ABSTRACT

SAINI, NADISH. High-fidelity Interface Capturing Simulations of the Post-LOCA Dispersed Flow Film Boiling Regime in a Pressurized Water Reactor Sub-channel (Under the direction of Dr. Igor A. Bolotnov).

In the dispersed flow film boiling (DFFB) regime, which exists under post loss-of-coolant accident (LOCA) conditions in PWRs, droplet dynamics play a critical role in heat transfer. The DFFB regime is characterized by a very high void fraction, such that the flow regime is akin to a mist type flow. Consequently, the dominant heat transfer pathway under these conditions is to the entrained droplets, which is a strong function of the surface area of the droplets. The major heat transfer mechanisms include radiation from rods to droplet surface and convective heat transfer from bulk vapor to droplets. Evaporation of droplets also results in an increase in the local vapor velocity, further enhancing the heat transfer coefficients. Spacer grids and mixing vane structures play an especially critical role in the DFFB regime. Collision of the droplets with these structures results in an increase in their surface area, which causes a sharp increase in heat transfer immediately downstream of the mixing vanes. Thus, a detailed study of the droplet dynamics – its morphology, average diameter, interaction with surrounding flow and spacers, is indispensable to understanding the intricacies of the DFFB regime.

With the advent of supercomputing and the development of highly scalable computer codes, it is becoming increasingly economical to run high fidelity, high resolution simulations of flow phenomena, wherein all relevant scales of the flow are resolved. PHASTA (Parallel Hierarchic Adaptive Stabilized Transient Analysis), a finite element method based Navier-Stokes solver, is one such numerical tool, used herein, with proven strong scaling on leading supercomputers. With the level-set method for interface capturing, PHASTA provides the capability of resolving two-phase flow phenomena. The level-set method implicitly captures the
interface between the phases, allowing for resolution of inherent complexities of the flow including droplet collision, breakup and coalescence.

In this research, detailed interface-resolved simulations are performed for simulating droplet dynamics in a prototypal reactor sub-channel with spacer grid and mixing vanes, under conditions representative of DFFB regime. Several ad-hoc functionalities are incorporated in PHASTA to enable the DFFB simulations and to enable high-resolution data collection from the simulations. Subsequent post-processing of the data provides the evolution of interfacial area, volume and Sauter mean diameter (SMD) of droplets along the axial length of the sub-channel domain. The SMD of the droplets at the downstream location of the mixing vanes is compared with existing empirical correlations, showing good agreement. Further, a comparative study of the upstream and downstream mean velocity and Reynolds stress tensor profile is presented to emphasize the effect of spacer-grid and mixing vane structures on the bulk flow, with and without the presence of droplets. The high spatial and temporal resolution database from both single-phase and two-phase simulations enable the prospect of data driven turbulence and system thermal hydraulic modeling.

Recognizing the prospect of level-set formulation for two-phase flows to simulate complex nuclear reactor regimes, efforts were made in this research to incorporate the formulation in another strong scaling flow solver, Nek5000. A spectrally vanishing viscosity (SVV) approach was implemented to stabilize the re-distancing equation. An improved multi-dimensional filter kernel for SVV is formulated and shown to provide adequate stabilization for liner/non-linear hyperbolic problems. Finally, the level-set formulation was coupled with an existing low Mach number solver in Nek5000 and demonstrated for the solution of 2D two-phase flow problems.
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High-fidelity Interface Capturing Simulations of the Post-LOCA Dispersed Flow Film Boiling Regime in a Pressurized Water Reactor Sub-channel

by
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DEDICATION

Dedicated to my parents,
Mrs. Anu Saini and Mr. Swaroop Saini
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Any Man’s thoughts and ideas, let alone achievements, are a superposition of the ideas of the great minds that one has the privilege and opportunity to come across or the ideas passed through generations of rigorous research and scientific study. This work has been made possible through the ideas contributed by several mentors who have guided me through my Ph.D. research.

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Chapter 1: Introduction

1.1 Research Scope and Overall Objective

The Ph.D. research is a part of larger integrated research project (IRP: 16-10918) sponsored by the Department of Energy’s Nuclear Energy University Program (DOE-NEUP). The overall objective of the project can be encapsulated as “the development and demonstration of a data driven methodology for validation of advanced computer models for nuclear power plant safety analysis” developed to support risk informed safety margin characterization (RISMC) [1], an integrated deterministic/probabilistic safety analysis methodology developed under the Department of Energy’s Light Water Reactor Sustainability (LWR-S) program [2]. Two system level computer codes are considered in this validation framework: NEUTRINO and COBRA-TF (or CTF) [3]. The former is a smooth particle hydrodynamics (SPH) code, to be validated for flooding scenarios [4]. The latter is a system-level code, a widely accepted industry standard for pressurized water reactor (PWR) and boiling water reactor (BWR) thermal hydraulic, steady state and transient, analysis. The *a priori* identified models for validation in CTF pertain to the post-LOCA (loss-of-coolant accident) PWR regime, particularly the dispersed flow film boiling (DFFB) regime. For addressing these models, *ad hoc* validation experiments and high-fidelity computer simulations were formulated and designed, to serve as a high spatial and temporal resolution data source, under the broader RISMC framework.

The rapid advent of technology in the high-performance computing (HPC) arena, resulting in a decrease in the cost of large-scale computations, has enabled high resolution studies of complex flow phenomena which hitherto remained elusive, or prohibitively expensive, to be scrutinized by experiments. Direct numerical simulations (DNS) enable resolution of all relevant scales of turbulence without resorting to any closure models, thus providing high fidelity
computations of the phenomena under investigation. Recently, DNS coupled with interface capturing method have been used to simulate two-phase flows in reactor sub-channels [5]. There have been simultaneous concerted advances in the development of data driven modeling frameworks, geared towards augmenting closure relations for thermal hydraulics, such as boiling heat transfer [6] and turbulence closure models [7], using data generated by DNS simulations.

The overarching objective of this work is conducting high-fidelity, interface capturing, representative simulations of the post-LOCA DFFB regime. More specifically, the simulations herein are designed to resolve the droplet and fluid dynamics in the vicinity of spacer-grids, which are quintessential structures in PWR subchannels from both a mechanical perspective, providing structural integrity to the fuel rod bundle, and a thermal hydraulic perspective, providing significant heat transfer augmentation. For DFFB regime, especially, the importance of the heat transfer supplement provided by spacer-grids and mixing vanes has been identified and emphasized by several prior experiments [8-10]. Inertial impact of entrained droplets on these structures results in a dramatic increase in their overall surface area, which manifests a sharp increase in the heat transfer to these suspended droplets. Thus, for modelling these phenomena or reducing the uncertainty of related models in system thermal hydraulic (STH) codes, highly detailed insights into the droplet and fluid dynamics is imperative. Large scale simulations are performed, realized by PHASTA [11], a strong scaling finite element method based numerical solver for the Navier-Stokes equations, on the Mira supercomputer at Argonne National Laboratory [12]. Through the implementation of advanced data collection tools, high fidelity data is collected from the simulations enabling unprecedented insight into the flow physics of a PWR subchannel under representative post-LOCA conditions.
1.2 Phenomenology of post-LOCA PWR Flow Regimes

Nuclear reactor power plants are designed with safeguard systems to withstand and/or mitigate the effects of several accident scenarios which are anticipated or postulated to occur during its lifecycle [9]. Among them, the most challenging accident to analyze is the large break loss-of-coolant accident (LOCA), wherein the core gets depressurized and loses its coolant due to a piping failure, referred to as a blowdown [13]. Owing to the deprivation of adequate coolant in the core, the thermal hydraulics during the blowdown phase is characterized by post-CHF (critical heat transfer) regimes, viz., transition boiling or film boiling (Figure 1). The former regime is highly unstable and features intermittent contact of the coolant with the walls, with dry regions exhibiting very high wall temperatures. The wet regions rapidly evaporate, establishing a continuous vapor film over the surface. Subsequent wall temperature is maintained consistently above the Liedenfrost limit [14], precluding any possibility of coolant contact with the rods. Since the thermal conductivity of vapor is significantly lower as compared to that of water, under the same conditions, the heat transfer coefficient for post-CHF boiling regimes is significantly lower, resulting in very high wall temperatures.
Figure 1: Pool boiling curve for water at 1 atm. Wall heat flux as a function of superheat [15].

Rehabilitation of core cooling depends on the safeguard systems (pumps), responsible for re-flooding the core after the failure is detected. Thermo-hydraulic characteristics of the reflood phase are highly dependent on the initial conditions i.e., the state of the core after blowdown and the inlet flooding rate of coolant. For the case of high flooding rates (~ 0.15 m/s [16]) an inverted annular flow boiling (IAFB) regime persists in the core, characterized by a void fraction of less than 50% [17,18]. While for low flooding rates (~ 0.025 m/s [16]), resulting in very high void fractions, dispersed flow film boiling (DFFB) is the dominant regime in the reactor channels [17,19,20]. A representative rendering of these two post-LOCA regimes is shown in Figure 2. Both regimes manifest a progressing quench front, ensued downstream by a continuous vapor film enveloping the fuel rods. In the IAFB regime, a reasonably integrated coolant core exists downstream of the quench front, which disintegrates further downstream to liquid slugs and then to smaller droplets, owing to the high interfacial shear rate [21]. The DFFB regime is essentially
characterized by dispersed droplets and may exist immediately beyond the quench front, as shown in Figure 2, or may succeed the IAFB regime, depending on the inlet flow conditions. In addition, the blowdown phase also results in a DFFB regime, thus, serving as the initial condition for the reflood transient analysis [13].

The most comprehensive experiments dedicated to studying the post-LOCA regimes were the FLECHT-SEASET [8] tests and, more recently, the experiments conducted at the Rod Bundle Heat Transfer (RBHT) facility at Pennsylvania State University [9]. As unanimously reported by these experiments, in most reactor reflood conditions, the flooding rates are typically low, resulting in DFFB conditions persisting for most of the axial length of the core. Therefore, the primary flow regime of interest for post-LOCA analysis and modeling is the DFFB regime. LOCA incidents impose the most limiting safety factors on the reactor total core power and the allowable peak linear fuel rod power [16]. These safety considerations ensure that the peak cladding temperature (PCT) remains reasonably below the Nuclear Regulatory Commission’s (NRC) established limit of $1477.6 \, K (2200^\circ F)$. A thorough understanding and subsequent modeling of the thermal-hydraulic phenomenon pertinent to the DFFB regime is, therefore, imperative for PWR safety margin characterization.
Figure 2: Representative rendering of the prominent post-LOCA flow regimes in reactor channels, DFFB (left) and IAFB (right). Preponderance of any of the two flow regime types is a strong function of the inlet flooding rate conditions [22].

1.3 Salient Observations from DFFB Experiments

Hochreiter et al [16] assembled the observed conditions for reflood transients from Westinghouse, Framatome and Siemens to design their test matrix for the DFFB regime. Consolidated parameters for the operating range were:

- Vapor Reynolds number, \( Re_v \in (2500,9500) \).
- System pressure, \( P[psi] \in (20,45) \)
- Wall superheat, \( T_w - T_{sat}[^0F] \in (400 - 1900) \)
- Difference b/w wall and vapor temperature, \( T_w - T_v[^0F] < 1800 \)

The DFFB regime is inherently transient, characterized by both mechanical and thermal non-equilibrium [8,10]. Phenomenologically speaking, it is best conceptualized by a mist type
flow, with polydisperse droplets, corresponding to high void fractions (> 0.8). Heat transfer in the DFFB regime is a convoluted interplay of several different mechanisms. There is not an apparent single dominant heat transfer path, which, understandably, renders extreme complexity to the task of modeling/accounting for these phenomena in STH codes. As noted by Hochreiter et al [23], these mechanisms include:

- Convection to superheated vapor from rod surface.
- Surface radiation from rods to vapor and droplets.
- Interfacial heat transfer between droplets and superheated vapor.
- Direct contact heat transfer between the wall and entrained liquid (quenching).
- Convective enhancement of the vapor by the entrained droplets.
- Impact of spacer-grids to heat transfer enhancement due to flow acceleration and droplet break-up.

A common implicit determinant governing all the above-mentioned heat transfer modes is the size and shape (interfacial area) of the entrained droplets. Thus, a detailed study of the droplet dynamics – its morphology, average diameter, interaction with surrounding flow, interfacial area evolution, is indispensable to understanding the intricacies of the DFFB regime. The importance of droplet dynamics to the DFFB regime is further reinforced by considering the PIRT analysis. Phenomena identification and ranking table (PIRT) was developed by the NRC under the code scaling, applicability and uncertainty (CSAU) initiative [24]. It assigns a priority order to all phenomena relevant to a complex system. Built on the observations from the FLECHT-SEASET experiments, Hochreiter et al [16] provided a phenomena identification and ranking table (PIRT) for the different heat transfer mechanisms relevant to the DFFB regime, reproduced in Table 1.
Barring convection to superheated vapor, all processes related to heat transfer with a high rank have a direct proportional dependence on the interfacial area.

Table 1: PIRT analysis of the DFFB regime. Results compiled by Hochreiter et al [23].

<table>
<thead>
<tr>
<th>Process/Phenomena</th>
<th>Ranking</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decay power</td>
<td>H</td>
<td>Energy source which determines the temperature of the heater rods, and energy to be removed by the coolant</td>
</tr>
<tr>
<td>Fuel Rod/heater Rod properties</td>
<td>L</td>
<td>The exact properties can be modeled and stored energy release is not as important</td>
</tr>
<tr>
<td>Dispersed Flow Film Boiling</td>
<td>H</td>
<td>DFFB modelling has a high uncertainty which directly effects the PCT</td>
</tr>
<tr>
<td>(components given below)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Convexion to superheated vapor</td>
<td>H</td>
<td>Principle mode of heat transfer as indicated in FLECHT-SEASET experiments</td>
</tr>
<tr>
<td>• Dispersed phase enhancement of convective flow</td>
<td>H</td>
<td>Models indicate that the enhancement can be over 50 % in source cases</td>
</tr>
<tr>
<td>• Direct wall contact</td>
<td>L</td>
<td>Wall temperatures are significantly above the Liedenfrost limit. No contact is expected</td>
</tr>
<tr>
<td>• Dry wall contact</td>
<td>M</td>
<td>This mechanism is less important than vapor convection</td>
</tr>
<tr>
<td>• Vapor to droplet interfacial heat transfer</td>
<td>H</td>
<td>The interfacial heat transfer reduces the vapor temperature which is the heat sink for the wall heat flux</td>
</tr>
<tr>
<td>• Radiation heat transfer to</td>
<td>H/M</td>
<td>This is important at higher bundle elevations (H) where the convective heat transfer is small since the vapor is so highly superheated. Very important for BWR reflood with sprays, and colder surrounding can. Large uncertainty.</td>
</tr>
<tr>
<td>o Surfaces</td>
<td>H/M</td>
<td></td>
</tr>
<tr>
<td>o Vapor</td>
<td>H/M</td>
<td></td>
</tr>
<tr>
<td>o droplets</td>
<td>H/M</td>
<td></td>
</tr>
<tr>
<td>• Gap heat transfer</td>
<td>L</td>
<td>Controlling thermal resistance is the dispersed flow film boiling heat transfer resistance. The large gap heat transfer uncertainties can be accepted, but fuel center line temperature will be impacted.</td>
</tr>
<tr>
<td>• Cladding Material</td>
<td>L</td>
<td>Cladding material in the tests is Inconel which has the same conductivity as Zircaloy nearly the same temperature drop will occur.</td>
</tr>
<tr>
<td>• Reaction Rate</td>
<td>M</td>
<td>Inconel will not react while Zircaloy will react and create a secondary heat source at very high PCTs, Zirc reaction can be significant</td>
</tr>
<tr>
<td>• Fuel Clad Swelling/Ballooning</td>
<td>L</td>
<td>Ballooning can divert flow from the PCT location above the ballooning region. The ballooned cladding usually is not the PCT location. Large uncertainty.</td>
</tr>
</tbody>
</table>

Andreani et al [25] provided a detailed account of the observed or postulated droplet entrainment mechanisms which precede the DFFB regime. The observations made by Hochreiter et al [16] confirmed that the DFFB conditions are a strong function of the upstream conditions,
near the quench front. The largest source of uncertainty for measurements made in the DFFB regime are propagated from the liquid entrainment sites. Some of the observed and accepted mechanisms governing droplet entrainment and subsequent morphology include:

- The semi-mechanistic theory of roll wave shearing by Kataoka et al [26] and Kocamustafaogullari et al [27].
- Wave shearing at the quench front location observed by Ardron et al [10], Peake et al [28] and Ihle et al [29].
- Spherical upper limit for droplet diameter for wake flow regime reported by Kocamustafaogullari et al [27] and observed by Lee et al [30]. To summarize, the observations essentially suggest that the largest stable spherical droplet diameter in churn-turbulent flow is much smaller than that observed by only considering entrainment mechanisms.
- Bubble bursting mechanism observed by Dhir et al [31] near the quench front location. Quantification of droplet population density to account for this phenomenon was provided by Lee et al [32].
- Droplet shearing in coaxial annular flow setup by Ishii et al [33]. They reported the breakup of liquid core into a homogeneous distribution of droplets and small ligaments.
- Downstream breakup of the droplets due to capillary and aerodynamic effects, as observed by Ardron et al [10], especially the latter, up to a distance of 1 m from the quench front. The aerodynamic breakup, also referred to as secondary breakup in the broader literature [34], is governed by the Weber number,

\[ We_a = \frac{\rho g D u_{rel}^2}{\sigma} \]  

(1.1)
where $\rho_g$ is the density of surrounding steam, $D$ is the equivalent diameter of the droplet, $u_{rel}$ is the velocity of the steam relative to droplet and $\sigma$ is the surface tension coefficient of the interface.

- Droplet breakup due to inertial impact with spacer-grids and mixing vanes

Although the entrainment and breakup procedures in the upstream regions are of significance, majority of the recent experiments have been devoted to the study of interaction of dispersed droplets with the spacer-grids structures. This phenomenon requires more extensive discussion and is addressed in the following section.

### 1.3.1 Impact of spacer-grids and mixing vanes on the DFFB thermal-hydraulics

In a recent publication Bajorek et al [35] presented their observations from the RBHT experiments, summarizing key results from almost a decade of experimental tests of the post-LOCA regime. They emphasized the predominant effect of spacer-grids on the thermal hydraulics of the DFFB regime. All of the tests conducted at the RBHT facility, irrespective of high or low flooding rates, recorded a sharp increase in the heat transfer coefficient in the immediate downstream vicinity of the spacer-grid structures, contributing a significant proportion to the overall heat transfer of the core. Convective heat transfer enhancement was also recorded for the initial single-phase experiments by Hochreiter et al [36], based on which Miller et al [37] and Riley et al [38] developed empirical correlations to account for the phenomenon in system thermal hydraulic codes.

It is evident that the recorded heat transfer coefficient for the two-phase flow tests are significantly higher as compared to the experiments with only steam as coolant [35,39]. For the DFFB regime, several additional factors provide a positive feedback to heat transfer near the spacers, all owing to the droplet interaction with spacer-grid structures. Note that based on the
flooding rate conditions, the phenomenology at the spacer-grids is quite different, resulting in different heat transfer mechanisms [40]. For high flooding rates, a film of coolant encapsulates the spacer grid structure due to de-entrainment from the bulk flow. High shear between this film and the surrounding vapor results in the formation of a liquid sheet at the trailing edge of the spacer [39]. Relatively large droplets and ligaments get re-entrained from this sheet which eventually breakup further downstream into smaller droplets, due to aerodynamic effects, resulting in a high increase in surface area. In the experiments by Miller et al [39] this manifested as a “second-stage” heat transfer augmentation observed about ten hydraulic diameters from the trailing edge of spacers, while the “first-stage” augmentation occurred at the trailing edge. Kang et al [41] provided a detailed mechanistic analysis and corresponding correlation for the shearing of droplets from this water sheet.

For low flooding rates, on the other hand, the void fraction in the bulk is too high for a stable water film to develop on the spacer surface. Sharp heat transfer augmentation is observed at the trailing edge of spacers, decaying exponentially with respect to the downstream distance [39,40,42]. The primary contribution comes due to the inertial impact of the droplets on the spacer-grid, resulting in breakup or deformation of the droplets and a drastic increase in the overall surface area. The heat transfer increase has been correlated with the observed decrease in the Sauter mean diameter (SMD) of the droplets, a statistical measure to characterize the volume of the droplets relative to their surface area, defined as [43],

\[
SMD = \frac{\sum_{j=1}^{N} n_j d_j^3}{\sum_{j=1}^{N} n_j d_j^2}
\]  

(1.2)

where, \( N \) is the total number of diameter groups, \( n_j \) is the number of droplets belonging to the group and \( d_j \) is the equivalent diameter of the group. Ratio of the immediate upstream and
downstream SMD, with respect to the spacer-grids, is an extremely important parameter used in modeling of the DFFB regime. A simplified mechanistic model was developed by Cheung et al. [43] to predict the downstream SMD of the droplets based on conservation of mass, kinetic and surface energies. A limited number of empirical correlations also exist in literature for SMD, subsequently used in modelling the interfacial source terms for closure relations in thermal hydraulic codes.

Other components, besides convective enhancement and decreasing SMD, through which the spacer-grids contribute, directly or indirectly, to the overall heat transfer in the DFFB regime, include direct radiation from the fuel rods to the spacer surface, thermal boundary layer separation and re-attachment and quenching due to impacting droplets. As a testament to their significance, not accounting for the spacer-grids in STH codes results in an over-prediction of the cladding temperature [22].

### 1.4 Modeling DFFB Regime in STH Codes

Although high-fidelity simulations provide a viable alternative to real world experiments, which are often more expensive and more limiting in their resolution capacity, they are yet prohibitively expensive to be used as industrial standards for predicting thermal-hydraulic response. These simulations are, therefore, intended as alternative databases to aide in the model development for the system thermal hydraulic codes (STH), which are more accessible and computationally magnitudes cheaper. A brief account of the models used for the DFFB regime in the STH code – COBRA-TF (Coolant Boiling in Rod Arrays-Two Fluid, also abbreviated as CTF) [44], is provided in this section with the objective of bringing into perspective the models that may be improved from the data generated herein.
CTF is built on a two-fluid, Eulerian-Eulerian approach for the governing equations with consideration for three separate fields, viz., vapor (includes bubbles and continuous vapor phase), liquid film and liquid droplets. Each field is modeled with a separate set of mass and momentum conservation equations. The energy conservation equation, however, is written only for two fields, with droplets and liquid film assumed to be in thermal equilibrium [45]. The governing equations of mass, momentum and energy, respectively, for a field $k$ are:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k) = L_k + M^T_e$$

$L_k \rightarrow$ Interfacial mass transfer

$M^T_e \rightarrow$ Mass transfer due to turbulent mixing

$$\frac{\partial \alpha_k \rho_k \vec{v}_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k \vec{v}_k) = -\alpha_k \nabla p + \nabla \cdot [\alpha_k (\tau^{ij}_k + T^{ij}_k)] + \vec{M}^k + \vec{M}^d + \vec{M}^T_k$$

$\tau^{ij}_k \rightarrow$ Viscous stress

$T^{ij}_k \rightarrow$ Turbulent shear stress

$\vec{M}^k \rightarrow$ Momentum source/sink due to phase change and entrainment

$\vec{M}^d \rightarrow$ Interfacial drag

$\vec{M}^T_k \rightarrow$ Momentum transfer due to turbulent mixing

$$\frac{\partial \alpha_k \rho_k h_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k h_k \vec{v}_k) = -\nabla \cdot [\alpha_k (\vec{Q}_k + \vec{q}_k)] + \Gamma_k h_k^i + q'''_{wk} + \alpha_k \frac{\partial P}{\partial t}$$

$\vec{Q}_k \rightarrow$ Conduction heat flux

$\vec{q}_k \rightarrow$ Turbulent heat flux

$\Gamma_k h_k^i \rightarrow$ Energy transfer due to phase change, from $i$

$q'''_{wk} \rightarrow$ Volumetric wall heat transfer

$\frac{\partial P}{\partial t} \rightarrow$ Pressure work

where $\alpha_k$ is the volume fraction of phase $k$. All the terms on the right-hand side of the equations are modeled mechanistically or empirically. The equations are subsequently reduced to sub-channel form, where only two flow directions are considered – axial and lateral, the latter implying all directions orthogonal to the vertical axis (refer to Salko & Avramova [45] for details). For
improved modeling of the DFFB regime Ergun et al [46] recommended splitting the droplet field equations into two separate fields representing small and large droplets. In addition to the conservation equations, the interfacial area for the droplet field is tracked using an explicit transport equation,

\[
\frac{\partial A''''_{i,d}}{\partial t} + \nabla \cdot (A''''_{i,d} \vec{v}_d) = A''''_{i,E} + A''''_{i,I}
\]

\(A''''_{i,d}\) → Interfacial area per unit volume
\(A''''_{i,E}\) → Interfacial area generation rate per unit volume due to entrainment
\(A''''_{i,I}\) → Interfacial area generation rate per unit volume due to evaporation

The interfacial area is subsequently used for the construction of several closure relations for the DFFB regime, including interfacial drag, interfacial heat transfer and radiative heat transfer to droplets.

Hochreiter et al [23] assembled data for measurement uncertainties, from prior experiments, related to all high ranking phenomena mentioned in Table 1 and their subsequent impact on the peak cladding temperature (PCT). Further, the uncertainties related to the models representing the phenomena in CTF were also quantified (see Table 2). Among the enumerated phenomena in Table 2, convective enhancement of heat transfer due to dispersed droplets and the effects of spacer-grids and mixing vanes are directly relevant in context of the simulations presented in this research. The uncertainty in the experimental measurement to isolate the effects of these phenomena is very large, owing to the implicit complexly woven multi-physics. Moreover, the uncertainty involved in the models formulated, empirical or mechanistic, in CTF is very high for convective enhancement while they are unaccounted for spacer-grid related models (as reported by Hochreiter et al [23] in 2010. More recent study dedicated to uncertainty quantification due to spacer-grid related models was not found by the author).
Table 2: Measurement uncertainties, based on prior experiments, associated with high-ranking phenomena. Reproduced from Hochreiter et al [23].

<table>
<thead>
<tr>
<th>High-ranking phenomena</th>
<th>Impact on PCT</th>
<th>Measurement uncertainty</th>
<th>Model uncertainty in CTF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decay power</td>
<td>Source of energy for rods, boundary conditions for tests.</td>
<td>Minimum</td>
<td>Input</td>
</tr>
<tr>
<td>Convection to superheated vapor</td>
<td>Principal mode of heat transfer, directly impacts PCT</td>
<td>Large</td>
<td>15%</td>
</tr>
<tr>
<td>Drop sizes, droplet number density, interfacial area</td>
<td>Determines the interfacial heat transfer in the DFFB Region.</td>
<td>Large</td>
<td>-</td>
</tr>
<tr>
<td><strong>Dispersed phase enhancement of convective heat transfer</strong></td>
<td>Important impact on PCT as the enhancement can be over 50 % in some cases.</td>
<td>Large</td>
<td>&gt;100%</td>
</tr>
<tr>
<td>Direct wall contact heat transfer</td>
<td>Quenching. Directly affects PCT</td>
<td>-</td>
<td>&gt;100%</td>
</tr>
<tr>
<td>Droplet to vapor interfacial heat transfer</td>
<td>The interfacial heat transfer reduces the vapor temperature.</td>
<td>Large</td>
<td>30%</td>
</tr>
<tr>
<td>Radiation heat transfer between surfaces, vapor, and droplets</td>
<td>Very important at high bundle elevations where the convective heat transfer is small due to large vapor superheat.</td>
<td>Large</td>
<td>~20% for transfer to surfaces 50% for transfer to vapor 50% for transfer to droplets</td>
</tr>
<tr>
<td>Interfacial shear and droplet velocity</td>
<td>Effects the void fraction distribution and resulting droplet velocity in the entrained flow.</td>
<td>Large</td>
<td>-</td>
</tr>
<tr>
<td><strong>Effects of spacer grids on droplet deposition, breakup, and heat transfer</strong></td>
<td>Important enhanced cooling mechanism especially in the DFFB region due to their effects in droplet evolution and flow restructuring.</td>
<td>Large</td>
<td>-</td>
</tr>
<tr>
<td>Gap heat transfer</td>
<td>-</td>
<td>-</td>
<td>100%</td>
</tr>
</tbody>
</table>

The following sections introduce some of the closure models pertinent to the DFFB regime. Discussion is limited to the closures necessary to account for spacer-grids and mixing vanes, which are directly relevant to the present research. For an exhaustive discussion of all correlations for the DFFB regime, the reader is directed to Salko et al [45] and cited literature therein.

**1.4.1 Convective heat transfer enhancement due to spacer-grids**

For single-phase steam flow, a range of experiments were conducted by Kidd et al [47], Rehme et al [48] and Yao et al [49] for varied spacer-grid and mixing vane configurations. Yao
et al proposed the following relationship for the Nusselt number enhancement due to turbulence mixing in the downstream vicinity of spacer-grids,

\[
\frac{Nu_x}{Nu_0} = 1 + 5.55 \epsilon^2 \exp \left( -\frac{0.13x}{D_h} \right)
\]  

(1.7)

where, \( Nu_0 \) is the immediate upstream Nusselt number, while \( Nu_x \) is the downstream Nusselt number, a function of distance, \( x \), from the trailing edge of spacers. \( \epsilon \) is the ratio of the cross-sectional area of the spacer-grid to the total cross-sectional area of the sub-channel. \( D_h \) is the hydraulic diameter of the sub-channel, not considering any obstacles. The above relation was valid for the configuration without any adjunct mixing vanes. Presence of the mixing vanes provides an additional swirl component to the flow, further enhancing heat transfer. The following modified relation was recommended by Yao et al to account for this swirl effect,

\[
\frac{Nu_x}{Nu_0} = \left[ 1 + \epsilon^2 \tan \Phi \exp \left( -\frac{0.034x}{D_h} \right) \right]^{0.4}
\]  

(1.8)

where \( \Phi \) is the angle of the mixing vanes with respect to the axial direction. These correlations, however, produced discrepancies with respect to the recent experimental data from the RBHT facility. Miller et al [37] proposed an improved correlation which also accounts for the Reynolds number of the flow,

\[
\frac{Nu_x}{Nu_w} = 1 + 465.4Re^{-0.5} \epsilon^2 \exp \left( -7.31 \times 10^{-6} Re^{1.15} \frac{x}{D_h} \right)
\]  

(1.9)

here \( Nu_w \) is the upstream Nusselt number evaluated from the Weismann correlation,

\[
Nu_w = \left[ 0.042 \left( \frac{P}{D_h} \right) - 0.024 \right] Re^{0.8} Pr^{0.4}
\]  

(1.10)
where $P$ is the rod bundle pitch and $Pr$ is the steam Prandtl number. Although the above correlations were developed based on empirical data from single-phase experiments, they are also directly used as a heat transfer enhancement component for two-phase simulation with droplets. The presence of droplets throttles the cross-sectional flow area further, resulting in increased turbulent kinetic energy (see Chapter 5), and is expected to provide an additional feedback to the downstream Nusselt number.

### 1.4.2 Dry spacer-grid droplet breakup

Collision of dispersed droplets with the spacer-grid structures results in a sharp increase in the interfacial area of the droplet field. An additional source term is, thus, added to the interfacial area transport equation (1.6) to account for this phenomenon. Existing correlation in CTF uses the empirical data from Wachters et al [50] and Senda et al [51] to estimate the ratio of downstream to upstream Sauter mean diameter,

$$\frac{SMD_o}{SMD_i} = 6.167 We_c^{-0.53} \quad (1.11)$$

Here $We_c$ is the collision Weber number of the impinging droplets, based on its absolute velocity (as opposed to aerodynamic Weber number which is based on the relative velocity of surrounding fluid, equation (1.1)),

$$We_c = \frac{\rho_l D u_{ad}^2}{\sigma} \quad (1.12)$$

where $\rho_l$ is the density of the liquid droplet, $D$ is its equivalent spherical diameter, $u_{ad}$ is the absolute velocity of the droplet and $\sigma$ is the surface tension coefficient of the interface. Cheung et al [43] later confirmed the model form of equation (1.11) through an extensive mechanistic
analysis. They also suggested an improved correlation, which provided a better fit for the RBHT data,

\[
\frac{SMD_o}{SMD_i} = (1 + 0.1803 \epsilon W e_0^{0.558})^{-1}
\]  

(1.13)

where, \(\epsilon\) is the blockage ratio of spacer-grid. It is important to emphasize that the above models are valid only for dry spacer-grids. In CTF the models are turned on only if less than 99% of the spacer-grid is quenched [45]. In contrast, for wet spacers, the droplets get de-entrained on the film enveloping the surface of the structures.

