ABSTRACT

SRIVASTAVA, SHUBHAM. A Hybrid Coarse-Fine grained Upscaling Scheme for Reacting Flows Using Kalman and Particle Filters. (Under the direction of Dr. Tarek Echekki).

A multi-scale combustion model involving the Kalman and Particle filters is developed and validated. The coarse-scale model consists of 1D grid which handles the mass conservation and momentum equations. In 3D this model emulates Large Eddy Simulation (LES) for turbulent variable density flow. The fine scale solution is handled using the Linear Eddy Model (LEM). The fine scale processes combine a deterministic implementation of reaction, diffusion and large scale transport with a stochastic implementation of fine scale transport. Here, turbulent stirring is represented by random, instantaneous rearrangements of the fields of transported variables along a one dimensional line via ‘triplet maps’, which emulate the rotational effect of turbulent eddies. The algorithm has the continuity equation and the Burger’s equation on the coarse scale and the temperature equation with heat release on the fine scale.

The density computed on the fine scale has to be passed from the fine scale to the coarse scale. This density passed contributes directly to the accuracy of the solution. The behavior of finer scale data also depends on the number of points embedded in each coarse grid cell. Therefore the values being passed should be spectrally smooth.

This work has been carried out in two parts. In the first part Kalman filter has been employed to combine these two scale solutions and in the second part Particle filter has been used to do the same. These filters have been used to remove the statistical errors in the data being passed and to make them as accurate as possible. The results convincingly establish the
potential role of Kalman and Particle filters in coupling the deterministic coarse grained solutions and stochastic fine-grained solutions in reacting flow applications.
A Hybrid Coarse-Fine Grained Upscaling Scheme for Reacting Flows Using the Kalman and Particle Filters

by
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DEDICATION

I dedicate this thesis to my parents for their unconditional love and continued support
BIOGRAPHY

Shubham Srivastava was born on 29th May 1984 in Agra, the city of the famous Taj Mahal, in India. He obtained his Bachelor of Science degree in Mechanical Engineering from Manipal Institute of Technology, India in 2007. To advance his knowledge in Thermal Science he enrolled as a Masters student in North Carolina State University in Fall 2009. Owing to his deep interest in research he has been working under the guidance of Dr. Tarek Echekki since Spring 2010.
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To begin with, I owe an enormous debt to Dr. Tarek Echekki for giving me the opportunity to undertake this research. His guidance, inspiration and patience have been a major contributing factor to the completion of this work. To him, I owe the vital learning from this research.

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Chapter 1

Introduction

The discovery of fire has been accentuated as the single most significant event in the human evolution which propelled the development of the species and culture. Fire provided our ancestors with heat and protection from predators. Its transition into our modern times has been accompanied with the discovery of fossil fuels which to this day remain our primary source of heating and power generation. Thus combustion technology has been an indispensable part of our lives and will remain for the years to come. Combustion being fundamentally important to our existence postulates a thorough understanding of the phenomenon.

Combustion can be either laminar or turbulent but more often than not it is encountered in its turbulent state because of two reasons: 1) the flow instability caused by the heat release in combustion facilitates transition to turbulence, and 2) the enhanced mixing processes due to turbulence stir up combustion. Turbulence is still far from being understood, having become one of the most significant unresolved problems in physics. With the arrival of computer technology and its subsequent exponential rise it has been possible to delve deeper into its mysteries making it possible to solve the turbulent flow equations numerically. There are three principle numerical techniques employed in the study of turbulent combustion. They are Direct Numerical Simulation (DNS), Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES). Each of them differs in their temporal and spatial resolutions and has different accuracies (Oran and Boris 2001).
DNS has a well refined temporal and spatial scale on the grid. It is the most accurate numerical method and can provide complete information regarding turbulent flow by directly computing the scalars. RANS is based on time averaged equations of fluid flow. Due to this averaging, unresolved details in the scales are lost which result in unclosed terms. These terms have to be modeled separately for closure. The third numerical approach is LES. In LES the large scale transport is explicitly modeled while closure is obtained by sub-grid scale models (Poinsot and Veynante 2001).

1.1 Background

From the vantage point of numerical schemes for turbulent flows, LES represents a midway between DNS and RANS. DNS requires numerical resolution of various scales of flow whereas RANS involves modeling of these turbulence scales. LES on the other hand postulates simulating the large scale transport numerically while the closure for sub-grid unresolved terms is obtained through modeling (Pope 2000). A comparison between them is crucial to gain a complete perspective of the numeric schemes.

Among the discussed methods DNS is the most accurate, albeit computationally expensive. DNS dwells on the concept of very fine discretization of temporal and spatial scales to model the turbulence characteristics. This places a restriction on the Kolmogorov length scale being modeled, which is defined by the Reynolds number. High Reynolds number translates into extremely fine grid which increases the complexity many folds making it difficult to monitor flows with larger physical dimensions and complex chemistry. On the other hand LES can provide almost the same flow information at a fraction of the cost. The enormous cost
involved in DNS modeling restricts it to flows with relatively low Reynolds number confined to small geometries.

RANS caters to equations that have been obtained after averaging of governing equations and flow properties. Consequently this leads to potential loss of data and details between the fine scales of chemical interactions. These have to be modeled separately in the governing equations. Comparatively RANS requires computational effort that is many orders lower than that of LES but the results provided by LES are far more accurate and reliable especially in unsteady flows.

1.2 Motivation

A principal challenge in modeling turbulent combustion flows is associated with their complex, multiscale nature (Peters 2009; Echekki 2009; Echekki and Mastorakos 2010). Turbulent combustion flows exhibit a broad range of length and time scales spanning over several decades even within the continuum limit. Traditional paradigms in turbulent combustion modeling have sought to bridge the gap of scales through various approaches (e.g. fast chemistry, thin flamelets relative to turbulence scales). However, many of these approaches are largely dependent on the combustion regime (e.g. flamelet vs. distributed reaction) and mode (e.g. premixed vs. non-premixed), which govern the combustion process. However, numerous challenges remain where a combustion process does not fit into a single combustion regime or mode. LES is gathering prominence as a mode for modeling of turbulent flows owing to its affordable computational cost and reasonable ability to render accurate solutions. LES has been developed and studied as a
turbulent flow prediction tool for the past three decades and the application of LES to chemically reacting flows is attracting considerable attention in the turbulence community. LES has been applied to non-premixed turbulent flames (Ihme and Pitsch 2008). LES is employed to model the turbulent transport on the large scale but the small scale chemistry has to be handled by a sub-grid closure model.

Appreciable progress has been made in the field of large eddy simulation, more so lately, principally owing to the recent advancements in the field of computational resources. Coupled with several sub-grid scale models LES has been successfully employed to model turbulent flows where the relationship between small and large scales of motion has been subject of many studies (Meneveau and Katz 2000). Moin, et al. have investigated the implementation of dynamic subgrid-scale model for LES of compressible flows and growing popularity of LES as a credible tool to simulate turbulent combustion can be attributed to the development of dynamic Smagorinsky model (DesJardin and Frankel 1998), PDF methods (Pope 1985 and Pope 2000).

With the emergence of large-eddy simulation (LES) as a viable modeling approach in combustion, additional challenges arose. In LES, large-scale physics is captured through spatial filtering of the solution and the governing equations. Meanwhile, scales below the spatial filter have to be modeled. However, important physics resides at these small scales and often combustion in thin flame structures cannot be resolved in LES. Closure for these finer scales is the primary scope of the state-of-the-art turbulent combustion models today, and this closure has been approached through different strategies. One promising class of strategies seeks to directly simulate the sub-filter scale physics through
low-dimensional or low-order models. Such strategies include for example, the tracking of notional particles and the solution of their joint scalar or scalar-velocity probability density functions (Pope 1985). Alternatively, the LEMLES (Menon and Kerstein 2010) and the ODTLES (Cao and Echekki 2008) approaches involve the coupling of LES with 1D fine-grained (FG) stochastic models using the linear-eddy model (LEM) (A. R. Kerstein 1991) and the one-dimensional turbulence model (ODT) (A. R. Kerstein 1999). These models potentially offer the ability to capture different combustion model (e.g. premixed vs. non-premixed reactants) and regimes because of their deterministic implementation of reaction-diffusion coupling, albeit in 1D.

Numerous issues arise with the coupling of LES with low-dimensional stochastic models. One issue is how they are coupled. The first issue is related to the layout of grid structures of LES and the layout of low-dimensional stochastic models. Recently, Cao and Echekki (Menon and Kerstein 2010; Cao and Echekki 2008) proposed a fixed lattice of ODT domains embedded on the LES grid. Alternatively, ODT domains may be embedded normal to a tracked flame brush and allowed to be advected with the flow. A second issue is to decide which equations or quantities to solve by both solutions. This decision also determines the degree of coupling and the redundancies between them. As proposed by Cao and Echekki (Menon and Kerstein 2010; Cao and Echekki 2008) a reasonable choice is to allow the LES to capture the flow (i.e. continuity and momentum), while ODT is tasked with the solution for the thermo-chemical scales (e.g. composition, temperature). In the Cao and Echekki model, both LES and ODT solve for a momentum equation. The momentum equation in ODT features contributions from large-scale transport through the
filtered velocity field and small-scale advective transport through a stochastic implementation of stirring events using the ODT model (A. R. Kerstein 1999).

ODT is a stochastic stand-alone turbulence model which is used to gather statistical properties of velocity and scalar fields turbulent flows. A series of random sequence of maps are used to represent turbulent advection and a variety of phenomena like small scale advection, molecular transport can be captured (A. R. Kerstein 1999). Punati et al. 2010 applied ODT Eulerian model to a planar nonpremixed turbulent jet flame and obtained good agreement with the DNS results. ODT has also been convincingly applied to autoignition of hydrogen/carbon monoxide in a turbulent jet (Gupta and Echekki 2011) and earlier attempts have been made to employ ODT as a robust high-fidelity subgrid closure for LES with a substantial reduction in computational cost (A. R. Kerstein 2002). This work is an effort in that direction.

1.3 Objective

The present work focuses on enhancing the coupling of LES and ODT to obtain accurate solutions to turbulent flow problems. An effort has been made to reduce the statistical errors associated with the flow of information between the multi-scale models by applying Kalman and Particle filtering techniques. A simplification of LES and ODT has been presented for the sake of validating the new filtering techniques by representing LES as a single dimensional coarse grid and a fine grid acts as a surrogate to ODT by enforcing mixing events through Linear Eddy Model.
CHAPTER 2
LES-ODT Coupling

This chapter deals with the principles and the issues being faced in coupling the solution schemes of LES and ODT. It sheds some light into the complex nature of interactions between the resolution scales. The interactions include the passing of various stochastic data and flow variables.