1.4.3 Grid quench front model and heat balance

CTF features a quenching model dedicated to spacer-grids which tracks the location of the quench front based on a heat balance. A simple geometric view of the spacer-grids, plate type obstacles, is assumed for the ensuing discussion (see Avramova [52]). The model is constructed based on partitioning the spacer-grid surface into dry and wet region and treating heat transfer in each region separately. The rate of deposition of water on the spacer surface is based on the following mass rate balance,

\[
\dot{m}_R = \dot{m}_{DE} - \dot{m}_{evap} = \frac{A_{grid}}{A_{flow}} \dot{m}_E - \frac{\left( (q''_{rad,w} + q''_{conv,w})P_{grid} f_w L_{grid} \right)}{h_f g}
\]  

(1.14)

where, \(\dot{m}_{DE}\) is the de-entrainment rate of the dispersed droplets onto the spacer surface, which is simplistically given by fraction of the droplet mass rate, \(\dot{m}_E\), that encounter the spacer surface. \(\dot{m}_{evap}\) is the mass rate loss from the liquid film on the wet portion of the spacer, determined by the combination of the radiative heat flux from the rod walls to the wet portion of the spacer, \(q''_{rad,w}\), and the evaporative flux from the wet portion, \(q''_{conv,w}\). \(P_{grid}\) and \(L_{grid}\) are the perimeter and length of the spacer, respectively, while \(f_w\) represents the fraction of the spacer that is wet.
Realistically, some additional liquid is lost from the surface due to sputtering near the quench front. It was accounted for by Avramova [52], making the resultant mass transfer to wet region of the spacer,

\[ \dot{m}_{QF} = \dot{m}_R \exp \left( 1 - \frac{T_{\text{dry}}}{T_{\text{sat}}} \right)^2 \]  

(1.15)

where, \( T_{\text{dry}} \) is the temperature of the dry portion of the spacer and \( T_{\text{sat}} \) is the saturation temperature of the liquid. Consideration of energy conservation provides an upper bound for the energy released at the quench front and, by extension, the quench front velocity, \( v_{QF} \),

\[ \rho_{\text{grid}} C_{p,\text{grid}} P_{\text{grid}} L_{\text{grid}} v_{QF} \left( T_{\text{dry}} - T_{\text{sat}} \right) \leq \dot{m}_{QF} h_f \]  

(1.16)

where the left hand side of the above inequality is the energy stored in the spacer-grid, with \( \rho_{\text{grid}} \) and \( C_{p,\text{grid}} \) being the density and the specific heat of the grid material, respectively. Note the above expression assumes that the temperature of the grid in the wet surface is equal to the saturation temperature of the liquid. Thus, the velocity of the *advancing* quench front is,

\[ v_{QF} \leq \frac{\dot{m}_{QF} h_f}{\rho_{\text{grid}} C_{p,\text{grid}} P_{\text{grid}} L_{\text{grid}} \left( T_{\text{dry}} - T_{\text{sat}} \right)} \]  

(1.17)

Several other constraints are imposed on the heat transfer to get an estimate for the advancing quench front velocity (see Avramova [52] or Salko et al [45] for details). On the other hand, if the film evaporation rate exceeds the de-entrainment rate, the quench front recedes. The receding velocity for this case is given by,

\[ v_{QF} = \frac{(\dot{m}_{DE} - \dot{m}_{evap}) h_f}{\rho_{\text{grid}} C_{p,\text{grid}} P_{\text{grid}} L_{\text{grid}} \left( T_{\text{dry}} - T_{\text{sat}} \right)} \]  

(1.18)
The quench front location, or the length of wet portion of the spacer, is evolved in time using,

$$L_{QF}^{n+1} = L_{QF}^n + v_{QF} \Delta t$$  \quad (1.19)

Finally, the energy balance for the dry and wet portions of the grid are given, respectively as,

$$\rho_{grid} C_{p,grid} \frac{\partial T_{grid}^{dry}}{\partial t} = \frac{P_{grid}}{A_c} (q_{rad}'' - q_{conv}'') - q_{dcht}'')$$  \quad (1.20)

$$\dot{q}_w = (q_{conv,w}'' + q_{rad,w}'') P_{grid} L_{QF}$$  \quad (1.21)

where, $q_{rad}''$ and $q_{conv}''$ are the radiative heat transfer from rod surface to dry portion of the spacer surface and convective heat transfer from dry surface to steam, respectively. $q_{dcht}''$ is the heat transfer partition due to droplets impacting the dry surface due to lateral migration (for detailed model forms for all heat transfer terms refer Salko et al. Here we maintain the focus of the discussion on a holistic view of the spacer-grid thermal hydraulic model). Heat balance equations (1.20) and (1.21) are solved in conjunction with the mechanics described by (1.17) - (1.19) to describe the thermal-hydraulics of the spacer-grids in CTF.

### 1.5 Research Objectives and Dissertation Outline

The preceding discussion in this chapter establishes the significance of droplet dynamics and the role of spacer-grids and mixing vanes to the overall thermal hydraulic response in the DFFB regime. From this vantage point, the key research objectives can be established as:

- Perform high fidelity simulations, both single phase and two-phase, of PWR sub-channel with spacer grids and mixing vanes to support models in CTF.
- Development and incorporation of \textsl{ad-hoc} functionalities in PHASTA to make the simulations feasible on state-of-the-art supercomputers (e.g. Mira at Argonne National Lab).
- Development and incorporation of scalable MPI routines in PHASTA for high resolution data collection.
- Implementation of local time stepping algorithm for the level-set re-distancing equation in PHASTA.
- Implementation of parallel droplet injection mechanism in PHASTA for two-phase simulation

- Detailed analysis of the effects of spacer-grids and mixing vanes on single phase turbulence.
- Detailed analysis of droplet dynamics from two-phase simulations representative of DFFB regime.
  - Capturing axial evolution of droplet interfacial area and Sauter mean diameter to study the effect of spacer-grids on these quantities.
  - Effect of the presence of droplets on turbulence and comparative study with single phase results.
- Comparison of the single and two-phase results with existing CTF correlations and propositions for improvement.

The two-phase simulations with PHASTA demonstrate the effectiveness of large-scale interface capturing simulations in resolving complex phenomena for key applications. The simulations are a progeny of excellent scaling numerical codes and state-of-the-art HPC architecture. To diversify interface capturing capability beyond PHASTA, the level-set method has also been implemented in Nek5000 [53], a spectral element method based code that also scales very well on supercomputers. The key objectives associated with this endeavor are encapsulated as:
• Implementation of spectrally vanishing viscosity (SVV) for stabilization of pure hyperbolic problems, necessary for re-distancing equation.
  o Improvements on the filter kernel design for complicated 2D problems
  o Demonstration of the implementation on challenging linear and non-linear hyperbolic problems.
• Implementation of level-set and re-distancing equations in Nek5000.
  o Coupling of the level-set method with existing low Mach number solver in Nek5000.
• Demonstration of the implementation on some archetypal two-phase problems e.g., Rayleigh-Taylor instability and recognizing current challenges to make Nek5000 a viable tool for large-scale two-phase flow simulations.

The essentials of the numerical methods in PHASTA are explained in reasonable detail in Chapter 2. Further, several additional ad-hoc numerical tools and data collection methodologies were implemented in PHASTA which made the ensuing large-scale simulations possible, expounded in Chapter 3. Statistical data collected from the single-phase simulations, at high spatial resolution and the temporal resolution equivalent of the simulation time step size, allowed the extraction of key turbulent flow features, viz., mean velocities, Reynolds Stresses and turbulence invariants. The quantitative effect of spacer-grids and mixing vanes on these turbulent features were studied in unprecedented detail and are reported in Chapter 4. The wealth of data collected from these simulations also contributed to the development of novel machine learning based turbulent models, demonstrating their capability of capturing the anisotropies and history effects at the downstream location of spacer-grids. The axial evolution of droplet morphology, quantified by means of instantaneous droplet volume, interfacial area and Sauter mean diameter was studied from
simulations with a range of upstream droplet Weber numbers, the critical dimensionless parameter characterizing droplet dynamics in the DFFB regimes, as identified by experiments. All two-phase simulation results are documented in Chapter 5. Primary challenge with the implementation of the level-set formulation in Nek5000 was posed by the re-distancing equation. Spectral methods are not well suited for purely hyperbolic problems due to minimal numerical dissipation, especially problems with non-smooth solutions. Therefore, an artificial viscosity stabilization technique was implemented in Nek5000, especially for stabilizing the level-set re-distancing equation. Details on this implementation and subsequent two-phase solver implementation are presented in Chapter 6. Recommendation on future work, including identification of the shortcomings and sources of uncertainty of the present DFFB simulations are presented in Chapter 7. Finally, a succinct summary of the research and conclusions are presented in Chapter 8.
Chapter 2: Numerical Method

This chapter provides a description of the governing equations used for the single- and two-phase simulations in this work. A brief history and overview of the computational tool, PHASTA, is outlined, which emphasizes the reason for its selection as the CFD code for large-scale simulations. Further, finite element discretization and its implementation in PHASTA are discussed in detail, important for understanding the underlying numerical method and the functionalities implemented in PHASTA, discussed in Chapter 3.

2.1 Essentials of the Computational Tool - PHASTA

The finite-element method based code, PHASTA (Parallel, Hierarchic, higher-order accurate, Adaptive, Stabilized, Transient Analysis) [54] is used for all large-scale computational studies in this work. Owing to the finite element formulation, the input mesh for PHASTA is unstructured with a range of allowable element shapes, including tetrahedrons, hexahedrons, wedges and prisms, a tremendous advantage for the computation of flows in complex geometries [55]. Advanced domain decomposition strategies – hypergraph partitioning method, implemented by Sahni et al [56], provide efficient load balancing of the degrees-of-freedom (dofs), which provide excellent strong scaling properties to the PHASTA solver, especially on the IBM BlueGene/Q architecture based supercomputer, Mira, at Argonne National Lab [57]. Further, PHASTA uses a fully implicit solver for the incompressible Navier-Stokes equations, which impart stability to the solver for time step size corresponding to a relatively large CFL. The resulting linearized matrix system of equations is solved using the GMRES (Generalized Minimal Residual) algorithm [58], the state-of-the-art, parallelizable, matrix solver in literature for sparse matrix systems.
PHASTA has, thus, been used for a range of studies pertinent to several disciplines, viz.,
aeronautics [59], biomedical [60], nuclear engineering [5] on meshes with dofs of the order of billions (92 billion is the largest reported mesh element size used with PHASTA [59]). The implementation of the interface capturing level-set method enabled the computation of two-phase flows in PHASTA [61]. In the level-set method a contour field is superimposed over the computational domain and the zero contour of the field is ordained the interface between the two phases [62]. Properties are transitioned across the interface, which allow for the computation of two-phase flow using an effectively single-phase flow solver.

Thus, the finite element and the level-set method are the foundational numerical ingredients which make the ensuing, DFFB simulations, possible. This chapter provides details on the formulation of these methods. In addition, however, several essential computational tools were also incorporated in PHASTA, required both for the feasibility of the simulations and for an in-depth scientific analysis of the results yielded from them. These adjunct tools are discussed in detail in Chapter 3.

2.2 Governing Equations

For the applications under consideration, the compressibility effects can be neglected (low Mach number). Thus, the Navier-Stokes equations are solved in the incompressible format, for which the governing equations are,

\[
\begin{align*}
\nabla \cdot \vec{u} &= 0 \\
\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) &= -\nabla p + \nabla \cdot \vec{\tau} + \vec{f} \\
\vec{\tau} &= \mu (\nabla \vec{u} + \nabla \vec{u}^T)
\end{align*}
\]

where \( \vec{u} \) is the three-dimensional velocity field, \( \rho \) is the fluid density, \( \vec{\tau} \) is the deviatoric stress tensor, \( \vec{f} \) is the body force and \( p \) is the pressure. Since the density is independent of the pressure
field, it does not have spatial-temporal dependence resulting in the devolution of the continuity equation into a divergence free constraint on velocity, Eq. (2.1).

Two-phase flow capabilities are embedded in PHASTA using the level-set (LS) interface capturing method [62]. In the LS approach the interface between the two phases is implicitly captured by the zero of a contour field, \( \phi \). The formulation allows for both phases to be solved by a “one-fluid” approach by transitioning properties across the interface using a smoothed Heaviside function,

\[
\gamma(\phi) = \gamma_1 H(\phi) + \gamma_2 (1 - H(\phi))
\]

where \( \gamma \) represents any of the flow properties of the either phase. Note that the regularization of the Heaviside function is essential for continuous Galerkin (CG) formulation, as implemented in PHASTA. A step/sharp transition of properties across the interface would, otherwise, result in inexorable numerical instabilities. Therefore, the Heaviside function is designed such that it is smeared out across a small finite length, \( \epsilon \),

\[
H(\phi) = \begin{cases} 
0 & \phi < -\epsilon \\
\frac{1}{2} \left[ 1 + \frac{\phi}{\epsilon} + \frac{1}{\pi} \sin \left( \frac{\pi \phi}{\epsilon} \right) \right] & |\phi| < \epsilon \\
1 & \phi > \epsilon 
\end{cases}
\]

where \( \epsilon \) is of the order of average mesh element length. The entire LS contour field is advected under the influence of the flow field using a transport equation,

\[
\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0
\]

The contour field, however, holds meaning only in the vicinity of the zero contour, acting as the interface between the phases. The level-set advection equation is coupled with the Navier-Stokes equations by means of the surface tension force. A continuum surface tension model, developed
by Brackill et al [63], allows for it to be smeared out across the length $\varepsilon$, using the gradient of the Heaviside function,

$$\nabla H = \delta(\phi) \vec{n} \tag{2.6}$$

$$\delta(\phi) = \begin{cases} 0 & \phi < -\varepsilon \\ \frac{1}{2\varepsilon} \left[ 1 + \cos \left( \frac{\pi \phi}{\varepsilon} \right) \right] & |\phi| < \varepsilon \\ 0 & \phi > \varepsilon \end{cases} \tag{2.7}$$

The surface tension source term is then added to the momentum equation,

$$\vec{f}_s = \kappa \delta(\phi) \vec{n} \tag{2.8}$$

where $\kappa$ is the curvature of the interface, given by,

$$\kappa = \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \tag{2.9}$$

Advection operation using Eq. (2.5) results in the level-set field losing its property as a signed distance function. It is essential to restore this distance function property for accurate calculation of curvature and subsequent coupling with the momentum equations. This is done by solving a Hamilton-Jacobi type equation after each advection solve [64],

$$\frac{\partial \phi_d}{\partial \tau} = \text{sign}(\phi_0)(1 - |\nabla \phi_d|) \tag{2.10}$$

where, $\phi_d$ is the distance field variable and $\phi_0$ is the field obtained after advection step, serving as input to the above equation. Quite often, Eq. (2.10) is re-formulated in the advection form,

$$\frac{\partial \phi_d}{\partial \tau} + \vec{w} \cdot \nabla \phi_d = \text{sign}(\phi_0) \tag{2.11}$$

$$\vec{w} = \text{sign}(\phi_0) \frac{\nabla \phi_d}{|\nabla \phi_d|}$$
where $\vec{w}$ is the advection velocity, zero only at the interface, positive unity $\forall \phi_0 > 0$ and negative unity $\forall \phi_0 < 0$. However, in accordance with property smearing, the signed distance function, $\text{sign}(\phi_0)$, and hence the advection velocity, is also smeared out across the interface for numerical stability,

$$\text{sign}(\phi_0) = \begin{cases} 
\frac{-1}{\epsilon} + \frac{1}{\epsilon} \sin \left( \frac{\pi \phi_0}{\epsilon} \right) & |\phi_0| < \epsilon \\
1 & \phi_0 > \epsilon 
\end{cases}$$  \tag{2.12}

Equation (2.11) is a non-linear hyperbolic, where $\vec{w}$ gives the direction of characteristic curves, which are outward pointing normals on each side of the interface. Further discussion on the re-distancing equation is continued in Section 3.4.

2.3 Finite Element Discretization

2.3.1 Streamline Upwind Petrov Galerkin (SUPG) Formulation

The underlying formulation of PHASTA is based on the finite element method (FEM). FEM employs a weighted residual formulation, Galerkin method, where the weighting and interpolation functions belong to the same functional space over the computational domain, $\Omega$, i.e., Sobolev space, defined as, [65],

$$H^1_0(\Omega) = \left\{ v(\Omega), v \in L^2(\Omega), \nabla v \in L^2(\Omega), v|_{\Gamma_D} = 0 \right\}$$  \tag{2.13}

where $\Gamma_D$ represents the boundary of the domain where Dirichlet boundary conditions are specified. Note that in FEM the weighting functions, $v(\Omega)$, necessarily vanish at Dirichlet boundaries, emphasized by the zero subscript in the above equation. $L^2(\Omega)$ is the functional space with L2 norm defined over $\Omega$,

$$L^2(\Omega) = \left\{ u(\Omega), \int_{\Omega} |u(\Omega)|^2 \, d\Omega < \infty \right\}$$  \tag{2.14}
Thus, Eq. (2.13) implies that the functional space chosen for FEM has both the weighting functions and its derivatives in $L^2(\Omega)$ space.

Standalone Galerkin methods are highly successful for diffusion (parabolic) problems, yielding a symmetric matrix system from the spatial discretization. For convection dominated problems, however, the Galerkin formulation yields spurious oscillations in the flow. An analogy between the standard FEM and finite volume method reveals its equivalence to a second order central difference discretization scheme, as applied to the latter. This discretization choice does not yield a monotone, or a total variation diminishing (TVD) scheme in time [66], which results in the manifestation of unphysical oscillations for convection dominated flows, especially near Dirichlet boundaries. For finite volume methods the remedy is the construction of upwind schemes, which consider the local direction of velocity, yielding TVD schemes. Analogous to upwind schemes, streamline upwind Petrov-Galerkin (SUPG) was conceptualized by Brooks et al [67] for FEM, wherein additional weights are imposed on the standard Galerkin weighting function to favor the upwind direction. In 1D the Petrov-Galerkin weights are envisioned as shown in Figure 3.

Figure 3: Comparison of 1D Petrov-Galerkin and standard Galerkin weighting functions, as shown by Brooks et al [68].
The new weight function is formulated as,
\[ \tilde{v} = v + \tilde{p} \]  \hspace{1cm} (2.15)

where, \( v \) is the weight owing to the standard Galerkin formulation, which is continuous across element boundaries and \( \tilde{p} \) is the weight introduced to skew the overall weighting function in the upwind direction. Note that \( \tilde{p} \) acts only on element interiors, thus, not affecting continuity conditions across the element interface.

For illustration, weak formulation of the general advection-diffusion equation,
\[ \frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = \nabla \cdot \mu \nabla \phi + f \]  \hspace{1cm} (2.16)
is given by,
\[ \int_{\Omega} \left( \frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi - f \right) v \, d\Omega + \int_{\Omega} \mu \nabla \phi \cdot \nabla v \, d\Omega + \int_{\Gamma_N} \mu v \nabla \phi \cdot \mathbf{n}_N \, d\Gamma \]
\[ + \sum_{e} \int_{\Omega_e} \tau_s \vec{u} \cdot \nabla v \left( \frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi - \nabla \cdot \mu \nabla \phi - f \right) \, d\Omega = 0 \]  \hspace{1cm} (2.17)

where, the first three terms result from the standard FE Galerkin formulation, while the third term, evaluated element wise, is the SUPG stabilization term. The third integral, resulting from the Laplacian term, is over the Neumann boundaries and is zero if only Dirichlet boundary conditions are specified. \( \tau_s \) is an adjustable stabilization parameter, a function of the local Peclet number (see Whiting [54] for exact definition). The dot product, \( \vec{u} \cdot \nabla w \), in the SUPG term corresponds to the skewed weight, \( \tilde{p} \), in Eq. (2.15). Owing to weighing in the direction of local convection velocity, SUPG yields minimal cross-wind diffusion as elucidated by Brooks et al [68]. Note the weak formulation for the advection, Eq. (2.5), and re-distancing, Eq. (2.11), equation is also
encapsulated by Eq. (2.17), albeit they lack the integrals due to the Laplacian term (second and third terms). Finally, it is important to note that the SUPG construction is multiplied by the strong form residual of the original advection-diffusion PDE, evaluated pointwise at the Gauss quadrature integration points. This ensures that the SUPG stabilization is consistent with the original governing equation (i.e., the term vanishes as the approximation approaches the exact solution).

2.3.2 Pressure Stabilization for Incompressible Navier-Stokes Equation

For the incompressible Navier-Stokes equations the approximating polynomials for pressure and velocity have to be chosen carefully, such that the Brezzi-Babuska or the inf-sup condition is satisfied (for details refer to [69]). In the context of FEM the problem can be better explained by considering the discretization of steady incompressible Stokes problem,

\[ \mu \nabla^2 \vec{u} - \nabla p + \vec{f} = 0 \]
\[ \nabla \cdot \vec{u} = 0 \]  

(2.18)

Weak formulation and subsequent expansion of the linear finite element basis yields a matrix system given by (details on the process of construction can be found in Gresho et al [70]),

\[
\begin{bmatrix}
K & G \\
D & 0
\end{bmatrix}
\begin{bmatrix}
\vec{u} \\
\vec{p}
\end{bmatrix}
=
\begin{bmatrix}
\vec{f} \\
0
\end{bmatrix}
\]  

(2.19)

where \( K \) is the stiffness matrix which is always of full rank and symmetric positive definite (SPD), owing to the finite element basis. \( G \) and \( D \) are the matrices resulting from the discrete gradient and divergence operators, respectively. Note that \( G = D^T \) and \( \vec{u}, \vec{p} \) are the vector of coefficients, for velocity and pressure respectively, resulting from the approximating polynomials, while \( \vec{f} \) is a similar vector resulting from the approximation of the forcing function. The above matrix system belongs to a special class of linear algebra problems, called the saddle-point problems [71]. The matrix system on the left-hand side is of full rank, and hence invertible, only if \( G \) (and \( D \)) is of full rank.
rank. This, consequently, puts a constraint on the finite element spaces that can be selected for $\mathbf{u}$ and $p$, described mathematically as the inf-sup condition. Gresho et al [70] present an extensive exposition of the inf-sup condition and the allowable finite element interpolation spaces (see Appendix A.1 for further discussion). Here, it suffices to note that equal order interpolation for velocity and pressure yield a singular matrix system, thus making them an infeasible choice. Although viable mixed interpolations exist which produce a full rank matrix, they require the construction of an extremely complex code, severely limiting their applicability to complex geometries (Aside: mixed interpolations are analogous to a staggered grid formulation for finite volume methods [72]).

Through the use of bubble functions, Brezzi et al [69] showed that the selection of equal order interpolation for pressure and velocity for the solution of Navier-Stokes equations lead to residual terms. These residual terms can be effectively countered using appropriate stabilization terms. A detailed mathematical analysis for the functional form of stabilization terms is given by Franca et al [73]. Referring Eq. (2.24), the stabilization terms force the matrix system to be of full rank,

$$
\begin{bmatrix}
K & G \\
D & -S
\end{bmatrix}
\begin{bmatrix}
\mathbf{u} \\
\mathbf{p}
\end{bmatrix} = \begin{bmatrix}
\mathbf{f} \\
0
\end{bmatrix}
$$

(2.20)

where $S$ is the discrete operator resulting from the pressure stabilization term. Analogous treatment in finite volume method for stabilization of the pressure field in collocated (equal order interpolation) grids was established by Rhie and Chow [74].
2.3.3 Discretization of Navier-Stokes equations in PHASTA

Narrowing discussion to the particular formulation of the Navier-Stokes equation in PHASTA, pressure stabilization is achieved by adding an additional term to the weak form of the incompressibility constraint (Eq. (2.1)),

\[
\int_{\Omega} (\nabla \cdot \mathbf{u}) v \, d\Omega + \sum_{e} \int_{\Omega_e} \tau_{PSPG} \nabla v \cdot \mathbf{L} = 0 \tag{2.21}
\]

Here, again, the construction of the stabilization term is performed elementwise using piecewise functions. This formulation, conceived by Tezduyar [75], is referred as the pressure stabilizing Petrov Galerkin (PSPG) method. \( \tau_{PSPG} \) is a stabilization parameter and \( \mathbf{L} \) is the strong form residual of the momentum equation, (2.2), evaluated at each numerical quadrature point,

\[
\mathbf{L} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nabla \cdot \mathbf{\tau} - \mathbf{f} \tag{2.22}
\]

The SUPG formulation of the Navier-Stokes momentum equation, as given by Tezduyar [75] and used in PHASTA, is,

\[
\int_{\Omega} \left[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \mathbf{f} \right) v + (-p \delta_{ij} + \mathbf{\tau}) \nabla v \right] d\Omega \tag{2.23}
\]

\[
- \int_{\Gamma} (-p \delta_{ij} + \mathbf{\tau}) v \cdot \mathbf{n} \, d\Gamma
\]

\[
+ \sum_{e} \int_{\Omega_e} \tau_{SUPG} (\mathbf{u} \cdot \nabla v) \mathbf{L} \, d\Omega
\]

\[
+ \sum_{e} \int_{\Omega_e} \tau_{LSIC} (\nabla v) (\nabla \cdot \mathbf{u}) \, d\Omega = 0
\]

Note that the weighting function, \( v \), for the momentum, Eq. (2.23), and continuity, Eq. (2.21) equations are the same. The first two terms in Eq. (2.23) arise from the standard Galerkin formulation. The boundary integral term in the second line results from application of the Gauss
theorem on the pressure and viscous term which reduces the restriction on the approximating polynomials to be twice differentiable. The SUPG stabilization term in the third line introduces appropriate artificial diffusion to achieve upwinding with minimal crosswind diffusion. The LSIC (least squares on incompressibility constraint) stabilization term in the fourth line was introduced by Tezduyar et al [76], responsible for providing additional stabilization of the pressure field for high Reynolds number cases.

In PHASTA the stabilization parameters, \( \tau_{SUPG} \) and \( \tau_{PSPG} \) are identical. For exact definitions of the stabilization terms and parameters, including \( \tau_{LSIC} \), refer to Whiting et al [77]. In Eqs. (2.2) and (2.23) the non-linear convection term in the momentum equation is considered in the advection form. Alternate construction of the non-linear term are discussed in Gresho et al [70]. Each yields a different discrete operator, offering certain unique properties. They are enumerated below, including the advective form:

- **Advective form** \( \rightarrow (\vec{u} \cdot \nabla)\vec{u} \): Does not conserve linear momentum or kinetic energy. Shows instabilities in the inviscid limit. Easiest construction of the discrete operator.
- **Divergence form** \( \rightarrow \nabla \cdot (\vec{u}\vec{u}) \): Conserves global linear momentum but not kinetic energy.
- **Rotational form** \( \rightarrow \frac{1}{2} \nabla (\vec{u} \cdot \vec{u}) - \vec{u} \times \nabla \times \vec{u} \): Conserves global linear momentum and kinetic energy.
- **Skew-symmetric form** \( \rightarrow \frac{1}{2} (\vec{u} \cdot \nabla)\vec{u} + \nabla \cdot (\vec{u}\vec{u}) \): Conserves global linear momentum and kinetic energy. Yields the most expensive discrete operator.

To fully comprehend the differences in the behavior of the discrete operator from each formulation requires a plunge into the, rather esoteric, detailed eigen solution analysis (see Gresho et al [70] and cited literature therein). PHASTA offers the option of constructing the non-linear terms in advective and conservative forms, however the former is used for most applications. An
additional term which modifies the convective velocity was added by Taylor et al [78] to PHASTA to compensate for the lack of momentum conservation in the advective formulation,

\[
\sum_e \int_{\Omega_e} (\vec{u}_m \cdot \nabla \vec{u}) \nu + \bar{\tau}(\vec{u}_m \cdot \nabla \nu)(\vec{u}_m \cdot \nabla \vec{u}) \, d\Omega
\]  

(2.24)

where, \( \vec{u}_m = -\tau_{PSPG} \vec{L} \) is the supplementary velocity field. The second term in the above equation is added to stabilize this new advective term, with its corresponding stabilization parameter, \( \bar{\tau} \). Conservative discretization of the variables, obviously, does not require the above correction. Whiting et al [77] provides further details on this implementation.

Expansion of Eqs. (2.21) and (2.23) using the typical linear finite element basis functions and accumulating all terms yields corresponding residuals which can be expressed as,

\[
\begin{bmatrix} R_m \\ R_c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\]  

(2.25)

Or, more conveniently, the residual may be expressed as a function of velocity, acceleration (\( \vec{a} \)) and pressure coefficients evaluated at element nodes,

\[
R(\vec{u}, \vec{a}, p) = 0
\]  

(2.26)

The problem, thus, now reduces to finding the coefficients that minimize the above residuals. Time integration in PHASTA uses the generalized \( \alpha \)-method introduced by Jansen et al [79]. Details of the time integration scheme is not presented here for brevity. Here, we focus on obtaining the solution to Eq. (2.26) within a single time step. However, it must be noted that the time integration scheme is tightly coupled with the method for minimizing the residuals, implemented in a predictor-multicorrector based algorithm. Equation (2.26) contains non-linear contribution from the advective term and, thus, it is imperative to linearize the residuals using
Newton’s iteration. Residual at a given step of the Newton’s iterative algorithm may be represented as,

\[ R(\vec{u}_{n+1}^{l}, \vec{a}_{n+1}^{l}, p_{n+1}^{l}) = 0 \] (2.27)

Linearization of \( R \) with respect to acceleration variables yields a matrix equation, which is analogous to the matrix system resulting from the linearized Stokes equation (2.20),

\[
\begin{pmatrix}
K^i & G^i \\
D^i & C^i
\end{pmatrix}
\begin{pmatrix}
\Delta \vec{a}_{n+1}^{l} \\
\Delta p_{n+1}^{l}
\end{pmatrix}
= -
\begin{pmatrix}
\vec{R}_{m}^{l} \\
R_c^{l}
\end{pmatrix}
\] (2.28)

\[
K^i \approx \frac{\partial \vec{R}_{m}^{l}}{\partial \vec{a}_{n+1}^{l}}
\]

\[
G^i \approx \frac{\partial \vec{R}_{m}^{l}}{\partial p_{n+1}^{l}}
\]

\[
D^i \approx \frac{\partial \vec{R}_{c}^{l}}{\partial \vec{a}_{n+1}^{l}}
\]

\[
C^i \approx \frac{\partial \vec{R}_{c}^{l}}{\partial p_{n+1}^{l}}
\]

which is evaluated for each pass of the predictor-multicorrector algorithm. The above are described as tangent matrices and contain linearized approximation of the directional derivatives. Deriving approximations to directional derivatives is extremely complex and special care is required for their evaluation. The directional derivatives used in PHASTA are detailed in Whiting et al [77].

Finally, the linearized system of equation is solved using the GMRES algorithm for the acceleration terms, \( \Delta \vec{a} \) and \( \Delta p \), for each Newton’s step (inner iterations). After a specified convergence criterion is satisfied, the solution is advanced to the next simulation time step.

2.4 Chapter Summary

The discussion in this chapter gives a comprehensive view of the numerical method in PHASTA for simulating both single phase, Navier-Stokes equation, and two-phase flows, in which
case two additional transport equations are also solved including the level-set advection and the re-distancing equation. PHASTA’s specific finite element formulation, SUPG for upwinding and PSPG for enforcing the incompressibility constraint, is explained and the resulting weak form and subsequent matrix operations are specified. In addition, the SUPG formulation for the general advection-diffusion equation is also presented, which applies both to the level-set and its re-distancing equation.
Chapter 3: Enabling DFFB Simulations

Large scale simulations running on massively parallel supercomputers, which constitute the major objective of current research, pose several problems for their successful execution and subsequent, or in-situ, post-processing and data analysis. Major challenges with the simulations performed herein with PHASTA were, understandably, of a logistical nature, which required efficient data management code, either integrated as subroutines within PHASTA using advanced MPI libraries or developed as separate programs capable of handling large volumes of data. Further, initial and boundary conditions, representative of post-LOCA reactor conditions, were made feasible for both the single-phase and two-phase simulations by several integrated subroutines also requiring consideration of efficient implementation such that they do not deteriorate the scalability of the pristine code significantly. Two-phase simulations introduced additional challenges with respect to stabilization of the solver near fluid interfaces, owing to a density ratio of approximately 1000 across a relatively small length, $\epsilon$ (see Eqs. (2.4) and (2.7)).

This chapter documents all the code enhancements in PHASTA and auxiliary data processing programs, which were essential to the simulations and results presented in Chapter 4 and Chapter 5.

3.1 Boundary Condition Transient (BCT) Capability

DNS scale turbulent flow CFD simulations in reactor sub-channels are often performed on relatively long domains computational domains with periodic boundary conditions across the axial ends of the domain [RW.ERROR - Unable to find reference:1612] ($x/D_h \gg 1$). With a large enough domain, such that the largest scale eddies are reasonably resolved, periodic boundaries can emulate infinitely long sub-channels and generate a fully developed turbulent flow profile. For the ensuing DFFB simulations, however, we are concerned with droplet interactions with the
spacer-grids and mixing vane structures (Figure 4). The presence of these internal structures and axially evolving droplet dynamics compromises longitudinal periodicity of the domain, irrespective of the length used for the simulations.

Figure 4: PWR sub-channel geometry with spacer-grid and mixing vanes. Boundary conditions are annotated. Periodic condition across axial boundaries is infeasible due to the presence of spacer-grids and mixing vanes.

Figure 5: Sub-channel without spacer-grids. Quasi-steady turbulent flow can be developed through the application of periodic boundaries across axial ends. Cross-section for capturing velocity data for primary domain marked in red.
To address the issue of specifying inlet boundary condition we use the, so called, boundary conditions transient (BCT) suite of tools, initially developed by Feng [81] for studying the drag and lift forces acting on bubbles in free shear flows. The tools are further developed and enhanced for adaptation to large scale simulations on supercomputers. Straightforward conception of the application of BCT can be summarized as capturing the fully developed turbulent flow profile on the auxiliary flow domain, shown in Figure 5, and applying to the inlet cross-section of the primary domain, Figure 4. Details of the process require careful consideration of the mesh partitions of primary domain, outlined below:

1. Generate primary mesh and split into desired number of partitions, say numpe, for production runs.
2. Identify and print the coordinates of all nodes at the inlet of primary mesh:
   - All mesh nodes at an axial distance of $|x - x_0| < \epsilon_t$ are marked. $x_0$ is the location of the inlet patch and $\epsilon_t$ is a small tolerance value, while $x$ is the x-coordinate of primary mesh.
   - Print all marked nodes on a given processor, myrank, onto a separate file → bct.dat.`myrank`
3. Using an external program, generate a probe file, xyzts.dat, which consists of all nodes in bct.dat.`myrank` files merged onto a single file.
4. Advance the simulation on the auxiliary domain to achieve quasi-steady turbulence for the same Reynolds number as desired for the primary domain.
5. Capturing velocity information in auxiliary domain:
- Identify the processor rank and element index in which each probe resides on the auxiliary domain. Store this mapping in an array, \( \text{constatptts}(\text{nproctspts}, 2) \). Done once before the time loop.

- Calculate the instantaneous velocity at the probe location. Stored in \( \text{varts}(\text{nproctspts}, \text{nfield}) \).

- Assemble data from \( \text{varts} \) array on all processors and output to a single file (using MPI parallel I/O).

6. Post-process the data generated from step 5, using external programs. Here, it is imperative to map the respective node data to the processor id, \text{myrank}, of the primary mesh. Print the data on files, labeled corresponding to processor ids of primary mesh → \text{bctInput/nstep/bct.dat.'myrank'}

7. Run the simulation on the primary mesh. Data is read from \text{bctInput/nstep/bct.dat.'myrank'} and stored periodically, with a specified \( iBC{T}\text{step} \), on a specific array structure, \( BCt(\text{nptsmx}, iBC{T}\text{step}, \text{nfield}) \). Transient data in \( BCt \) is suitably interpolated in time and assigned to the corresponding node in primary domain. \( \text{nptsmx} \) is the number of nodes on \text{myrank} and \( \text{nfield} \) is the number of fields captured (3 velocity + \( \Delta t_a \)).

For the two-phase simulations shown in Chapter 5, the primary mesh was split into 131,072 partitions (\text{numpe}). The inlet cross-section of the domain is, thus, split into reasonably large number of processors, with random processor ids. The process of writing coordinate data in step 2 and reading the transient data in step 7 (see A.2.1 ), are performed independently by each processor, not requiring any inter-processor communication for the primary mesh. For the
geometry configuration shown in Figure 4, identification of mesh nodes that lie on inlet cross-section is trivial. Since all inlet nodes lie on the plane $x_0$, they can be identified using:

$$|x - x_0| < \epsilon_t$$  \hspace{1cm} (3.1)

where $\epsilon_t = 10^{-8}$ suffices. More advanced implementations for marking inlet boundaries are also possible using the surfID boundary condition available in SimModeler, which is the pre-processing tool used with PHASTA [82]. On the auxiliary domain, assuming the mesh consists of all tetrahedral elements, the element in which a given probe, $(x_p, y_p, z_p)$, resides is identified by computing its Barycentric coordinates with respect to the element,

$$\begin{bmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3
\end{bmatrix} = \begin{bmatrix}
x_1 - x_4 & x_2 - x_4 & x_3 - x_4 \\
y_1 - y_4 & y_2 - y_4 & y_3 - y_4 \\
z_1 - z_4 & z_2 - z_4 & z_3 - z_4
\end{bmatrix}^{-1} \begin{bmatrix}
x_p - x_4 \\
y_p - y_4 \\
z_p - z_4
\end{bmatrix}$$  \hspace{1cm} (3.2)

where $x_{1-4}, y_{1-4}, z_{1-4}$ are the coordinates of tetrahedron vertices and $\lambda_{1-3}$ are the corresponding Barycentric coordinates. The condition for the probe to be inside the volume is,

$$0 < \lambda_1, \lambda_2, \lambda_3 < 1 \& \lambda_1 + \lambda_2 + \lambda_3 < 1$$  \hspace{1cm} (3.3)

The value of instantaneous fields is computed at the element level through the interpolating polynomial (or basis) functions,

$$\phi_p = \sum_{i=1}^{4} \phi_i B_i$$  \hspace{1cm} (3.4)

where, $\phi$ represents any scalar and $B_i$ are the standard finite element basis functions. The subroutine for the above operation is included in Appendix A.2.4. The most expensive part of entire process is writing the collected data to file. This requires a more detailed explanation and is, therefore, addressed in Section 3.2
Through further post-processing, the collected data from the auxiliary domain is segregated into separate files corresponding to the processor rank on primary domain where the node lies in. The necessary array structures for storing this data for primary domain simulation were specified in an external Fortran module, included in A.2.2. The transient data is split into \( iBCT \text{step} = 200 \) time steps, which provided a reasonable memory allocation size for the \( BCt \) array. The routine for specifying the boundary condition, \( BCint \), is called at every simulation time step from the primary time loop. See Appendix A.2.3 for the implementation of \( BCint \) routine. Linear interpolation maps the instantaneous velocity at each node (or probe from the perspective of auxiliary domain) from the time step resolution of the simulation in auxiliary mesh, \( \Delta t_a \), to the time resolution of simulation in the primary domain, \( \Delta t_p \). \( \Delta t_a / \Delta t_p = 2 \) was used as the maximum ratio for capturing velocity from the auxiliary mesh.

### 3.2 MPI Sub-communicators and MPI Parallel I/O

File I/O remains the most expensive operations for large-scale computations. For this reason the simulation restart files are, often, sparingly written to the disk [83]. This, for obvious reasons, imposes constraints on the post-processing analysis and the meaningful information that can be extracted from the simulations. In order to capture the turbulent velocity profile without loss of spatial resolution, as discussed in the previous section, all the computational nodes at the inlet cross-section of the primary mesh are used as velocity capturing probes on the auxiliary mesh, shown in Figure 6. Data must be captured at every time step of the auxiliary domain simulation at each of these probes, to avoid any loss in the temporal resolution. This results in very large I/O buffers to be written to disk at each simulation step, which, understandably, severely exacerbates the overall computational cost of the code. Further, as will be discussed in greater detail in Chapter 4 and Chapter 5, to extract temporal statistics for a comprehensive analysis of turbulence flow.
features, a yet greater amount of probes are required, distributed across the axial length of the primary domain ($\sim 10^5$).

Figure 6: Mesh nodes (29,389 in total) at the inlet cross-section of the primary mesh, used as the virtual probes to capture instantaneous velocity in the auxiliary domain.

To address these, otherwise inhibiting, logistical problems, advanced MPI libraries were implemented in PHASTA to greatly enhance the speed of write operations. The implementation involves a combination of MPI Sub-communicators and MPI parallel I/O. The ensuing design of the pertinent algorithm is based on the following deliberations:

- All processors writing their probe data to separate files is too expensive. The average number of probes that reside on a given processors are too low ($<10$). The I/O overhead dominates in this situation. Further, post-processing of thousands of separate files using this method is unwieldy and prohibitive.

- A single processor (say master) collecting data at each time step from all other processors and writing to single file is also prohibitive. The buffer required on the master processor
to receive information is too large, even exceeding the total memory available on a compute node for large number of probes. Further, the I/O buffer from master to write to disk is also too large, making the process extremely slow.

- An optimal mechanism is desired to collect data from a reasonable number of processors, labeled hereafter `nvartsdiv`, onto a designated number of processors responsible for writing to disk, labeled hereafter `nvartsproc`.

- All the `nvartsproc` processors must write to a single file, to make the following post-processing easier.

The algorithm is represented by Figure 7, wherein the boxes represents the processors and are marked with their global id numbers, starting from zero. On initiation all the processors are encompassed by the MPI_COMM_WORLD communicator. Before the main time iteration loop this communicator is split into two sets of groups. The first set consists of `nvartsproc` number of sub-groups, represented by each row in Figure 7. Data is collected on an array defined on the first processor in each of these groups though intra-broadcast operations (highlighted in red). The second set consists of just one group, responsible for writing the data to the disk. It includes all processor ranks in the first column in Figure 7. The essential MPI calls for defining these two sets of groups and their corresponding communicators are shown in Code Excerpt 1.
call MPI_COMM_GROUP(MPI_COMM_WORLD, worldgroup, ierr)

c Groups and Communicators for data collection

! call MPI_GROUP_INCL(worldgroup, nvartsdiv, nvartsranks, 
&             nvartsgroup, ierr)

! call MPI_COMM_CREATE(MPI_COMM_WORLD, nvartsgroup, 
&             nvartscomm, ierr)

c Group and communicator for writing to disk

! call MPI_GROUP_INCL(worldgroup, nvartsproc, iwriteranks, 
&             iwritegroup, ierr)

! call MPI_COMM_CREATE(MPI_COMM_WORLD, iwritegroup, 
&             iwritecomm, ierr)

Code Excerpt 1: MPI calls for defining subgroups and corresponding communicators

Figure 7: Representation of the splitting process of MPI_COMM_WORLD into sub-groups for data collection, represented by each row, and writing data to disk, represented by the first column.

The entire purpose of defining sub-communicators is the subsequent ease of broad casting
data among the members of the group. Further, the number of probes residing in any given
processor is variable. To collect the data on the first rank of the sub-group it is imperative to
initialize a buffer on this rank (labeled \textit{vartsout}), compute the size of the buffer (labeled
*vartsbuffer* to be received from all other processors in the group and calculate the exact location in the buffer where data will be placed (stored in *idispranks*). The essential MPI calls for these operations are included in Code Excerpt 2.

```c
Gather the number of probes on each processor in sub-group
    call MPI_ALLGather(nproctspts, 1, MPI_INTEGER,
            & nproberanks, 1, MPI_INTEGER, nvartscomm, ierr)

Gather data from all processors in sub-group on a buffer defined on the first rank
    call MPI_Gatherv(vartsbuffer, nproctspts*numvarc,
            & MPI_DOUBLE_PRECISION, vartsout, nproberanks,
            & idispranks, MPI_DOUBLE_PRECISION, 0,
            & nvartscomm, ierr)
```

**Code Excerpt 2: MPI calls for collecting data from members in a sub-group**

The *iwritecomm* group facilitates operations for writing the data to disk. Only the processors in this group are assigned visibility of the output (*vartsfile*) file, representation shown in Figure 8. The number of probes from each contributing processor is variable, therefore, it is necessary to explicitly specify the location in the output file where each processor will subsequently write. Finally, the MPI_FILE_WRITE_AT command directs all the processors to write onto the output file. All essential MPI calls relevant to the write operation are included in Code Excerpt 3.

![Figure 8: Representation of *iwritecomm* group and parallel write operation to *vartsfile*](image)

47
c Parallel file open by all ranks in iwritecomm
   if(MPI_COMM_NULL .ne. iwritecomm) then
      call MPI_FILE_OPEN(iwritecomm,fvartsb,
     &   MPI_MODE_WRONLY + MPI_MODE_CREATE, MPI_INFO_NULL,
     &   vartsfile,ierr)
   endif

c Calculate offset location for each processor in iwritecomm
   if(MPI_COMM_NULL .ne. iwritecomm) then
      call MPI_ALLGATHER(isum*realsize, 1, MPI_INTEGER,
     &   iwriteoffset, 1, MPI_INTEGER, iwritecomm,
     &   ierr)
      call MPI_ALLREDUCE(isum*realsize, iwriteinc, 1,
     &   MPI_INTEGER, MPI_SUM, iwritecomm, ierr)
      offset = 0
      if(myrank .ne. master) then
         do i = 1, nvartsproc
            if(i .le. myrank/nvartsdiv) then
               offset = offset + iwriteoffset(i)
            endif
         enddo
      endif
      iwrittenum = isum
   endif

c Write to a single file on disk
   if(MPI_COMM_NULL .ne. iwritecomm) then
      call MPI_FILE_WRITE_AT(vartsfile,
     &   offset,vartsout,
     &   iwrittenum,
     &   MPI_DOUBLE_PRECISION,MPI_STATUS_IGNORE,ierr)
      offset = offset + iwriteinc
   endif

Code Excerpt 3: MPI calls for collecting data from members in a sub-group.

Table 3: Time taken for writing data to disk for 29,389 probes and one time step.

<table>
<thead>
<tr>
<th>Number of processors selected for recording data (nvartsproc)</th>
<th>CPU Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without Probes</td>
<td>1.184</td>
</tr>
<tr>
<td>Original Code (1 processor)</td>
<td>429.39</td>
</tr>
<tr>
<td>10</td>
<td>90.24</td>
</tr>
<tr>
<td>171</td>
<td>55.546</td>
</tr>
<tr>
<td>1000</td>
<td>58.267</td>
</tr>
<tr>
<td>5000</td>
<td>83.436</td>
</tr>
</tbody>
</table>

Table 3 shows the performance of the above implementation, measured by CPU time to complete one time step of the simulation, for writing data to the disk with different number of
This analysis was conducted on an auxiliary mesh with ~17 M element mesh on the Cetus supercomputer at Argonne National Lab, running on 256 BG/Q nodes with the mesh partitioned into 16,384 parts. Optimum performance was seen when the probes were distributed on $\sqrt{ntspts}$ processors, where $ntspts$ is the total number of probes. For future usage it is, however, recommended that $nvartsproc = 2^n \approx \sqrt{ntspts}$. The performance increase in contrast to a single processor writing to file is significant, emphasizing the importance of MPI I/O for large scale simulations. The decrease in computational time compounds for simulations running for a larger number of steps, since data is recorded at every simulation step. Table 4 shows the performance comparison of I/O operation using 171 processors against a single processor writing to file, for one hour of simulation time. The penalty factor to the code for each case is also shown with respect to a simulation where no data is recorded. As the number of probes increase the penalty to the code increases exponentially with a single processor, however, with 171 processors writing in parallel, the penalty increase is very gradual. For capturing velocity profile at the spatial resolution of the mesh (28389 probes), the write operation with a single processor was prohibitive, advancing only nine time steps in an hour. With the implementation of MPI I/O the number of time steps were increased by a factor of 160.

Table 4: Number of time steps performed during 1 hour of wall-clock time on Cetus.

<table>
<thead>
<tr>
<th>Number of probes</th>
<th>Single Processor</th>
<th>171 Processors</th>
<th>Speed up ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time steps</td>
<td>Penalty factor</td>
<td>Time steps</td>
</tr>
<tr>
<td>0 (No recording)</td>
<td>2887</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5000</td>
<td>1267</td>
<td>2.28</td>
<td>2027</td>
</tr>
<tr>
<td>10000</td>
<td>75</td>
<td>38.5</td>
<td>1920</td>
</tr>
<tr>
<td>29839</td>
<td>9</td>
<td>320.78</td>
<td>1440</td>
</tr>
</tbody>
</table>
3.3 Droplet Injection Routine for DFFB Simulations

In addition to specifying inlet turbulent velocity profile, it is also required to introduce droplets at the upstream location of the spacer grid structure for simulating DFFB conditions. An ad hoc droplet injection routine was, therefore, added to PHASTA, which manipulates the local level-set field to introduce new droplets periodically in the domain. For context, it is worthwhile to recall Eq. (2.3), used for specifying properties in the computational domain. To regard the volume enclosed by the zero contour \( \phi < 0 \) as a droplet in Figure 9, for instance, impose \( \gamma_2 = \{\rho_l, \mu_l\} \), while \( \gamma_1 = \{\rho_g, \mu_g\} \) in Eq. (2.3). Given the coordinates of the center, spherical droplets can be easily initialized by manipulating the local level-set field in the domain,

\[
\phi(\vec{x}) = \min \left( \phi(\vec{x}), \sqrt{(x - x_s)^2 + (y - y_s)^2 + (z - z_s)^2} - r_s \right)
\]

where \((x_s, y_s, z_s)\) are the coordinates of the ‘seed’ point for the droplet and \(r_s\) is the desired radius.

![Figure 9: A simple 2D example to illustrate property assignment using the level-set contour field, \(\phi\).](image)

It is required to initialize droplets at the upstream location (with respect to spacer-grid) in the primary domain (Figure 4). To achieve this, ‘seed’ points is selected, based on a uniform
random distribution, on the inlet cross-section of the primary domain. All mesh node points at the inlet cross-section are considered as inputs to the random sampling routine, for choosing a single seed point. However, since the cross-section is partitioned into numerous processors, assembling the inputs for random seed point selection poses a challenge. The detailed algorithm for the process is outlined below:

- **Pre-processing (before primary time loop):**
  - Initialize the intrinsic random number generator in Fortran. It requires a random seed to initialize specified as,

    ```fortran
    call random_seed()
    allocate(seed(1))
    call system_clock(COUNT=clock)
    seed = clock + 37 * (myrank+1)
    call random_seed(PUT = seed)
    ```

  - All relevant data structures are defined in a global module, *injectorData*, included in Appendix A.3.1. Identify the coordinates on the inlet cross-section, to be used as ‘seed’ points. Owing to the orientation of the inlet (perpendicular to x-axis), this operation is trivial, however more complicated implementations are feasible using *surfID* (see discussion in section 3.1 for generating probes). Seed points that are too close to the wall, as shown in Figure 10, are deleted. For all simulations in Chapter 5, this offset distance from the wall is $1.25r_s$. The index of the coordinates that qualify as the seed nodes on a given processor are stored in an array in the module, viz., *seednodes*. Note that the visibility of this array is limited to a single processor. Further, all processor ranks which have at least one active seed are considered active; their ids are collected (MPI_GATHER) and then broadcast to all processors (MPI_BCAST), stored in *availproc* array. The subroutine, *identifyInjectorPatch*, performs all the above operations, included in Appendix A.3.2.
If the simulation is being restarted, the history information of the injector is read from file and stored in `activenodes` arrays (read further for more information).

![Contour map](image)  
**Figure 10:** Contour map showing division of nodes on the inlet cross-section among processors. Also shown, using the black demarcation line, regions close to wall not considered as ‘seed’ area for introducing droplets.

- **Injector Operations (Inside primary time loop):**
  - For the first time step of the simulation, minimum number of droplets are initialized using an input parameter, `minseeds`. A special data array, `activenodes(1:N,1:7)`, shared and synchronized among all processors keeps track of the ‘active’ seed points. $N$ is the total number of active seeds, while the second index of `activenodes` stores the initial coordinates of the seed, the initial velocity assigned to the droplet begot from the seed and the simulation time stamp when the seed is initialized.
  - As time advances, new seed points are introduced in the domain at periodic intervals, controlled by an input parameter `tperiodinj`. Thus, a new droplet is initialized when the following condition is satisfied,
\[ t - t_s^N \geq t_{\text{periodinj}} \]  

where, \( t \) is the simulation time and \( t_s^N \) is the time at which the last droplet was initialized. The algorithm for selecting a seed point (and deleting it) and adding it to the \textit{activenodes} array is outlined in Figure 11. After condition (3.6) is detected, the uniform random number generator selects a processor id from the list of \textit{availproc}. From the chosen processor, a point is again sampled randomly from the list of eligible \textit{seednodes}. The seed point is discarded if its distance from the nearest ‘active’ node is less than a specified length (here chosen as \( 3r_s \)). In case the seed is discarded, the selection process is repeated until a qualifying seed location is found. On successful selection, a user specified velocity, \( \vec{v}_i \), is assigned to the seed and the axial position is adjusted (by \( 2r_s \)), so that the resulting droplet is completely inside the computational domain. The coordinate and the velocity information along with the simulation time stamp are added to the top of the \textit{activenodes} array. Thus, the array will have the oldest seeds always stored at the last index. The selected processor broadcasts the \textit{activenodes} information to all processors and then a new droplet is initialized using equation (3.5). Note that this equation only changes the level-set contour field in the immediate vicinity of the seed point, therefore existing droplets are not affected by the initialization process. The subroutine to add seed point on \textit{activenodes} array is included in Appendix

- At each time step the algorithm also checks for potential de-activation of the last seed point in \textit{activenodes} array, condition shown in Figure 11. The seed is deactivated after it has advected a specified distance into the computational domain, estimated from its velocity at inception. For the simulations herein this distance was chosen arbitrarily to be \( 5r_s \). Deletion of the entry from \textit{activenodes} is straightforward, i.e., does not require inter-processor communication since all processors already share the same information.
Figure 11: Algorithm for adding and deleting ‘active’ seed points to the `activenodes` array.

The velocity assigned to the seed point, $\vec{v}_i$, is calculated from the desired collision Weber number, $W_{ec}$, for droplets, given by Eq. (1.12),

$$v_x = \sqrt{\frac{W_{ec} \sigma}{\rho_i 2r_s}}$$  \hspace{1cm} (3.7)

where, $\vec{v}_i = (v_x, 0, 0)$ is assumed to have a non-zero component only in the axial direction. Note that the flow field, as specified on the inlet cross-section, is highly turbulent. In practice, abruptly changing the velocity in the volume of the domain where new droplet is initialized and assigning liquid properties to it (increasing the density ratio by a factor of 1000), resulted in solver instability. To address this, the velocity was initialized to $\vec{v}_i$ in the region $\phi < 2\epsilon$ in the local vicinity of the droplet (see Figure 12). Blending $v_i$ with the initial velocity using an implementation similar to
Eq. (2.3) was also found to solve instability issue. Further, since the domain is periodic across lateral ends, care must be taken while reinitialization of level-set field using Eq. (3.5). Periodicity of the level-set field must be ensured, failing which subsequent level-set re-distancing iterations causes inexorable oscillations. For further details on the implementational nuances related to droplet injection, the reader is directed to the file, *incompressible/injector.f* [84].

![Figure 12: Velocity contours at the inception point of the droplets. The velocity inside the volume of newly initialized droplet (shown on right) is reset to \( \mathbf{v}_i \), while the velocity field outside the droplet is highly turbulent.](image)

**3.4 Local Time Stepping for Re-distancing Equation**

As briefly introduced in Section 2.2 the level-set function is initialized as a signed distance function. It is essential that the signed distance property is maintained throughout the simulation for accurate calculation of curvature, which couples the level-set advection with the Navier-Stokes equations. The re-distancing equation (2.11), formulated using a pseudo-time \( \tau \), is responsible for
restoring the signed distance property of the level-set field. The importance of this procedure is highlighted in Figure 13, featuring an initial circular level-set field advecting under the effect of a prescribed parabolic velocity profile. Without re-distancing equation, the calculation of curvature, and subsequently the surface tension force (Eq. (2.8)), would be error prone.

![Figure 13: Level-set field, advected by a parabolic velocity profile, without and with re-distancing performed after every advection step.](image)

Detailed exposition of the behavior of the re-distancing equation was presented by Russo et al [85], wherein they showed that \( n \) iterations of the re-distancing equation restored the distance field up to \( n\Delta t \) normal distance on either side of the interface. In practice 15-20 iterations of the re-distancing solve are generally performed, with a nominal CFL of 1-2 using an implicit solver, after the level-set advection step, to ensure that the signed distance field is corrected in the vicinity of the zero contour.

### 3.4.1 Challenges accompanying level-set re-distancing in large-scale simulations

#### 3.4.1.1 Volume loss due to re-distancing

The advection velocity for the re-distancing equation is formulated such that it is zero at the exact interface location (\( \phi = 0 \)) and directed along normal outside from the interface in either direction, with a unit magnitude. Thus, solution of the re-distancing equation, in the strong form, does not move the interface. In the numerical implementation of the equation, however, the velocity is smeared by means of the smoothed implementation of the sign function, equation
Irrespective of how sharp the smearing length is, subsequent discretization of the sign function results in a non-zero velocity at the interface. Therefore, the re-distancing equation has the tendency to move the interface in a preferential direction [86]. This problem is recognized and well documented in literature. It is the primary cause of mass loss with the level-set method, a long standing critique concerning the method’s applicability to two-phase flow problems [87]. Sussman et al [88] introduced a mathematical fix to this issue by imposing that the volume enclosed by the level-set remain constant across re-distancing iterations at any simulation step,

\[
\frac{\partial \int_{\Omega} H(\phi)}{\partial \tau} = 0
\]  

(3.8)

where \( H(\phi) \) is the Heaviside function, Eq. (2.4). This alleviates the volume loss issue but does not eliminate it entirely. Discrete implementation of Eq. (3.8), in the context of finite element method, was introduced in PHASTA by Nagrath et al [89].

More sophisticated implementations for two-phase flow have been introduced in literature, which are better at mass conservation. For instance, the conservative level-set formulation by Olsson [82], implemented in the context of finite volume method, uses the Heaviside function, instead of the signed distance field as the phase identifier. Thus, it is the Heaviside function which is advected by the underlying velocity field. The implementation, however, relies on maintaining a sharp gradient, or a shock, at the interface. An equation similar to the classic re-distancing equation is used to restore this sharp transition, which is smoothed out due to advection of the phase indicator function. The method is shown to yield excellent volume conservation properties over long time integrations. However, owing to the presence of discontinuity, the method is not amenable to the continuous Galerkin (CG) formulation.
Other techniques successful at preventing volume loss include alternate methods of restoring the distance field, not involving partial differential equation. The earliest of such methods, applicable to structured meshes was the fast march method for computing geodesics [90]. The fast march method, however, is extremely complicated to adopt for unstructured grids, with heterogenous elements and limited to second order accuracy. Recently, a direct re-distancing method was introduced by Greene et al [91], capable of achieving arbitrary order of accuracy, based on a Lagrange multiplier optimization algorithm. The method is especially suited for high order Galerkin projection methods, e.g., discontinuous Galerkin (DG) and spectral element methods (SEM). The disadvantage, however, is that the method is expensive as it involves Newton’s iteration to find the optimum solution for each $dof$ independently. Further, expensive inter-processor communication is required for distributing the information of the zero-contour. This raises reasonable concern for the scalability of the method and its feasibility for large-scale simulations.

3.4.1.2 Spurious interfaces in large domain

For simulations in long computational domain, where the characteristic length of the domain is significantly greater than the droplet or bubble diameter, the level-set method presents another challenge, especially when the flow is highly turbulent. Typically, it suffices to perform re-distancing iterations until the signed distance is reset upto $\epsilon$ distance from the interface. However, it was observed for turbulent simulations that not restoring level-set field completely in the peripheral regions of the domain results in the development of spurious interfaces over time. Arbitrary contortion of the level-set field due to the underlying flow solution results in the level-set value going negative. Wherever this situation occurs, surface tension forces also come into play, thus polluting the flow solution, eventually causing the solver to diverge. This affliction is
visually described in Figure 14, resulting from simulation in the primary domain with insufficient re-distancing. The simulation is initialized with a constant velocity throughout the domain and a turbulent velocity profile at the inlet, using the BCT capability described in Section 3.1. Severe deformations in the level-set field are highlighted in the figure, observed near the inlet where velocity field is turbulent. Note that once the level-set field gets contorted to the point that spurious interfaces appear, the interfaces persist thereafter, even if the number of re-distancing iterations are drastically increased to attempt correction of the distance field, since the re-distancing velocity is zero at the zero-contour.

An explanation for this phenomenon can be provided by recalling the properties of the re-distancing equation. As discussed before, the characteristics emanate from the zero contour in the normal direction, travelling at unit speed [85]. If the total time, $\Delta \tau$, of the re-distancing iterations is small such that the information conveying characteristic waves do not reach the peripheral regions, the level-set field in these regions never gets the information about the topography of zero-contour. The contour field in these regions is, therefore, left defenseless against whimsical manipulation by local turbulence, invariably resulting in excessive contortion.
3.4.1.3 Re-distancing near collision events

Another issue, pertaining the re-distancing equation, of significance to the ensuing DFFB simulations manifested during the collision of droplets with the spacer-grid structure. To describe the problem, consider the simulation setup shown in Figure 15. A 1\textit{mm} droplet is initialized at the upstream location of a rectangular obstacle, with its center being 1.55\textit{mm} from the incident face of obstacle. Width of the obstacle is 0.5\textit{mm}, same as the dimension of spacer-grid strap in the primary domain. The density ratio of the droplet to the gas is 1000, while the viscosity ratio is 48. A uniform velocity of 7 \textit{m/s} is specified at the inlet cross-section and the lateral faces are periodic. In the interior of the domain, including the droplet volume, the velocity is initialized to be 2 \textit{m/s}. Based on this velocity, the collision Weber number for the droplet, $W e_c = 52.14$, while the surface tension coefficient, $\sigma = 1/11 \text{ N/m}$. The simulation parameters were designed to simulate similar conditions as expected for the large-scale case in Chapter 5, albeit with the absence of turbulent inflow boundary condition. The re-distancing time-step for the case was fixed.
at $\delta \tau = 5 \times 10^{-6}$, equivalent to a maximum CFL of ~ 0.5. Both property smearing length and the sign function smearing length, for the re-distancing equation, were fixed at $\epsilon = 8.75 \times 10^{-2} \text{mm}$.

Figure 15: Simulation setup to test the dynamics of droplet collision for conditions similar to the large-scale representative DFFB simulations in Chapter 5.
Figure 16: Time evolution of the level-set field contours and velocity contours during droplet collision. Perturbations on the interface due to re-distancing results in unphysically high velocities.
Both level-set advection and re-distancing equations are initial value problems (IVP). Accordingly, there are no natural boundary conditions that can be imposed for either of the equations. The interface is mass less and advects only under the effect of the fluid velocity. Momentarily disregarding re-distancing; since the advection velocity near the walls is zero, the level-set contours ‘accumulate’ near the obstacle wall as the droplet approaches it, resulting in increasing level-set gradient near the incident wall. Recall that the gradient magnitude for a correct distance field is 1. Re-distancing of the level-set field in this region, between the incident wall and the droplet interface, has the effect of dilating the contours to restore the gradient magnitude. However, when the interface is very close to the wall, advection results in accumulation of contours and high gradients in the vicinity of the zero-contour. The sign function, given by Eq. (2.12), for the re-distancing equation therefore becomes smeared across an increasingly small spatial region. Re-distancing under these conditions results in unphysical perturbations near the interface, due to spatial discretization of \( \text{sign}(\phi) \). This phenomenon is illustrated in Figure 16.

The problem is further exacerbated due to subsequent action of surface tension force on the momentum equation, since the curvature corresponding to the perturbed regions will be extremely high. The momentum solve will, therefore, result in very high local velocity magnitude. The high velocity regions can be distinctly seen, next to sharp corners in interface, at \( t = 3.2 \times 10^{-4} \text{s} \) onwards (middle image), in Figure 16. From a physics perspective, note that perturbations on a droplet surface are unstable, and thus more difficult to resolve numerically, as compared to perturbations on a bubble surface, due to the stabilizing effect of the outer denser fluid in case of bubbles[92]. This dichotomy in the dynamics of droplets and bubbles can be explained mathematically using the Rayleigh-Taylor instability analysis [93].
3.4.2 Local Time Step (LTS) Implementation in PHASTA

Two of the problems described in the previous sections, especially peripheral level-set field contortion and interface perturbation during collision events, preclude the target representative DFFB simulations. This section describes the cure for these problems, i.e., local time stepping for the re-distancing solver and its implementation in PHASTA. The realization for the need of a local time step is based on the following deliberations:

- To prevent excessive level-set field contortion, such that spurious interfaces do not manifest, it is imperative to convey the interface information to the peripheral regions. Thus, re-distancing must be advanced for a sufficiently large total time, Δτ, after every level-set advection step. Re-distancing iterations account for a considerable amount of total computational time. Thus, a large CFL is desired such that the characteristic waves travel reasonable distance (comparable to the domain size) in 15-30 re-distancing iterations.

- Choosing a high re-distancing CFL results in severe mass loss. It is desirable to effectively ‘freeze’ the zero-contour during re-distancing iteration, similar, in principle, to the strategy described by Sussman et al [88].

- To avoid compounding perturbations near the interface during collision events a small time step, δτ, (or low CFL) is required for the re-distancing equation.

\[
|\nabla \phi| = 1
\]

(3.9)

The salvaging property of the re-distancing equation is that it is formulated in pseudo time, therefore each \textit{dof} can be evolved at a different rate. FEM-SUPG formulation of the re-distancing equation gives,
On expansion of the linear basis, \( \nu \), and the solution approximation, \( \phi_d \approx \sum_{i=1}^{4} \phi_i B_i \) (considering tetrahedral elements), we get a system of ordinary differential equations,

\[
M \frac{d\Phi_d}{d\tau} = R \Phi_d
\]  

(3.11)

where \( M \) is the mass matrix and \( R \) is the matrix obtained from the combination of convection, force and SUPG stabilizing term, while \( \Phi_d \) is the vector of expansion coefficients. Considering explicit forward Euler time integration (note that PHASTA also has implicit backward Euler time integrator, not shown here for ease of representation. Implementation details with respect to local time stepping are the same for implicit time integration),

\[
\Phi_d^{n+1} = \Phi_d^n + T(\Phi_d^n)_{CFL}M^{-1}R\Phi_d
\]  

(3.12)

where \( T(\Phi_d^n)_{CFL} \) is an array consisting of time multiplier corresponding to each dof. Note that linear finite element basis are nodal, i.e., the expansion coefficients \( \Phi_d^n \) are the values of the scalar at element nodes. For the following studies the time array is defined as,

\[
T(\Phi_d^n)_{CFL} = \begin{cases} \delta\tau_b \frac{CFL_{LTS}}{CFL_b} & |\Phi_d^n| < 1.5\varepsilon \\ \delta\tau_b & \text{otherwise} \end{cases}
\]  

(3.13)

where, \( CFL_b \) is either the user defined CFL for the re-distancing equation (and \( \delta\tau_b \) is the corresponding calculated time step) or the maximum of CFL values calculated for all elements in case a constant time step, \( \delta\tau_b \), is specified by the user. \( CFL_{LTS} \) is a user defined CFL value for the
local time step, imposed up to a distance of $1.5\epsilon$ on either side of the interface. The subroutine to calculate $T(\Phi_n^{i})_{CFL}$ in PHASTA is included in Appendix A.4.1. Further, an additional routine was added to implement Eq. (3.12), which makes use of the variable time array, included in Appendix A.4.2.
Figure 17: Time evolution of the level-set field contours and velocity contours during droplet collision with the LTS implementation. Perturbations on the interface do not compound with time.
Figure 17 shows the resolution of the collision event for the same simulation setup as introduced in section 0. The CFL for near interface (< 1.5ε) region was specified to a small value of 5 × 10⁻⁴, while the re-distancing time step in the rest of the domain was kept the same as the previous setup, δτ = 5 × 10⁻⁶. Twenty-two re-distancing iterations were performed after each advection step. It is clearly seen that the perturbations near the interface are stable over time from Figure 17, while preserving the distance field quite well throughout the simulation. It should be emphasized that introducing a local time-stepping (LTS) mechanism for re-distancing does not alter the physics, i.e., the momentum or level-set advection equation.

Another benefit of the LTS mechanism is its potential to ameliorate volume conservation problem. By definition, Equations (3.12) and (3.13) greatly reduce the movement of the zero contour across re-distancing iterations, thus providing superior volume conservation. As discussed in some length in Section 3.4.1.1, there have been several implementations in literature for addressing the issue of volume loss due to the application of re-distancing equation. However, most of these implementations focus on the treatment of spatial discretization. LTS provides an easy mechanism to achieve the same goal with the treatment of the temporal discretization. Demonstration of volume conservation with LTS is provided using the following setup. A 2 mm sphere was initialized at the center of a rectangular domain of 30 mm with periodic boundaries (lateral width was 5 mm). A uniform underlying velocity field of 1 m/s in the x-direction was specified. For all cases shown the advection time step was fixed, δt = 3 × 10⁻⁵ s. For the relevant cases, the sign function for the re-distancing equation was smeared across a distance of ε = 0.15 mm and 10 re-distancing iterations were performed after each advection step.