2.1 Coupling for Eulerian LES ODT Set Up

(Cao and Echekki 2008) applied the Eulerian formulation of the LES-ODT approach to the turbulent combustion. The ODT model forms the closure for the small scales, including key processes in combustion (e.g. resolution of flame structures). The model proposed by Cao and Echekki has a fixed lattice of ODT domains embedded in the LES grid. The ODT lattices are fixed in the LES computational domain for simulating with full spatial and temporal resolution, the turbulent transport and dynamic fluctuations in velocity and fluid properties. The flow properties are thus updated in time with respect to fixed position vectors. Figure 2.1 shows a layout of the LES-ODT configuration. ODT elements can be laid on a 3D lattice on LES grids or in between.
Umpteen issues arise when the information is being dealt by the two models. The LES captures the flow i.e. continuity and momentum, while the ODT handles the finer thermo-chemical scales i.e. for composition and temperature. The ODT also solves for the momentum equation which takes contributions from the LES by taking the filtered velocity field from the large-scale transport. The small-scale transport is taken care of by a stochastic implementation of stirring events in the ODT model.

2.2 Variables and Information Passed in LES-ODT Formulation

The coupling between LES and ODT necessitates a downscaling and an up scaling of information. The downscaling process involves the transfer of information from the coarse grid LES to the fine grid ODT. In this operation the intention is to bring the large-scale component of transport in ODT in agreement with the LES resolved velocity field since LES
takes care of the momentum transport. This enforcement of data is carried out by *interpolation* as shown in section 3.1.

The up scaling of data is just reverse of the downscaling process. In this process information is moved from ODT to LES grid. The ODT keeps track of the small-scale transport and chemistry. The chemical interactions at this level impact the heat release which in turn affect the mixture density. The ODT calculates scalars and transmits the density data to the LES. These changes in density then used by the LES impacts the overall flow. The following figure explains this flow of information.

![Flow of variables between LES and ODT](image)

**Figure 2.2**: Flow of variables between LES and ODT

The accuracy of the filtered density from ODT depends on the number of ODT points in the lattice embedded in each LES cell as the statistics are derived from them. This can be a source of sampling error/noise resulting from a limited resolution. The remedy to this problem can be by adding more number of ODT points in each cell. Alternatively statistical behavior of the data can be observed and passed through a filter for a broad range of wave numbers. The removal of this sampling error is the scope of this study. In the following text
the LES-ODT simplified model is presented to simulate a reacting flow and efforts have been made to eliminate the error in the variables passed. The model here includes the coupling between a coarse grained deterministic solution (denoted by CG) and the fine-grained stochastic solution (denoted by FG). The Kalman filter (Kalman 1960; Kalman and Bucy 1961) and Particle filter are used to combine the densities between these two scales such that both the mass conservation and the heat release are satisfied.
CHAPTER 3
Model Formulation

The model consists of a 1 D domain which comprises of a coarse grain scale (CG) and a fine grain scale (FG). The CG handles the solution for the momentum equation and the continuity equation and the FG deals with the solution of the temperature equation. Both solutions are implemented on the same physical 1 D domain. Since the FG is embedded inside the CG the FG has finer resolution. Owing to the difference in resolution the time-steps used in FG are smaller than that in CG.

The CG provides the large-scale advection for FG transport. The FG monitors the sub grid heat release processes thereby affecting the temperature. The density derived from these temperature fluctuations is obtained from the ideal gas equation. The sub grid scale advective transport is implemented through the LEM stirring events as explained in Section 5.1 while the reaction, molecular diffusion and large-scale advection are implemented deterministically. The velocity field originating from CG is interpolated into FG. This interpolation is a simple implementation of inverse spatial filtering within the context of LES.

3.1 Interpolation

Interpolation is an inverse LES filter. The interpolation is conducted in one direction using linear interpolation which is quite similar to bilinear interpolation (Press, et al. 1996). The linear interpolation is represented in a discretized way as follows:
Let us assume a variable $g$ that has to be interpolated from $f$ on the CG into the FG. Let the point where it has to be interpolated be denoted by $x$. Firstly the distance of $x$ from the starting point of the cell that contains $x$ is calculated. Let that be denoted by $\alpha$

$$\alpha = \frac{x - x_{min}}{\Delta x}$$  \hspace{1cm} (3.1)

$x_{min}$ denotes the starting point of the cell and $\Delta x$ denote the size of the cell. Then the interpolation equation is given as:

$$g = (1 - \alpha)f_i + \alpha f_{i+1}$$  \hspace{1cm} (3.2)
Chapter 4
Coarse Grained Implementation

The CG solution only resolves at the large-scale physical phenomena. It does not resolve the heat release, yet it needs that information through density and transport properties’ variation due to this release. Hence the CG solution is based on the 1D solution of continuity for density and the momentum (Burgers’) equation for one component of the velocity field that is aligned with the domain.

In their dimensionless form, these equations are written as:

- Continuity Equation

\[
\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u})}{\partial x} = 0
\]  
(4.1)

- Momentum (Burger’s)

\[
\frac{\partial \tilde{u}}{\partial t} + \tilde{u} \frac{\partial \tilde{u}}{\partial x} = \left( \frac{\mu}{\tilde{\rho}} + \frac{1}{\text{Re}} \right) \frac{\partial^2 \tilde{u}}{\partial x^2}
\]  
(4.2)

In the above equations, \(t\) and \(x\) refer to the time and the 1D spatial coordinate, respectively. The dependent variables are the filtered density, \(\tilde{\rho}\) and the filtered velocity, \(\tilde{u}\). \(\text{Re}\) is the reference Reynolds number used for the non-dimensionalization of the governing equations based on a reference length and velocity scales and the molecular kinematic viscosity of the fluid.
\[
\text{Re} = \frac{U_{\text{ref}} L_{\text{ref}}}{\nu}
\] (4.3)

In the dimensionless form of the governing equations, it represents the kinematic viscosity. \(\mu_t\) represents the turbulent viscosity. It is treated as a constant independent of the heat release process during the computation. This enables the explicit incorporation of the filtered density in the Burgers’ equation.

This filtered density is the result of application of the Kalman and Particle filters to the output densities from the CG and FG. This \(\bar{\rho}\) is the corrected density from the filters and helps to steer the final flow solution in the right direction. The Kalman filter and the Particle filter are designed to generate a reasonably “smooth” density that can be used within the context of a deterministic and potentially high-order discretization scheme. The ratio of the turbulent viscosity and the filtered density is the turbulent kinematic viscosity, \(\nu_t\), which varies as the reaction/heat release process (discussed within the context of the FG solution) evolves. The over-bar corresponds to a spatial filter. For a quantity \(q\), its spatial filter \(\bar{q}\) is expressed as follows:

\[
\bar{q}(x) = \int_{\Delta} q(x') G(x - x') dx',
\] (4.4)
where $\Delta$ is the filter size and $G$ is the filtering function. The filtered density at a prescribed position $x$ from the LEM solution is spatially filtered with a top hat profile of size $\Delta$ and centered at $x$. Favre-filtering is implemented for the velocity $u$ such that:

$$\tilde{u}(x) \equiv \frac{\rho u}{\rho} = \frac{1}{\Delta} \int_{\Delta} \rho(x') u(x') G(x-x') \, dx'. \quad (4.5)$$

As explained below, the solution for the filtered density in Equation (4.1) constitutes the prediction of forecasting step for the evaluation of the filtered density. In the spirit of the introductory remarks of the various filtered densities, this density may be labeled as $\tilde{\rho}_{c}$. 
Chapter 5

Fine-grained Implementation

The temperature resides on the finer scale with all its minute variations being monitored. The heat generation is taken care by a source term in the temperature equation. On the 1D solution of the finer scale the molecular diffusion, the large-scale advection and reaction are implemented deterministically whereas the sub grid turbulent transport is enforced stochastically. This has been made possible through the Linear Eddy Model (LEM) using the triplet maps to imitate stirring events. The 1D transport equation for temperature, $T$, in dimensionless form is written as follows:

\[
\frac{\partial T}{\partial t} + \bar{u} \frac{\partial T}{\partial x} = \frac{1}{Re \text{ Pr}} \frac{\partial^2 T}{\partial x^2} + Da \ T (1-T) + \Omega,
\]

This equation is non-dimensionalized such that $T$ ranges from 0 (unburned reactants) to 1 (burned products). In this expression, the term $\bar{u} \frac{\partial T}{\partial x}$ corresponds to large-scale transport, where the advective velocity $\bar{u}$ is obtained by interpolating the filtered velocity field from CG onto the FG grid.

The term $\frac{1}{Re \text{ Pr}} \frac{\partial^2 T}{\partial x^2}$ corresponds to the molecular diffusion term, where Pr is the Prandtl number assumed here to be unity. Re here is the turbulent Reynolds number calculated from the flow parameters at each step.
The term $Da \ (1-T)$ is a heat release term where $Da$ is a reaction Damköhler number and serves to modulate the rate of conversion from un-burnt reactants to burnt products.

The last term on the right-hand side corresponds to the stochastic sub-filter scale transport.

The combination of large-scale and sub-filter scale transport make up the essential contributions of all relevant scales in this problem.

The instantaneous density from the FG solution is obtained using the ideal gas state equation:

$$\rho = \frac{1}{1 + \beta T}.$$  \hspace{1cm} (5.2)

Here, $\beta$ is a heat release parameter. It may be expressed in terms of the dimensional temperatures as follows:

$$\beta = \frac{T_b - T_u}{T_b}.$$  \hspace{1cm} (5.3)

where the subscripts $u$ and $b$ refer to the unburned and burned gas states, respectively. The density is spatially-filtered at the end of a full step, $\Delta t$, to yield the observation value for the filtered density, $\bar{\rho}_f$. The filtering operation is implemented here using the top-hat spatial filter.

As stated above, the last term in the governing equation for temperature is implemented in parallel with the deterministic solution associated with the remaining terms of the temperature equation. The stochastic implementation of turbulent advection involves mapping events applied to the computed 1D scalar field. Each mapping event is a ‘triplet
map’ (Kerstein, Ashurst, et al. 2001) applied to a sampled segment (eddy) of size \( \hat{l} \) and left boundary location, \( \hat{x} \), such that the eddy spans the range \([\hat{x}, \hat{x} + \hat{l}]\).

5.1 Stirring Processes Applied through LEM

To seize all the complexities of turbulence all the eddy events should be modeled. Turbulent eddies result in mass transport and increase mixing and thereby affect the flow parameters significantly. This process is emulated through ‘triplet maps’. Triplet maps are random instantaneous maps applied to the fields in the interval domain of stirring motions to simulate eddies though stochastic processes. A conservative rearrangement is done which results in the redistribution of energy (A. R. Kerstein 1988).