Figure 18 shows the state of the level-set contours, for four different cases, after the simulation is advanced for 5000 time-steps, equivalent to 5 complete flow throughs of the length
of the computational domain. The case setups include pure advection (Case 1), advection and a re-distancing CFL of 0.1 (Case 2), advection with a re-distancing CFL of 0.9 (Case 3) and advection with a re-distancing CFL of 0.9 with a local time-step CFL of $10^{-4}$ (Case 4). For each image the initial zero contour, a circle on the shown cross-section, is highlighted with a solid black line. Considerable mass loss and zero-contour deformation are observed even for the case with pure advection indicating that the mesh is relatively coarse. For Case 2 it is evident that the re-distancing CFL is very low, such that the re-distancing iterations are incapable of restoring the distance property in the peripheral regions. This is the same problem, described in section 3.4.1.2, which eventually leads to spurious interfaces under the effect of a turbulent velocity field. Case 3 proves that a large CFL for the re-distancing equation maintains the distance field in the peripheral regions, however, the volume loss for this case is severe. The contours of the level-set field for Case 4, as shown in Figure 18, are maintained to a proper distance field in the peripheral regions and the volume loss of the enclosed volume is also, relatively, benign. The mass loss for all cases was also recorded though the simulations and is shown in Figure 19. It is evident that LTS implementation preserves the enclosed volume well. Increase in enclosed volume for Case 3 is seen due to contortions of the far-field which, evidently, deforms the zero-contour, reinforcing the significance of adequate re-distancing.
Figure 18: Level-set contours, shown on the longitudinal cross-section plane, after advecting through 5 times the length of the domain, for four different case setups.
3.5 Chapter Summary

Successful representative simulations of the DFFB regime, discussed in Chapter 5, present considerable challenges with respect to inlet boundary conditions, re-distancing equation and its implementation on large domains and for resolving droplet collision events and the, widely recognized, volume loss problem during re-distancing iterations. This chapter details the new computational solutions that were implemented in PHASTA for the resolution of these problems as part of this thesis work. Large-scale data collection from the simulations were made viable through the implementation of MPI sub-communicators and MPI parallel I/O in PHASTA. Problems related to re-distancing in large domains and near the droplet interface were jointly addressed through the implementation of local time stepping mechanism for the re-distancing equation in PHASTA. This implementation was also shown to better conserve the volume of enclosed interfaces through re-distancing iterations, demonstrated by a simpler advection test case. Further, large scale implementation details of the droplet injection routine, required particularly for the DFFB regime simulations, are also detailed in this Chapter.
Chapter 4: Analysis of Single-phase Turbulence in a PWR Sub-channel

4.1 Introduction: Need for high-fidelity DNS Data

Developing a universal turbulence model remains an ever-elusive objective for researchers. In complicated geometries, more relevant to industrial applications, the inhomogeneous anisotropic nature of turbulence dictates the local flow features and hence the transport properties affecting momentum transfer, heat convection, etc. Moreover, as noted by Wilcox [95], owing to the transport of large eddies, the state of turbulence is not only a function of local strain rate, but also depends on the upstream history. In most CFD codes, commercial or open-source, two equation linear eddy viscosity RANS models remain the de-facto turbulence modeling approach. However, linear formulation of the Reynolds stress terms simply lacks the required dimensionality to capture secondary flow structures, as encountered in the curved geometry of a PWR sub-channel.

Various higher-order models exist in literature for RANS, broadly classified under two categories, viz., the algebraic stress models (ASM) and the Reynolds-stress models (RSM). The former class of methods has a simpler model-form; the anisotropic components of the Reynolds stress tensor are modeled by a non-linear constitutive relation, a function of the local mean strain rate and rotational rate tensor [96,97]. Determining the values of the coefficients in these correlations, however, remains a challenge, resulting in ad hoc, tinkered values for ‘fitting’ a particular application (e.g., [98]). On the other hand, in RSM the turbulent transport and pressure strain terms are explicitly modeled [99]. As a result, convection and diffusion of all terms of the Reynolds stress tensor, \( \langle u'_i u'_j \rangle \), are automatically accounted for, a necessary model form to account for upstream history effects. The resulting Reynolds stress transport equations are, however, formidable to model, involve questionable assumptions, have limited applicability, and are
plagued with stability and conservation issues while increasing the computational cost significantly.

Owing to shortcomings of the traditional RANS models, machine learning (ML) based methods have, in recent years, invited significant attention. Recently Chang et al [7] documented an extensive list of possible frameworks and their finer nuances, for a data-driven modeling approach. Their work concretizes the role of machine learning as a viable turbulence modeling alternative. Deep neural networks (DNNs) are purported to be universal approximators [100], thus they have the tantalizing potential to implicitly capture the underlying complexity of turbulent flows, given enough training data. The seminal work of Ling et al [101], for example, uses local mean and rotation rate tensors, with embedded invariance, to predict the Reynolds stress tensor terms. The method showed promising results in capturing the anisotropic behavior of turbulence, demonstrating that DNNs can offer similar dimensionality as the ASM or RSM models. Several researchers have later built upon this work (see e.g., [102,103]), adding more complexity to the input array provided to the DNNs. More recently, ML frameworks have also been used for other complex endeavors, such as boiling heat transfer prediction [104], mesh optimization [105] and coarse grid CFD error prediction [106].

Data collection, either from experiments or from high-fidelity simulations, poses a major bottleneck to the success of DNNs for turbulence modeling. Most of the aforementioned research on ML based modeling demonstrated their application to relatively simpler geometries, mostly 2D in nature. Extracting flow features from experiments, such as velocity and pressure gradients, with high spatial and temporal fidelity remains a challenge. Even with high fidelity DNS or LES simulations, data I/O significantly overshadows the scaling performance of the code, remaining the most time-consuming operations. For this reason, restart data from these simulations is
sparingly written to the disks. To extract the underlying statistical features of a turbulent flow, it is imperative to have data available at high temporal resolution. The limited availability of data precludes any data driven modeling of engineering flows (PWRs).

Using the MPI enabled data collection tools, introduced in Section 3.2 data is collected from the simulation in the primary domain (Figure 4) at high spatial and temporal resolution. The virtual probes are prudently located throughout the length of the domain to capture the bulk and near wall flow features. Extracting the instantaneous fluctuations in velocity, pressure and their gradients provided the requisite statistics to calculate mean velocity, Reynolds and anisotropic stress tensors at each of the probe locations. Further, an invariant analysis, following Lumley [107], using the eigenvalues of the Reynolds stress tensor, is presented which illuminates the evolution of the turbulence anisotropy along the axial length of the sub-channel. Similar in-depth analysis of the characterization of turbulence using the Lumley triangle was presented recently for a $5 \times 5$ rod bundle by Busco et al [108]. The data is archived and intended to be used for the development of data-driven turbulence models under the integrated research project (IRP)[109]. It should be noted that the simulation presented herein has the implicit assumption of periodic boundaries across the lateral faces, as opposed to the existence of crossflow in an actual PWR core, which remains a limitation of the current analysis.

This Chapter is organized as follows. Two simulations were performed, relevant to the operating conditions of the DFFB regime (see Section 1.3 , for bulk Reynolds numbers $Re_b = \{5000,11000\}$ (see definition in the following section). The simulation setup details are first described along with the data collection details. The first order statistics are compared with existing, and widely accepted, data in literature for DNS in a typical channel i.e., flow between parallel plates. Downstream axial evolution of the turbulence features is then discussed in detail
for $Re_b = 11000$ case. The emphasis on this Reynolds number value is because it’s near the higher DFFB operating spectrum. Further, the two-phase simulations in Chapter 5 were also performed for this Reynolds number. A short discussion of the remaining cases is presented at the end of the chapter.

4.2 Simulation Setup

Mesh used for all single-phase simulations in primary domain, Figure 4, is shown in Figure 20. The hydraulic diameter of the sub-channel, $D_h = 12.976 \text{ mm}$, given by,

$$D_h = \frac{4A_{in}}{P_w}$$  \hspace{1cm} (4.1)

where $A_{in}$ is the area of the inlet cross-section and $P_w$ is the wetted perimeter of the surface of the fuel rods. The bulk Reynolds number for the sub-channel is defined as,

$$Re_b = \frac{\rho u_{mean}^2 D_h}{\mu}$$  \hspace{1cm} (4.2)

It is important to emphasize that the internal structures, spacer-grids and mixing vanes, are not considered in the definition of the hydraulic diameter and bulk Reynolds number. For this reason, equation (4.2) is a better characterization for the accompanying auxiliary domain rather than the flow conditions in the primary domain. However, owing to the complex shape of the spacer-grids and mixing vanes, the above definition for $Re_b$ is also retained for characterization of flow in the primary domain [110]. For DNS simulations, it is essential to capture all the length scales of turbulence. This enforces cell size restrictions for near wall and bulk regions [111,112]. The same mesh is used for all cases with the first node point located at a wall distance of $\Delta y_w^+ = \{0.27, 0.53\}$ ($\Delta y = 10\mu m$), for respective $Re_b$ cases, on all wall surfaces including spacer-grids and mixing vanes, where,
\[ y^+ = y \frac{u_\tau}{v}; \quad u_\tau = \sqrt{\frac{\tau_w}{\rho}} \]  

(4.3)

\( y^+ \) is the dimensionless distance from the wall, normalized by the friction velocity, \( u_\tau \). \( \tau_w \) is the shear stress acting on the sub-channel rod walls, estimated from Darcy friction factor for a pipe domain of equivalent dimensions, \( f \) [113],

\[ f = 0.316 R e_b^{0.25}; \quad \tau_w = \frac{\rho u_{\text{mean}}^2 f}{8} \]  

(4.4)

Extended boundary layers are used near the walls, with a growth factor of 1.2. The mean bulk mesh resolution, \( \Delta y^+ = \{1.16, 4.61\} \). The mesh is unstructured, consisting of \( \approx 55.8 \) M purely tetrahedral cells. Mean velocity at the inlet cross-section is, \( u_{\text{mean}} = \{7.17, 15.77\} m/s \), while the kinematic viscosity of the fluid is \( 1.86 \times 10^{-5} m^2/s \). Total length of the domain, as shown in Figure 4, is \( 3.08 D_h \). The leading edge of the spacer grid block is at \( 0.23 D_h \), while the trailing edge of the mixing vanes is at a distance of \( 1.4 D_h \) from the inlet of the domain. The width of the spacer grid strap is 0.5 mm.

![Figure 20: Mesh for the primary domain consisting of \( \approx 55.8 \) million purely tetrahedral elements. Zoomed view shown for the boundary layer and bulk mesh near the inlet cross-section (left) and the longitudinal cross-section near the mixing vane location.](image)

Fully developed turbulent boundary conditions were specified at the inlet cross-section of the domain using the same strategy described in Section 3.1 The auxiliary domain, used for
capturing quasi-steady turbulence, has the same near wall and bulk mesh resolution as for the primary domain described above. The flow is developed to fully turbulent under a pressure gradient body force of \( \{77.03, 279.43\} \, kg/m^2 s^2 \) per unit volume, for the respective \( Re_b \) cases. Data was captured from the auxiliary domain using a constant simulation time size of \( \Delta t = \{5.0, 1.0\} \, \mu s \). The same constant time step size was used for corresponding simulations in the primary domain to avoid any loss in temporal or spatial resolution at the inlet boundary. The primary domain is initialized with a constant velocity of \( u_{\text{mean}} \) in the axial direction while zero in both transverse directions. Further, a constant pressure of zero is initialized throughout the domain and a zero-pressure boundary condition is specified at the outlet. Simulation is advanced to a long enough time for the turbulent inflow boundary to advect throughout the domain before commencing data collection.

4.3 Data Collection Method

To capture the full time-transient data from the primary domain, we select the location of the probes using a priori location estimates, independent of the underlying computational mesh. Figure 21 shows the configuration of probes used in this study. Thirty equidistant probe planes are placed in the domain, starting at the inlet cross-section. The axial distance between any two probe planes is, thus, \( \Delta x^+ = \{35.21, 70.14\} \). At each plane the probes are organized in 20 loci spanning each quadrant, from the rod walls to the center of the channel (three such loci are highlighted in the first quadrant in Figure 21). Each locus has 37 probe points which yields a homogeneous configuration of probes, with respect to distance from the wall, desirable for obtaining turbulence statistics. The first probe is at the same distance from the wall as the first mesh node point and the subsequent probes are placed at a distance corresponding to a growth factor of 1.2, consistent with
boundary layer meshing. Each plane has 2960 probes, while the entire domain has 84,908 probes, omitting the extraneous probes in the spacer grid and mixing vane ‘material’.

Figure 21: Probe configuration for data collection on a plane. The probes are organized into 20 loci in each quadrant, yielding a homogeneous distribution. All planes, along axial length, shown on right, totaling 84,908 probes.

Since the energy cascades from length scale of the largest eddies, an estimate for the Kolmogorov time scale, $\tau_\eta$, can be obtained from the corresponding bulk Reynolds number for each case, [114],

$$
\tau_0 \sim \frac{l_0}{u_0} = \frac{D_h}{u_{mean}}
$$

$$
\tau_\eta \sim Re_b^{-\frac{1}{2}} \tau_0 = \{25.6, 7.84\} \mu s
$$

where $\tau_0$ is the time scale for the largest eddies with corresponding length scale, $l_0$, equal to the hydraulic diameter and velocity scale, $u_0$, equal to the bulk mean velocity. Taylor microscale gives largest length scale at which dissipation occurs (scale of smallest eddies). As given by Pope [114], the time scale corresponding to the Taylor microscale is given by,

$$
\sqrt{15} \tau_\eta = \{0.1, 0.03\} ms
$$
Data was collected and averaged from the simulations for a total time of $\{13, 4.6\}$ ms, equal to approximately $\{508, 586\} \tau_\eta$ for the respective $Re_b$ cases based on equation (4.5), amounting to over 80 GB of data for all probes from each case. A constant time step size of $\{5.0, 1.0\}$ $\mu$s was used for both simulations during the duration of data collection. Note that for obtaining average quantities, all probes in a loci at corresponding locations (recall that each locus has 37 bins) are accumulated from all 80 loci in a plane, shown in Figure 21. This groups all probes with the same approximate perpendicular distance to the nearest wall in one bin. However, this may not be necessarily true for bins that correspond to probes located near the center of the subchannel, as can be deduced from Figure 21 by the ‘shape’ of different loci.

4.4 Upstream Turbulence – Comparison with Existing DNS Simulations

For comparison with existing DNS data, we focus on the results obtained for the plane at $x = 0$ (or equivalently from the auxiliary domain). Most widely used benchmark DNS data in literature is provided by Lee et al [115] for a typical flow channel. To enable a direct comparison with this data, the coordinate system is rotated, for each probe location, as shown in Figure 21, from $y - z$ to $t - n$, (rod) wall tangential-normal direction, with the normal pointing into the sub-channel. It is important to clarify the definition of the friction Reynolds number used here for the sub-channel,

$$Re_{\tau} = \frac{u_\tau D_h}{3v} \quad (4.7)$$

The perpendicular dimensionless wall distance from the center of the sub-channel to the rod walls, given by Eq. (4.3) is $\Delta y^+ = \{114.61, 228.47\}$. For the typical flow channel [111,116], the rationale for the definition of friction Reynolds number is that it yields a value close to the dimensionless wall distance from the center of the channel, making subsequent analysis intuitive.
and convenient. Maintaining a similar convention provides the explanation for the factor of 1/3 in Eq. (4.7), which gives $Re_\tau \approx \{110, 230\}$.

### 4.4.1 Mean Velocities

Figure 22 shows the comparison of normalized mean streamwise components of velocity ($U^+ = U/u_\tau$), obtained with PHASTA from the auxiliary domain, with the results obtained from DNS simulations by Fang et al [117] for a similar sub-channel and with that of Lee et al [118] for a typical channel (flow between parallel plates). Excellent agreement is obtained near the wall ($y^+ < 5$) for both cases with existing DNS data, ensuring that the mesh resolution and selected probe resolution captures the essential viscous sub-layer profile. Two different $Re_\tau$ cases are shown from the data by Lee et al to illuminate the effect of increasing Reynolds number on the $U^+$ profile. The sub-channel results show the same trend of a decrease in the $U^+$ value with increasing Reynolds number as that of channel data in the log-layer region ($30 < y^+ < 100$). However, comparison with the sub-channel data of Fang et al [117] seems to violate this trend. The $Re_\tau = 110$ case shows better agreement with the $Re_\tau = 530$ case by Fang et al [117] which is unexpected. Nevertheless, the present results show good agreement in the trends observed in the log layer region. Discrepancies in the log layer profiles with the channel data of Lee et al can also be owed to the difference in geometrical configuration (also noted by Fang et al [117]). The Log law of the wall is given by,

$$U^+ = \frac{1}{\kappa} \log(y^+) + B \quad (4.8)$$

The above relation was fitted for both cases using the data in $30 < y^+ < 100$ region. A value of $\kappa = 0.44$ and 0.43 was obtained for $Re_\tau = 110$ and 230, respectively, shown in Figure 22. As pointed by Lee et al [118], the choice of the above parameters is arbitrary. Different values have
been reported by different researchers, from experimental and DNS sources. For instance, the high
Reynolds number cases reported by Lee et al [118] gave a better fit with the parameters, $\kappa = 0.384, B = 4.27$. The earliest DNS simulation for a channel by Kim et al [111], for a modest
Reynolds number of 3300, showed a better fit with $\kappa = 0.4, B = 5.5$. Bailey et al [119] determined
$\kappa = 0.4$ for pipe flow from experimental observations. Pope [114] provided a value of $\kappa = 0.41, B = 0.52$, with an uncertainty of 5% for wall flows, in general. Nagib et al [120] consolidated
experimental data for channel and pipe flows in their study, reaching the conclusion that there is
no consistent value for $\kappa$ and that it is dependent on the geometry of the flow. More relevant to the
present study, Fang et al [121] provided $\kappa = 0.43$ and 0.42, while $B = 6.7$, for their simulations
in a PWR sub-channel with similar dimensions, for $Re_b = 29,079$ ($Re_\tau = 530$) and 80,774
($Re_\tau = 1300$), respectively.

Figure 22: Comparison of the present simulations with DNS data for a sub-channel by Fang et al [121] and channel data by Lee et al [118]. Note that the plot on the right shows a zoomed view, limiting $y^+$ to 300.

4.4.2 Reynolds Stresses

The profile obtained for the normalized principal Reynolds stresses, defined as,
\[ R_{ij} = \frac{\langle u'_i u'_j \rangle}{u^2_\tau} \]  

is given in Figure 23. For a comparison of the trendline, the profile obtained from the data provided by Lee et al [118] is also shown. Note that a direct comparison of Reynolds stress magnitude with the channel data is infeasible due to the difference in geometry and the length scales used to define the friction Reynolds number, which for a channel is equal to its half-width. Nevertheless, juxtaposition of the current results with the channel data reveals important similarities in the profiles, especially in the near wall region for all principal components. The wall normal component, \( R_{nn} \), shows a tendency for steeper gradients in the viscous sub-layer region, while the streamwise component, \( R_{xx} \), and tangential component, \( R_{tt} \), have a very similar growth trend to the channel data. Similar to a simple channel, most of the energy for the sub-channel geometry is contained in the streamwise fluctuations. Further, the \( R_{xx} \) value peaks at approximately the same wall distance, \((10 < y^+ < 15)\), and then decline through the log-layer region. The wall normal component, \( R_{nn} \), on the other hand shows a significantly different behavior in the log-layer region for the sub-channel. For the \( Re_\tau = 230 \) case the \( R_{nn} \) profile plateaus in the log-layer-region, while for \( Re_\tau = 110 \) the energy in \( R_{nn} \) continue to increase through the log-layer region up to \( y^+ \sim 80 \) and then declines thereafter. The log-layer trend for the tangential component \( R_{tt} \) is also very similar to the channel data, with a peak obtained at \( y^+ \sim 40 \) for both geometries. However, the \( R_{tt} \) profile plateaus towards the outer layers for the sub-channel more rapidly as compared to the channel data. The turbulent kinetic energy (TKE), given by the trace of the Reynolds stress tensor,

\[ k = \frac{1}{2} \langle u'_i u'_i \rangle \]  

(4.1)
is normalized by the friction velocity \( k^+ = k/u^+_r \) and shown in Figure 24. The TKE data provided by Fang et al [121] is also included in the comparison. Since the streamwise fluctuations contain most of the energy, the profile is very similar to \( R_{xx} \) profile for all cases. The TKE profile increases for increasing Reynolds number for both sub-channel and channel cases, as expected. Note that the sub-channel study by Fang et al did not provide the results for individual Reynolds stress components. The secondary Reynolds stresses, \( R_{xt} \) and \( R_{nt} \), have negligible energy contained in them for both channel and sub-channel geometries and therefore can be justifiably neglected from a modeling perspective. The trendline for \( R_{xn} \) component shows a more coherent profile for the channel geometry, while for the sub-channel cases the energy contained in \( R_{xn} \) was found to be negligible. All normalized secondary stress profiles and their comparison with channel data are shown in Appendix A.5 Their discussion, however, becomes more important for the downstream location in the primary domain due to the effects of mixing vanes, as shown in the Section 4.5
Figure 23: Normalized principal Reynolds stress profile obtained from the simulations. Profile from the channel data by Lee et al [118] also shown for comparing trends.
4.4.3 Invariant Analysis

The Reynolds stress tensor can be decomposed into isotropic and anisotropic components,

$$\langle u'_i u'_j \rangle = 2k \left( \frac{1}{3} \delta_{ij} + b_{ij} \right)$$

(4.11)

where, $\delta_{ij}$ is the Kronecker delta and $b_{ij}$ is the normalized anisotropy tensor,

$$b_{ij} = \frac{\langle u'_i u'_j \rangle}{\langle u'_l u'_l \rangle} - \frac{1}{3} \delta_{ij}$$

(4.12)

The eigenvalues associated with $b_{ij}$ are given by the characteristic polynomial,

$$\det(B - \lambda I) = 0 \Rightarrow \lambda^3 - I \lambda^2 + II \lambda - III = 0$$

(4.13)

where, $B$ is the matrix representation of the tensor $b_{ij}$ and $I$, $II$ and $III$ are the coefficients of the characteristic equation. Owing to the Cayley-Hamilton theorem [122], which states that the matrix $B$ satisfies its own characteristic equation, the coefficients of the above equation can be calculated as (see Pope [114] for details),
\[ I = \text{tr}(B) = \lambda_1 + \lambda_2 + \lambda_3 \]  
\[ II = \frac{1}{2} (\text{tr}(B)^2 - \text{tr}(B^2)) = \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_1 \lambda_3 \]  
\[ III = \det(B) = \lambda_1 \lambda_2 \lambda_3 \]  

where \(\lambda_{1-3}\) are the eigenvalues of \(b_{ij}\). The coefficients of the characteristic equation are also referred to as the tensor invariants, since they remain unchanged under coordinate transformations. Owing to its definition, equation (4.12), \(b_{ij}\) has zero trace, implying \(I = 0\) and that only two independent eigenvalues exist. Further, Lumley [122] showed that none of the eigenvalues of \(b_{ij}\) can be smaller than \(-1/3\) nor greater than \(2/3\), as that would result in either one or two of the principal Reynolds stress components being exactly zero. Therefore, owing to Eq. (4.14), the second and third invariants are also constrained and can be represented by a, so called, turbulence triangle, shown in Figure 25 on a (-II, III) coordinate system. All realizable turbulence must lie within the turbulence triangle, otherwise the eigenvalues of the anisotropic stress tensor \(b_{ij}\) are negative or complex [114]. A more convenient representation was introduced by Choi [123] on a \(\xi - \eta\) coordinate system, defined as,

\[ \xi^3 = III/2 \]  
\[ \eta^2 = -II/3 \]  

The above transformation also yields a triangle, famously known as the Lumley triangle, which demarcates all realizable turbulence by straight lines, zoomed view shown in Figure 26 (for a full view of the Lumley triangle boundaries see Appendix A.6). The annotations shown on the figures for the boundaries of the triangles are for the shape of the Reynolds stress tensor, as opposed to the shape of the turbulent eddies (see Simonsen [124] for details on how the shape of a tensor is evaluated). The origin of the triangles represents 3D isotropic turbulence, wherein all eigenvalues are exactly zero. The left and the right boundaries, emanating from origin, both correspond to
axisymmetric turbulence, with two equal eigenvalues. For the left face, one eigenvalue is smaller than the other two, resulting in a pancake shape for the stress tensor, while the right face has one eigenvalue larger than the other two, resulting in a cigar shape. The extremity of the left face, thus, results in the smaller eigenvalue approaching zero, a 2D isotropic state. The right face extremity results in the two smaller eigenvalues reducing to zero, resulting in a 1D turbulence. The line connecting the two extremities have two prominent, although unequal eigenvalues, indicating anisotropy. Choi et al [125] and Lee et al [126] collected experimental data for different conditions, expected to yield different anisotropic states, and characterized them on the Lumley triangle. Here we keep the discussion focused on the state of turbulence in channel and sub-channel flows.

Figure 25: Turbulence triangle analysis for the current simulation with $Re_{110}$ (left) and $Re_{230}$ (right), compared with channel data of Lee et al [126].
Figure 26: Lumley triangle analysis for the current simulation with $Re_\tau = 110$ (left) and $Re_\tau = 230$ (right), compared with channel data of Lee et al [126]. Zoomed view of the right corner of the triangle is shown. (See Appendix A.6 for the complete Lumley triangle)

In Figure 25 and Figure 26 the profile obtained from the channel data by Lee et al [118] is compared with the $Re_\tau = 110$ and 230 cases for sub-channel geometry, from present simulations, on the turbulence and Lumley triangle, respectively (Note that Lee et al [118] did not present this analysis. It has been extracted from the data available openly [127]). The data by Lee et al is mapped onto the triangle such that the near the wall, $y^+ < 5$, turbulence is 2D anisotropic, almost coinciding with the line joining the two extremities of the triangles. Combining the knowledge from the trends observed in Figure 23, the eigenvalues are expected to correspond to the streamwise and tangential directions, with the major eigenvalue (and hence energy) corresponding to the streamwise direction. As distance from the wall increases, turbulence tends towards a 1D state, corresponding to maximization of energy in the streamwise component of stress tensor, peaking at around $y^+ = 7$. Further away from the wall the turbulence tends towards an axisymmetric shape, with the streamwise component being larger than the other two, while the magnitude of the tangential and wall normal components are comparable, also affirmed by Figure 23. Towards the center of the channel the state, running along the axisymmetric line, tends towards isotropy. It is interesting to note the effect of Reynolds number of the flow on the state on the
Lumley triangle. For \( Re_\tau = 550 \) channel case, the near wall turbulence has a stronger 2D anisotropic character as compared to the \( Re_\tau = 180 \) case, implying that the latter case predominantly contains energy in the streamwise component. Further, in the transition region and beyond, \( Re_\tau = 180 \) case shows a stronger axisymmetric character than the \( Re_\tau = 550 \) case. The \( Re_\tau = 180 \) case also reaches a closely isotropic state near the channel center as compared to the \( Re_\tau = 550 \) case.

For the current sub-channel simulations, the invariants were extracted for the center locus, highlighted in Figure 21 in red, and the resultant profile, as a function of wall distance, is plotted in Figure 25 and Figure 26, for both \( Re_\tau = 110 \) and 230 cases. Near the wall, the trend matches that of the channel data, a 2D profile tending to a 1D state with increasing distance from the wall, although for \( Re_\tau 110 \) case the trend was found to reverse at \( y^+ < 11 \). Further away from the wall the profile, similar to channel data, follows the 2D axisymmetric border closely. For \( Re_\tau = 110 \) case the profile in the transition layer region is more axisymmetric than for \( Re_\tau = 230 \) case. Into the log-layer region the anisotropy for the latter case is even stronger, exhibiting a more random variation as we move further along the distance to the wall. Overall observation of the profile with increasing Reynolds number suggests the same conclusion as the channel data, i.e., the turbulence gets more anisotropic, both in the near wall region and away from the wall, as the Reynolds number is increased.

4.5 Downstream Evolution of Turbulence for \( Re_b = 11000(Re_\tau = 230) \) Case

4.5.1 Mean Velocities

From the perspective of modeling the effects of spacer grids and mixing vanes on the convective heat transfer enhancement, it is imperative to understand their effect on the downstream dynamics of the flow. Figure 27 shows the normalized mean velocity profiles at two upstream
(including the inlet) and six successive downstream locations. Note here that the wall distance \( y^+ \) is normalized by the friction velocity based on the bulk Reynolds number at the inlet. Thus, the classifications of \( y^+ \) into viscous sub-layer, transition layer and log-layer regions is not directly applicable for local downstream conditions. However, we retain this normalization, for lack of a better alternative and to maintain uniformity throughout the axial length. Recall that the leading edge of spacer grid is at the normalized coordinate, \( \frac{x}{D_h} = 0.23 \), while the trailing edge of mixing vanes is at \( \frac{x}{D_h} = 1.4 \). Evidently, the mixing vanes transfer a significant amount of axial momentum of the flow to wall normal and tangential components. The change in the streamwise velocity profile is not very significant in the near wall region \( (y^+ < 30) \), however, it is significantly reduced in the immediate wake of the mixing vanes. The axial momentum is recovered to some extent as we move further downstream from the trailing edge. The mixing vanes, both, force the fluid towards the wall from the bulk, as can be seen by a negative \( U_n^+ \) at the sub-channel center, and induce a swirl or tangential component. There is a distinct transition in the lateral velocity profiles at a half distance, \( y^+ \approx 100 \), from the wall. The wall normal velocity component switches sign near this location, while the gradient of the tangential component undergoes a sharp change. This trend is sustained for the downstream locations, although the magnitudes are attenuated. The tangential velocity witnesses a very sharp increase in the near wall region \( (y^+ < 20) \), followed by a decline in the transition layer region. It is interesting to note that the direction of tangential velocity changes its direction at downstream locations, at progressively lower wall distances. At further distance downstream, the tangential velocity in the near wall regions approaches zero, however, it is sustained in the bulk, in the opposite direction.

A more intuitive understanding of the mixing vane effect is provided by the contour plots of mean velocities, with respect to \( x-y-z \) coordinate system, shown in Figure 28. Note that the data
is reconstructed for the entire plane of probes, Figure 21, at downstream locations using a linear interpolation of data at each probe location. The induced swirl is evident in the mean normalized streamwise component at $\frac{x}{D_h} = 1.54$, the immediate downstream location of the mixing vanes, with a distinct core region where the streamwise momentum is transferred to lateral momentum. $U^+$ progressively diffuses as we move downstream, leaving a primary vortex kernel at the sub-channel center. The sharp momentum imparted to $V^+$ and $W^+$ component at the center also diffuses progressively downstream.

Figure 27: Comparison of upstream and downstream, relative to spacer grid, normalized mean velocity profiles (lateral coordinates are rotated to $t - n$).
Figure 28: Normalized mean velocity contours at inlet and successive downstream locations. Front view of the geometry (x-axis pointing outward) is shown for reference.
4.5.2 Reynolds Stresses

Observing the normalized principal Reynolds stress profiles, shown in Figure 29, it is evident that the mixing vanes impart a significant increase in energy to all components at the downstream location. The gradients of $R_{xx}$ and $R_{tt}$ are increased in the near wall regions ($y^+ < 10$), as compared to the upstream profile, and decrease progressively downstream. Further from the wall ($30 < y^+ < 100$) the trend for downstream profiles of $R_{xx}$ is similar to the upstream profile, however, further towards the center of the sub-channel another component is added due to the presence of mixing vanes. An especially sharp increase can be seen in the immediate wake of the mixing vanes. However, this additional component attenuates relatively rapidly as we move further downstream. The wall normal and tangential components are relatively insignificant in the upstream region. $R_{tt}$ component shows an almost five magnitude order increase in the region $y^+ \sim 10$, while the increase in $R_{nn}$ are more gradual as we move away from the wall. Major enhancement for both $R_{tt}$ and $R_{nn}$ are seen in the wake region, with each gaining 30-40 times of magnitude increase, even greater than the enhancement of the stream-wise component, $R_{xx}$. Note that in alignment with the change in gradient of the normalized velocities, Figure 27, the normalized principal stresses also witness a change in their profile in the vicinity of $y^+ \sim 100$, which indicates the boundary of the wake region. Although insignificant for the upstream region, the secondary stress components acquire significant energy in the downstream region, shown in Figure 30, especially towards the center of the sub-channel. This is indicative of a highly anisotropic flow, as further explored in Section 4.5.3.

The contour plots of the normalized Reynolds stress components in Figure 31, reveal their organizations at successive downstream locations ($y – z$ co-ordinate system). The wake region of the mixing vane at $\frac{x}{D_h} = 1.54$ is distinctly identifiable from the $R_{xx}$ profile and coincides with the
corresponding low velocity regions for the streamwise component of velocity shown in Figure 28. Clearly an organization of the momentum in these regions results into immense attrition, manifested as high Reynolds stresses in local regions. Similar enhancement of energy is also seen for the $R_{yy}$ and $R_{zz}$ components. Since the contour profiles are extracted at successive downstream locations, deductions can be made about the transport of Reynolds stresses. A massive production source is contributed by the mixing vanes, however, further downstream locations are characterized by a dominant dissipation term for all principal components. Their evolution is also, evidently, controlled by the mean convection term, since the high intensity regions tend to rotate clockwise, suggesting a centrifugal effect due to the swirl caused by the mixing vanes, as seen in Figure 31. These observations suggest the importance of, often ignored, history effects for modeling turbulence in complicated geometries. It must be emphasized here that all existing and recognized wall-bounded DNS simulations in literature were performed on simple geometries, for example flow between parallel plates [118], Couette flow [128] or flow in a pipe [129,130], where turbulence retains homogeneity in, at least, the streamwise direction. For the present domain, however, internal structures inhibit homogeneous and isotropic turbulence, its state being a strong function of the upstream conditions (see Section 4.5.3). The secondary stress contours, shown in Figure 32, show a similar massive production source contribution from the mixing vanes at the immediate downstream location. Their downstream evolution is, again, controlled by advection, in both axial and lateral directions (clockwise rotation) and dissipation terms.
Figure 29: Comparison of upstream and downstream normalized primary Reynolds stress profiles (lateral coordinates are rotated to $t - n$).
Figure 30: Comparison of upstream and downstream normalized secondary Reynolds stress profiles (lateral coordinates are rotated to $t - n$).
Figure 31: Normalized principal Reynolds stress contours at inlet and successive downstream locations. Front view of the geometry (x-axis pointing outward) is shown for reference.
Figure 32: Normalized secondary Reynolds stress contours at inlet and successive downstream locations. Front view of the geometry (x-axis pointing outward) is shown for reference.
4.5.3 Invariant Analysis

Invariant analysis, following Section 4.4.3, reveals interesting insights into the evolution of the state of turbulence at the downstream locations. Figure 33 shows the results obtained for the center locus (highlighted in red) in Figure 21, plotted on the turbulence and Lumley triangles. For elucidation, the results are separated into the first probe point off the wall, the region $1 < y^+ < 7$, $7 < y^+ < 30$ and the core regions of the domain, $y^+ > 30$. Observing the nearest probe point off the wall we observe that the turbulence gets shifted across the line joining the extremities, 1D-2D, line towards the 2D end, as we move downstream from $\frac{x}{D_h} = 1.54$ to 2.16. Thus, the near wall state tends to become 2D isotropic, implying that the streamwise and tangential eigenvalues are almost identical, containing equal energy. However, this state seems unstable as the near wall behavior traces its path back on the 2D line from $\frac{x}{D_h} = 2.16$ to 2.47. This behavior was also discussed in Section 4.4.3 for increasing Reynolds number for both channel and sub-channel, thus suggesting an increase in the local Reynolds number of the flow at the immediate downstream location followed by a subsequent decrease further downstream. The same behavior is also seen for the $1 < y^+ < 7$ region, i.e., it traces to the left along the 2D line and returns as we move further downstream. The region $7 < y^+ < 30$ at the immediate downstream location resides on right border, indicating an axisymmetric stress tensor profile. Moving downstream up to $\frac{x}{D_h} = 2.47$, the entire profile for this wall region gets shifted to the left, suggesting an increase in the anisotropic behavior. The profile returns to the axisymmetric line from $\frac{x}{D_h} = 2.47$ to 2.77. The above discussion suggests a dissonance or a lag in the near wall behavior, $y^+ < 7$, and the ‘transition’ layer behavior $7 < y^+ < 30$, i.e., the near wall region returns to a 1D profile faster than the following layer. The points corresponding to the outer layers $y^+ > 30$ are shown by disjointed
points on the triangle due to a more chaotic behavior in this region. It is interesting to note that the state in the core, for some locations, gets shifted all the way to the left border, which represents axisymmetric stress tensor shape with two equal eigenvalues greater than the third one. This is typically not observed in channel data (Lee et al [118]) or even sub-channel simulations (as shown in Section 4.4.3). As opposed to typical wall bounded flows, this state is more representative of axisymmetric contraction experiments from Choi et al [125] or turbulent mixing layer experiments by Bell et al [131]. For $\frac{x}{D_h} = 2.47$, this re-organization of state to the left end of axisymmetric line is seen even for the $7 < y^+ < 30$ region.

![Figure 33: Turbulence triangle (left) and Lumley triangle (right) analysis for the $Re_\tau 230$ case at successive downstream locations.](image)

### 4.5.4 Axial Evolution of Mean Velocity and Mean Reynolds Stresses

A relatively dense distribution of probe planes, as shown in Figure 21, allows the study of axial evolution of turbulence features. This data is, potentially, pertinent to modeling in system thermal hydraulic codes, like CTF, since they involve cross-sectionally averaged governing equations. Figure 34 shows the evolution of normalized streamwise velocity, averaged over entire cross-section of probe plane, for the case $Re_\tau = 110$ and $Re_\tau = 230$. Sharp increase in the average velocity can be seen corresponding to the leading edge of spacer, for both cases, followed by a
sharp decrease at its trailing edge, where the flow encounters the mixing vanes. Beyond the mixing vane edge the streamwise velocity recovers, showing a tendency to asymptote to a value slightly lesser than that at the inlet cross-section. Similar expected trends are also seen for the plane averaged normalized principal Reynolds stresses and turbulent kinetic energy (TKE), shown in Figure 35 for both cases. All three principal components, for both cases, follow similar trends along the axial length. $Re_\tau = 230$ case experiences a sharper increase in Reynolds stresses at the leading edge of spacer as compared to the $Re_\tau = 110$ case, suggesting a Reynolds number dependency that should be accounted for while modeling for STH codes. Further along the mixing vane profile the energy increases continuously for both cases, followed by a consistent decrease in the downstream region. It is interesting to note here that Miller et al [37], based on RBHT data, also modified the original correlation by Yao et al [49] for convective heat transfer enhancement to include a Reynolds number dependency. The plots in Figure 35 suggest that this dependency is due to the TKE added at the leading edge of the spacer, rather than the mixing vane effect. The TKE decreases linearly in the downstream region for both Reynolds number cases. Figure 36 shows the plane averaged secondary stress profile for both cases. The mixing vane effect provide a sharp increase to the lateral shear stress component, however, $\overline{R_{xy}}$ and $\overline{R_{xz}}$ remain relatively unchanged throughout the axial length.
Figure 34: Axial evolution of plane averaged, normalized mean streamwise velocity.

Figure 35: Axial evolution of plane averaged, normalized principal Reynolds stresses for $Re_{\tau} = 110$ (top) and $Re_{\tau} = 230$ cases.
Figure 36: Axial evolution of plane averaged, normalized secondary Reynolds stresses for $Re_\tau = 110$ (top) and $Re_\tau = 230$ cases.

### 4.6 Chapter Summary

Development of turbulence models for flows characterized by anisotropy and non-linearity remains an open challenge. Machine learning based turbulence models offer considerable promise owing to their ability to be universal approximators. However, a major bottleneck to the construction of such models is the sparsity of high-fidelity data from experimental or computational resources. This Chapter details high fidelity data collection and its subsequent analysis for single phase simulations in a PWR sub-channel. Two simulations are performed for
bulk Reynolds number of $Re_b = 5000$ and 11000 and their results are processed and rigorously compared with existing DNS data for flow between parallel plates and for a sub-channel. The downstream axial evolution of turbulence statistics highlights the importance of spacer-grids and mixing vane structures and their contribution to turbulent mixing. An invariant analysis is also performed using the collected data to study the evolution of turbulence anisotropy at upstream and downstream locations. Finally, cross-sectionally averaged profiles for mean streamwise velocity and Reynolds stresses are presented, pertinent to modeling the convective heat transfer enhancement provided by spacer-grids in STH codes.
Chapter 5: Representative DFFB Simulations

5.1 Introduction

The importance of spacer-grids and mixing vanes on the thermal hydraulics of post-LOCA regime was highlighted in Chapter 1. Among the critical observations and results presented by Bajorek et al [35] for experiments conducted at the RBHT facility, the effect of heat transfer enhancement due to droplet collision with spacer-grid and mixing vane structures was particularly underscored. Reiterating briefly from Chapter 1; all experiments at RBHT reported a sharp increase in the heat transfer coefficient at the immediate downstream location of spacer-grids, for both single phase and droplet-laden experiments. Droplet collision and subsequent breakup and/or deformation results in a very sharp increase in the interfacial area, which provides a positive feedback to several heat transfer paths, including convective heat transfer from droplet to vapor, radiative heat transfer to droplet surface, convective enhancement due to droplet evaporation and local steam de-superheating due to droplet evaporation. Thus, droplet topology, characterized by the Sauter mean diameter (SMD) is extremely important for prediction of heat transfer coefficients. For this reason, a set of experiments at the RBHT facility, documented by Cheung et al [43], were dedicated to characterizing the SMD of droplets at the immediate upstream and downstream location of spacer-grids. They constructed the model form for correlating SMD with the upstream collision Weber number, Eq. (1.12), based on a mechanistic analysis and provided its coefficients based on experimental data.

Further, owing to the axiomatic complexity involved in measuring the state of turbulence statistics for two-phase flows, most of the existing correlations in STH codes rely on data collected from separate effect tests. For instance, the convective heat transfer enhancement, Eq. (1.8), which implicitly correlates Nusselt number enhancement to the turbulent kinetic energy (TKE)
enhancement due to spacers for single-phase steam flow, is also used in CTF for the DFFB regime. The presence of the droplets, however, decreases the effective cross-sectional area for steam flow, which is expected to increase the overall TKE, an additional feedback to convective heat transfer enhancement.

This Chapter documents details of two-phase interface capturing simulations performed using PHASTA. Four simulations are performed with varying upstream collision Weber numbers and flow conditions. The setup for the simulations, its assumptions and the rationale for the selected parameters are described in detail. Through the implementation of ad-hoc subroutines in PHASTA, instantaneous axial evolution of droplet dynamics, its volume, interfacial area and SMD was recorded. Subsequent post-processing reveals the time averaged SMD values, which agree well with the existing CTF and RBHT correlations. Following the method described in Chapter 4, data is collected from both single and two-phase simulations with a high spatial and temporal resolution. The statistics reveal the effect of the presence of the droplets and the effect of changing collision Weber number on the mean velocity and Reynolds stress profiles.

5.2 Simulation Setup

5.2.1 Information from experimental observations

The simulations presented herein were designed to emulate droplet spacer-grid interaction in the upper regions of the reactor channels, near the peak power profile location. It is important to revisit and emphasize reported experimental observations to justify the rationale for selected parameters for representative DFFB simulations, enumerated below:

- Andreani et al [25] provided a detailed account of the observed or postulated droplet entrainment mechanisms which precede the DFFB regime. The observations made by Hochreiter et al [16] confirmed that the DFFB conditions, i.e., droplet diameter
distribution, their velocities and void fraction, are a strong function of the upstream conditions, near the entrainment sites.

- The relatively larger droplets and/or ligaments that are entrained near the quench front undergo aerodynamic breakup, also referred to as secondary breakup in the broader literature [34], for a distance of up to 1 m from the quench front, as observed by Ardron et al [10], governed primarily by the aerodynamic Weber number, Eq. (1.1).

- As reported by Cheung et al [43] and Jin et al [132], the droplet size near the peak power profile ranges from 0.4 – 1.5 mm and they retain high sphericity, suggesting a low aerodynamic Weber number (also confirmed by Andreani et al [133]). Thus, droplets in the upper regions of the core are not expected to undergo breakup due to surrounding flow.

- For the experiments conducted at the RBHT facility at low re-flood conditions [43], the reported droplet collision Weber numbers were in the range, $W e_c = \{54.14, 59.4\}$.

- Ardron et al [10] observed that droplets travel with roughly similar velocities, irrespective of their size differences. The droplets remained in mechanical non-equilibrium, not reaching their terminal velocity through the length of the core.

- For the DFFB regime the wall temperature near the peak power profile is maintained above the Leidenfrost limit. Thus, any direct contact of the droplets with the heated rod wall is precluded [23]. Droplets remain confined to the core regions of the sub-channel.

### 5.2.2 Mesh Specifications

Interface capturing two-phase flow simulations impose additional constraints on mesh requirements besides the usual constraints for resolving all length scales of single-phase turbulence, discussed in Section 4.2, primarily to calculate the numerical curvature, Eq. (2.9), with a reasonable degree of accuracy. Prior investigations on two-phase flow using the level-set method
have established guidelines for required cell size [110]. Accordingly, the bulk mesh resolution in
the primary domain (Figure 4) was set to 43.75μm (Δy⁺ = 2.45) up to an axial distance of 2.0Dₕ
(26 mm from the inlet), equivalent to ~23 elements across the droplet diameter at their inception
location (D = 1mm, see Table 5). Maximum bulk mesh resolution in the domain was 87.5μm
(Δy⁺ = 4.9), near the outlet. The first mesh node off the walls, including rod surfaces and internal
surfaces, was placed at a distance of 10μm (y⁺ = 0.561). Extended boundary layers were applied
at the internal surfaces for capturing collision events, stretching up to a distance of 0.763 mm,
with a growth factor of 1.2, as shown in Figure 37. The resulting mesh had 367.5 M purely
tetrahedral elements.

Note that the primary mesh for the single-phase case, listed in Table 5 had the same mesh
specifications as described in Section 4.2, consisting of 55.8 M tetrahedral elements. The essential
difference between the meshes for the single-phase and two-phase cases was that the former had a
minimum bulk resolution of 87.5μm and lacked the extended boundary layer region near the
internal surfaces.

Figure 37: Primary mesh for two-phase flow simulations. Fine mesh region extends up to a distance of
2.0Dₕ. Extended boundary layers, up to a distance of 0.763mm, are designed on all internal surfaces to
resolve collision events. Mesh consists of 367.5 M purely tetrahedral elements.

Fully developed turbulent velocity profile was prescribed at the inlet cross-section of the
primary domain, Figure 4, using similar method as described in Section 3.1 with probes
corresponding to exact mesh node coordinates of the primary domain placed in a periodic auxiliary domain. The pressure gradient specified in the auxiliary domain for reaching quasi-steady turbulent state was 79.396 \( kg/m^2 s^2 \). All two-phase cases enumerated in Table 5 use the same data repository for specifying the turbulent velocity profile at the inlet cross-section. The bulk Reynolds number, defined at the inlet (or in auxiliary domain), is \( Re_b = 11822 \) (Eq. (4.2)) for all cases, corresponding to a friction Reynolds number of \( Re_f = 242.539 \) (Eq. (4.7)). The mean velocity of the gas at the inlet cross-section was \( u_{mean} = 7 \text{ m/s} \).

### 5.2.3 Flow properties and characteristic dimensionless numbers

Table 5 shows the parameters for single-phase and all two-phase simulations discussed in this Chapter. As mentioned in Section 1.3 the system pressure of the core under post-LOCA conditions is near atmospheric, 20-45 psi. Under these conditions the density ratio of steam-water system is \(~1000\), while the dynamic viscosity ratio \(~10\). For the first simulation conducted under this research the property ratio resembled that of air-water system, with viscosity ratio being higher, equal to forty-eight, than the steam-water system under typical DFFB conditions. The following studies were conducted for exact property ratios for steam-water system at 30 psi system pressure. The droplet dynamics are not expected to be significantly affected by a higher viscosity ratio, since the dominant force acting on the droplets is due to inertial impact, as also corroborated by the mechanistic treatment and experiments of Cheung et al [43], where they identified the collision Weber number, \( We_c \), as the primary determinant of downstream SMD.

The controlled parameters in all two-phase simulations are the bulk Reynolds number, \( Re_b \), and the collision Weber number, \( We_c \), of the injected droplets. To obtain a desired \( We_c \), the surface tension coefficient is varied for different cases, shown in Table 5. The upstream injected droplets are assumed to be monodisperse and spherical, i.e., they all have a diameter equal to 1mm.
Further, the properties are chosen such that they result in an initial velocity of the droplets, $u_d$, close to the terminal velocity, estimated from the following drag correlation by Morrison [134] developed for spherical solid objects in free stream,

$$C_D = \frac{24}{Re_d} + \frac{2.6(Re_d)^{1.52}}{1 + (Re_d)^{5.0}1.52} + 0.411 \left( \frac{Re_d}{263000} \right)^{-0.94} + 0.25 \frac{Re_d}{10^6} \left( \frac{Re_d}{263000} \right)^{-8} + \frac{Re_d}{10^6} \left( \frac{Re_d}{263000} \right)^{-8} + 0.25 \frac{Re_d}{10^6}$$

(5.1)

where $Re_d$ is the droplet Reynolds number, based on the relative velocity of the surrounding flow with respect to absolute droplet velocity, $u_{rel} = u_{mean} - u_d$, given by,

$$Re_d = \frac{\rho_d u_{rel} D}{\mu_g}$$

(5.2)

Above correlation yields an absolute velocity of $2.05\,m/s$ for the air-water system case (labelled We55-Air in Table 5) and $1.97\,m/s$ for the steam-water system cases. The maximum aerodynamic Weber number, $We_a$, of the flow based on the above parameters is 0.507 for the We80 case, given as

$$We_a = \frac{\rho_d D u_{rel}^2}{\sigma}$$

(5.3)

The experiments conducted by Wierzba [135] on free stream droplet breakup established the critical aerodynamic Weber number, i.e., the value at which droplet breakup occurs, in the range 11-14. Thus, the current designed conditions ensure that the droplets will not undergo aerodynamic breakup, also affirmed by the aforementioned experimental observations of the DFFB regime.

As described in Section 3.3, the droplets are initialized ensuring their center is at a minimum distance of $0.75\,D$ from the rod walls and that their initial velocity has a non-zero component only in the axial direction. This assumption is in accordance with the experimental observation that the droplets do not contact the rod walls due to Leidenfrost effect in the upper regions of the core.
Finally, it is assumed that the droplets at the injection plane do not intersect. A minimum distance of $1.5D$ is maintained between the active droplet seed points. This assumption along with an axial injection velocity ensures that the droplets do not coalesce at the upstream location, before they collide with the incident face of the spacer-grids.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Single phase</th>
<th>We55-Air</th>
<th>Properties @ 30 psi, steam superheat (100K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>We40 (Steam)</td>
</tr>
<tr>
<td>Density ratio ($\rho_l/\rho_g$)</td>
<td>$\rho_g = 1.185 \text{ kg/m}^3$</td>
<td>1000</td>
<td>1029.59</td>
</tr>
<tr>
<td>Viscosity ratio ($\mu_l/\mu_g$)</td>
<td>$\rho_g = 9.1 \times 10^{-6} \text{ Pa.s}$</td>
<td>48</td>
<td>13.49</td>
</tr>
<tr>
<td>Bulk Reynolds number, $Re_b$</td>
<td></td>
<td></td>
<td>11822</td>
</tr>
<tr>
<td>Friction Reynolds number, $Re_f$</td>
<td></td>
<td></td>
<td>242.539</td>
</tr>
<tr>
<td>Mean inlet gas velocity, $u_{\text{mean}} (m/s)$</td>
<td>7.0</td>
<td>55</td>
<td>40</td>
</tr>
<tr>
<td>Collision Weber number, $We_c$</td>
<td>-</td>
<td>55</td>
<td>40</td>
</tr>
<tr>
<td>Aerodynamic Weber number, $We_a$</td>
<td>-</td>
<td>0.319</td>
<td>0.253</td>
</tr>
<tr>
<td>Injected droplet Reynolds number, $Re_d$</td>
<td>-</td>
<td>643.71</td>
<td>654.67</td>
</tr>
<tr>
<td>Injected absolute droplet velocity, $u_d (m/s)$</td>
<td>2.05</td>
<td>1.97</td>
<td></td>
</tr>
<tr>
<td>Injected droplet diameter, $D (mm)$</td>
<td>-</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>Surface tension coefficient, $\sigma (N/m)$</td>
<td>0.091</td>
<td>0.118</td>
<td>0.086</td>
</tr>
<tr>
<td>Droplet Ohnesorge number, $Oh$</td>
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<td>0.001</td>
<td>3.23 $\times$ 10^{-4}</td>
</tr>
<tr>
<td>Gravity, $g (m/s^2)$</td>
<td>-</td>
<td>-9.81</td>
<td></td>
</tr>
</tbody>
</table>

5.2.4 PHASTA setup details

The primary mesh for two-phase simulations was split into 131072 partitions, using the load balancing PUMI tool [136], distributed on 2048 Mira BlueGene/Q nodes [137], each node consisting of 16 processing cores. The simulation was run with four MPI threads per core, which
has been shown to yield super-scaling on the Mira supercomputer [138]. At each time step of the simulation the staggered flow level-set iteration approach, described by Nagrath et al [61], was used to advance the solution. Four non-linear iterations were performed at each time step, which involved flow solve followed by the level-set advection solve. The linearized system of equations obtained from the tangent matrices, described in Section 2.3.3, was solved using the GMRES matrix solver [58]. Ten to thirty Newton’s iterations were performed for each non-linear iteration. The tolerance on both momentum and continuity equations was specified to be $10^{-8}$. Finally, the level-set re-distancing was performed before advancing the solution to next time step. Here, 20-22 re-distancing iteration steps were performed at each time step for all two-phase simulations. Maximum time-step size for the simulations was $1\mu s$, while the re-distancing solve was also assigned a constant pseudo time-step size of $5\mu s$. As described in Section 3.4.2, a local time stepping CFL of $5 \times 10^{-4}$ was assigned for the region $1.5\epsilon$, where $\epsilon$ is the property smearing length for the level set field, Eq. (2.4). A length of $87.5\mu m$, equal to the maximum resolution of the primary mesh, was chosen as $\epsilon$. Note that the same smearing length was also used for the $\text{sign}$ function for re-distancing equation, Eq. (2.12). For the We55-Air case the total wall clock time was ~195 hours, equivalent to approximately 6.4 M core hours (or 0.4 M node hours) on the Mira system.

5.3 Results and Discussion

Instantaneous velocity contours for the single-phase simulation in primary domain is shown in Figure 38. Contours at the inlet cross-section, which is essentially the velocity profile captured in the auxiliary domain, and at the axial location $x/D_h = 1.85$ are also shown. Recall that the trailing edge of the mixing vane is at $x/D_h = 1.4$. The juxtaposition of these planes makes the mixing vane effect evident. The contours at the downstream cross-section are characterized by
a central wake region with a reduced velocity magnitude. Figure 39 shows the time evolution of droplets for the We55-Air case. Starting from a single-phase solution, droplets were introduced in the domain at regular intervals, consistently increasing the droplet volume fraction. This simulation was run for a total of 14.125 ms, at which time the recorded droplet volume fraction was 2.77%.

Figure 38: Velocity contours for the single-phase simulation. Cross-sections at the upstream (inlet) and downstream ($x/D_h = 1.85$) locations are shown.

Figure 39: Droplet evolution for We55-Air case at time $t = 8.1, 10.1$ and 13.1 ms. Cross-section at ($x/D_h = 1.85$) is shown on the right.
The steam-water system cases were run for a total simulation time of $t = 14.75, 13.65, 13.35\, ms$ for We40, We55 and We80 cases, respectively. The droplet volume fraction for the cases at these time stamps were $[3.14, 3.12, 2.91]\\%$, respectively. Instantaneous velocity contours for the steam-water system case with $We_c = 40$ at $t = 14.75\, ms$ and $We_c = 80$ at $t = 13.35\, ms$, are shown in Figure 40. Simultaneous examination of the two cases reveals important differences in the droplet dynamics, emphasizing the role of upstream collision Weber number on the axial evolution of the droplet morphology. For the We40 case the observed diameter of the droplets at the downstream location is evidently larger than the We80 case. For the former case the droplets tend to coalesce into larger blobs while for the We80 case smaller droplet diameters, but a larger number of individual droplets can be perceived in the domain. This is tantamount to a smaller downstream SMD of the droplets for the We80 case. Although the current simulations are adiabatic, but it can be undoubtedly conjectured that the We80 case will register a higher heat transfer coefficient near the spacer-grid location as compared to the We40 case. Further, for the We40 case the droplets show a greater tendency to develop a liquid film over the leading edge of the spacer-grid structure, owing to a higher surface tension coefficient. It can therefore be conjectured that for lower collision Weber numbers the grids will be better quenched and the droplets in the bulk will have a higher tendency to get de-entrained onto the spacer surface.

Velocity contours at the downstream lateral cross-section at $x/D_h = 1.85$ are also shown in Figure 40. The zero contour, or the droplet interface, is highlighted in black. Note that the mixing vane profile has the tendency to push the droplets into the peripheral regions of the domain. In actual DFFB experiments the droplets would likely not contact the rod walls due to Leidenfrost effect. Thus, a lack of numerical modeling of this phenomenon remains one of the implicit assumptions of the present simulations. Nevertheless, the Leidenfrost effect is only expected to
affect the lateral distribution of droplets, rather than their axial evolution. The difference in the velocity contour profile inside the volume of the droplets and the outside gas can be perceived from the lateral cross-sections. Due to the higher density of liquid in the droplet volume, the velocity contour profile in the volume is expected to be more uniform as compared to the more turbulent profile in the bulk gas flow.

It is evident that a quantitative description of droplet dynamics is required to gain a more in-depth understanding of the effect of spacer-grids and upstream $W_{e_c}$. The data collection mechanism and subsequent presentation of results detailed in the following section addresses this desired knowledge base.

Figure 40: Instantaneous state of droplets and velocity contours for the We40 (top) and We80 case at $t = 14.75 \, ms$ and $13.35 \, ms$, respectively.
5.3.1 Axial evolution of droplet dynamics

One of the advantages of the level-set formulation is that it offers a convenient mechanism for calculating enclosed droplet volume and interfacial area, which enables insight into the effect of spacer-grids, mixing vanes and local flow on droplet morphology. Here, we analyze the axial evolution of droplets by partitioning the domain into 20 equi-spaced regions, as shown in Figure 41. In each partition the droplet volume and interfacial area are evaluated as,

\[
V_p = \sum_{e} \int_{\Omega_e} (1 - H(\phi)) \, d\Omega \tag{5.4}
\]

\[
A_p = \sum_{e} \int_{\Omega_e} \nabla H(\phi) \cdot \vec{n} \, d\Omega \tag{5.5}
\]

where \(H(\phi)\) is the Heaviside function. Eq. and \(\vec{n}\) is the normal to the interface,

\[
\vec{n} = \frac{\nabla \phi}{|\nabla \phi|} \tag{5.6}
\]

The above integrals are evaluated element wise, at each time step, through summation over numerical quadrature points. Only the elements with their centroid inside the partition boundaries contribute to the total volume or interfacial area for that partition. Sauter mean diameter, which effectively characterizes the morphology of the interface, can be calculated for a partition, analogous to Eq. (1.2) for discrete droplets, as,

\[
SM D_p = 2 \frac{r_V^3}{r_A^2} = \frac{6V_p}{A_p}; \quad r_V^3 = \frac{3V_p}{4\pi}; \quad r_A^2 = \frac{A_p}{4\pi} \tag{5.7}
\]

where \(r_V\) is the equivalent radius for the entire enclosed volume in each partition and \(r_A\) is the equivalent radius corresponding to the interfacial area.
Figure 41: Domain partitions for evaluating droplet dynamics. Axial inception location and droplet size is annotated. Each partition has a width of 2mm.

Figure 42: Axial evolution of total droplet volume in partitions for the We55-Air case. Time averaged value for each partition is annotated with dashed blue line.
Figure 43: Axial evolution of total droplet interfacial area in partitions for the We55-Air case. Time averaged value for each partition is annotated with dashed blue line.

Figure 44: Axial evolution of SMD in partitions for the We55-Air case. Time averaged value for each partition is annotated with dashed blue line. Existing CTF correlation and correlation by Cheung et al [43] is also annotated at downstream partitions.

Figure 42 shows the instantaneous and time averaged axial evolution of aggregate droplet volume in successive partitions for the We55-Air case. Note that the data collection for the plots was commenced after 8.3 ms, after the initial droplets reach downstream of mixing vanes (as can
be discerned from Figure 39). The fluctuations seen in Partition 1 result from the departure and periodic inception of droplets. Consistency in the time period of fluctuations is progressively lost in the downstream partitions due to changes in morphology and velocity of droplets. A sharp increase in the droplet volume is seen in Partition 2, where the incident surface of the spacer-grid resides, due to the deceleration of droplets upon collision. Collision of the droplets causes rapid morphological transformation or breakup, transferring the kinetic energy to surface energy, resulting in an increase in surface area. This causes an increase in the relative drag force acting on the new droplets, since,

$$\frac{F_d}{F_g} \sim \frac{\text{Surface Area}}{\text{Volume}} \sim \frac{1}{\text{SMD}}$$

(5.8)

Therefore, the droplets experience greater acceleration following Partition 2, which is manifested as a monotonous decrease in droplet volume in the subsequent partitions. The evolution of surface area, Figure 43, in the partitions follows a similar trend as the droplet volume. Note that the time averaged value shown for partitions in Figure 42 and Figure 43 excludes the period when the partition is empty.

From a STH modeling perspective, the axial evolution of SMD is more desirable. Based on mechanistic considerations and RBHT experiments Cheung et al [43] proposed the following correlation for predicting the downstream SMD of droplets,

$$SMD_d = SMD_u (1 + 0.1803eW e_c^{0.558})^{-1}$$

(5.9)

where $\epsilon$ is the blockage ratio of the spacer grids, maintained at 0.362, same as described by Cheung et al. Further, the existing correlation in the STH code, COBRA-TF (or CTF) [44], was designed using experimental data from Wachters et al [50],

$$SMD_d = SMD_u 6.617W e_c^{-0.53}$$

(5.10)
The SMD data obtained from the We55-Air case and the value obtained from the above correlations, with $We_c = 55$ and $SMD_u = 1\text{mm}$, is shown in Figure 44. It should be noted that despite instantaneous fluctuations, the time averaged SMD in Partition 1 is approximately equal to $1\text{mm}$, equal to the diameter of the droplets at inception which is expected since the droplets in this partition are approximately spherical. In contrast to the droplet volume or interfacial area profile, the time averaged SMD in Partition 2 drops sharply, owing to the collision of droplets and their consequent increase in surface area. Along the profile of the spacer-grids and mixing vanes, up to Partition 10, the SMD value is constant, close to 0.5 $\text{mm}$. In the downstream region, beyond Partition 12, the SMD increases. This can be attributed to deformed droplets regaining their sphericity in this region, owing to surface tension forces, and the droplets coalescing due to the mixing vane profile. In Partition 15 and 17 the averaged SMD coincides with the existing CTF correlation, Eq. (5.10), establishing confidence in the predictive capability of present simulations. In general, the SMD value in the downstream partitions is close to the experimentally correlated values.

Figure 45 shows the axial evolution of droplet volume in partitions for all steam-water system cases, with prescribed upstream collision Weber numbers of 40, 55 and 80. Comparison of the instantaneous droplet volume profile for the We55 case and the We55-Air case, shown in Figure 42, reveals that the injected droplet for the former case are more prone to deformation as compared to the air-water system. This is likely owing to the Ohnesorge number for the steam-water system being an order of magnitude lower than the air-water system, listed in Table 5. The Ohnesorge number of a droplet depends only on its dynamic properties, defined as,

$$Oh = \frac{\mu_l}{\sqrt{\rho_l D \sigma}}$$  \hspace{1cm} (5.11)
Guildenbecher et al [139] documented findings from several experiments on breakup of droplets under the effect of aerodynamic forces. They concluded that an increase in the Ohnesorge number results in an increase in the critical Weber number of droplets, i.e., the aerodynamic Weber number at which droplets break. Although, their focus was specifically on breakup, it can be conjectured that an increase in Ohnesorge number also makes droplets more resistant to deformation. It is also due to this reason that the recorded SMD of the droplets in Partition 1 for the We40 and We55 cases, shown in Figure 47, is slightly greater than 1, implying that the droplets undergo deformation as soon as they are injected due to impinging turbulence. As we move to the higher $We_c$ case, We80, the fluctuations in Partition 1 are smoother, similar to the We55-Air case, owing to a high surface tension coefficient for this case. The time averaged volume of the droplets in Partition 1 for all steam-water system cases is comparable, indicating droplets are injected in the domain for all three cases with the same time period. Note that the frequency of droplet injection for We55-Air case, as evident from Figure 42, was higher than the steam-water system cases. Increase in the time-averaged droplet volume in Partition 2, due to collision, is also comparable for all steam-water cases, although the instantaneous fluctuations in droplet volume are expectedly different in their amplitude. Further, downstream the time-averaged volume follows the same axial trend as for the We55-Air case. The instantaneous fluctuations in droplet volume also lose their periodicity, becoming increasing chaotic downstream. Note, however, that the We40 case loses periodicity in fluctuations more rapidly than the We50 or We80 case, owing to a lower surface tension coefficient. The trends seen in the axial droplet interfacial area, shown in Figure 46, can also be explained by the rationale in the preceding discussion.
Figure 45: Axial evolution of total droplet volume in partitions for We40, We55 and We80 steam-water system cases (top to bottom).
Figure 46: Axial evolution of total droplet interfacial area in partitions for We40, We55 and We80 steam-water system cases (top to bottom).
Figure 47: Axial evolution of SMD in partitions for We40, We55 and We80 steam-water system cases (top to bottom). For each case the value obtained from empirical correlations with the corresponding upstream $W_{e_c}$ are also shown.
Figure 47 shows the axial evolution of SMD for all steam-water system cases. The Figure also shows the values obtained from the RBHT correlation, Eq. (5.9), and from the existing CTF correlation, Eq. (5.10), at the downstream partitions, evaluated using corresponding upstream $W\epsilon_c$ (40, 55 and 80) for the cases. Best agreement, for any case, is obtained in Partitions 14-17 with the RBHT correlation. For low $W\epsilon_{40}$ and $W\epsilon_{55}$ case the existing correlation in CTF, Eq. (5.10), is found to overpredict the SMD values.

The time averaged profiles can be discerned more clearly from Figure 48 and Figure 49. As mentioned before, after droplet collision with the leading edge of the spacer-grid both droplet volume and interfacial area follow an almost monotonous decreasing trend. Only a slight disruption to this trend is seen near the trailing edge of the mixing vane for the steam-water system case. In Figure 49 only the SMD values obtained from the RBHT correlation by Cheung et al [43] are shown for comparison, since they agree better than the existing CTF correlation. It is worthwhile to emphasize again that a sharp increase in droplet SMD is seen at some distance downstream from the mixing vane trailing edge (Partition 14, $x/D_h\sim 2.16$), since the droplet regain their sphericity around this region after collision with mixing vanes. For the steam-water system cases, a decreasing trend is seen in the downstream SMD, moving from $W\epsilon_{40}$ to $W\epsilon_{80}$, as expected. The $W\epsilon_{55}$-Air case, however, matches more closely with the $W\epsilon_{40}$ steam-water system case, indicating that viscosity ratio, or Ohnesorge number, is also an important consideration for correlating downstream SMD, in addition to the upstream $W\epsilon_c$. The RBHT experiments by Cheung et al [43] were all performed under similar conditions, thus similar thermodynamic properties, which might be the reason that this dependence on $Oh$ remained undiscovered.
Figure 48: Axial profile of time averaged droplet volume (left) and interfacial area in domain partitions for all two-phase cases.