5.2 Triplet Maps

Triplet maps are stochastic rearrangements of fields so that all the flow fields are altered but the properties still satisfy the mass, momentum and energy conservation laws. This reorganization takes place in a single dimension and creates a rotational effect. The description that follows gives a precise algorithm for prescribing of triple maps stochastically on a 1D field (Cao and Echekki 2008). A triplet map applied on a segment of 1D domain (i.e. an eddy) of length \( \hat{l} \) may be expressed as:
\[
f(x) = x + \begin{cases} 
3(x-x) & \text{if } x \leq x \leq x + \frac{\hat{l}}{3} \\
2\hat{l} - 3(x-x) & \text{if } x + \frac{\hat{l}}{3} \leq x \leq x + \frac{2\hat{l}}{3} \\
3(x-x) - 2\hat{l} & \text{if } x + \frac{2\hat{l}}{3} \leq x \leq x + \hat{l} \\
x-x & \text{otherwise}
\end{cases}
\]

(5.4)

The figure below shows the transformation that this function brings in a 1 D scalar field.

![Figure 5.1- Application of Triplet maps on scalar field](image)

When applied to a segment of a field of span \( \hat{l} \) this mapping increases the gradient to impose turbulence effects. It consists of the replacement of 1D profile on the sampled segment, \( \hat{x} \), by three identical copies compressed to span one-third of their original size. So initially the line segment is replicated into three copies of identical characteristics. These are then compressed to one-third size and placed against each other. Finally the middle copy is inverted to combine with the first two. This inversion helps to maintain the continuity of the values on the new profile. However, derivatives at the interfaces of the three sub-intervals are not continuous.
5.3 Implementation of Triplet Maps

The location of the position of the triplet map is chosen randomly from the entire domain length using a uniform distribution. The size of the stirring events is governed by an eddy size distribution, \( f(l) \) which is prescribed by a chosen spectrum of the kinetic energy distribution. Here we chose the familiar inertial range form and obtain an expression for \( f(l) \) of the form:

\[
    f(l) = \frac{5}{3} \frac{1}{L_t[L_t / \eta]^{-5/3} - 1} \left( \frac{1}{L_t} \right)^{-8/3}
\]

where \( L_t \) and \( \eta \) are the integral scale and Kolmogorov scale of the turbulence, respectively.

Sizes subject to stirring events are prescribed by sampling from the distribution \( f(l) \) and ranging from \( \eta \) to \( L_t \). Because stirring events address sub-filter scale physics, the integral scale should be of the order of the filter size or the CG solution grid size, \( \Delta x_c \), where the subscript “c” refers to the CG solution. Because of the considerations of the Nyquist limit (Schmidt, Kerstein and McDermott 2010) of the range of physics addressed by CG grid, a size of \( L_t = 2\Delta x_c \) is adopted. In practical terms the smallest eddy adopted in the simulations corresponds to 6 FG grid points on a uniform grid structure. This is because a mapping with \( \hat{l} = 3 \) does not change the field and \( \hat{l} = 6 \) is the next available multiple of 3. Nonetheless, the smallest eddies have little effect on transport but have a significant effect on dissipation.

The eddy rate process is regulated by an event frequency parameter \( \lambda_r \) (A. R. Kerstein 1991) and it has the measure of \( 1/(\text{length} \times \text{time}) \). The eddy rate distribution is given by-
In this expression, we implicitly assumed that the turbulent thermal diffusivity is equal to the turbulent kinematic viscosity, which yields a unity turbulent Prandtl number. Again here the turbulent diffusivity $D_t$ is equal to- 

$$D_t = \frac{\mu_t}{\rho} = \frac{2}{27} \frac{\lambda}{\eta} \int l^3 f(l) dl$$

(5.7)

There is a time spread between two stirring processes which is determined by the stirring time-step as given below-

$$\Delta t_t = \frac{1}{\lambda_t X}$$

(5.8)

where $X$ is the entire domain size. Since $\lambda_t$ depends upon the transient turbulent viscosity it should be variable with time. The turbulent viscosity evolves with the heat release and this variation is incorporated into the stirring processes by adjusting the stirring time-step at each instant. With everything else maintained constant this time-step is inversely proportional to the turbulent kinematic viscosity. Figure 5.2 shows the structure of stirring processes in LEM.
Figure 5.2- Stirring process in LEM
5.4 Implementation of FG Model

As described above, stirring events are applied concurrently with the deterministic solution of unsteady 1D reaction-diffusion equations (without advective terms or pressure variations along the 1D domain). The random process governing these events is implemented numerically by a sampling procedure at successive time-steps, $\Delta t_s$. Its effects correspond to the dissipation term represented by the turbulent kinematic viscosity in the coarse-solution. In the CG solution, this viscosity is inversely proportional to the filtered density. However, in the FG solution, it is implemented uniformly in the 1D domain using the average of all the turbulent viscosities in the entire domain.

At the beginning of the algorithm the diffusion time-step is calculated based on the CFL conditions. Later, the time-step for stirring is computed as shown above, in equation (5.8). Comparison of these time-steps provides the information about the processes to be executed. Among them the operation, whether diffusion or stirring, which has a lower time-step is followed after which the timer is advanced by the prescribed time-step. This procedure is repeated until the FG cycle is completed and starting all over again when data from the CG is obtained for the next cycle. Figure 5.3 depicts the entire layout of the FG model.
Figure 5.3 - Implementation of FG model
Chapter 6

The Kalman Filter

The Kalman filter is a recursive filter which is based on the principal of mean square error minimization technique (Welch and Bishop 2006). It is used to estimate the state of a dynamic linear system which has been corrupted by random noise. All noise in the system is assumed to be white Gaussian noise. For rectifying its estimate it uses measurements as feedback which may again be disturbed by random noise (Whyte 2001).

It is typically used in a physical system (e.g. GPS, robots) which is driven by a set of external inputs or controls and its outputs are evaluated by measuring devices or sensors, such that the knowledge of the system’s behavior is solely given by the inputs and the observed outputs (Funk 2003). The observations convey the errors and the uncertainties in the process, namely the sensor noise and the system errors. Based on the available information it is required to obtain an estimate of the system’s state that optimizes a given criteria.

Figure 6.1- Application of Kalman Filter (Ribeiro 2004)
The Kalman filter follows two steps as also shown in figure 6.2-

- Prediction
- Correction

![Diagram of Kalman filter steps]

**Figure 6.2-** Scheme for Kalman filter

### 6.1 Assumptions in Kalman Filter

To be able to implement the Kalman filter, a number of assumptions must apply:

- All the dynamic systems handled by Kalman filter are linear. Therefore, the governing equations governing this system (in their differential, algebraic or other forms must be linear).
- The system noise and the observation noise have a Gaussian distribution.
- All conditional probability density functions are Gaussian for all time-steps.
- The mean, median and mode of the conditional probability densities coincide.

Important ingredients for the Kalman filter include a state vector, dynamic model and an observation model-

6.2 The State Vector

The state vector contains the variables which have to be estimated. The variables in the state vector cannot be measured directly but they can be inferred from values that are measurable. A higher number of variables in the state vector increase the complexity of the system. The state vector has two values in the Kalman filter algorithm, 1) the *a priori* value, the predicted value before the update and 2) *a posteriori* value, the corrected value after the update.

6.3 The Dynamic Model

The dynamic model describes the transformation of the state vector over time. A linear system model is written as-

\[ x^{n+1} = M^n x^n + B^n u^n + G \sigma^n \]

(6.1)

where \( x \) is the state vector, \( M \) is the variable state transition matrix, \( B \) is the control input model applied to the control vector \( u \) and \( n \) is the time-step.

Here \( x \in R^n \), \( u \in R^m \), \( \omega \in R^n \), \( \{ \omega \} \) is a sequence of white, zero mean, Gaussian noise for the dynamic model.

\[ E[\omega^n] = 0 \]
6.4 The Observation Model

The observation model represents the relationship between the state and the measurements. In the linear case the measurements can be described by a system of linear equations which depend on the state variable.

\[ y^n = Hx^n + \nu^n \]  

(6.2)

where \( y \) is the observation, \( H \) is the variable observation model and \( n \) is the time-step.

Here \( y \in R^r \), \( \nu \in R^r \) and \( \{\nu\} \) is a sequence of white, zero mean Gaussian noise for the observation model.

\[ E[\nu^n] = 0 \]

6.5 Noise and Error Covariance

The covariance matrix for the entire system (with models and observations) may be expressed as follows

\[
E\left[ \begin{pmatrix} \omega^n \\ \nu^n \end{pmatrix} \begin{pmatrix} \omega^n^T \\ \nu^n^T \end{pmatrix} \right] = \begin{bmatrix} S^n & 0 \\ 0 & R^n \end{bmatrix}
\]  

(6.3)

This specifies that the covariance of the model noise is \( S \) and the covariance of the measurements is \( R \). Also this is a diagonal matrix since the noise in both the models is assumed to be independent and uncorrelated.

Initially the exact state of the system is known. Hence for the initial state \( x^0 \) the estimate is \( E[x^0] = x^0 \). In this section the top hat denotes optimal estimate. Error covariance matrix is-

\[ E[(x^0 - \hat{x}^0)(x^0 - \hat{x}^0)^T] = \sigma^0 \]
6.6 The Kalman Filter Algorithm

Let \( p(x^n \mid y^n) \) signify the conditional probability of having an estimate \( x \) at time \( n \) after making observations \( y \) up to time \( n \).

Since all probability functions are Gaussian we can write

\[
p(x^n \mid y^n) \sim N(\hat{x}^{n|n}, P^{n|n})
\]

where

\[
\hat{x}^{n|n} = E[x^n \mid y^n] \\
P^{n|n} = E[(x^n - \hat{x}^{n|n})(x^n - \hat{x}^{n|n})^T]
\]

\( \hat{x}^{n|n} \), the state estimate also acts as the mean of the conditional pdf and \( P^{n|n} \) is the estimate error covariance which is a measure of the uncertainty of the estimate till time \( n \).

A very important property of the Kalman filter is its recursive nature. Its implications are profound, mainly being that only estimated state from the previous time-step and the current measurement are needed to compute the estimate for the current state. Therefore rather than propagating the entire conditional pdf, the Kalman filter only propagates its first and second moments. In contrast to batch estimation techniques, no history of observations or estimates is required (Ribeiro 2004).

Before going into a detailed discussion of the filter’s equations and the steps involved it is essential to introduce the inherent characteristics. The following derivations and equations have been adopted from Ribeiro 2004. This treatment closely follows the evolution of the Kalman filter equations and its inherent logic.

\[
p(x^n \mid y^n) \sim N(\hat{x}^{n|n}, P^{n|n}) \\
p(x^{n+1} \mid y^n) \sim N(\hat{x}^{n+1|n}, P^{n+1|n})
\] (6.4)
which tells that the current and the future states all have Gaussian nature.