Figure 49: Axial profile of time averaged SMD in domain partitions for all two-phase cases. The values obtained with the RBHT correlation by Cheung et al [43] are also annotated.

The evolution of the droplet volume in the domain for the We40 and We80 cases is shown in Figure 50 and Figure 51, respectively. Droplet volume in the entire domain and at the downstream portion of the domain, $x/D_h > 1.39$, are shown in the figures. Periodic increments in the total volume plot correspond to time windows in which the droplets are introduced in the domain. Decline in the total volume plot can be owed to numerical volume loss. Notice that in contrast to the total volume trend, the volume at the downstream portion of the domain shows a more consistent increase in droplet volume. It can, thus, be deduced that the maximum numerical loss in droplet volume is witnessed due to droplet collision at the leading edge of the spacer, as
expected due to the droplets breaking into fine ligaments (see single droplet collision, Figure 17). At the downstream locations, however, the numerical loss in volume of liquid is not appreciable. A pessimistic error estimate for the numerical volume loss can be calculated by considering the evolution of total droplet volume. One time period of droplet injection is considered for the We40 (11.526 – 12.275 ms) and We80 case (11.101 – 11.925 ms), during which 15 droplets were initialized at the upstream location for each case. The error in volume can be calculated as,

\[
\%error = \frac{V_{new} - (V_{final} - V_{initial})}{V_{new}} \times 100
\]  

where, \( V_{new} \) is the additional volume added to the domain, equal to 15 droplets, during the time window. \( V_{initial} \) and \( V_{final} \) are the total volumes recorded at the initial and final timestamps, respectively. The resulting volume error was \{19.01, 16.16\}% for the We40 and We80 cases, respectively.

Figure 50: Evolution of droplet volume in the entire domain (left) and at the downstream location, \( \frac{x}{D_h} > 1.39 \) (right), for the We40 case.
Figure 51: Evolution of droplet volume in the entire domain (left) and at the downstream location, $\frac{x}{D_h} > 1.39$ (right), for the We80 case.

### 5.3.2 Turbulence statistics and their axial evolution

The characteristic friction Reynolds number for the simulations in this Chapter, defined at the inlet, is $Re_\tau = 243$ (see Eq. (4.7)). Probe configuration shown in Figure 21 was used for data collection for both single and two-phase simulations, amounting to 84,908 total probes and 30 axial probe planes. The time scale for the simulations corresponding to the largest eddy size, assumed comparable to hydraulic diameter, and bulk mean velocity is $\tau_0 = 1.85 \text{ ms}$. The corresponding Kolmogorov time scale, as estimated from Eq. (4.5), is $\tau_\eta = 17.05 \mu\text{s}$. The scale of the smallest eddies at which dissipation occurs or the Taylor microscale is, thus, $\sim 0.06 \text{ ms}$ (see Eq. (4.6)). Data was collected, and subsequently time averaged, for the We40 and We80 case for an approximate time window of 3.38 ms, ensuring that the eddies corresponding to Taylor length scale are sufficiently resolved ($\sim$ factor of 56). Considering local flow conditions near internal structures and the presence of the droplets, the above estimates are no longer valid. However, since the data is collected for a relatively long time period (equal to 5000 simulation time steps), we assume that the first order turbulent statistics are sufficiently captured.
5.3.2.1 Verification of inlet turbulent flow features

Figure 52 shows the mean streamwise velocity profile captured at the inlet cross-section of the two-phase cases, We40 and We80. For details on the spatial averaging procedure for obtaining this (and the following) profile see Section 4.3. Note that the droplets are initialized with their center at a distance of 1 mm from the inlet. Thus, the velocity profile at the inlet cross-section is not affected by the presence of the droplets and can thus be regarded as the fully developed turbulent profile in auxiliary domain. The inlet profile is compared with DNS profile for typical channel by Lee et al [118] and the sub-channel profile by Fang et al [117], showing excellent agreement in both the near wall and log-layer regions. The parameters obtained for the log-law of the wall, Eq. , are $\kappa = 0.41, B = 5.96$, which agree well with the existing parameter values in literature and the values for the single phase simulation results presented in Chapter 4.

Figure 52: Comparison of mean normalized streamwise velocity profile at the inlet cross-section for all two-phase cases with channel data of Lee et al [117,118] and sub-channel data of Fang et al [117].
Figure 53: Comparison of normalized principal Reynolds stress profile at the inlet cross-section for all two-phase cases with channel data of Lee et al [117,118] (lateral coordinates are rotated to $\xi - \eta$).

The normalized Reynolds stress profiles obtained at the inlet are also compared with the channel data of Lee et al [118], shown in Figure 53. For further discussion on these results and their comparison with existing DNS data, the reader is referred to Section 4.4.
5.3.2.2 Effect of droplets on turbulence features

The presence of droplets in the computational domain decreases the effective hydraulic diameter for the steam/vapor flow. Thus, for the same flow rate maintained at the inlet cross-section, the droplets throttle the bulk flow, which is expected to increase the overall turbulent kinetic energy. Figure 54 shows the mean normalized velocity component profile for the We80 case compared with the single-phase simulation, both in primary domain. Profile at three successive downstream locations, $\frac{x}{D_h} = 1.54, 2.16$ and $2.77$, are also shown for both cases. Recall that the trailing edge of the mixing vane is location at $\frac{x}{D_h} = 1.4$. The profile at the inlet cross-section is also shown for reference. It is evident that the presence of droplets increases the streamwise velocity magnitude in the near wall region. The effect is more pronounced for the immediate downstream location $\frac{x}{D_h} = 1.54$ and the further downstream location past the vanes, with the near wall $U_x^+$ profile at $\frac{x}{D_h} = 2.77$ being almost identical. For the tangential component, however, the presence of droplets attenuates the momentum imparted due to mixing vanes, as compared to single phase case, in the wall region at $\frac{x}{D_h} = 1.54$. Away from the wall the droplets do not seem to have a significant effect on the mean components besides some re-origination of momentum.
Figure 54: Comparison of normalized mean velocity components for single phase simulation, in the primary domain, with the We80 two-phase case. Profiles at three downstream probe planes are shown (lateral coordinates are rotated to $t - n$).

The effect of droplets on the normalized principal stress components is more interesting, as shown in Figure 55. The presence of droplets imparts a significant positive feedback, across the $y^+$ distance, to all principal components, especially at the immediate downstream location. Only the wall normal component, $R_{nn}$, is slightly attenuated at the center of the sub-channel. The feedback is attenuated as we move further downstream, nevertheless an increase in the streamwise
and tangential components is registered even at the $x/D_h = 2.77$ location. The massive feedback at the immediate downstream location can be owed to the mixing vane profile, which forces both the droplets and the bulk flow towards the peripheral regions. Note that the profile trend for the two-phase case is similar to the single-phase case for all components, especially in the near wall region, which bolsters confidence in the time averaging width selected for the two phase case (3.38 ms).

Figure 55: Comparison of normalized principal stress component profile for single phase simulation, in the primary domain, with the We80 two-phase case. Profiles at three downstream probe planes are shown (lateral coordinates are rotated to $t - n$).
Figure 56: Normalized mean velocity contours at the inlet and successive downstream location for the We80 case. Front view of the geometry (x-axis pointing outward is shown for reference).
Figure 57: Normalized principal Reynolds stress contours at the inlet and successive downstream location for the We80 case. Front view of the geometry (x-axis pointing outward is shown for reference).
Figure 56 shows the contours of mean velocity at the inlet and successive downstream probe planes for the We80 case. Although droplets cause a random re-distribution of the momentum, similarities can be chalked on comparison with the contours obtained for the single-phase case, shown in Figure 28. An identifiable core region, similar to single phase case, can also be seen for the two-phase case at all downstream locations in the streamwise component. The lateral components have an even stronger resemblance to the single-phase case, with the effect of droplets being barely identifiable at the downstream locations from the contour plot. Figure 57 shows the normalized Reynolds stress contour on probe planes. It is evident that the presence of droplets results in a more uniform lateral distribution of energy as compared to the single-phase case, shown in Figure 31. For the single-phase case, distinct mixing-vane wake regions of high energy were clearly discernible, which are smeared out for the We80, two-phase case, albeit the overall magnitude of energy is higher. However, similar to the single-phase case, downstream evolution of Reynolds stresses is dominated by transport, induced swirl, and dissipation for the two-phase case.

5.3.2.3 Effect of upstream collision Weber number on turbulence

As observed in the experiments by Cheung et al [43] and the results presented in Section 5.3.1, the droplet SMD at the downstream location is governed by the upstream collision Weber number. Specifically, an increase in $We_c$ results in a decrease in the downstream SMD since droplets breakup into smaller volumes on collision. Since the droplets, their size and distribution, provide a feedback to the surrounding flow, it is worthwhile to observe the effect of changing collision $We_c$ on the downstream turbulence behavior. Figure 58 shows the mean normalized components of velocity for the We40 and We80 case. Minor changes are seen in the streamwise velocity profile between the two cases, however, the tangential and wall normal components show
some appreciable difference. An increase in $We_c$ results in a decrease in the positive tangential momentum imparted to the flow by mixing vanes, possibly due to the greater resistance offered by a larger droplet population, albeit the individual droplets might be smaller volumes. The migration of droplets towards the periphery due to mixing vanes, on the other hand, results in a greater positive wall normal momentum to the flow for the We80 case (note that the wall normal axis is pointed into the domain). A larger wall normal component, pushing flow to the periphery, is also observed in the core region for the We80 at the immediate downstream location.

Figure 58: Comparison of normalized mean velocity components for the We40 and We80 cases. Profiles at three downstream probe planes are shown (lateral coordinates are rotated to $t-n$).
Figure 59: Comparison of normalized principal stress component profile for the We40 and We80 cases. Profiles at three downstream probe planes are shown (lateral coordinates are rotated to $t-n$).

Analysis of the normalized Reynolds stresses, as shown in Figure 59, reveals a minor magnitude decrease in energy for $R_{tt}$ and $R_{nn}$ component for the We80 case in the near wall region. Towards the sub-channel core, at the immediate downstream location, the We80 case, however, records a significant positive feedback to the streamwise and tangential components while an attenuation is registered for the wall normal component. Further downstream, the core region profile for the cases are comparable.
5.3.2.4 Lateral averaged evolution of turbulence

As briefly alluded to in Section 4.5.4, the governing equations in STH codes are usually laterally averaged. Thus, it is important to analyze the axial evolution of turbulence features for the droplet laden cases and their comparative study with the single-phase simulation.

Figure 60 shows the axial evolution of cross-sectionally averaged normalized mean velocity. Accumulation of the droplets near the leading edge of the spacers due to collision results in a more pronounced increase in the streamwise velocity in the vicinity as compared to the single-phase case. Along the spacer and mixing vane profile the trend followed by single phase simulation and both the two-phase cases is similar, including the magnitude of velocity drop near the spacer trailing edge. Further downstream all cases asymptote to comparable velocity, although reduced as compared to average velocity at the inlet cross-section.

Figure 60: Comparison of axial evolution of plane averaged normalized mean streamwise velocity profile for the single phase, We40 and We80 cases.
Figure 61: Comparison of axial evolution of plane averaged normalized Reynolds stress components and turbulent kinetic energy profile for the single phase, We40 and We80 cases.
Figure 61 shows the axial evolution of plane averaged normalized Reynolds stress profile for the single phase and two-phase case. The dominant effect of the presence of droplets on turbulence enhancement is evident. It is important to emphasize that no correlations exist in CTF, to the author’s best knowledge, that account for this positive feedback provided by the droplets. However, the importance of the consideration of droplets is clearly conveyed by Figure 61. The increase in $TKE^+$ at the leading edge of the spacer is almost 25-35 times, that of single-phase case, with the enhancement for We80 case being higher. Further downstream, however, the TKE rapidly dissipates, reducing to a value close to that of single-phase case at the furthest downstream location. Further, it should be highlighted that the void fraction of the droplets, at the end of the two-phase simulations, is ~3%. It can be conjectured that the increase in energy of the principal stress components will be even greater for a higher population density.

5.4 Chapter Summary

This Chapter details the design and analysis of high-fidelity interface capturing simulations of droplet dynamics in a PWR sub-channel under representative post-LOCA DFFB conditions. Prior experimentation has firmly established the importance of spacer-grids and mixing vanes, specifically due to their effect on droplet dynamics, for characterizing the overall heat transfer coefficient of the DFFB regime. The downstream droplet conditions have been shown to strongly correlate to the upstream collision Weber number. Thus, in this Chapter presents four sets of simulations with different property ratio for droplet-gas system and different $We_c$. Data collection tools for recording the axial evolution of SMD of droplets are detailed. The results affirm the dependence of downstream SMD on upstream $We_c$ and are compared with existing empirical correlations. Further, using the data collection tools and mechanism described in Chapter 3 and Chapter 4, a detailed analysis of turbulence flow features is presented. The effect of the presence
of droplets on mean velocity profiles and Reynolds stresses is highlighted by comparison with the single-phase flow and comparison of two upstream $We_c$ cases. Cross-sectionally averaged axial profiles of Reynolds stresses and TKE emphasize the importance of accounting for the effect of droplets on convective heat transfer enhancement in the STH codes.
Chapter 6: Level-set Formulation - CG Spectral Element Method

Nek5000 [53] is a spectral element method based CFD code which, same as PHASTA, has also been shown to exhibit strong scaling on petascale supercomputers [140]. As shown in Chapter 5, the level-set interface capturing method shows tremendous promise in simulating complex flow regimes in nuclear reactors. This Chapter details the research conducted to incorporate the level-set based two-phase flow formulation in Nek5000, owing to the potential of interface capturing methods on strong scaling codes. As explained in the following sections, the SEM is not particularly well suited for pure hyperbolic problems, due to its minimal dissipation which does not offer any stability. This proved to be the major challenge in the successful implementation of level-set method, since it involves solving two additional hyperbolic problems, viz., the level-set advection and re-distancing equations. Thus, an artificial viscosity method, termed the spectrally vanishing viscosity, was implemented in Nek5000 for stabilization of pure hyperbolic problems. The implementation is demonstrated successfully on some challenging linear/non-linear hyperbolic problems. Further, the resulting level-set formulation is coupled with the existing low Mach number solver in Nek5000 [141] for a two-phase flow formulation and tested on a few typical 2D problems.

6.1 Basics of Spectral Element Method

Introduced by Patera [142], the spectral element method (SEM) is another major branch of numerical methods for the solution of incompressible Navier-Stokes equation, besides the finite element method (FEM), finite volume method (FVM), the finite difference method (FDM) and the more recently developed discontinuous Galerkin method (DGM). The SEM is very similar in its formulation to the FEM – both are constructed from a continuous Galerkin (CG) projection technique, the solution is approximated by a Lagrangian interpolation formula and they both have
local support i.e., the basis functions for both methods are non-zero in the interior of local element, \( \Omega_e \), and zero in the rest of domain, \( \Omega \) [143]. The basis functions used for the approximation of solution, however, dichotomizes the two methods. Specifically, the SEM methods are characterized as the collocated or pseudo-spectral methods, wherein the solution approximation is,

\[
I_N u(\xi) = \sum_{j=0}^{N} u_j \pi_j(\xi)
\]

(6.1)

where the basis, \( \pi_j(\xi) \), are defined such that \( I_N u(\xi_j) = u_j \), \( \xi_j \) being the \( N+1 \) Gauss quadrature points defined in the standard 1D element \( \hat{\Omega} \in [-1,1] \), and \( I_N \) is the interpolation operator. The simplest and most widely used basis for the SEM are constructed from Legendre polynomials, \( L_N \), defined on Gauss-Lobatto-Legendre (GLL) quadrature nodes in \( \hat{\Omega} \) [144],

\[
\pi_j(\xi) = \frac{1}{N(N+1)} \frac{(1-\xi^2)L'_N(\xi)}{(\xi-\xi_j)L_N(\xi_j)}, \quad 0 \leq j \leq N, \quad \xi \in \hat{\Omega}
\]

(6.2)

The SEM basis are orthonormal, i.e., the inner product on the standard element, \( \hat{\Omega} \), is defined as,

\[
(\pi_i, \pi_j)_{\hat{\Omega}} = \int_{\hat{\Omega}} \pi_i \pi_j \, d\Omega = \begin{cases} 1 & i = j \text{ otherwise} \
0 & \text{otherwise} \end{cases}
\]

(6.3)

which, upon subsequent expansion for all GLL points, yields a diagonal mass matrix. This is an extremely beneficial property of the Legendre SEM basis, from a computational perspective, since the inversion of mass matrix is trivial [143]. Note that a linear FEM basis also results in a collocated expansion, with the element nodes as quadrature points. Extension of the FEM basis to higher order, however, is not straightforward. Thus, most implementations of FEM are restricted to quadratic basis, limiting the accuracy of the method. Moreover, mesh refinement with FEM yields only an algebraic convergence rate. Nevertheless, FEM reigns in its generality and ease of
application to all elements, viz., tetrahedrons, prisms and wedges, which makes it ideal for complex geometries. In contrast, although SEM does provide spectral or exponential convergence for smooth solutions ($C_\infty$), its applicability is limited to hexahedral elements in 3D [142].

6.2 Stabilization of Pure Hyperbolic Problems within the SEM Framework

Spectral element method is particularly suited for linear/non-linear transport problems, in contrast to FEM, FDM or FVM, owing to minimal numerical dissipation. As a result, SEM allows long time integrations without significant decay or energy loss, as compared to its contenders. While a highly desirable feature, this property of SEM also makes its problematic for pure hyperbolic or even convection dominated problems. The reader is referred to the eigensolution analysis presented in the text by Deville et al [143] or a recent comprehensive analysis by Moura et al [145]. As shown by the latter study, for pure hyperbolic problems SEM discretization yields discontinuities in the eigensolution, especially for higher order approximations of the solution ($N > 6$). These discontinuities manifest in the higher wavenumbers and persist through time due to the absence of dissipation, resulting in spurious oscillations in the solution (primary wavenumber). Note that for parabolic problems, in contrast, the high wavenumber oscillations rapidly decay, smoothing out the solution.

Thus, the scourge of dispersion errors in advection dominated problems has been a continual source of vexation in the SEM framework. The problem is exacerbated if the underlying exact solution is discontinuous ($C_0$) or has discontinuities in its gradients ($C_1$), resulting in spurious oscillations in the vicinity, also referred to as the Gibbs phenomena [146]. Several techniques have been proposed in literature for stabilization of advection problems in the SEM framework, including, solution filtering [147], consistent integration of non-linear terms [148] and the class of methods characterized by augmenting the original PDE with second-order dissipative operators.
While the two former methods have been shown to be successful for advection-diffusion equations, they provide inadequate stabilization for purely hyperbolic systems.

Introduced by Maday and Tadmor [150] in the context of 1D non-linear conservation laws, the construction of spectrally vanishing viscosity (SVV) has since evolved to more complex systems [145,151,152] and applied to several engineering applications [153-155]. The SVV operator is imperatively built upon a Legendre basis, which provides a mechanism for it being activated only for high wave numbers, thus not affecting the convergence properties of the spectral approximation significantly [151]. Later, Kirby et al [152] developed the necessary matrix operators required for applying the SVV to any arbitrary orthogonal basis. Their construction allowed for a multi-dimensional formulation of SVV and ensured that the resulting matrix operator is symmetric and semi-positive definite. As mentioned before, Moura et al [145] presented a systematic analysis of the eigensolution resulting from the application of SVV to advection-diffusion equation. Their work also yielded an improved SVV “power kernel”, which provided a consistent increase in resolution power with increasing wave number, as opposed to the “exponential kernel” used in prior work [150,152].

Another branch of viscous regularization technique was introduced by Guermond et al [156] for CG methods, which hinges on the formulation of a non-linear viscosity coefficient based on local entropy production. Very recently Lu et al [157], enhanced and applied the concept to spectral element method (SEM), in particular, using a residual/filter-based scaling of the non-linear viscosity operator. They demonstrated the ability of the method to recover spectral convergence for smooth solutions and the effective stabilization of strong discontinuities through 1D and 2D examples.
In this work, we build upon the SVV construction of Kirby et al [152] using the “power kernel” of Moura et al [145]. A slightly modified construction of the SVV operator is introduced, which provides better stabilization, especially, for multi-dimensional problems. To the authors best knowledge SVV has not been tested on 2D linear/non-linear, purely hyperbolic, scalar convection problems. Thus, we demonstrate the stabilization and convergence properties of SVV on some archetypal hyperbolic systems with implicit discontinuities in solution, including, 2D linear system with strong initial discontinuity, shock capturing in 1D Burgers equation and resolution of discontinuous gradients in 2D Hamilton-Jacobi (level-set re-distancing) equation. For some cases, the results are also compared with non-linear artificial viscosity method by Lu et al [157], to elucidate the differences in the two approaches. The results show that the SVV construction adds a non-negligible viscosity only in the vicinity of discontinuities, thus not significantly affecting the accuracy of the solution in smooth regions. All work presented herein is built upon the foundations of the spectral element code Nek5000 [53].

6.3 Formulation of Spectral Vanishing Viscosity (SVV)

6.3.1 Preliminaries

Consider the general multidimensional scalar transport equation on a domain $\Omega$, complemented with initial condition,

$$\begin{align}
\frac{\partial u}{\partial t} + \vec{c} \cdot \nabla u &= f \\
u(\vec{x}, 0) &= u_0
\end{align} \quad (6.4)$$

where $\vec{x} \in \Omega \subset \mathbb{R}^d$, $\vec{c}$ is the convection velocity and $f$ is the forcing function, which may be linear/non-linear. In order to stabilize the system, equation (6.4) is augmented with an artificially constructed diffusion term [151],
\[
\frac{\partial u}{\partial t} + \vec{c} \cdot \nabla u = f + \mu \nabla \cdot (Q \nabla u) \tag{6.5}
\]

Limiting our discussion here to periodic domains, weak formulation of the above involves finding \( u(\vec{x}, t) \in V \) such that,

\[
\int_{\Omega} v \left( \frac{\partial u}{\partial t} + \vec{c} \cdot \nabla u \right) d\Omega = \int_{\Omega} vf d\Omega - \mu \int_{\Omega} \partial v \cdot (Q \nabla u) d\Omega \quad \forall \ v(\vec{x}) \in V \tag{6.6}
\]

where \( V = H^1(\Omega) \) is the space of square-integrable functions in \( \Omega \). Further, we divide \( \Omega \) into non-overlapping elements, \( \Omega_e \), such that \( \Omega = \bigcup \Omega_e \). In the spectral element method, the solution within a standard (2D) element, \( \hat{\Omega} \), is approximated by a tensor-product of 1D basis,

\[
u(r,s)|_{\hat{\Omega}} \approx \sum_{m=0}^{M} \sum_{n=0}^{N} u_{mn} \pi_{M,m}(r)\pi_{N,n}(s) = \sum_{i=0}^{P} u_i \phi_i(r,s) \tag{6.7}
\]

where \( \phi_i \) is the multi-dimensional expansion basis and \( u_i \) is the corresponding coefficient, while \( P = (M + 1)(N + 1) - 1 \). \( \pi_{M,m}(\pi_{N,n}) \) is the Lagrangian interpolant of degree \( M(N) \) based on Legendre polynomials, \( L(M) \) (equation (6.2)) [158]. The integrals in equation (6.6), written for each element \( \Omega_e \), are transformed via affine mapping to the standard element \( \hat{\Omega} \). Subsequent expansion of the basis using a standard Galerkin projection, wherein the test function is given by \( v = \sum_{j=0}^{P} v_j \phi_j \), yields the following matrix system of ordinary differential equations,

\[
v^T M \frac{du}{dt} = v^T (-C u + M \vec{f} - S_{vv} u) \tag{6.8}
\]

\( M \) and \( C \) are the mass and convective matrix operators, respectively. \( \underline{u} = (u_0, u_1, \ldots, u_{p+1})^T, \underline{f} = (f_0, f_1, \ldots, f_{p+1})^T \) and \( \underline{v} = (v_0, v_1, \ldots, v_{p+1})^T \) are the vector representations of coefficients corresponding to approximations of \( u, f \) and \( v \), respectively. The interested reader is referred to the text by Deville et al [158] for further details on the construction of these operators. Note that
owing to the aforementioned orthonormality property of the SEM basis, equation (6.2), both matrices, evaluated at GLL (Gauss-Lobatto-Legendre) quadrature points, are diagonal, greatly simplifying the system. Here, we focus discussion on the construction of the stiffness matrix, $S_{\nu\nu}$, pertinent to the application of the artificial viscosity.

### 6.3.2 Matrix Formulation of the SVV operator

Construction of the multi-dimensional SVV matrix was detailed by Kirby et al. [152]. Following the authors, we commence by introducing the rudimentary building blocks for constructing the diffusion term in equation (6.6). Introduce a (2D) basis matrix, $B$, which is composed of columns of multi-dimensional basis, $\phi_i$, evaluated at the GLL quadrature points, indexed as $j$, of the standard element, $\Omega$,

$$B[j][i] = \phi_i(x^j) = \psi_m(r^k)\psi_n(s^l)$$  \hspace{1cm} (6.9)

where $\psi$ represents any general expansion basis (modal or nodal). Considering the order of polynomial expansion basis in both directions $r$ and $s$ to be $N$, we have $0 \leq m, n \leq N$. Of particular importance is the mapping of the 2D index $i$ with respect to the 1D basis indices,

$$i = m(N + 1) + n + 1$$  \hspace{1cm} (6.10)

Further, a similar indexing pattern is also applied to the GLL point $j$ of $\Omega$ with respect to the point indices $(k,l)$ of 1D standard element,

$$j = (k - 1)(N + 1) + l; \hspace{0.5cm} 1 \leq k, l \leq N + 1$$  \hspace{1cm} (6.11)

Note that the above indexing is consistent with the current array structure in Nek5000, allowing for straightforward implementation of subsequent matrix-matrix/matrix-vector multiplications.

Similarly, the 2D derivative matrices are defined as,
\[ D_r[j][i] = \frac{\partial \phi_j}{\partial r} \bigg|_{x_i} = \psi'_m(r^k)\psi_n(s^l) \] (6.12)
\[ D_s[j][i] = \frac{\partial \phi_j}{\partial s} \bigg|_{x_i} = \psi_m(r^k)\psi'_n(s^l) \]

Finally, in accordance with the affine transformation, the matrix derivative operators for an arbitrary element, \( \Omega_e \), in global coordinates will be,

\[ D_x = G_r^x D_r + G_s^x D_s \] (6.13)

where \( G_r^d \) and \( G_s^d \) are diagonal matrices consisting of geometric factors at corresponding GLL points (\( d \) represents the global coordinates),

\[ G_r^d[j][j] = \frac{\partial r}{\partial d} \bigg|_{x_i}; \quad G_s^d[j][j] = \frac{\partial s}{\partial d} \bigg|_{x_i} \] (6.14)

Further, define a diagonal matrix \( W \), which contains quadrature weights multiplied by the Jacobian of the transformation matrix mapping from \( \Omega_e \) to \( \hat{\Omega} \). Momentarily ignoring \( Q \) from the diffusion term in equation (6.6), the discrete Laplacian term obtained from the following Galerkin approximation is,

\[ \int_{\Omega_e} \nabla v \cdot \nabla u \, d\Omega \approx v^T(D_r^x WD_x + D_s^x WD_s)u \] (6.15)

The key to implementing SVV, as expounded by Kirby et al [152], hinges on an, equivalent, alternate construction of the above system,

\[ D_r^x WD_d \equiv S_d^T M^{-1} S_d \]
\[ M = B^T WB; \quad S_d = B^T WD_d \]

where \( M \) is the usual mass matrix and \( S \) is an elemental matrix which is, essentially, defined by the following inner product,
\[ S_d = \left( \phi_j, \frac{\partial \phi_i}{\partial d} \right)_{\Omega_e} \]  

(6.17)

The general matrix definitions in equations (6.9) and (6.12) are now adapted for matrices built from a spectral element (nodal) and Legendre (modal) bases, denoting the latter by superscript (\sim) and retaining the notation for the former. Thus, the mass matrix associated with Legendre basis is,

\[ \tilde{M} = \tilde{B}^T \tilde{W} \tilde{B} \]  

(6.18)

The following definition of the elemental matrix allows the projection of the derivatives from nodal onto modal space,

\[ \tilde{S}_d = \tilde{B}^T \tilde{W} D_d \]  

(6.19)

through the subsequently derived operator \( \tilde{M}^{-1} \tilde{S}_d \). Filter kernels \( \tilde{Q}_d \) are then applied to the resulting modal projections, which allow preferential control of higher wave number terms. Finally, the artificial viscosity matrix operator in equation (6.8) is constructed as,

\[ S_{vv} = \mu (\tilde{S}_x^T \tilde{Q}_x \tilde{M}^{-1} \tilde{S}_x + \tilde{S}_y^T \tilde{Q}_y \tilde{M}^{-1} \tilde{S}_y) \]  

(6.20)

\( \tilde{Q} \) is a diagonal matrix with entries given by the array \( \hat{q} \), corresponding to wave numbers of the modal basis. Note that the matrix operations required for the construction of \( S_{vv} \) are expensive. However, the operator is evaluated only once in the pre-processing stage of the simulation. At each simulation step, application of the operator requires one matrix-vector product (for each direction).

6.3.3 Construction of Filter Kernels for SVV

6.3.3.1 A brief history of kernel design

As noted earlier, the filter kernels are constructed in modal space, wherein the basis are hierarchical, thus allowing explicit control over desired wave numbers. Early construction of the filter was introduced by Maday et al [151] in a 1D context and applied to cases where the solution
space was also modal. The filter, as defined below for a given polynomial order $N$, was activated only for modes with indices, $m > N_{SVV}$,

$$
\hat{q}^m = \exp\left(-\frac{(m - N)^2}{(m - N_{SVV})^2}\right); \quad m > N_{SVV}
$$

(6.21)

$N_{SVV} \sim \sqrt{N}$ or $N$ are used most commonly in literature [151,152]. Moura et al [145] presented a detailed analysis of the solution of advection-diffusion equation with the above kernel design. They observed that for convection dominated flows the kernel yielded spurious oscillations with increasing polynomial order. This was reported even for the choice of $N_{SVV} = 0$, the asymptotic limit, which introduces the highest dissipation attainable for a given polynomial order, indicative of inadequate stabilization properties of the kernel. The trend of the above kernel is shown in Figure 62. To overcome stability issues, the authors proposed a new “power” kernel design,

$$
\hat{q}^m = \left(\frac{m}{N}\right)^{N_{SVV}}
$$

(6.22)

also shown in Figure 62 for $N_{SVV} = N/2$ and $N$, which provides a consistent increase in viscous effect with increasing wavenumber for a given polynomial order $N$, as opposed to a cut-off value for the exponential kernel. It is important to note, that this filter affects all but the zeroth mode, however, the magnitude becomes increasingly small as $N$ is increased for the smaller wavenumbers. The authors [145] analyzed the effect of this design on the convergence behavior, for a Fourier series expansion basis. Their results indicated algebraic convergence for a fixed $N_{SVV}$, while an exponential convergence for $N_{SVV} \propto N$.

The multi-dimensional extension of the filter is based on the tensor product formulation of the multi-dimensional basis. The ordering of the orthogonal basis products, consistent with equation (6.10), is used as the indexing order for populating the 2D filter matrix $\tilde{Q}$. Note that the
matrix is necessarily diagonal and has non-negative entries, by design. This ensures that the resulting $S_{νν}$ operator is positive semi-definite [152], i.e.,

$$\hat{φ}^T \tilde{S}^T \tilde{Q} \tilde{M}^{-1} \tilde{S} \hat{φ} \geq 0; \quad \forall \hat{φ} \neq 0$$  \hspace{1cm} (6.23)

since $\tilde{M}$ is always diagonal due to the orthogonal nature of the Legendre basis. The diagonal array for 2D form of the exponential filter, as given by Kirby et al [152] is,

$$\hat{q}[i] = \begin{cases} 0 & m + n \leq N_{SVV} \\ \exp\left(-\frac{(m + n - N)^2}{(m + n - N_{SVV})^2}\right) & \text{otherwise} \end{cases}$$  \hspace{1cm} (6.24)

Moura et al [145] presented an updated formulation, where the 2D filter was a product of corresponding 1D kernels,

$$\hat{q}[i] = \begin{cases} 0 & m, n \leq N_{SVV} \\ \exp\left(-\frac{(m - N)^2}{(m - N_{SVV})^2}\right) \exp\left(-\frac{(n - N)^2}{(n - N_{SVV})^2}\right) & \text{otherwise} \end{cases} \quad (6.25)$$

$$\hat{q}[i] = \left(\frac{m}{N}\right)^{N_{SVV}} \left(\frac{n}{N}\right)^{N_{SVV}}$$

for exponential and power kernels, respectively.

Figure 62: Comparison of filter trend with increasing wave number index, $m$, for exponential (left) and power (right) kernels.

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6.3.3.2 Scaling the viscosity amplitude, $\mu$

In early implementations of SVV, the amplitude of viscosity factor was scaled inversely with the polynomial order [151,152]. Moura et al [145] suggested a more consistent implementation, such that the local Peclet number is kept constant across different mesh sizes and local convection velocity. In addition, elaboration of the discrete terms in the SVV operator (6.20) reveal that for consistency in amplitude scaling across polynomial orders, the following should be kept constant,

$$Pe^* = \frac{Pe}{N}$$ (6.26)

where $Pe$ is the local Peclet number,

$$Pe = \frac{|\vec{c}|h}{\mu}$$ (6.27)

Thus, a base scaling factor $\mu_0$ is used as an input parameter, such that the resulting amplitude is independent of mesh size, local convection velocity and polynomial order,

$$\mu = \mu_0 \frac{|\vec{c}|h}{N}$$ (6.28)

which results in $Pe^* = \mu_0^{-1}$.