\( \hat{x}^{n|n} \) is the \textit{a priori state estimate} where \( \hat{x}^{0|n} \) and \( \hat{x}^{n+1|n} \) are given by

\[
\begin{align*}
\hat{x}^{0|n} &= E[x^n | y^n] \\
\hat{x}^{n+1|n} &= E[x^{n+1} | y^n]
\end{align*}
\]  
(6.5)

and

\[
\begin{align*}
P^{0|n} &= E[(x^n - \hat{x}^{0|n})(x^n - \hat{x}^{0|n})^T] \\
P^{n+1|n} &= E[(x^{n+1} - \hat{x}^{n+1|n})(x^{n+1} - \hat{x}^{n+1|n})^T]
\end{align*}
\]  
(6.6)

\( P^{n+1|n} \) is the \textit{a priori estimate error covariance} i.e. without the knowledge of the current observations. \( \hat{x}^{n+1|n} \) is the estimate of \( n+1 \) state without current observations.

Assumption: \( p(x^n | y^n) \) is known i.e. \( \hat{x}^{0|n} \) and \( P^{0|n} \) are known from the previous deductions and the objective is to estimate \( p(x^{n+1} | y^{n+1}) \)

\subsection*{6.6.1 Dynamic Model Prediction}

Since the mean value operator is a linear operator, calculating the expected value of equation (6.1) yields:

\[
E[x^{n+1} | y^n] = M^n E[x^n | y^n] + B^n E[u^n | y^n] + G E[\omega^n | y^n]
\]  
(6.7)

Considering equations (6.4) and (6.5) and since \( \omega^n \) being a 0 mean white Gaussian noise we have

\[
\hat{x}^{n+1|n} = M^n \hat{x}^{0|n} + B^n u^n
\]  
(6.8)

There are two kinds of errors in this estimation \textit{the prediction error} and \textit{the filtering error}

These errors are defined as follows:

\textit{Prediction error}: \( \tilde{x}^{n+1|n} = x^{n+1} - \hat{x}^{n+1|n} \)  
(6.9)
Filtering error:  \( \tilde{x}^{0|n} = x^n - \hat{x}^{0|n} \)  \( (6.10) \)

From equations (6.8) and (6.9) we can say
\[
\tilde{x}^{n+1|n} = M^n x^n + B^n u^n + G^n \omega^n - M^n \hat{x}^{0|n} - B^n u^n
\]
\( (6.11) \)

Next, using equation (6.10) in equation (6.11) we get
\[
\tilde{x}^{n+1|n} = M^n \tilde{x}^{0|n} + G^n \omega^n
\]
\( (6.12) \)

Now
\[
E[\tilde{x}^{n+1|n}(\tilde{x}^{n+1|n})^T] = M^n E[\tilde{x}^{0|n} \mid y^n](M^n)^T + G^n S^n (G^n)^T
\]
\( (6.13) \)

Including equation (6.6)
\[
P^{n+1|n} = M^n P^{0|n} (M^n)^T + G^n S^n (G^n)^T
\]
\( (6.14) \)

Equations (6.8) and (6.14) give the estimated state and the estimate error covariance of the system at time \( n \) before making any observations for time \( n+1 \).

### 6.6.2 Observation Model Prediction

Taking into consideration equation (6.2) we can say that
\[
p(y^{n+1} \mid y^n) = p(H^{n+1} \tilde{x}^{n+1} + \nu^{n+1} \mid y^n)
\]
\( (6.15) \)

Thus the predicted observation mean is
\[
\hat{y}^{n+1|n} = E[y^{n+1} \mid y^n] = H^{n+1} \tilde{x}^{n+1|n}
\]
\( (6.16) \)

Prediction error:  \( \tilde{y}^{n+1|n} = y^{n+1} - \hat{y}^{n+1|n} \)  \( (6.17) \)

Using equation (6.16) and equation (6.2) the Prediction error is
\[
\tilde{y}^{n+1|n} = H^{n+1} \tilde{x}^{n+1|n} + \nu^{n+1}
\]
\( (6.18) \)

The error covariance matrix for equation (6.18) is
Multiplying $\chi^{n+1}$ with $(y^{n+1|n})^T$ and using equation (6.18)

$$\chi^{n+1}y^{n+1|n,T} = \chi^{n+1}(\chi^{n+1|n})^T(H^{n+1})^T + \chi^{n+1}(v^{n+1})^T$$

Finally

$$E[x^{n+1}(\tilde{y}^{n+1|n})^T] = P^{n+1|n}(H^{n+1})^T$$

Equation (6.16) elicits the predicted observation before taking the actual measurement.

### 6.6.3 Correction

As the information contained is alike, we can write

$$E[x^{n+1} | y^{n+1}] = E[x^{n+1} | y^n, \tilde{y}^{n+1|n}]$$

Also, since $y^n$ and $\tilde{y}^{n+1|n}$ are independent it follows that

$$\hat{x}^{n+1|n+1} = E[x^{n+1} | Y^n] + E[x^{n+1}, \tilde{y}^{n+1|n,T}]P^{-1}_{y^n, \tilde{y}^{n+1|n}}$$

Now using equations (6.17), (6.19) and (6.21)

$$\hat{x}^{n+1|n+1} = \chi^{n+1|n} + P^{n+1|n}(H^{n+1})^T[H^{n+1}P^{n+1|n}(H^{n+1})^T + R]^{-1}[y^{n+1} - H^{n+1}\hat{x}^{n+1|n}]$$

The term $P^{n+1|n}(H^{n+1})^T[H^{n+1}P^{n+1|n}(H^{n+1})^T + R]^{-1}$ is called the Kalman Gain written as $K^{n+1}$

$$\hat{x}^{n+1|n+1} = \hat{x}^{n+1|n} + K^{n+1}[y^{n+1} - H^{n+1}\hat{x}^{n+1|n}]$$

In simple terms this expression concludes that

$$\text{Filtered state estimate} = \text{Predicted state estimate} + \text{Gain} \times \text{Error}$$

Filtering error:

$$\hat{x}^{n+1|n+1} = x^{n+1} - \hat{x}^{n+1|n+1}$$
Using this in equation (6.24)
\[
\hat{x}_{n+1|n} = \hat{x}_{n+1|n} - P_{n+1|n} (H_{n+1})^T [H_{n+1} P_{n+1|n} (H_{n+1})^T + R]^{-1} [H_{n+1} \hat{x}_{n+1|n} + v_{n+1}]
\] (6.27)

Taking the expected value of the above expression we finally have
\[
P_{n+1|n+1} = P_{n+1|n} - P_{n+1|n} (H_{n+1})^T [H_{n+1} P_{n+1|n} (H_{n+1})^T + R]^{-1} H_{n+1} P_{n+1|n}
\] (6.28)

Simplifying this expression
\[
P_{n+1|n+1} = (I - K^{n+1} H_{n+1}) P_{n+1|n}
\] (6.29)

Equation (6.29) provides the estimation error covariance of the \textit{a posteriori} estimated state.

In equation (6.25) the expression \(y_{n+1} - H_{n+1} \hat{x}_{n+1|n}\) is called the \textit{measurement error}. The error reflects the discrepancy between the predicted measurement \(H_{n+1} \hat{x}_{n+1|n}\) and the actual measurement \(y_{n+1}\) at time-step n+1. An error of zero means they are in complete agreement.

Looking at the expression of Kalman Gain in equation (6.25) certain conclusion can be inferred.
\[
K^{n+1} = \frac{P_{n+1|n} (H_{n+1})^T}{H_{n+1} P_{n+1|n} (H_{n+1})^T + R}
\]

As the measurement error covariance \(R\) approaches zero we have-
\[
\lim_{R \to 0} K^{n+1} = [H_{n+1}]^{-1}
\]

As the \textit{a priori} estimate error covariance \(P_{n+1|n}\) approaches zero-
\[
\lim_{P_{n+1|n} \to 0} K^{n+1} = 0
\]

The \(K\) here acts as a weighting factor. As the measurement error covariance \(R\) approaches zero, the actual measurement \(y_{n+1}\) is trusted more, while the predicted measurement \(H_{n+1} \hat{x}_{n+1|n}\) is trusted less. In contrast, as the \textit{a priori} estimate error covariance \(P_{n+1|n}\)
approaches zero the actual measurement $y^{n+1}$ is trusted less while the predicted measurement $H^{n+1}\hat{x}^{n+1|n}$ is trusted more (Welch and Bishop 2006). Figure 6.3 summarizes the steps and equations involved in the Kalman filter.

6.7 Summary of the Kalman Filter

**Update “Prediction”**

1) Advance the state

$$\hat{x}^{n+1|n} = M^n \hat{x}^n + B^n u^n$$

2) Advance the estimate error covariance

$$P^{n+1|n} = M^n P^n (M^n)^T + G^n S^n (G^n)^T$$

**Measurement “Correction”**

1) Kalman Gain

$$K^{n+1} = \frac{P^{n+1|n} (H^{n+1})^T}{H^{n+1} P^{n+1|n} (H^{n+1})^T + R}$$

2) Update estimate with measurement

$$\hat{x}^{n+1|n+1} = \hat{x}^{n+1|n} + K^{n+1} [y^{n+1} - H^{n+1} \hat{x}^{n+1|n}]$$

3) Update the estimate error covariance

$$P^{n+1|n+1} = (I - K^{n+1} H^{n+1}) P^{n+1|n}$$

**Figure 6.3**- Summary of Kalman filter equations
Chapter 7

The Particle Filter

In the previous chapter, we have discussed the Kalman filter. This filter may be implemented for linear dynamic systems with Gaussian noise. However, not all dynamical systems are subject to these constraints. A more general filter is the Particle filter. Particle filters are used to predict accurately the underlying dynamics of a non-linear system which are subject to non-Gaussian random noise (Thrun 2000). The Particle filter is a nonparametric implementation of the Bayes filter. It is a technique of implementing the required posterior density function by a set of random samples with associated weights and to compute estimates based on these samples and weights. It weights particles based on a likelihood score and then propagates these particles according to a motion model (Maskell 2001).

The Particle filter too is recursive in nature, tracking a state variable as it evolves in time by constructing a sample based representation of the entire probability density function. With large number of samples, this Monte Carlo characterization becomes an equivalent representation to the usual functional description of the posterior probability density function. The pdf here can also be a multi-modal pdf (Mukherjee and Sengupta 2010).

Particle filtering assumes a Markov Model for system state estimation which implies that past and future states are conditionally independent, given the current state (Chen, Morris and Martin n.d.). Thus observations are dependent only on the current state. The characterizing sample of states is taken from a proposal and not a posterior density for estimation. For this reason the samples have to be likelihood weighted by the ratio of
posterior and proposal distribution (Gordon, Salmond and Smith 1993). A discrete set of samples or particles represents the object state and evolves over time driven by the means of “survival of the fittest” principal. More details and explanations have been given in subsequent sections. The derivations, equations and strategies that follow have been obtained from Thrun 2000. The details and the elaborate discussions can be found in the text.

7.1 Dynamic Model

The dynamic model equation helps in propagating the state variable and the system samples as shall be shown later. A non-linear system is represented as-

$$x^n = f(x^{n-1}, u^{n-1}) + \omega^n$$  \hspace{1cm} (7.1)

where $x^n$ is the state vector, $u^n$ is the control vector and $f$ is the non-linear system equation. System noise $\omega^n$ represents disturbances, all unmodeled dynamics and any mismatch between the process and the model. Unlike most other state estimation methods, process noise does not necessarily have to be assumed to be Gaussian, rather any standard or non-standard distribution can be assumed depending on the behavior of the process noise.

7.2 Observation Model

The observations provide feedback for the model state. A non-linear observation equation is written as-

$$y^n = h(x^n) + \nu^n$$  \hspace{1cm} (7.2)
where \( y^n \) is the measurement vector and \( h \) is the non-linear measurement equation. The measurement noise \( \nu^n \) captures the inaccuracy in the measurement system. Again, this noise is *not* necessarily Gaussian. It can have *any arbitrary distribution*. Our goal is to estimate \( x^n \) from the set of all available measurements.

### 7.3 Noise Covariance

The covariance of the model and measurement noises is given by-

\[
E \begin{pmatrix} \omega^n \\ \nu^n \end{pmatrix} \begin{pmatrix} \omega^n \strut & \nu^n \strut \end{pmatrix} = \begin{pmatrix} S^n & 0 \\ 0 & R^n \end{pmatrix}
\]

(7.3)

Hence, \( S^n \) and \( R^n \) are model error covariance and measurement error covariance respectively. They are considered to be independent and uncorrelated and hence the noise covariance matrix is also a diagonal matrix.

### 7.4 Steps for the Particle Filter

There are three steps involved in the Particle filter scheme –

- Prediction
- Correction
- Resampling

Detailed schematics of the Particle filter have been described in figure 7.1.
In contrast, to the Kalman filter algorithm additional complexities characterize the Particle filter algorithm. They are detailed in the following discussion.

**Model Equation**: \( x^n = f(x^{n-1}) + \omega^n \)

In the Particle filter, samples characterizing the posterior distribution are drawn which are called ‘particles’ and the set is denoted as \( \mathcal{X}^n = x^{n[1]}, x^{n[2]}, \ldots, x^{n[M]} \). There are \( M \) samples of the state \( n \) in this sample set (Thrun 2000).

Each particle \( x^{n[m]} \) is a hypothesis as to what the true world state may be at time \( t \).

The objective of the Particle filter implementation is to capture the best estimate of the state variable using the various drawn out samples. The expected value of a distribution is calculated as-

\[ \hat{x} = \frac{1}{M} \sum_{m=1}^{M} x^{n[m]} \]
\[ E(x) = \int x p(x) dx \]  

(7.4)

Similarly for the estimation of our posterior distribution \( p(x^n | y^n) \) we have to evaluate

\[ E[x^n] = \int x^n p(x^n | y^n) dx^n \]  

(7.5)

\( n \) is the time-step, \( x \) is the model state and \( y \) are the observations. \( p(x^n | y^n) \) is the probability of estimating \( x \) at time-step \( n \) after having observations \( y \) till current time-step \( n \) (Imtiaz, et al. n.d.).

But there are two issues associated with the evaluation of the above equation

- It is not possible to directly sample from \( p(x^n | y^n) \)
- It has to be calculated in an online recursive manner

For this purpose the Particle filter employs a technique called Importance Sampling. Importance Sampling is a discrete method for approximating \( E(x) \) by replacing \( p(x) \) with a similar, but easily sampled distribution \( q(x) \) and then correcting for the error introduced by this switch (Owen and Zhou 2000).

### 7.5.1 Importance Sampling

If a set of sample \( x^{[m]} \) is generated from a given probability distribution \( p(x) \) then the expectation expression in (7.4) can also be calculated by the average of \( x \) evaluated with those samples.

\[ E(x) = \int x p(x) dx \]

\[ \approx \frac{1}{M} \sum_{m=1}^{M} x^{[m]} \]  

(7.6)
As discussed earlier, it is not possible to draw samples from \( p(x) \). Therefore another distribution \( q(x) \) is introduced, called the Importance Density, to draw samples from.

\[
E(x) = \int x \cdot \frac{p(x)}{q(x)} \, q(x) \, dx \\
\approx \frac{1}{M} \sum_{m=1}^{M} \frac{p(x^{[m]})}{q(x^{[m]})} \cdot f(x^{[m]})
\]

\[
E(x) = \frac{1}{M} \sum_{m=1}^{M} w^{[m]} x^{[m]}
\] (7.7)

where \( w^{[m]} \propto \frac{p(x^{[m]})}{q(x^{[m]})} \) is the normalized weight of the \( m \)th particle.

Now within context of our Particle filter if \( x^{[m]} \) are the samples drawn from an importance density, \( q(x^n \mid y^n) \) then the weights defined by (7.8) are

\[
w^{[m]} \propto \frac{p(x^{[m]} \mid y^n)}{q(x^{[m]} \mid y^n)}
\] (7.8)

We have samples constituting an approximation to \( p(x^{n-1} \mid y^{n-1}) \) and want to approximate \( p(x^n \mid y^n) \) with a new set of samples from an importance density \( q \) such that

\[
q(x^n \mid y^n) = q(x^n \mid x^{n-1}, y^n)q(x^{n-1} \mid y^{n-1})
\] (7.10)

Hence we can obtain samples \( x^{n[m]} \sim q(x^n \mid y^n) \) by augmenting each of the existing samples \( x^{n-1[m]} \sim q(x^{n-1} \mid y^{n-1}) \) with the new state \( x^{n[m]} \sim q(x^n \mid x^{n-1}, y^n) \).

Now expressing \( p(x^n \mid y^n) \) in terms of \( p(x^{n-1} \mid y^{n-1}), p(y^n \mid x^n) \) and \( p(x^n \mid x^{n-1}) \).
\[ p(x^n \mid y^n) = \frac{p(y^n \mid x^n, y^{n-1}) p(x^n \mid y^{n-1})}{p(y^n \mid y^{n-1})} \]
\[ = \frac{p(y^n \mid x^n, y^{n-1}) p(x^n \mid x^{n-1}, y^{n-1}) p(x^{n-1} \mid y^{n-1})}{p(y^n \mid y^{n-1})} \]
\[ = \frac{p(y^n \mid x^n) p(x^n \mid x^{n-1})}{p(y^n \mid y^{n-1})} p(x^{n-1} \mid y^{n-1}) \]
\[ \propto p(y^n \mid x^n) p(x^n \mid x^{n-1}) p(x^{n-1} \mid y^{n-1}) \] (7.11)

By substituting (7.10) and (7.11) in equation (7.9) the weight update equation can then be shown to be

\[ w^{[m]}_n \propto \frac{p(y^n \mid x^{[m]}_n) p(x^{[m]}_n \mid x^{n-1 \mid [m]}) p(x^{n-1 \mid [m]} \mid y^{n-1})}{q(x^{[m]}_n \mid x^{n-1 \mid [m]}, y^n) q(x^{n-1 \mid [m]} \mid y^{n-1})} \]
\[ = w^{n-1 \mid [m]} n \frac{p(y^n \mid x^{[m]}_n) p(x^{[m]}_n \mid x^{n-1 \mid [m]})}{q(x^{[m]}_n \mid x^{n-1 \mid [m]}, y^n)} \] (7.12)

Thus the expression

\[ w^{[m]}_n \propto w^{n-1 \mid [m]} n \frac{p(y^n \mid x^{[m]}_n) p(x^{[m]}_n \mid x^{n-1 \mid [m]})}{q(x^{[m]}_n \mid x^{n-1 \mid [m]}, y^n)} \] (7.13)

and the posterior filtered density \( p(x^n \mid y^n) \) can be approximated as

\[ p(x^n \mid y^n) \approx \sum_{m=1}^{M} w^{[m]}_n \delta(x^n - x^{[m]}_n) \] (7.14)

As \( M \to \infty \) the approximation (8.14) approaches the true posterior density \( p(x^n \mid y^n) \).

### 7.5.2 Sequential Importance Sampling (SIS) Algorithm

\[ \left[ \{ x^{[m]}_n, w^{[m]}_n \} \right]_{m=1}^{M} = \text{SIS} \left[ \{ x^{n-1 \mid [m]}, w^{n-1 \mid [m]} \} \right]_{m=1}^{M}, y^n \]

1: for \( m = 1 \) to \( M \)
2: draw $\chi^{n[m]} \sim q(x^n | x^{n-1[m]}, y^n)$

3: assign the particle a weight $w^{n[m]}$ according to equation (7.13)

4: end for

Particle filters construct the particle set $\chi^{n[m]}$ recursively from the set $\chi^{n-1[m]}$. The input to this algorithm is the particle set $\chi^{n-1[m]}$ along with the most recent measurement $y^n$. Line 2 generates a hypothetical state $\chi^{n[m]}$ for time $n$ based on the particle $\chi^{n-1[m]}$. The resulting sample is indexed by $m$ because it is generated from the $m^{th}$ particle of the set $\chi^{n-1[m]}$. Line 3 calculates for each particle an importance weight. This is used to incorporate the measurement $y^n$ into the particle set. In a way it gives us the proximity of the priori estimate to the observation. The SIS algorithm thus consists of recursive propagation of the weights and samples as each measurement is received sequentially (Arulampalam, et al. 2002).

### 7.5.3 The Degeneracy Problem

A common problem with the SIS algorithm is the *Degeneracy* phenomenon. If it were to occur, then after a few iterations, all but one particle will have negligible weight. This happens because the variance of the importance weights only increases over time and thus it is impossible to avoid this problem. The degeneracy implies that a large computational effort is devoted to updating particles whose contribution to the approximation of posterior density counts to almost zero (Andrieu, et al. 2004).
7.5.4 Resampling

Resampling is a method by which the effect of degeneracy can be reduced. It can be applied whenever a significant degeneracy is observed. If resampling is not performed many samples might be wasted in the regions of low probability (Thrun 2000). A standard approach to determine whether or not resampling should be performed is to measure the variance of the importance weights. The variance of the weights relates to the efficiency of the sample based representation. If all weights are identical, then the variance is zero and no resampling is required. If on the other hand, the weights are concentrated on a small number of samples, then the weight variance is high and resampling should be performed.