6.3.3.3 Modified multi-dimensional filter

In our experimentation with the aforementioned 2D filters, the stabilization properties were found to be inadequate, especially for the more demanding 2D cases (as in Section 6.5.4). According to equations (6.24) and (6.25), the same matrix operator $\tilde{Q}$ is applied to the construction of the Laplacian operators in both orthogonal directions in equation (6.20). We further note that the wavenumber for the 2D tensor product form is dictated by higher of the two 1D wavenumbers, which contribute to the product. Thus,
\[ p(i) = \max (m, n) \tag{6.29} \]

where \( i \) is the index given by equation (6.10) and \( p \) represents the apparent wavenumber of the 2D Legendre basis. From this vantage point, the limitation of the construction in equations (6.24) and (6.25) becomes apparent. For the same wavenumber, the magnitude of viscosity introduced for the 2D construction is scaled down by the product of the contribution from the smaller mode, as compared to the corresponding 1D kernel. Based on this realization we propose the construction of independent kernel matrices for the Laplacian term for each direction, as already alluded to in equation (6.20). Thus, the exponential and power kernels used in this work are given, respectively, as,

\[
\hat{q}_x[i] = \begin{cases} 0 & m \leq N_{SVV} \\ \exp \left( -\frac{(m - N)^2}{(m - N_{SVV})^2} \right) & \text{otherwise} \end{cases} \tag{6.30}
\]

\[
\hat{q}_y[i] = \begin{cases} 0 & n \leq N_{SVV} \\ \exp \left( -\frac{(n - N)^2}{(n - N_{SVV})^2} \right) & \text{otherwise} \end{cases} \tag{6.31}
\]

Note that the diagonal index in each of the directional kernel arrays, \( \hat{q}_d \), is still governed by equation (6.10). Thus, the definitions in equations (6.30) and (6.31) amount to applying artificial viscosity in each direction independently. Consequently, the same magnitude of viscosity is applied to a particular wavenumber, as the corresponding 1D construction. Finally, note that this deconstruction of kernels is possible due to the very nature of the Laplacian term itself, equation (6.15), since it involves a dot product of the expansion basis.
6.4 Non-Linear Artificial Viscosity Method

An alternate branch of artificial viscosity stabilization for CG projection methods was introduced by Guermond et al [156]. Lu et al [157] recently improved upon the original method and demonstrated its application to SEM, in particular. We briefly introduce their implementation, hereon represented by the acronym AVM. Slightly contrary to SVV, AVM introduces a non-linear viscosity coefficient into the artificially constructed diffusion term, as described below in the weak form,

$$\int_{\Omega} \mu_a(\vec{x}) \nabla v \cdot \nabla u \, d\Omega$$

The method hinges on the design of $\mu_a$, defined by Lu et al as,

$$\mu_a = \min(\mu_E, \mu_h)$$  \hspace{1cm} (6.33)

where $\mu_E$ scales with an error indicator function, $r_E(u)$,

$$\mu_E = c_E h^2 r_E(u)$$  \hspace{1cm} (6.34)

c_E being an input control coefficient and h being the mesh size. $\mu_h$, in equation (6.33), is an upper bound of viscosity, defined as follows,

$$\mu_h = \gamma h |\vec{c}|$$

Several implementations of the error indicator function $r_E(u)$ were enumerated by Lu et al. We introduce one of those implementations, which was used for comparative studies presented herein. Ignoring the forcing function from the original governing equation for simplicity, the semi-discrete form, similar to the one shown in equation (6.20), for pure advection equation is,

$$\frac{du}{dt} = -M^{-1}Cu$$

(6.36)
Fisher et al [147] presented the construction of a low-pass filter, designed to eliminate spurious oscillations from the highest frequency modes, given by \( F(u) \) (see cited paper for details on the construction of \( F \)). The filter provides a mechanism for the approximation of the residual in equation (6.34), constructed from the difference between the filtered and original solution as,

\[
R(u) = M^{-1}C(I - F)u
\]

which provides a reliable error indicator function,

\[
r_E(u) = \frac{R(u)}{\|u - \overline{u}\|_\infty}
\]

where \( \overline{u} \) is the globally space averaged value of \( u \). We make a final note that the default values provided by Lu et al [157] for the construction of filter \( F \) are retained in all subsequent comparative studies, i.e., a linear low-pass filter is constructed with a cut-off wave number of \( N_c = N/5 \) and \( \alpha = 0.5 \) for the transfer function in local modal space.

6.5 Computational Experiments

6.5.1 Convergence behavior for Smooth Solution

It is imperative to the design of any stabilization method that the convergence behavior of the solution is not affected significantly in smooth regions of the solution. Thus, to analyze the error decay behavior of aforementioned methods, we setup a 1D linear transport problem with initial solution defined by \( u(x, 0) = \sin(\pi x) \) in \( x \in [-1,1] \). Periodic boundaries are specified at the edges and the domain is discretized into 5 spectral elements. The convection speed is fixed at \( c = 1 \). The simulation is allowed to run for \( t = 1s \), with a fixed \( \Delta t = 10^{-5}s \) for all cases. Second order explicit Runge-Kutta time integration is used to advance the solution, which precludes the complexities of implicit discretization of diffusion terms, albeit at the trade-off of imposing CFL constraints. We note here that explicit RK2 is also used for all other cases shown in this work. The
base amplitude factor of the SVV term, $\mu_0$, is 0.1 for all cases. The parameters for the AVM, as in equations (6.34) and (6.35) are, $c_E = 0.5, 2$ and $\gamma = 0.5$.

Figure 63: Convergence behavior for 1D smooth sine wave obtained from errors measured at $t = 1s$ with different SVV kernels, up to polynomial order $N = 11$.

Figure 63 shows the globally measured $L_2$-norm of the error plotted against polynomial order, defined as,

$$
\|e\|_{L_2} = \frac{\sqrt{\int_{\Omega} (u - u_{exact})^2 d\Omega}}{\int_{\Omega} d\Omega} \quad \text{(6.39)}
$$

Both exponential and power kernels, as in equations (6.21) and (6.22), respectively, were tested for different $N_{SVV}$ values. Consistent with prior discussion, the exponential kernel with $N_{SVV} = 0$ affects all but the zeroth mode, consequently, providing maximum dissipation of all SVV kernels (recall Figure 62). The decay rate for the power kernel is more consistent, as evident by a more linear profile in Figure 63, with increasing polynomial approximation, as compared to the exponential kernel. For higher values of $N$, both exponential kernels add inordinately more dissipation to lower wavenumbers, resulting in a sharp change in decay rate at $N = 5$ and 6 for $N_{SVV} = 0$ and $N/2$, respectively. Nevertheless, the exponential kernel with $N_{SVV} = N/2$ shows
the closest decay rate to the pure advection case among all SVV kernels and AVM cases. The AVM shows the most desirable profile for this case, yielding a consistent spectral decay rate profile, with parameter $c_E$ only having the effect of scaling the dissipation term.

### 6.5.2 Non-linear Advection, Capturing Shock: Burgers Equation

The augmented inviscid Burger’s equation is given by,

$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = L(u)$$

where $L(u)$ represents the source term yielded by either the SVV or AVM operators. The initial condition, following Maday et al [151], is $u(x, 0) = 1 + 0.5 \sin (\pi x)$ on $x \in [-1,1]$. Periodic boundary conditions are specified across the domain extremes. The characteristic curves intersect at $t_c = 2/\pi$ yielding a shock discontinuity at $x_c = (2 - \pi)/\pi$. To obtain error decay trends for the case, an extensive array of tests was performed with meshes consisting of 10-80 elements ($N_{el}$) for each of the following mentioned SVV and AVM operators. For all the SVV cases $\mu_0$ is maintained at 0.1. Further, all cases were run with a constant time step size of 50$\mu$s, ensuring a low CFL even for the highest resolution cases.

Figure 64 shows the solution obtained at $t = 1s$ for meshes with 10, 40 and 80 elements. The exponential and power kernels both have an $N_{SVV} = N/2$ for the plots shown in this Figure, while the residual scaling parameter for the AVM case is $c_E = -0.5$. Evidently, the AVM kernel is more effective at eradicating oscillations in the vicinity of the discontinuity than either of the SVV kernels, albeit resulting in a worse convergence trend in the smooth regions of the domain as seen in Figure 65. The effect of SVV kernels is more localized as compared to the AVM operator, as can be deduced from the trend of absolute errors at collocation points shown in Figure 66 at $t = 1s$. For the SVV kernels the errors are concentrated near the discontinuity, at $x = 0$. Moreover, the power kernel exhibits a superior localization than the exponential kernel, however
the error magnitude is smaller for the latter. For the AVM operator, on the other hand, the errors diffuse away from the discontinuity onto smoother regions. This behavior can be owed to the difference in construction of the SVV (equation (6.20)) and AVM (equation (6.32)) operators. *AVM uses residual to scale the viscosity coefficient $\mu_a$, while the SVV filter, $Q$, operates on the gradients itself.* Note that the mesh with 10 elements is too coarse to observe the aforementioned error localization trends. Nevertheless, the error trends for the finer meshes elucidate that with increasing mesh refinement, the SVV operator yields increasing localization, while this desirable trend is not observed with the AVM operator.
Figure 64: Solution obtained with SVV exponential kernel (top), SVV power kernel (middle), both with $N_{SVV} = N/2$, and AVM operator (bottom) at $t = 1s$ with polynomial order $N = 7$, for three meshes with 10, 40 and 80 elements
Figure 65: Pointwise L1-norm of error with different SVV and AVM operators for polynomial orders 5 and 7, in the region $|x| > 0.2$.

The convergence trends are shown in the log-line plot, Figure 65, for varied SVV and AVM kernels, obtained from the point-wise $L_1$ norm of error,

$$L_1 = \frac{1}{N_T} \sum_{n=1}^{N_T} \Delta h |u_n - u_n^{\text{exact}}|$$

(6.41)

where $N_T$ is the total number of collocation points in the smooth region $|x| > 0.2$ and $\Delta h$ is the length of an element. Consistent with prior discussion, the AVM kernel yields algebraic convergence, again, owing to the diffusion of errors. Increasing the viscosity scaling factor, $c_E$, only reduces the error but does not affect the convergence trend. The SVV power kernel exhibits geometric convergence with the kernel $N_{SVV} = N$ and an algebraic trend with $N_{SVV} = N/2$. The latter kernel gives a lower value for the error norm, which seems to contradict the trends obtained for the smooth case presented in Section 6.5.1. The reason for this is revealed by comparing the error plots in Figure 66 and Figure 67. The point-wise error for the kernel $N_{SVV} = N$ are lower, however, $N_{SVV} = N/2$ results in better localization, yielding a lower overall norm. Similar rationale explains the lower value of error norm obtained from the exponential kernel $N_{SVV} = 0$ as
compared to $N_{SVV} = N/2$, although the former provides stronger overall dissipation. The behavior of the exponential kernel is less consistent as compared to the power kernel (Figure 65). A geometric trend is observed with $N_{SVV} = 0$ for the polynomial order of 5, while an algebraic with an order of 7. For $N_{SVV} = N/2$ the trend is, at least up to $N_{el} = 60$, geometric for both polynomial orders.
Figure 66: Log of errors at collocation points obtained from the SVV exponential kernel (top), SVV power kernel (middle), both with $N_{SVV} = N/2$, and AVM operator (bottom) at $t = 1s$ with polynomial order $N = 7$, for three meshes with 10, 40 and 80 elements.
6.5.3 Linear Advection of Discontinuous Solution: Zalesak Pole Problem

In this section, advancing into 2D simulations, we examine the rigid body linear advection problem, specifically the Zalesak pole problem, which has been extensively used in literature as a rigorous test case for stabilizing schemes [157,159]. For a more veritable analysis of the construction of the multi-dimensional SVV matrix operator (equation (6.20)) and its kernels (equations (6.30) and (6.31)), the computational domain is rotated at an angle of $\theta = 45^\circ$. The slotted pole is initialized as,

$$ x_c = 0.5\cos\theta - 0.5\sin\theta; \ y_c = 0.5\sin\theta + 0.75\cos\theta $$

$$ \phi = \sqrt{(x - x_c)^2 + (y - y_c)^2} - 0.15 $$

$$ u(x,y) = \begin{cases} 1 & \phi \leq 0 \ & (|x| < 0.025 \ & y < 0.5\sin\theta + 0.85\cos\theta) \\ 0 & otherwise \end{cases} $$

Figure 67: Log of errors at collocation points obtained from the SVV exponential kernel $N_{SVV} = 0$ (top) and power kernel $N_{SVV} = N$ (bottom) at $t = 1s$ with polynomial order, $N = 7$, for three meshes with 10, 40 and 80 elements
while the underlying velocity field is rotational, given by,

\[
\begin{align*}
v_x &= \pi (0.5(\cos\theta - \sin\theta) - y) \\
v_y &= \pi (x - 0.5(\cos\theta + \sin\theta))
\end{align*}
\]  

(6.43)

The domain is periodic across opposite ends. Studies were performed on two different meshes with 20 and 40 elements in each direction and with polynomial orders of 5 and 7. A fixed time step size of $2 \times 10^{-4}$ s was chosen for all cases, which corresponds to a CFL of 0.392 for the highest resolution case (note that CFL is calculated based on the GLL point location). The base viscosity factor, $\mu_0 = 1$ for all SVV cases. Note that the SVV kernel construction given in equation (6.25) were found to provide inadequate stabilization for $\mu_0 = \{0.01, 0.1, 1, 100, 1000\}$ for this study. Moura et al [145] demonstrated the applicability of this construction for the stabilization of advection-diffusion equation. However, in our experiments for the stabilization of pure hyperbolic systems, it did not provide reliable stabilization and, thus, has been abandoned.

Figure 68 and Figure 69 show the solution obtained after one complete rotation, $t = 2s$, with different SVV kernels for the 40 element mesh with polynomial order of 7. Also shown in the figures is the source term, $S_{vv}(u)$, obtained from the SVV operator, which gives an intuitive understanding of the effect of stabilizing term, represented by a uniformly scaled extrusion surface. It is evident that the effect of the operator is more localized for the power kernel as compared to the exponential kernel. The power kernel with $N_{SVV} = N/2$, consistent with previous cases, is more dissipative resulting in less pronounced undershoots and overshoots compared to the $N_{SVV} = N$ kernel. Similarly, the exponential kernel with $N_{SVV} = 0$ introduces more overall dissipation as compared to $N_{SVV} = N/2$, consequently providing better amelioration of overshoots and undershoots near the discontinuity. AVM on the other hand, as seen in Figure 70, with the aforementioned default parameters for the construction of filter and $c_E = 0.5$, eliminates spurious oscillations near the discontinuity. However, AVM introduces sustained perturbations in the
smooth regions, relatively further from the discontinuity, as can be observed in Figure 71 or more clearly in Figure 72. The former figure shows a line plot of the solution at the location \( y = 0.89 \) for all the cases, illuminating the difference in the behavior of all methods near the discontinuity. Note that the central notch in the mesh with 20 elements along each dimension is resolved with less than one element width. Nevertheless, SVV with the power (\( N_{SVV} = N \)) and exponential (\( N_{SVV} = N/2 \)) kernels capture the discontinuity very well even for the coarsest case. In Figure 72 errors are extruded with a uniform scale factor for the SVV, with \( N_{SVV} = N \) power kernel, and AVM operators for the 40 element mesh and polynomial order of 7. This result clearly shows the superior localization property of the SVV operator.

We make a final note that the solution obtained with SVV can be post-processed with a low-pass filter, similar to approach adopted by Maday et al [151], to eliminate oscillations. Here, however, we defer that task to focus on the results obtained from the pristine artificial viscosity formulation.
Figure 68: Solution and the $S_{uv}(u)$ source term obtained with SVV using two different power kernels, $N/2$ (top) and $N$ (bottom), after one rotation, $t = 2s$. 
Figure 69: Solution and the $S_{\nu_0}(u)$ source term obtained with SVV using two different exponential kernels, 0 (top) and $N/2$ (bottom), after one rotation, $t = 2s$. 
Figure 70: Solution obtained with AVM after one rotation, \( t = 2s \), with \( c_E = 0.5 \).

Figure 71: Solution plotted on the line \( y=0.89 \), at \( t = 2s \), for all cases with different stabilization methods. \( N = 5 \) (top) and \( N = 7 \) (bottom) polynomial order shown for 20 (left) and 40 (right) element meshes.
Figure 72: Errors obtained at $t = 2s$ for SVV, with $N_{SVV} = N$ power kernel (left), and AVM, with $c_E = 0.5$ (right), operators for polynomial order 7 and 40 element mesh. Error magnitude is extruded uniformly for both cases.

6.5.4 Hamilton-Jacobi Equation, Discontinuous Gradients: Level-set Re-distancing

For a final demonstration of the SVV, we present its application to the stabilization of Hamilton-Jacobi type equation (HJE). One of the popular applications of the HJE in fluid dynamics is the re-distancing of level-set field, used for capturing the interface between immiscible liquids [160]. The re-distancing PDE, augmented with the stabilizing Laplacian operator, is given as,

$$\frac{\partial \phi}{\partial t} = \text{sign}(\phi)(1 - |\nabla \phi|) + L(\phi)$$
(6.44)

The complexity of the re-distancing PDE lies in that the convection speed depends on the local gradient, elucidated when written in advection form,

$$\frac{\partial \phi}{\partial t} + \vec{w} \cdot \nabla \phi = \text{sign}(\phi)$$
(6.45)

$$\vec{w} = \text{sign}(\phi) \frac{\nabla \phi}{|\nabla \phi|}$$
Simulations of enclosed surfaces, such as bubbles and droplets, using the level-set method ensures that there will be a discontinuity in the gradients of the level-set field, although the solution itself is always continuous. Subsequent application of re-distancing equation, essential for maintaining accurate curvature in the vicinity of the interface, results in spurious oscillations in the vicinity of these gradient discontinuity sites, progressively ravaging the level-set field.

![Figure 73: Level-set field contours for the intersecting circles problem, initial (left) and exact (right)](image)

We use the non-smooth intersecting circles test described by Karakuş et al [161]. The initial condition features a skewed level-set field described as (see Figure 73),

\[
\phi_\varepsilon(x, y) = \begin{cases} 
\max \left( -\sqrt{x^2 + \left( y \pm \sqrt{r^2 - a^2} \right)^2} \right) & a - x \geq \frac{a}{r} \text{ and } a + x \geq \frac{a}{r} \\
\min \left( \sqrt{(x \pm a)^2 + y^2} \right) & \text{otherwise}
\end{cases} 
\]

\[
\phi_0(x, y) = ((x - 1)^2 + (y - 1)^2 + 0.1)\phi_\varepsilon(x, y)
\]
The circles have a radius $r = 1$ and $a = 0.7$. The re-distancing equation, run for a sufficient number of iterations, corrects $\phi_0$ to the signed distance field, given by $\phi_e$. Note that the exact solution has a line gradient discontinuity across portions of $x=0$ and $y=0$ lines. Further, the initial solution has gradients ranging from very high to very low along the zero-contour line, making this an extremely challenging test case for the re-distancing equation. The $sign(\phi)$ in equation (6.44) changes abruptly across the zero contour of level-set, which would lead to inexorable oscillations in CG formulation. Thus, it is smeared across the zero contour as,

$$\text{sign}(\phi) = \tanh\left(\frac{\pi \phi}{\epsilon}\right)$$

(6.47)

where $\epsilon$ is a user defined smearing length, chosen herein equal to $\frac{\Delta h}{N+1}$, $N$ being the polynomial order.
Figure 74: Solution (left) and error (right) contour obtained on a 40X40 mesh for two polynomial orders, $N = 5$ (top) and $N = 7$ (bottom), with the SVV operator using the $N_{SVV} = N/2$ power kernel.
Figure 74 shows the solution obtained from the SVV operator on a 40X40 uniform mesh with polynomial orders of 5 and 7. Power kernel was used for this case with $N_{SVV} = N/2$, which was found to be the most robust among all the aforementioned kernels. Even the power kernel with $N_{SVV} = N$ yielded spurious oscillations along the discontinuities as the simulation proceeded, and thus has not been shown. The base amplitude factor was chosen to be $\mu_0 = 0.5$. The simulation was initiated with a relatively low CFL of 0.01, which was stepped up to a CFL of 0.1 after a few iterations.

Recall that the characteristics for the re-distancing equation, as evident from equation (6.45), originate at the zero contour and travel away along the direction of normal to the zero contour. Similar behavior is exhibited by the absolute errors in Figure 74, measured at quasi-steady state. Figure 75 shows the source term yielded by the SVV operator at quasi-steady state for the two polynomial orders. Diffusion is essentially added in the vicinity of kinks, as evident from the
contour map, especially for the $N = 7$ case, bolstering confidence in the localized action of the SVV diffusion term.

6.6 Two-phase formulation in Nek5000

The low Mach number solver was introduced in Nek5000 by Tomboulides et al [141] for the simulation of reactive flows. The attractive feature of the formulation for present application is that it allows for both variable density and viscosity implementation in Nek5000. Originally the low Mach number solver requires the specification of thermal divergence, $Q_T$, as source term to the incompressibility constraint,

$$\nabla \cdot \vec{u} = Q_T$$

(6.48)

However, for adiabatic two-phase formulation which does not involve any mass transfer across the interface, (as, for example, in phase change problems), the thermal divergence supplied to the low Mach number solver will be zero. The momentum equation retains its original form, with the added regularized surface tension force [63],

$$\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p + \nabla \cdot \tau + \vec{f} + \vec{f}_s$$

(6.49)

where, $\vec{f}_s$, is the surface tension force, given by Eq. (2.8). Note that both density and viscosity in the momentum equation are functions of the level-set scalar, $\rho(\phi)$ and $\mu(\phi)$. Similar to the formulation described in Section 2.2 the properties are smeared across the interface using a smooth Heaviside function, Eq. (2.3).

6.6.1 Rayleigh-Taylor instability problem

To test the level-set two-phase formulation in Nek5000, we perform a 2D simulation of Rayleigh-Taylor instability for parameters described by Karakus et al [162]. The rectangular domain, as shown in Figure 76, has a width of $D/2$ and length of $4D$, where the characteristic
length $D = 1$. Symmetry boundary conditions are specified on the left and right faces, while no-slip boundary condition is specified at the top and bottom faces. A heavier fluid is initialized over a lighter fluid, with the Atwood number for the setup being equal to 0.5, defined as,

$$At = \frac{\rho_l - \rho_g}{\rho_l + \rho_g}$$  \hspace{1cm} (6.50)

where $\rho_l$ and $\rho_g$ represent the denser and lighter fluids, respectively. The dynamic viscosity for both fluids is equal. The Reynolds number of the flow is 3000, defined as,

$$Re = \rho_l D^{1.5} g^{0.5} / \mu_l$$  \hspace{1cm} (6.51)

The initial level set field is given by,

$$\phi_0(x, y) = y - (2D + 0.1 \cos(2\pi x))$$  \hspace{1cm} (6.52)

which also describes the initial location of the interface, as shown in Figure 76. A mesh with 16 X 128 elements was created and a polynomial order of 7 was used for the simulations. The CFL for the flow solver was limited to a maximum value of 0.5, while the CFL for the re-distancing equation was limited to a maximum value of 0.01. Thirty re-distancing iterations were performed at each time step after level-set advection solve. SVV stabilization was applied only to the re-distancing equation using a power kernel with an amplitude factor, $\mu_0 = 3$, and $N_{SVV} = N/2$. For both property transition, Eq. (2.3), and smearing the sign function across the interface for re-distancing equation, Eq. (6.47), a length of $\epsilon = \Delta h / N$ was chosen, where $\Delta h$ is the edge length of a cell and $N$ is the polynomial order. The evolution of interface topology compares well with the results shown by Karakus et al [162] (their results are included in Appendix A.7). Note the authors used an adaptive discontinuous Galerkin method for their simulations with a polynomial order of 3, which could explain the differences observed in topology. Figure 77 shows the evolution of
level-set contours and the SVV stabilization term, Eq. (6.20). It is evident that a non-zero SVV diffusion is added only in the vicinity of discontinuous gradients of level-set at each time step. The magnitude of SVV term in the rest of the domain is negligible. Figure 77 highlights the localized stabilization feature of the SVV construction.

Figure 76: Evolution of interface for Rayleigh-Taylor instability problem. Images shown at $t = 0, 0.55, 0.69, 0.81, 1.01, 1.2$ and $1.3$ s.
Figure 77: Evolution of level-set contours (zero contour highlighted in white, rest in black) and SVV stabilization term (color contour map) for Rayleigh-Taylor instability problem. Images shown at $t = 0, 0.55, 0.69, 0.81, 1.01, 1.2$ and $1.3$ s.

6.7 Chapter Summary

This Chapter details the implementation of spectrally vanishing viscosity (SVV) in the spectral element method based code, Nek5000. Specifically, SVV is introduced for the stabilization of pure hyperbolic problems which accompany the level set formulation, including the level-set advection and re-distancing equation. The effectiveness of SVV is demonstrated with problems including the inviscid Burger’s equation, linear advection of discontinuous solution and re-distancing for highly skewed initial level-set field around intersecting circles. Further, continuum surface tension force was implemented in Nek5000 for two-phase formulation and coupled with the existing low Mach number solver. The formulation is demonstrated using a Rayleigh-Taylor instability simulation with good agreement with existing simulation in literature.
Chapter 7: Avenues for Future Research

The primary objective of the present research is interface capturing simulations to represent conditions in the DFFB regime, in the vicinity of spacer-grids and mixing vanes. Although the high resolution simulations presented in Chapter 5 and subsequent analysis of the results is a tremendous leap forward in understanding the intricacies of the dynamics of droplets in the DFFB regime, yet the implicit or explicit assumptions of the simulation setup make them far from representing the actual DFFB conditions.

This Chapter presents discussion on the knowledge gaps between the simulations and DFFB regime and the source of uncertainty that may introduce errors in the results presented in Chapter 5. The identification of the limitations of the current simulations then enables us to create a roadmap for future research into enhancing the understanding of the DFFB regime. Further, recommendation on improving the LTS formulation is discussed which is expected to provide a smoother implementation for time advancement of the re-distancing equation. Finally, the Chapter also presents discussion on the current challenges with the successful implementation of the level-set method in Nek5000 and provides recommendations for overcoming these challenges.

7.1 Reflections on Knowledge Gaps and Sources of Uncertainty

Taking into the perspective the phenomenology of the DFFB regime, described in Section 1.2, and the simulation setup of the current two-phase interface capturing simulations, described in Section 5.2, provides us with a vantage point to address the following questions:

- What are the gaps in the physics being modeled and the actual conditions of the DFFB regime – model form uncertainty?
- What are the sources of uncertainty, including model form, and how can they be quantified?
All possible sources of uncertainty are identified and enumerated in Table 6 and discussed in detail in the following sections.

7.1.1 Uncertainty due to lack of heat transfer modeling

Using a top down strategy to address these questions, we start by eliminating the most obvious assumption viz., the adiabatic isothermal nature of the present simulation. The ideal objective of the simulations would be to evaluate the axial heat transfer coefficient in the DFFB regime. However, recognizing the lack of energy equation solver as a model form uncertainty, the objective of the present study is reduced to understanding the droplet dynamics in, perhaps, the most significant section of the DFFB regime i.e., the immediate vicinity of the spacer-grid and mixing vane region. The following discussion, therefore, centers on the recognition of downstream SMD as the quantity of interest for the present (and future) interface capturing simulations.

As evident from prior experimental observations, heat transfer in the DFFB regime is a complex interplay of several different mechanisms, with no clear dominant path [22,23]. Droplet dynamics and local heat transfer coefficients are strongly coupled providing a feedback to one another. Therefore, it is of note to identify the physics that is not being resolved by excluding thermal effects, which has a potential impact on droplet dynamics. The phenomena include:

- Quenching of the spacer-grid and mixing vane structures, resulting in boiling of droplets.

  The uncertainty depends on flooding rate conditions. For low flooding rates (the more significant case with respect to safety margin characterization), the droplets will rapidly lose mass due to quenching, resulting in a relative overall increase in surface area of droplets. Any daughter droplets that survive the collision and quenching events and reach downstream will provide a negative feedback to the SMD (i.e., decrease the overall SMD).
• Loss of droplet mass to evaporation due to surrounding superheated steam. The experimental correlation by Lee et al [163] is widely used for droplet evaporation in superheated steam. The experimental data collected by them falls well within the operating conditions of the DFFB regime, barring the high superheats near the rod walls. Thus, it can be used to get an estimate of the amount of droplet mass loss due to evaporation expected in the simulation domain. The residence time for droplets in the domain under consideration, not considering collision with the spacer grid or mixing vane structures, is in the order of $10^{-3}$ s. For the millisecond interval and for superheats up to $61^\circ F$ and relative vapor velocity up to 5 m/s, the expected mass loss for a droplet with initial radius of 1 mm is less than 1%. Thus, the uncertainty introduced due to evaporation of droplet in bulk superheated steam is expected to be small and can be ignored.

• Enhancement of droplet evaporation by heat flux due to radiation. There is high uncertainty in the radiation heat transfer to droplets. As reported by Andreani et al [164], the radiation heat transfer to the droplets is often considered negligible. In contrast, other authors report that the radiation heat transfer to the droplets may be as significant as heat transfer via convection to vapor [165]. In any event the partitioned effect of the change in downstream SMD, in the vicinity of the spacer-grids, due to enhancement in evaporation is expected to be insignificant due to high droplet velocity.

7.1.2 Uncertainty due to upstream droplet conditions

The design of the droplet injection routine, Section 3.3, adds determinism due to the way droplets are initialized at the spacer-grid upstream location. Currently, all droplets are initialized with an assumed spherical shape, with an equal diameter of 1 mm and an equal terminal velocity, calculated with respect to mean gas velocity at the domain inlet. Thus, the collision Weber number,
$We_c$, of all droplets impacting the spacer-grids is equal. Prior experimental studies, however, support the assumption that $We_c$ lies in a narrow range. The experiments conducted by Cheung et al [43] reported $We_c = \{54.14, 59.49\}$. The range of SMD reported by most experiments in the spacer upstream region is 0.4-1.2 mm [43,132,166]. Further, as reported by Ardron et al [10], small and large droplets travel with roughly the same velocity, albeit lower than the average terminal velocity. An easily apparent reason for this is the momentum transfer between droplets which attenuates the difference between droplet velocities travelling in close vicinity. Further reason noted by Andreani et al [19] is the radial migration of small and large droplets. The small droplets, with a higher velocity in the lower axial regions are carried by turbulent eddies towards the wall where they lose part of their axial momentum. In contrast the larger droplets, due to their large Stokes number remain in the central part of the channel where they experience continuous acceleration due to drag. Based on these observations considering terminal velocity as the initiation condition for the droplets, in so far, we are simulating the conditions close to the peak power profile, seems reasonable.

Another possible source of distortion in the SMD results is the frequency with which droplets are introduced in the domain. As a first implementation, the algorithm is designed to introduce droplets in batches. A specified maximum number of droplets are maintained in the inlet region based on a required minimum distance between the seed points (3 droplet radii). This resulted in a void fraction, close to 97 % in the overall domain. DFFB regime’s signature starts at the mark of 80%. Higher frequency of droplet initiation will increase the droplet concentration and the resulting positive feedback to the gas turbulent kinetic energy. A void fraction of 97 % is very high and would correspond to very low flooding rates. From the results it is evident that the presence of droplets significantly enhances turbulent mixing, even for such high void fractions.
Thus, it will be of tremendous significance, from a modelling perspective, to quantify the relationship of TKE to changing void fraction. Further, higher void fractions are likely to result in the formation of a persistent wetting layer over the spacer grid and mixing vane structures. Under these conditions the dynamics of droplets are significantly altered. Droplets get re-entrained from the water sheet at the trailing edge of the mixing vane resulting in an increase in the downstream SMD [41]. Additionally, the increased concentration of the droplets increases the probability of coalescence, providing an additional positive feedback to SMD.

7.1.3 Uncertainty due to numerical discretization and mesh resolution

Uncertainties must be accounted for due to the inherent two-phase modelling methodology of the numerical method, i.e., the level-set method. Properties are smeared out across the interface by means of a Heaviside function which provides numerical stability to the solver. In the current simulation, a constant smearing length equal to 175\(\mu m\) is applied (equal to 4 times the cell length in the bulk mesh). This may be a significant source of distortion, especially in the near wall region during collision event. Further, as discussed in Section 3.4.1.1, discretization of the \(\text{sign}\) function for the re-distancing equation causes the interface to move, resulting in volume loss. The LTS method introduced in Section 3.4.2, is shown to ameliorate the problem. However, more rigorous testing is required to quantify the mass loss with LTS and its dependence on spatial resolution.

The breakup or coalescence of the interface is limited by the mesh resolution. In the mesh for the two-phase simulations the highest bulk resolution is 43.75\(\mu m\), which may be regarded as the limiting length for droplet breakup. Note that this limiting length also depends on the underlying numerical discretization. The manufactured solution by Ito et al [167] is an effective strategy for characterizing the dependence of breakup and coalescence on numerical discretization and mesh resolution.
Table 6: Various sources contributing to uncertainty in the present representative DFFB simulations. The quantity of interest for the present simulations is the downstream SMD.