A suitable measure of degeneracy of the algorithm is the effective sample size $M_{\text{eff}}$ which is defined as

$$
\hat{M}_{\text{eff}} = \frac{1}{\sum_{m=1}^{M} (w_{m}^{n})^{2}} \tag{7.15}
$$

Resampling can be done whenever $\hat{M}_{\text{eff}}$ falls below a threshold. The basic idea of resampling is to eliminate particles that have small weights and to concentrate on particles with large weights. The following section gives a resampling algorithm which can be appended to the SIS algorithm to avoid the degeneracy problem (Arulampalam, et al. 2002).

7.5.5 The Resampling Algorithm

The resampling algorithm may be summarized as follows:

$$
\left[ \left\{ x_{m}^{n[m]}, w_{m}^{n[m]} \right\}_{m=1}^{M} \right] = \text{RESAMPLE} \left[ \left\{ x_{m}^{n[m]}, w_{m}^{n[m]} \right\}_{m=1}^{M} \right]
$$
1: Initialize the CDF- \( c_1 = 0 \)

2: for \( i = 2 \) to \( M \)

3: Construct the CDF- \( c_i = c_{i-1} + w^{n[i]} \)

4: end for

5: Start at the bottom of the CDF- \( i = 1 \)

6: Draw a starting point- \( u_1 \sim \bigcup [0,M^{-1}] \)

7: for \( j = 1 \) to \( M \)

8: Move along the CDF- \( u_j = u_i + M^{-1}(j-1) \)

9: while \( u_j > c_i \)

10: \( i = i + 1 \)

11: end while

12: Assign sample- \( x^{n[j]} = x^{n[i]} \)

13: Assign weight- \( w^{n[j]} = M^{-1} \)

14: end for

The algorithm draws with replacement \( M \) particles from the temporary set. The probability of drawing each particle is given by its importance weight. Resampling transforms a particle set of \( M \) particles into another particle set of the same size. In fact, the resulting sample set usually possesses many duplicates, since particles are drawn with replacement. This step in a way imposes the idea of “Survival of the fittest”.
7.6 Summary of Steps in Particle Filtering

Finally we present a summary of the Particle filter implementation. The implementation consists of 3 principal steps:

1) The Prediction Step
   - Initialization: Draw sample of $x^{0[m]}$ from the initial pdf $p(x_0)$
   - Prediction: Draw sample of $x^{n[m]}$ from the transition pdf $p(x^n | x^{n-1[m]})$

2) The Correction Step
   - Evaluate the importance weights $w^{n[m]} = w^{n-1[m]} p(y^n | x^{n[m]})$
   - Normalize the importance weights $\tilde{w}^{n[m]} = \frac{w^{n-1[m]}}{\sum_{m=1}^{M} w^{n[m]}}$

3) The Resampling Step
   - Calculate the effective particle set size $\hat{M}_{eff}$ as in equation (7.15)
   - If $\hat{M}_{eff}$ is smaller than the resample threshold, resample the particles according to their weights $\tilde{w}^{n[m]}$
   - For $m = 1$ to $M$, reset $w^{n[m]} = \tilde{w}^{n[m]} = 1 / M$
   - Calculate the filtered state estimation $\hat{x} \approx \frac{1}{M} \sum_{m=1}^{M} x^{n[m]}$

There is no specific assumption about the model characteristic (e.g. linear or non-linear) and the probability distribution (Gaussian or non-Gaussian) of the noise in the Particle filter, so it can handle any form of pdf even if it is multimodal. The flow of algorithm is shown below.
Figure 7.2- Algorithm of the Particle filter
7.7 Advantages and Disadvantages of Particle Filter

As discussed above, the Particle filter can address a broader range of applications than the Kalman filter. However, it generality comes at a cost. The principal advantage of the Particle filter is its ability to represent any arbitrary distribution (e.g. Gaussian and non-Gaussian, uni-modal or multi-modal).

The principal disadvantages of the Particle filter are 1) its higher computational complexity, 2) difficulties in determining the optimum number of particles 3) the number of particles increases with increasing model dimension, and 4) the potential risk of degeneracy and loss of diversity of the samples as time advances.
Chapter 8

Coupling of Coarse-Grained and Fine-Grained Solutions

Using Kalman and Particle Filters

To provide accurate solutions to the combustion process CG and FG regimes have to work in tandem. The small scale variations in density and temperature which are overlooked by CG are monitored by the FG and reported back to CG, helping it to provide meaningful large scale solutions. This process of capturing of physics on the fine scale is accompanied with statistical sampling error due to a limitation on the number of FG points embedded in each CG cell. This dearth of information is reflected in erroneous nature of FG chemistry being passed over to CG. The Kalman and Particle filters have a potential role in this regard. They attempt at better coupling of the solutions by predicting the correct probabilistic nature of the captured density and removing this statistical error.

The coupling of the CG and the FG solutions is implemented through

1) The interpolation of the filtered velocity field from the CG solution on to the FG solution for large-scale advection.

2) The spatial filtering of the instantaneous density from the FG solution to the CG solution.

3) The implementation of Kalman and Particle filter on the filtered densities.

The filtered velocity from CG solution is interpolated onto the FG LEM solution using linear interpolation to account for the large-scale advection term. This linear interpolation amounts to an approximation of an inverse filtering operation. The interpolation is carried out at the end of a CG time-step and at the beginning of the FG sub-steps or cycles.
A principal challenge in the present study, of course, is the use of the spatially-filtered density field from the FG solution. The resulting density contributes to the solution of the CG momentum equation and affects its accuracy. The FG solutions also constitute statistical data whose behavior over all scales and sampling error depends on the density of this data (e.g. how many LEM solution grids are within a given coarse cell). To address the potential limitations of a limited statistical sample of density values from LEM and its effect on the accuracy of the density field in the CG solution, the Kalman filter (KF) (Section 8.2) and Particle filter (PF) (Section 8.3) are used.

Because of the use of filtering, it is important to distinguish 3 different densities:

- The density $\bar{\rho}_c$ is the solution of the continuity equation in the CG solution prior to KF. Here the subscript “c” refers to the CG solution and the over-bar denotes spatial averaging/filtering.

- The density $\bar{\rho}_f$ is the spatially-filtered density from the LEM solution. This density is obtained using an equation of state by prescribing the pressure and the computed temperature field. A top-hat filter is adopted for the spatial average. Here the subscript “f” refers to the FG solution and the over-bar again denotes spatial averaging/filtering.

- The density $\bar{\rho}$ is the density obtained after filtering, which combines the values obtained for $\bar{\rho}_c$ and $\bar{\rho}_f$. Again, the over-bar denotes spatial averaging/filtering.
8.1 Numerical Implementation

The continuity equation (4.1) in the CG solution is discretized using a uniform grid $\Delta x_c$ and a time step $\Delta t_c$, where the subscript $c$ refers to the CG solution. The central difference scheme is used for spatial discretization, and forward Euler is used for time advancement:

$$\bar{\rho}^{n+1}_{ci} = \bar{\rho}^n_{ci} - \left( \frac{\Delta t_c}{2\Delta x_c} \right) \left( \bar{\rho}^n_{ci+1} \bar{u}_{i+1}^n - \bar{\rho}^n_{ci-1} \bar{u}_{i-1}^n \right)$$  \hspace{1cm} (8.1)

The Burger’s equation (4.2) in the CG solution is discretized using a similar scheme as follows:

$$\bar{u}_{i+}^{n+1} = \bar{u}_{i}^{n} + \left( \frac{\Delta t_c}{\Delta x_c^2} \right) \frac{1}{\bar{\rho}^n_{ci}} \left( \bar{u}_{i+1}^n - 2\bar{u}_{i}^n + \bar{u}_{i-1}^n \right) - \left( \frac{\Delta t_c}{2\Delta x_c} \right) \bar{u}_{i}^n \left( \bar{u}_{i+1}^n - \bar{u}_{i-1}^n \right)$$  \hspace{1cm} (8.2)

The temperature equation (5.1) in the FG solution is solved on a finer grid $\Delta x_f$ using parallel implementations of a deterministic solution for reaction, diffusion and large-scale advection combined with the implementation of stirring events. The deterministic solution is discretized as follows:

$$T_{i}^{n+1,s} = T_{i}^{n,s} + \left( \frac{\Delta t_f}{\Delta x_f^2} \right) \frac{1}{\text{Re Pr}} \left( T_{i+1}^{n,s} - 2T_{i}^{n,s} + T_{i-1}^{n,s} \right) - \left( \frac{\Delta t_f}{2\Delta x_f} \right) u_{i}^n \left( T_{i+1}^{n,s} - T_{i-1}^{n,s} \right) + D_{1}T_{i}^{n,s} \left( 1 - T_{i}^{n,s} \right) \Delta t_f$$  \hspace{1cm} (8.3)
The time-steps $\Delta t_f$ are treated as sub-cycles within a CG time-step. The cycles are denoted with the superscript $s$ in the discretized equations. This temperature field in the ODT scale has stirring processes which results in random perturbations in the density field in the ODT scale. The turbulence model is implemented as a series of independent operations on the scalar field. First, the time until the next eddy event is determined and the diffusion process is advanced until this time is reached. Next, the eddy location and eddy size are selected and the triplet map is performed until the simulation ending time is reached. The different time scales of CG and FG models are shown in the figure below.

![Comparison of time-steps for FG and CG processes](image)

**Figure 8.1-** Comparison of time-steps for FG and CG processes

### 8.2 Implementation of the Kalman Filter

This section discusses about the methodology followed to use the Kalman filter as an error prediction tool. This implementation exploits the linearity of the Continuity equation in density and also assumes that the distribution of the FG densities and errors to be Gaussian or at least unimodal.
In accordance with the discussion in Chapter 6, the inclusion of Kalman filter requires three basic ingredients-

- **A State Vector**: This is the solution vector to be rectified by the Kalman filter. In the present model, it corresponds to the filtered density over the discrete grid of the coarse-solution. The state vector can be written as:

\[
\bar{\rho} = (\bar{\rho}_1, \bar{\rho}_2, \ldots, \bar{\rho}_{N_c}, \bar{\rho}_{N_c})^T
\]  

where \(N_c\) is the number of coarse-grid cells in the computational domain.

- **A Model Equation**: This is the equation governing the evolution of the state vector. In the present model, it corresponds to the continuity equation (8.1). Potential errors within the model equation may be attributed to discretization errors. However, an important uncertainty in the model solutions may be attributed to the fact that the coarse-solution only accounts for fluid dynamics effects and do not consider the mechanism of density change due to heat release.