<table>
<thead>
<tr>
<th>Source</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Heat Transfer</strong></td>
<td></td>
</tr>
<tr>
<td>• Quenching of Spacer-grid and mixing Vanes</td>
<td>Depends on flooding rate conditions. For low flooding rates, rapid evaporation of droplets is expected on collision. This would significantly affect the resultant downstream SMD</td>
</tr>
<tr>
<td>• Loss of droplet mass to evaporation due to energy transfer by superheated steam.</td>
<td>A rough estimate can be obtained from experimental correlation by Lee et al [163]. The resulting effect on SMD is expected to be small</td>
</tr>
<tr>
<td>• Evaporation enhancement due to radiation</td>
<td>Effect on the downstream SMD should be insignificant</td>
</tr>
<tr>
<td><strong>Droplet Initialization</strong></td>
<td>Downstream droplet SMD is a strong function of the upstream SMD and collision Weber number</td>
</tr>
<tr>
<td>All droplets are currently initialized with constant velocity and diameter (identical collision Weber number). This reduces the inherent stochasticity of droplet distribution in the DFFB regime</td>
<td></td>
</tr>
<tr>
<td><strong>Droplet Breakup</strong></td>
<td>The breakup of zero level set is mesh dependent. The lowest resolution of mesh is 10 μm and the highest ‘bulk’ resolution is 43.75 μm.</td>
</tr>
<tr>
<td><strong>Void Fraction</strong></td>
<td>Higher droplet concentrations increase the probability of droplet coalescence. Also, if a film develops over the spacer grid structure the resulting downstream SMD reportedly increases[132].</td>
</tr>
<tr>
<td>The frequency with which droplets are introduced governs the resultant void fraction and droplet concentration</td>
<td></td>
</tr>
<tr>
<td><strong>Level-Set Method</strong></td>
<td>Unavoidable in fixed-mesh simulations and helps with numerical stability. Distorts the physics in the interface region but have been shown to have negligible effect on many important parameters, such as drag force estimate on a bubble [168].</td>
</tr>
<tr>
<td>• Property smearing across the interface</td>
<td></td>
</tr>
<tr>
<td>• Volume loss due to re-distancing</td>
<td>Spatial discretization of the characteristic velocity in the re-distancing equation causes the interface to move. More rigorous testing of the LTS required to characterize volume loss.</td>
</tr>
<tr>
<td><strong>Droplet Contact Angle</strong></td>
<td>Distortion to droplet collision events is uncertain. Effect might be insignificant as compared to inertial and aerodynamic forces under DFFB conditions.</td>
</tr>
<tr>
<td>Contact angle controls the liquid spreading onto a surface (Rein et al [169])</td>
<td></td>
</tr>
</tbody>
</table>
7.2 Recommendations for future research

Figure 78 shows an overview of the research during the course of author’s Ph.D. and recommendation for extending the present research. The droplet simulations presented herein showcase the potential of interface capturing methods for large-scale simulations of nuclear reactor flow regimes. Straightforward extension of the present research may involve modification of the droplet injection routine to study the more realistic scenario of polydisperse droplets. A larger $We_c$ and $Re_b$ space may also be chosen by varying droplet and flow properties to cover a wider range of conditions in the DFFB regime (see Section 1.3).

Accounting for heat transfer will, however, require more extensive development efforts in PHASTA. For instance, including phase change at the droplet interface modifies the saddle point problem, Eq. (2.19), due to an additional source term in the incompressibility constraint [170],

$$\nabla \cdot \vec{u} = \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \vec{m} \vec{n} \nabla H(\phi) = \Gamma_m$$ (7.1)

where, $\vec{m}$ is the mass flux across the interface due to phase change,

$$\vec{m} = \frac{k \nabla T|_l \cdot \vec{n} - k \nabla T|_v \cdot \vec{n}}{h_{fg}}$$ (7.2)

where, $k \nabla T|_l$ and $k \nabla T|_v$ is the heat flux on the liquid and vapor side, respectively, and $h_{fg}$ is the latent heat of vaporization (for details see Son et al [170]). Subsequent expansion of the basis leads to the saddle-point problem,

$$\begin{bmatrix} K & G \\ D & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} \vec{f} \\ \Gamma_m \end{bmatrix}$$ (7.3)

where $\Gamma_m$ is the discrete operator for the source term in Eq. (7.1). For equal order pressure-velocity interpolating functions, as used in PHASTA, additional terms are required for stabilization of
pressure oscillations at the interface. In addition a sharp treatment of the interface is required in the FEM context, similar to that described by Nagrath et al [171]. Initial efforts for modeling phase change problems in PHASTA were made by Li et al [172]. Further, to account for quenching effect and wall heat transfer, development and integration of conjugate heat transfer (CHT) is essential.

Droplet breakup and coalesce is a microscale phenomenon and requires a very fine mesh for its resolution [173]. Adaptive mesh refinement (AMR) was implemented recently in PHASTA by Rodriguez et al [174], a promising tool for resolving collision events in the DFFB regime. Application of AMR to large-scale problem with interface capturing methods remains to be properly explored.

Further, the high-resolution data collected from the present simulations offers substantial potential for data driven modeling. The configuration of probes shown in Figure 21, essentially captures instantaneous point data for the entire simulated sub-channel domain. The normalized distance between any two probes for the \( Re_b = 11000 \) case was \( \Delta x^+ \sim 70 \). Thus, the volumetric evolution of Reynolds stresses and mean velocities, essential for turbulence modeling can be reconstructed with a reasonable degree of accuracy. This massive volume of data opens opportunities for developing machine learning based turbulence models for nuclear reactor sub-channels, especially accounting for the effect of spacer-grids and mixing vanes on turbulence. The arrangement of the probes on cross-sections also allows for extracting laterally averaged information for developing correlation for system thermal hydraulic codes, like CTF.
Figure 78: An overview of present research and recommendation for future research.
7.2.1 Improved LTS operator for re-distancing equation

As detailed in Section 3.4.2, an operator to modify the time multiplier based on the level-set distance field helps eliminate perturbations on the droplet interface during collision events. The objective while constructing the operator is to ‘freeze’ re-distancing at the exact location of the interface. Current construction of the operator uses a step function, re-written below (Eq. (3.13)),

\[ T(\Phi_d^n)_{CFL} = \begin{cases} \delta\tau_b \frac{CFL_{LTS}}{CFL_b} & |\Phi_d^n| < 1.5\epsilon \\ \delta\tau_b & \text{otherwise} \end{cases} \tag{7.4} \]

Thus, the pseudo time step \( \delta\tau_b \) experience a step change at the location \( |\phi_d| = 1.5\epsilon \). A much better implementation of the above is possible using the already available \( \text{sign}(\phi_d) \) function. The following is suggested,

\[ T(\Phi_d^n) = \text{abs}(\text{sign}(\Phi_d^n))^p \delta\tau_b \tag{7.5} \]

where \( p > 1 \) may be any exponent, depending on application and stability requirement. Figure 79 shows comparison of new implementations Eq. (7.5), with \( p = 2 \) and 4, with the existing operator, Eq. (7.4). It is evident that the new implementation will ensure that the exact time multiplier operator at the interface location will be zero, while it asymptotes to one at \( |\phi_d| = \epsilon \). The power \( p \) may be increased for improving the stability during collision events or for improved volume conservation.
Figure 79: Comparison of existing and improved implementation for local time stepping operator for re-distancing equation. The plot assumes that the smearing length $\varepsilon = 1$. 
Chapter 8: Synopsis and Conclusions

Dispersed flow film boiling (DFFB) is the primary flow regime which exists under post-LOCA conditions in nuclear reactor cores during the re-flood transients. Safety considerations to accommodate for the eventuality of post-LOCA incidents impose the most limiting constraints on the peak power profile of PWRs. Therefore, predicting the thermal hydraulic response of the DFFB regime is extremely critical from a safety margin characterization perspective due to the potential of rod temperatures reaching beyond the NRC established peak cladding temperature limit. Prior experimentation has, unequivocally, established the dominant role of spacer-grids and mixing vanes on the overall thermal-hydraulics of the DFFB regime. Sharp augmentation in the heat transfer coefficients were experimentally recorded at the immediate downstream location of the spacer-grids. Heat transfer in the vicinity of spacers is a complex interplay of several mechanism. However, the breakup of dispersed droplets on collision with spacer-grids, which results in a sharp increase in their interfacial area, is identified as the primary contributing phenomena to the positive heat transfer feedback.

Single phase DNS and two-phase high fidelity, interface capturing, simulations in a prototypal nuclear reactor sub-channel, with spacer-grids and mixing vanes, constitutes the bulk of present research. A finite element method based numerical tool, PHASTA, optimized for strong scaling on the Mira supercomputer at Argonne National lab, was used for all large-scale simulations in this research. Interface capturing simulations to represent DFFB conditions in the vicinity of spacer-grids required special numerical and logistical considerations. Thus, several ad hoc functionalities were implemented in PHASTA, including,
• Large-scale implementation of boundary condition transient (BCT) suite of tools for specifying fully developed turbulent flow conditions at the upstream location of spacer-grids.

• MPI sub-communicators and MPI Parallel I/O for large-scale high-resolution data collection.

• Large-scale parallelized droplet injection routine for initializing droplets at the upstream location of spacer-grids

• Local time stepping algorithm for the re-distancing equation for resolving droplet collision with spacer-grids and mixing vanes.

High resolution data capturing from the single-phase simulations reveal the quantitative effect of spacer-grids and mixing vanes on turbulent statistics. Results from simulations at two bulk Reynolds numbers, which lie at the extremes of the operating range of DFFB regime, are rigorously compared with the existing, and widely accepted, data in literature for DNS of flow between parallel plates. Comparative study of the upstream and downstream conditions, with respect to spacer-grids, was performed, with unprecedented spatial resolution, providing details on the axial evolution of mean velocity and Reynolds stress profiles. Further, an invariant analysis of turbulence was performed which sheds light on the role of mixing vanes in changing turbulence anisotropy state at the downstream location. All results highlight the importance of spacer-grids and mixing vanes to the convective heat transfer enhancement, which is currently empirically modelled in system thermal hydraulic code -CTF.

As reported by experiments, the droplet dynamics at the downstream location of spacer-grids is primarily governed by the upstream collision Weber number, $\text{We}_c$. Following guidelines from experimental observations, a set of two-phase simulations for varying $\text{We}_c$ were performed
in this research. High spatial and temporal resolution data collected from these simulations illuminates the effect of spacer-grids and mixing vanes on the downstream Sauter mean diameter (SMD), a measure for characterizing the morphology of droplets. The time averaged SMD results were compared with empirical correlation, derived from experiments at RBHT facility, and existing empirical correlation in CTF, showing good agreement. Further, extensive analysis of turbulence statistics reveals the effect of droplets on turbulent energy and emphasize the importance of developing correlations to account for this effect in STH codes. Axial evolution of the first order statistics is presented which gives a quantitative measure of the combined effect of spacer-grids and droplets on turbulence.

Interface capturing simulations in this and prior work highlight the potential of the level-set method for incompressible flows to perform large scale two-phase simulations for nuclear reactor regimes of key interest. The strong scaling, highly optimized libraries of PHASTA are a key ingredient to the success of these simulations on large supercomputers. Recognizing this potential, this research also documents efforts towards the incorporation of the level-set method in another widely recognized, strong-scaling, CFD code – Nek5000. The key challenge for successful implementation of level-set method in Nek5000 pertains to the stabilization of pure hyperbolic equation systems, viz., the level-set advection and re-distancing equation. Thus, a spectrally vanishing viscosity (SVV) formulation, introduced by Tadmor [150], was implemented in Nek5000 for stabilization of hyperbolic or convection dominated systems. An improved multi-dimensional filter kernel was developed for the SVV formulation and shown to provide effective stabilization for some very challenging linear/non-linear hyperbolic problems, including a problem involving the solution of the re-distancing equation. Further, the level-set formulation was coupled
with the existing low Mach number solver in Nek5000 and the resulting two-phase implementation was demonstrated on some archetypal problems.

The key conclusions from the present research are enumerated below:

- The research herein highlights the capability of PHASTA, coupled with level-set method, to simulate the post-LOCA DFFB regime. Simulations with unprecedented resolution and fidelity were performed to illuminate droplet dynamics in this critical PWR regime.

- Advanced high-resolution data collection tools are implemented in PHASTA which enable detailed study of turbulence from DNS scale simulations, optimized for large scale supercomputers.

- The high spatial and temporal resolution of data collected from the single-phase and two-simulations is archived and would, potentially, serve as a data mine for the development of machine learning based turbulence and STH models.

- The results from single-phase simulations highlight the effect of spacer-grids and mixing vanes on convective enhancement. Further, invariant analysis of the data reveals that the mixing vanes modify the state of turbulence in the downstream region.

- The results from two-phase simulations emphasize the importance of considering droplet feedback to turbulence, in addition to the enhancement provided by spacer-grids and mixing vanes. The SMD results at the downstream locations match well with experimental data, establishing confidence in PHASTA and the incorporated level-set method in simulating the DFFB regime.

- All tools are in place for a more extensive parametric study of the DFFB regime, with a range of bulk Reynolds number and collision Weber numbers. Single droplet collision
studies are recommended for characterizing uncertainties associated with collision events.

- The most limiting assumption of the current simulations, in contrast to the real DFFB conditions, is the lack of heat transfer modeling. Consideration of heat transfer mechanisms requires more extensive development efforts in PHASTA, including methods for phase change, conjugate heat transfer and modeling of radiative heat transfer.

- Successful implementation of the level-set formulation in Nek5000 requires further development efforts. The most challenging problem to be addressed is the re-distancing equation. Re-distancing near interface breakup or coalescence events with artificial viscosity for stabilization results in the diffusive terms dominating near the zero contour. This cause unphysical stretching of the interface and prevents the interface from rupturing, for breakup events, or merging, for coalescence events. Direct re-distancing methods or SUPG type stabilization methods are recommended for future work.
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APPENDICES
A.1 Explanation of the inf-sup condition

The discrete system of equation resulting from the incompressible Stokes problem, Eq. (2.9), is,

\[
\begin{bmatrix}
  K & D^T \\
  D & 0
\end{bmatrix}
\begin{bmatrix}
  u \\
  p
\end{bmatrix}
=
\begin{bmatrix}
  f \\
  0
\end{bmatrix}
\tag{0.1}
\]

Considering, \( u \in V, p \in Q \) and \( f \in F \), where \( V, Q \) and \( F \) are finite element functional spaces equipped with the norms \( \| \cdot \|_V, \| \cdot \|_Q \) and \( \| \cdot \|_F \), respectively. Boffi et al [175] showed that the system of equations in (0.1) is stable if,

\[
\| u \|_V + \| p \|_Q \leq c \| f \|_F
\tag{0.2}
\]

where \( c \) is a positive constant. The above puts the following constraint on the matrix \( D \),

\[
u^T D^T p \geq \beta \| u \|_V \| p \|_Q
\tag{0.3}
\]

where \( \beta \) is a positive constant independent of the mesh size. Reformulating the above as,

\[
\frac{u^T D^T p}{\| u \|_V} \geq \beta \| p \|_Q
\tag{0.4}
\]

we realize that to ensure the above inequality always holds, it is best to consider the supremum of the left hand side. Thus, given \( p \in Q \), choose \( u \in V \) such that,

\[
\forall p \in Q \quad \sup_{u \in V} \frac{u^T D^T p}{\| u \|_V} \geq \beta \| p \|_Q
\tag{0.5}
\]

Thus, the above inequality puts a constraint of the choice of \( u \in V \). The condition clearly holds for the trivial case, \( p = 0 \), however constraints must also be placed on \( p \in Q \). Thus rewriting as,

\[
\forall p \in Q \quad \frac{1}{\| p \|_Q} \sup_{u \in V} \frac{u^T D^T p}{\| u \|_V} \geq \beta
\tag{0.6}
\]
The worst possible value for $p$ is the one that minimizes the left hand side. Thus, in order for the above to be always true, $p \in Q$ must be chosen such that it must hold for the infimum of the left hand side,

$$\inf_{p \in Q} \sup_{u \in V} \frac{u^T D^T p}{\|u\|_V \|p\|_Q} \geq \beta \quad (0.7)$$

The above is popularly referred to as the inf-sup condition in the finite element literature for the saddle point problem, Eq. (0.1). As illustrated, it effectively puts constraints on the choice of $u \in V$ and $p \in Q$. Gresho et al [70] showed that equal order interpolations for velocity and pressure violate the above inf-sup condition.

A.2 Boundary Condition Transient (BCT) Code

A.2.1 Subroutine to read BCT file (incompressible/readBCT.f)

```fortran
subroutine readBCT(iBC, BC, x)
use specialBC
include "common.h"

integer iBC(numnp)
real*8 x(numnp,nsd)
real*8 BC(nshg, ndofBC)
logical extsbct
character*80 :: filenum1
integer k
integer stat1
integer ic
real*8 x1, x2, x3
real*8 dd
real*8 epsd
character*80 iBCTStepName
character*80 infile

c You must advance to the next BCT file when this routine is called
iBCTstep = iBCTstep + iBCTReadGap

epsd=1.0d-9

if( myrank.ge.0 .and. myrank.le.9)then
    write(filenum1,'(i1.1)')myrank
else if(myrank.ge.10 .and. myrank.le.99)then
    write(filenum1,'(i2.2)')myrank
else if(myrank.ge.100 .and. myrank.le.999)then
    write(filenum1,'(i3.3)')myrank
else if(myrank.ge.1000 .and. myrank.le.9999)then
    write(filenum1,'(i4.4)')myrank
else if(myrank.ge.10000 .and. myrank.le.99999)then
```

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write (filenuml, '(i5.5)' ) myrank
else if (myrank.ge.100000 .and. myrank.le.999999) then
write (filenuml, '(i6.6)' ) myrank
else if (myrank.ge.1000000 .and. myrank.le.9999999) then
write (filenuml, '(i7.7)' ) myrank
else if (myrank.ge.100000000 .and. myrank.le.99999999) then
write (filenuml, '(i8.8)' ) myrank
else if (myrank.ge.1000000000 .and. myrank.le.999999999) then
write (filenuml, '(i9.9)' ) myrank
derend
endif
if (iBCTstep.ge.0 .and. iBCTstep.le.9) then
write (iBCTStepName, '(i1.1)' ) iBCTstep
else if (iBCTstep.ge.10 .and. iBCTstep.le.99) then
write (iBCTStepName, '(i2.2)' ) iBCTstep
else if (iBCTstep.ge.100 .and. iBCTstep.le.999) then
write (iBCTStepName, '(i3.3)' ) iBCTstep
else if (iBCTstep.ge.1000 .and. iBCTstep.le.9999) then
write (iBCTStepName, '(i4.4)' ) iBCTstep
else if (iBCTstep.ge.10000 .and. iBCTstep.le.99999) then
write (iBCTStepName, '(i5.5)' ) iBCTstep
else if (iBCTstep.ge.100000 .and. iBCTstep.le.999999) then
write (iBCTStepName, '(i6.6)' ) iBCTstep
derend
endif
infi le =
& 'bctInput/ //trim(iBCTStepName) // bct.dat. //
& trim(filenuml) //''

inquire (file=trim(infile), exist=extsbct)
if (extsbct) then
  iextsbct = 1
derend
if (iextsbct .eq. 1) then
  open (1899, file=infile)
  read (1899, *) nptmax, ntv
  ic=0
do k=1, nptmax
    read (1899,*, IOSTAT=stat1) x1, x2, x3, nptpts
    if (stat1 .gt. 0) then
      write (*,*) 'Read error', myrank
      write (*,*) x1, x2, x3
      write (*,*) myrank, k, nptmax
    enddo
  do i=1, numnp
    if (ibits (ibc(i), 3, 2) .eq. 7) then
      dd = distds(x1, x2, x3, x(i, 1), x(i, 2), x(i, 3))
      if (dd .lt. epsd) then
        ic = ic+1
        nBct(ic)=i ! the pointer to this point
        numBct(ic)=nptpts ! the number of time series
      do j=1, nptpts
        if (tvbcswlch.eq.0) then
          if (solheat .gt. 0.00d0) then
            read (1899,*) (Bct(ic,j,n), n=1,5)
          else
            read (1899,*) (Bct(ic,j,n), n=1,4)
          endif
          Bct(ic,j,1)=Bct(ic,j,1)+shvebct
        else
          read (1899,*) (Bct(ic,j,n), n=1, ndof+1)
          Bct(ic,j,1)=Bct(ic,j,1)+shvebct
        endif
      enddo
A.2.2 Module to store BCT data structure (common/bctint.f)

module specialBC

  real*8, allocatable :: BCt(:,:,:), acs(:,:), spamp(:)
  real*8, allocatable :: ytarget(:,:)
  integer, allocatable :: nBCt(:), numBCt(:)
  integer ntv, nptsmax
  integer iextsbct
  integer iBCTstep

end module

A.2.3 Subroutine to impose BCT (common/bctint.f)

subroutine BCint(timel,shp,shg,shpb,shglb,x,BC,iBC)
  use specialBC
  include "common.h"
  real*8 BC(nshg,nshg,nsd), timel, t
  real*8 x(numnp,nsd),
  & shp(MAXTOP,maxsh,MAXQPT),
  & shgl(MAXTOP,nsd,maxsh,MAXQPT),
  & shpb(MAXTOP,maxsh,MAXQPT),
  & shglb(MAXTOP,nsd,maxsh,MAXQPT)
  integer iBC(numnp),nlast,i,j,nper
  real*8 wr
  integer foundflag

c -----------------------------------------------
do i = 1, itvn
  nlast=numBCt(i)
  if (tvbcswitch.eq.0) then
c -----------------------------------------------
    foundflag=0
    nper=timel-BCt(i,nlast,4)
    t=timel-nper*BCt(i,nlast,4)
    if (timel .gt. BCt(i,nlast,4)) then
      call readBCT(iBC, BC, x)
      nlast = numBCt(i)
    else
      foundflag = 1
    endif
c -----------------------------------------------
  endif
c -----------------------------------------------
do j=2,nlast
  if (BCt(i,j,4) .gt. t) then
    wr=(timel-BCt(i,j-1,4))/(BCt(i,j,4)-BCt(i,j-1,4))
    BC(nbct(i),3:5) = BCt(i,j-1,1:3)*(1.0-wr)
    + BCt(i,j,1:3)*wr
  endif
end subroutine

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if(solheat .gt. 0.0d0) then
  BC(nbct(i),:) = BCt(i,j-1,1)*(1.0-wr)
  + BCt(i,j,1)*wr
  exit
endif
endif
return
enddo

C
else
nper=timel/BC(i,nlast,1)
t=timel-nper*BC(i,nlast,1)
do j=2,nlast
  if(BC(i,j,1).gt.0.0d0) then
    wr=(t-BC(i,j-1,1))/(BC(i,j,1)-BC(i,j-1,1))
    BC(nbct(i),1:,:) = BC(i,j-1,1:,:)*(1.0-wr)
    + BC(i,j,1:,:)*wr
  endif
endif
endo
dreso
return
end

A.2.4 Subroutine to record instantaneous fields (common/timeseries.f)

subroutine timeseries(ycl, xl, ien, sgn, n_0, n_1)
use timedata
include "common.h"
dimension shape(nshl), ycl(npro,nshl,2),
& ien(npro,nshl), xl(npro,nenl,nsd),
& sgn(npro,nshl)
real*8 al(npro,nenl,nsd),
& zi0(npro,nsd), detai(npro), dzi0(npro,nsd),
& m1(npro), m2(npro), m3(npro), m21(npro), m22(npro),
& m23(npro), m31(npro), m32(npro), m33(npro),
& r1(npro), r2(npro), r3(npro), shgradl(nshl,nsd)
real*8 xts1, xts2, xts3
real*8, allocatable, dimension(:) :: soln
integer e, founde, n_0, n_1, ndiff

ndiff = n_1 - n_0 + 1
allocate(soln(ndiff))
if(size(varts) .eq. 0 .and. nproctspts .gt. 0) then
  allocate(varts(nproctspts,numvarc))
  allocate(comptts(nproctspts,nsd))
  allocate(comparptts(nproctspts,nsd))
  allocate(comstatptts(nproctspts,:))
i=1
do jj = 1,ntspts
  if(statptts(jj,2) .gt. 0) then
    comptts(i,:) = ptts(jj,:)
    comparptts(i,:) = parptts(jj,:)
  endif
endo
comstatptts(i,:) = statptts(jj,:)
i = i + 1
endif
enddo
write(*,*) nproctspts," probes found on ",myrank
C-------------------------------------------------------------
endif
do jj=1,nproctspts
founde = 0
if(comstatptts(jj,1).eq.0 .or. tssearch .eq. 0) then
  if(comstatptts(jj,1).eq.iblkts) then
    call shphex (ipord, comparptts(jj,:),shape(:,),
    &                 shgradl(:,;))
  elseif(lcsyst.eq.1) then
    call shptet (ipord, comparptts(jj,:),shape(:,),
    &                 shgradl(:,;))
  endif
founde = comstatptts(jj,2)
endif
if(founde.ne.0) then
  soln(1:ndiff) = zero
  do i = 1,nenl
    soln(1:ndiff) = soln(1:ndiff)*shape(i)
  enddo
  do i = 1+nenl,nshl
    soln(1:ndiff) = soln(1:ndiff)
    +ycl(founde,i,1:ndiff)*shape(i)*sgn(founde,i)
  enddo

  varts(jj,n_0:n_1) = soln(:)
C Write Coordinates
  if(n_1 .eq. numvar) then
    varts(jj,numvar+1:numvar+3) = comptts(jj,1:3)
  endif
endif
enddo
deallocate(soln)
return
end

A.3 Droplet Injection Code

A.3.1 Module to store injector data (incompressible/injector.f)

module injectorData
  real*8 pmaxb, pminb
  real*8 pmaxh, pminh
  integer, allocatable, dimension(:):: seednodes
  real*8, allocatable, dimension(:,::) :: activenodes
  integer injstart
  integer idelete
  integer, allocatable, dimension(:::) :: markpatchi
  integer, allocatable, dimension(:::) :: availproc
end module
A.3.2 Subroutine to identify injector seed nodes (incompressible/injector.f)

```fortran
subroutine identifyInjectorPatch(iBC, BC, mark, x, injectorDirect & markpatch)
  use injectorData
  include "common.h"
  include "mpif.h"
  real*8  BC(nshg, ndofBC), x(numnp, nsd)
  integer iBC(nshg)
  integer mark(nshg)
  integer markpatch(nshg)
  integer injectorDirect

  real*8 velmag
  integer node1, node2
  real*8 maxb(i), minb(i)
  real*8 maxh(i), minh(i)
  real*8 dist, dist1
  integer count
  integer flag
  integer procstat
  integer, allocatable :: gatherproc(:)
  integer navailproc

  mark = 0
  markpatch = 0
  do i=1, nshg
    velmag = sqrt((BC(i,3)**2.0 + BC(i,4)**2.0 + BC(i,5)**2.0)
    if(x(i,1) .lt. 1e-8) then
      mark(i) = 1
      markpatch(i) = 1
    endif
  enddo

  node1 = 0
  node2 = 0
  flag = 0
  do i=1, nshg
    if(mark(i) .eq. 1) then
      flag = 1
      exit
    endif
  enddo

  if(flag .eq. 1) then
    do i=1, nshg
      if(mark(i) .eq. 1 .and. node1 .ne. 0) then
        node2 = i
      elseif(mark(i) .eq. 1 .and. node1 .eq. 0) then
        node1 = i
      elseif(node1 .ne. 0 .and. node2 .ne. 0) then
        exit
      endif
    enddo
    if((node1 .ne. 0 .and. node2 .ne. 0) then
      if(abs(x(node1,1)-x(node2,1)) .lt. 1e-8) then
        injectorDirect = 1
      elseif(abs(x(node1,2)-x(node2,2)) .lt. 1e-8) then
        injectorDirect = 2
      else
        injectorDirect = 3
      endif
    endif
  endif
```

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if(myrank .ne. master .and. injectorDirect .ne. 0) then
   call MPI_Send(injectorDirect,1,MPI_INTEGER,master,myrank, MPI_COMM_WORLD,ierr)
elseif(myrank .eq. master) then
   call MPI_Recv(injectorDirect,1,MPI_INTEGER,MPI_ANY_SOURCE,
                MPI_ANY_TAG,MPI_COMM_WORLD,MPI_STATUS,ierr)
endif
call MPI_Bcast(injectorDirect,1,MPI_INTEGER, master,MPI_COMM_WORLD,ierr)
if(injectorDirect .eq. 1) then
   maxb = maxval(x(:,2))
   minb = minval(x(:,2))
   maxh = maxval(x(:,3))
   minh = minval(x(:,3))
elseif(injectorDirect .eq. 2) then
   maxb = maxval(x(:,1))
   minb = minval(x(:,1))
   maxh = maxval(x(:,3))
   minh = minval(x(:,3))
elseif(injectorDirect .eq. 3) then
   maxb = maxval(x(:,1))
   minb = minval(x(:,1))
   maxh = maxval(x(:,2))
   minh = minval(x(:,2))
endif
call MPI_ALLREDUCE(maxb, pmaxb, 1, MPI_DOUBLE_PRECISION, MPI_MAX, MPI_COMM_WORLD, ierr)
call MPI_ALLREDUCE(minb, pminb, 1, MPI_DOUBLE_PRECISION, MPI_MIN, MPI_COMM_WORLD, ierr)
call MPI_ALLREDUCE(maxh, pmaxh, 1, MPI_DOUBLE_PRECISION, MPI_MAX, MPI_COMM_WORLD, ierr)
call MPI_ALLREDUCE(minh, pminh, 1, MPI_DOUBLE_PRECISION, MPI_MIN, MPI_COMM_WORLD, ierr)
dist = 0.0
dist1 = 0.0
count = 0
k=0
flag = 0
do i=1,nshg
   if(mark(i) .eq. 1) then
      flag = 1
      exit
   endif
enddo
if(myrank .eq. master)write(*,*:"All communication done"
procstat = -1
if(myrank .eq. master)allocate(gatherproc(numpe))
if(flag .eq. 1) then
   do i=1,nshg
      if(mark(i) .eq. 1) then
         if(injectorDirect .eq. 1) then
            dist = min(abs(pmaxb-x(i,2)),abs(pminb-x(i,2))),
                     abs(pmaxh-x(i,3)),abs(pminh-x(i,3)))
            dist1 = sqrt((pmaxb-x(i,2))**2.0+(pminb-x(i,2))**2.0)
            dist1 = min(dist1,
$$\sqrt{\left(\max b - x(i, 2)\right)^2 + \left(\max h - x(i, 3)\right)^2}$$

dist1 = min(dist1,
$$\sqrt{\left(\min b - x(i, 2)\right)^2 + \left(\min h - x(i, 3)\right)^2}$$)

elseif(injectorDirect .eq. 2) then
    dist = min(abs(max b - x(i, 1)), abs(min b - x(i, 1)),
               abs(max h - x(i, 1)), abs(min h - x(i, 1)))
elseif(injectorDirect .eq. 3) then
    dist = min(abs(max b - x(i, 1)), abs(min b - x(i, 1)),
               abs(max h - x(i, 2)), abs(min h - x(i, 2)))
endif

if(dist .lt. 1.25*rinj .or.
    dist1 .lt. (1.0*rodradinj+2.0*rinj)) then
    mark(i) = 0
endif
A.3.3 Subroutine to add seed point to *activenodes* array

```fortran
subroutine addnode()
! The new node is added at the top of the list
! Previous ones are pushed down
use injectorData
include "common.h"
include "mpif.h"
real*, allocatable, dimension(:,1) :: tempnodes
integer newsize

newsize = size(activenodes,1) + 1
if(newsize .gt. 1) then
  allocate(tempnodes(newsize,7))
  tempnodes(2:newsize,:) = activenodes(1:newsize-1,:)
  deallocate(activenodes)
  allocate(activenodes(newsize,7))
  activenodes = tempnodes
  deallocate(tempnodes)
else
  allocate(activenodes(1,7))
endif
activenodes(1,:) = 0.0
activenodes(1,7) = time
end
```

A.3.4 Subroutine to delete seeds from *activenodes*

```fortran
subroutine deletenode(inode)
use injectorData
include "common.h"
include "mpif.h"
integer inode
integer isize, k
real*, allocatable, dimension(:,1) :: tempnodes

isize = size(activenodes,1)
k=1
if(isize .eq. 1) then
  deallocate(activenodes)
else
  allocate(tempnodes(isize-1,7))
  do i=1,isize
    if(i .ne. inode) then
      tempnodes(k,:) = activenodes(i,:)
      k=k+1
    endif
  enddo
  deallocate(activenodes)
  allocate(activenodes(isize-1,7))
  activenodes = tempnodes
  deallocate(tempnodes)
  if(myrank .eq. master) write(*,*) "Deleted seed number ",inode
endif
end
```

A.4 Local Time Stepping Code for Re-distancing Equation

A.4.1 Routine to populate time array, T(Φₙ) (incompressible/calc_delt.f)

```fortran
subroutine calc_redeltat(reDelt, cfl, x, y)
```
This routine calculates time step for each DOF for LTS of re-distancing equation

```fortran
use turbsa
include "common.h"

real*8 x(numnp, nsd)
real*8 y(nshg,ndof)
real*8 reDelt(nshg)
real*8 cfl(nshg)
real*8 epsilon_ls_tmp
real*8 dist
real*8 tmpcfl
real*8 slope

epsilon_ls_tmp = epsilon_lsd
dist = 1.5*epsilon_ls_tmp
slope = 5.0

do i=1,nshg
   if(abs(y(i,7)) .le. dist) then
      tmpcfl = re_lts_cfl
      reDelt(i) = tmpcfl/(cfl(i)*Dtgl)
   else
      reDelt(i) = 1.0/Dtgl
   endif
endo
dfcn
enddo

return
dend

A.4.2 Routine for time integration using $T(\Phi^n_{ij})$ (incompressible/itrPC.f)

```fortran
subroutine itrCorrectSclr_LTS(y,ac,solinc,reDelt)
include "common.h"

real*8 y(nshg,ndof), ac(nshg,ndof), &
  solinc(nshg), reDelt(nshg)

is=5+isclr

y(:,is) = y(:,is) + reDelt(:) * solinc(:)
ac(:,is) = ac(:,is) + solinc(:)

return
dend
```
A.5 Comparison of normalized Secondary stresses for sub-channel with channel data (Lee et al [118])
A.6 Lumley triangle and turbulence characterization

A.7 Evolution of interface topology for Rayleigh-Taylor instability simulation by Karakus et al [162]

Images shown at time $t = 0, 1.28, 1.71, 2.18$ and $2.7$ s from Karakus et al [162]