- **An Observation**: This is a set of data that is obtained independently for the state vector, which will be used to refine the state vector using the Kalman filter. In the present model, it corresponds to the filtered density from the FG LEM solution. Invariably, this observation has ‘errors’ associated with the limited sample of densities within a CG grid on which a filtered density is based. Since the FG solution is able to capture heat release and the resulting changes in the density field, the observation also serves to steer the CG solution. Also, because all the data on which the filtered density is available, a covariance matrix estimate of the error may be evaluated as well.
8.2.1 The Prediction Step

This step corresponds to the implementation of the model equation (the continuity equation) resulting in \( \bar{\rho}_c \). This step may be represented by the following matrix operation:

\[
\bar{\rho}^{n+1}_c = M^n \bar{\rho}^n + \epsilon^n_c
\]  

(8.5)

where \( \bar{\rho}^n \) is the vector made up of the solutions at the coarse-grid for the filtered density. \( M \) is the state transition \( N_c \times N_c \) matrix, which results from the discretization of the continuity equation (8.1). This equation is linear in \( \bar{\rho} \); however, it includes contributions from the velocity field, which evolves in both space and time. Therefore, this matrix must be evaluated at each time-step of the evolution of the density field. \( \epsilon^n_c \) is the vector of errors of length \( N_c \) associated with the determination of the filtered density from the continuity equation. Associated with this error vector is the symmetric error covariance matrix \( S = \langle \epsilon_c, \epsilon^T_c \rangle \) of dimensions \( N_c \times N_c \). The error may be attributed primarily to temporal and spatial discretization. The goal of the Kalman filter is to estimate the unknown true state \( \bar{\rho}^{n+1} \) when \( \epsilon \) is the Gaussian error.

For the Kalman filter operation, the model matrix is expressed as:
The symmetric covariance matrices associated with this error and the errors associated with the filtering of the density from the FG solution are expressed as:

\[
M^n = \begin{bmatrix}
1 & -\frac{\Delta t_c}{2\Delta x_c} u_2^n & 0 & \ldots & 0 & \frac{\Delta t_c}{2\Delta x_c} u_{N_c}^n \\
\frac{\Delta t_c}{2\Delta x_c} u_1^n & 1 & -\frac{\Delta t_c}{2\Delta x_c} u_3^n & 0 & \ldots & 0 \\
0 & 0 & \ddots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \ldots & 0 & 1 & -\frac{\Delta t_c}{2\Delta x_c} u_{N_c}^n \\
-\frac{\Delta t_c}{2\Delta x_c} u_1^n & 0 & 0 & 0 & \frac{\Delta t_c}{2\Delta x_c} u_{N_c-1}^n & 1
\end{bmatrix}
\]  

(8.6)

Here \( S \) is taken as a diagonal matrix since all noise is considered to be white noise. As stated earlier, the prediction error is associated with the temporal and spatial discretizations of equation (4.1). In the present simulation, we take it as primarily associated with the temporal discretization. The temporal integration is carried out with one half the time-step of the coarse-solution and the error is estimated by taking the difference between the full time-step and half the time-step. The same error estimate and associated covariance matrix is maintained throughout the simulation.
8.2.2 The Correction Step

This step involves an update of the filtered density field by incorporating the effects of the observations. The observation is based on filtering the density field using the FG solution. It too carries an error and is expressed as:

\[
\mathbf{p}_{f}^{n+1} = \mathbf{H}^{n} \mathbf{p}^{n} + \mathbf{e}_{f}^{n}
\]  

(8.8)

where the \( \mathbf{H} \) is the \( N_{c} \times N_{c} \) matrix, which relates the observations to the variable of the state-vector. Since both correspond to filtered densities, this matrix corresponds to the identity matrix. Therefore,

\[
\mathbf{p}_{f}^{n+1} = \mathbf{p}^{n} + \mathbf{e}_{f}^{n}
\]  

(8.9)

Again, \( \mathbf{e}_{f}^{n} \) is the vector of errors associated with the determination of the filtered from the spatially filtering the FG solution. Its covariance matrix is denoted as \( \mathbf{R} = \langle \mathbf{e}_{f}, \mathbf{e}_{f}^{T} \rangle \).

\[
\mathbf{R} = \langle \mathbf{e}_{f}, \mathbf{e}_{f}^{T} \rangle = \begin{bmatrix}
\mathbf{e}_{f_{1}}^{2} & \mathbf{e}_{f_{1}} \mathbf{e}_{f_{2}} & \cdots & \mathbf{e}_{f_{1}} \mathbf{e}_{f_{N_{c}}} \\
\mathbf{e}_{f_{2}} \mathbf{e}_{f_{1}} & \mathbf{e}_{f_{2}}^{2} & \cdots & \mathbf{e}_{f_{2}} \mathbf{e}_{f_{N_{c}}} \\
\vdots & \vdots & \ddots & \vdots \\
\mathbf{e}_{f_{N_{c}}} \mathbf{e}_{f_{1}} & \mathbf{e}_{f_{N_{c}}} \mathbf{e}_{f_{2}} & \cdots & \mathbf{e}_{f_{N_{c}}}^{2}
\end{bmatrix}
\]  

(8.10)

Again, \( \mathbf{R} \) is taken as a diagonal matrix since all noise is considered to be white noise.

The error covariance for the measurements (i.e. the filtered density from the FG solution) is estimated from the sample of FG densities on which the filtered density is based. The error associated with each CG cell is expressed as:
\[ e_i = \sqrt{\frac{\sum (\rho_f - \bar{\rho}_f)}{z}} \] (8.11)

where \( z \) is the number of FG points in one CG domain.

The proper analysis equation is written as follows:

\[ \bar{\rho}^{n+1} = \bar{\rho}_c^{n+1} + K^{n+1} (\bar{\rho}_f^{n+1} - H \bar{\rho}_c^{n+1}) = \bar{\rho}_c^{n+1} + K^{n+1} (\bar{\rho}_f^{n+1} - \bar{\rho}_c^{n+1}) \] (8.12)

where \( K \) is the Kalman gain matrix, which is expressed as:

\[ K^{n+1} = P^{n+1|n} H^T (H P^{n+1|n} H^T + R^{n+1})^{-1} = P^{n+1|n} (P^{n+1|n} + R^{n+1})^{-1} \] (8.13)

\( P^{n+1|n} \) is the *a priori estimate error covariance* as discussed in Section 6.6. In this context it is calculated as:

\[ P^{n+1|n} = M^n P^{n|h} (M^n)^T + S^n \] (8.14)

To be used in the next time-step the a priori error covariance is updated as:

\[ P^{n+1|n+1} = (I - K^{n+1}) P^{n+1|n} \] (8.15)

It follows from the above expressions that the final update of the solution may be expressed as:

\[ \bar{\rho}^{n+1} = (I - K) \bar{\rho}_c^{n+1} + K \bar{\rho}_f^{n+1} \] (8.16)

**8.2.3 The Solution Scheme**

The solution is implemented as follows:
8.2.3.1 Initialization

At \( t = 0 \), a smooth temperature field is prescribed on the FG grid. In the present study, we use a sinusoidal profile for the temperature. From this profile we compute the FG density and filter it onto the CG. The spatial filtering is implemented using the top hat filter around the CG grid point and with a width, \( \Delta x_c \), which corresponds to the CG solution uniform grid. The filtered velocity profile on the coarse-grid is initialized independently from the filtered density, and it too is prescribed with a sinusoidal profile as discussed in the next section.

8.2.3.2 Temporal Integration

With the initial solution provided, the solution proceeds at time-steps of \( \Delta t_c \), which corresponds to the CG solution time-step. Within this step, the FG solution is advanced at fractions of this step, \( \Delta t_f \) using the numerical discretization schemes discussed above. At the end of the coarse time-step between iteration at \( t^n \) and \( t^{n+1} \):

- The density is computed from the FG solution and filtered onto the coarse-grid and a solution for \( \tilde{\rho}_f^{n+1} \) is obtained.
- Also the density from the continuity equation is updated and a solution for \( \tilde{\rho}^{n+1} \) is obtained.
- With \( \tilde{\rho}_f^{n+1} \) and \( \tilde{\rho}^{n+1} \), an update for the filtered density \( \tilde{\rho}^{n+1} \) is obtained using KF. This density will be used in the following iteration in the right-hand side terms of the governing equations for continuity and momentum.
- The solution for the filtered velocity field from the CG solution is interpolated onto the finer grid and will be used to evaluate the large-scale advection term in the transport equation for the FG temperature.

The above procedure is repeated through the next time iterations until the final time-step is reached. The entire process is shown schematically in figure 8.2.
Figure 8.2- Schematic for coupling of CG and FG solutions using KF
Initialize temperature field $T^1$ on the FG

Initialize velocity field $u^1$ on the CG

Find initial density field $\bar{\rho}_i^1$ on FG from temperature field $T^1$ using eq. (5.2)

Average $\bar{\rho}_i^1$ for each CG to find the initial density on CG $\bar{\rho}_c^1$. This also serves as the initial state for KF i.e. $\bar{\rho}^1$

Advance $\rho^\prime_n$ to $\rho^\prime_{n+1}$ using the velocity field $u'$ in eq. (8.5)

Interpolate $u'$ from CG to FG

Start
Advance $T^n$ to $T^{n+1}$ with step $\Delta t_f$ using eq. (8.3) and applying stirring processes.

Convert $\Delta t_f$ into $\bar{\rho}_{i,i+1}$ using eq. (5.2).

Use $\bar{\rho}_{c,i+1}$ and $\bar{\rho}_{i,i+1}$ in the KF eq. (8.14) to come up with ideal estimate of density $\bar{\rho}^{n+1}$.

Advance $u^n$ to $u^{n+1}$ using eq. (8.2) and the KF estimated density $\bar{\rho}^{n+1}$.

All the CG time-steps complete?

Yes

End

No
8.3 Implementation of Particle Filter

In Section 8.2 Kalman filter was employed to attain a similar objective albeit with the assumption of Gaussian distribution of the model and process noise. In this section an attempt has been made to go a notch higher and handle the true nature of the noise covariance. As shown in Chapter 7 Particle filters can handle non-Gaussian and even multi-modal noise distributions. This provides the ability to include filtering of chemical source and heat release source terms from FG solutions.

As discussed in Section 7.2 the enforcement of Particle filter on a system requires three ingredients-

- **A State Vector**: The state vector is the variable of interest on which the Particle filter is applied. The objective to be achieved is the refinement of this vector by the Particle filter. In the present scenario the state vector is the filtered density on the CG i.e. \( \bar{\rho} \). Unlike the Kalman filter, here each CG grid density has been treated individually instead of a matrix of all the CG densities.

- **A Model Equation**: The discretized continuity equation (8.1) serves as the model equation as this is the equation that propagates the state vector in time to find the priori state of the variable and its samples. The errors in the model are partially ascribed to the discretization errors and partially to the absence of knowledge of fine scale chemistry.

- **An Observation**: The filtered density from the FG LEM solution functions as the observation for each state variable. This density, along with its sampling error due to dearth of LEM grid points, is combined with the CG solution using Particle filter to
give meaningful information about the density variations. This density after correction is used to advance the system in the right sense.

### 8.3.1 The Prediction Step

The prediction step results in the *a priori* state. Equation (8.1) which is also the continuity equation is utilized to obtain the predicted state of the state variable which is later combined with the observations. The prediction equation looks like:

\[
\vec{\rho}_{t+1}^{n+1} = \vec{\rho}_t^n - \left( \frac{\Delta t}{2 \Delta x} \right) \left( \vec{\rho}_{t+1}^n - \vec{\rho}_{t-1}^n \right) + \vec{e}_c^n
\]  

(8.17)

The input to this equation is the refined density field from the previous time-step. \( \vec{\rho}_t^n \) is the coarse grid density. \( \vec{e}_c^n \) represents any error type in the prediction equation, principally resulting from the temporal and spatial discretization. Inaccuracies resulting from temporal discretization techniques form the major segment of the errors. To ascertain this error, results are obtained with a full step and a half step discretization and the difference between these results gives the measure of the model error. An error variance \( S = \{ \vec{e}_c, \vec{e}_c^T \} \) is associated with the model error which is later used in the Particle filter algorithm.

The Particle filter needs a number of *sample particles* to represent the posterior density distribution. As the initial state is known with certainty, thus for the first step a random sample of particles is created around the initial state. This is done by assuming a Gaussian distribution for the model error and sampling states from this distribution. Although Particle
filters can handle errors with arbitrary distributions, this assumption is made solely for initialization purposes.

This set of particles is addressed as $\bar{\rho}_c^{n+1[m]}$ where $m$ is the index of the particle which ranges from 1 to $M$. $M$ being the total number of particles.

### 8.3.2 The Correction Step

The correction step incorporates the inclusion of observations so that the a priori state or predicted state can be rectified. In the present case the observations amount to the filtered density from FG solutions. The observation model follows the equation –

$$\bar{\rho}_f^{n+1} = h\bar{\rho}^n + \varepsilon_f^n$$  \hspace{1cm} (8.18)

The density here is being observed directly and there is no transformation function, hence equation (8.18) can be simply stated as-

$$\bar{\rho}_f^{n+1} = \bar{\rho} + \varepsilon_f^n$$  \hspace{1cm} (8.19)

$\varepsilon_f^n$ is the error in the FG filtered density resulting from the paucity to adequate LEM grid points. This sampling error is calculated as-

$$\varepsilon_i = \sqrt{\frac{\sum (\rho_f - \bar{\rho}_f)^2}{z}}$$  \hspace{1cm} (8.20)

$\rho_f$ are each of the FG densities and $z$ is the number of FG points in each CG domain. The error variance associated with this error is denoted as $R = \langle \varepsilon_f \varepsilon_f^T \rangle$. Sequential Importance
Sampling (SIS) algorithm is applied to this data set to acquire the optimum estimation of the posterior density $p(x^n | y^n)$ as explained in Section 7.5.2.

### 8.3.2.1 Selecting the Weight Function

The choice of the weight function is an enormous determining factor in the correct behavior of the Particle filter. Choosing the suitable weight function ensures that the changes in the error covariance and patterns are adequately reflected in the results and the weights give legitimate importance to model as well as observations. This also entails the assignment of importance weights to each particle of the particle set, weights being a measure of the proximity of the respective particle to the observations (Han and Li 2008). The choice of the weighing function is crucial to the algorithm. The weighing function should –

- Produce appreciable difference among particles of different importance so that significant distinction can be achieved while deciding the subsequent particle set for future iterations.
- Incorporate the error covariance of the observations so that the true nature of measurements can be captured.

Bearing in mind the above requirements, a Gaussian function is chosen to represent the weighing function with the covariance of observations i.e. $R$. Even though the observation error may be non-Gaussian, the weighing function does not have to be and can be Gaussian (Nagarajan, et al. 2011). This follows from the Central Limit Theorem which states that “The distribution of an average tends to be Normal, even when the distribution from which the normal is computed is decidedly non-Normal.” Thus-
The discussion in Chapter 9 convincingly establishes the choice of the above weight function.

### 8.3.3 The Resampling Step

To avoid any degeneracy problems creeping into the system the Resampling algorithm given in Section 7.5.5 is employed. This ensures a healthy propagation of particle set and an accurate estimation of posterior states.

### 8.4 The Solution Scheme

The solution is implemented follows in general the approach adopted for the Kalman filter, but invariably includes the additional details of the Particle filter implementation. It is implemented as follows:

#### 8.4.1 Initialization

At $t = 0$, a smooth temperature field is prescribed on the FG grid. In the present study, we use a sinusoidal profile for the temperature. From this profile we compute the FG density and filter it onto the CG. The spatial filtering is implemented using the top hat filter around the CG grid point and with a width, $\Delta x$, which corresponds to the CG solution uniform grid. The filtered velocity profile on the coarse-grid is initialized independently from the filtered density, and it too is prescribed with a sinusoidal profile as discussed in the next section.

\[
\omega^{n[m]} = \frac{1}{\sqrt{2\pi R}} e^{-\frac{(\hat{d}^{m})^2}{2R}}
\]  

(8.21)
8.4.2 Temporal Integration

With the initial solution provided, the solution proceeds at time-steps of $\Delta t_c$, which corresponds to the CG solution time-step. Within this step, the FG solution is advanced at fractions of this step, $\Delta t_f$ using the numerical discretization schemes discussed above. At the end of the coarse time-step between iteration at $t^n$ and $t^{n+1}$:

- The density is computed from the FG solution and filtered onto the coarse-grid and a solution for $\bar{\rho}_f^1$ is obtained.
- Also the density from the continuity equation is updated and a solution for $\bar{\rho}_c^{n+1}$ is obtained.
- With $\bar{\rho}_f^{n+1}$ and $\bar{\rho}_c^{n+1}$, an update for the filtered density $\bar{\rho}^{n+1}$ is obtained using Particle filter. This density will be used in the following iteration in the right-hand side terms of the governing equations for continuity and momentum.
- The solution for the filtered velocity field from the CG solution is interpolated onto the finer grid and will be used to evaluate the large-scale advection term in the transport equation for the FG temperature.

The above procedure is repeated through the next time iterations until the final time-step is reached as presented schematically in figure 8.3.
Figure 8.3- Schematic for coupling of CG and FG solutions using PF
Start

Initialize temperature field $T^1$ on the FG

Initialize velocity field $u^1$ on the CG

Find initial density field $\bar{\rho}^1$ on FG from temperature field $T^1$ using eq. (5.2)

Average $\bar{\rho}^1$ for each CG to find the initial density on CG $\bar{\rho}''$. This also serves as the initial state for KF i.e. $T''$

Advance $\rho''$ to $u''$ using the velocity field $\bar{\rho}''$ in eq. (8.4)

Interpolate $\bar{\rho}''$ from CG to FG

A

B
A

Advance $\tilde{\rho}_n^{n+1}$ to $T_n^{n+1}$ with step $\Delta t$, using eq. (10.3) and applying stirring processes

Convert $T_n^{n+1}$ into $\tilde{\rho}_t^{n+1}$ using eq. (5.2)

Use $\tilde{\rho}_n^{n+1}$ and $\tilde{\rho}_t^{n+1}$ in the PF algorithm to come up with ideal estimate of density $\tilde{\rho}_n^{n+1}$

Advance $\tilde{u}_n^{n+1}$ to $\tilde{\rho}_n^{n+1}$ using eq. (8.2) and the PF estimated density $\tilde{\rho}_n^{n+1}$

B

All the CG time-steps complete?

No

Yes

End
9.1 Run Conditions

Initial inputs to the algorithm include the velocity profile and temperature profiles and certain other parameters. Details of the initial conditions are mentioned below.

- The initial filtered velocity profile is a sinusoidal wave with three periods over the spatial domain and a peak magnitude of 0.5 in dimensionless form.
- A sinusoidal profile for the temperature in the FG solution is also imposed with a mean of 0.1 and a magnitude of 0.09 (i.e. the solution is provided with various degrees of preheat) and three periods over the spatial domain. Because of the sensitivity of the reaction rate to temperature, the higher temperature regions of the computational domain will undergo initially higher heat release than the remaining regions of the computational domain.
- The simulation parameters include a resolution of 90 grid points for the CG solution and 900 grid points for the FG solution, resulting in 10 FG cells per CG cell.
- The reference Reynolds number, based on a reference length and velocity scales and the kinematic viscosity, is 608.
- The number of dimensionless time-steps is 2,500.
- The Prandtl number is unity, $Pr = 1$.
- The heat release parameter, $\beta = 2$.
- The Damköhler number $Da$ in the heat release equation is $Da = 5$. 
• The initial turbulence Reynolds number is \( \text{Re}_t = 4,000 \). This value is used to determine the initial dimensionless turbulent kinematic viscosity, \( \nu^0 = \text{Re}_t / \text{Re} \). In subsequent time-steps, \( \nu_t \) is rescaled with the inverse of spatially-averaged filtered density field, \( \nu_t = 1/\langle \rho \rangle \), where the brackets “\( < > \)” denote an of the entire filtered density field.

In the following discussion, the results are presented first based on the FG temperature and density fields, and then for the CG profiles of the filtered velocity and density fields.

9.2 Results and Discussions for the Kalman Filtering

9.2.1 Evolution of the FG Fields

Figure 9.1 shows the evolution of the temperature field from the FG solutions of the LEM at 4 different times corresponding to the initial profiles \( t = 0 \) and \( t = 500, 1500 \) and 2500. The initial sinusoidal profile of temperature pertains to regions with different amount of heat. The troughs having a dimensionless temperature of 0.01 signify preheat and the peaks with temperature of 0.2 stand for relatively hotter regions. The figure shows the presence of contributions of the various terms to the governing equation of the temperature field. As higher temperature transforms into higher chemical activity, there is a significant and immediate rise in temperature of the hotter regions. The heat source term simulates the combustion process. Plots at subsequent time-steps show substantial fluctuations in the field while the general pattern of where the peaks are reflected in the profiles. These fluctuations are a consequence of stochastic stirring processes implemented through triplet maps imitating turbulent eddies. A wide range of eddies are observed in the temperature fields enhancing the
process of mixing beyond the role played by molecular diffusion and playing the equivalent role of turbulent diffusion on the CG scales. Equation (5.1) also has a diffusion term. The diffusion acts on the high gradients resulting from the triplet maps to smooth the fluctuations and attenuate the eddies. Another important observation is associated with the spread of the high-temperature zone and the thinning of the low-temperature zone, indicating a process of ignition propagation as hot layers contribute to the preheating of neighboring layers and the acceleration of their chemistry. The temperature ranges from 0 to 1 where 1 signifies complete combustion hence in the figure the temperatures plateau at 1 with advancing time-steps.

**Figure 9.1** - Evolution of the FG temperature field at 4 different times t=0, 500, 1500, 2500

Figure 9.2 shows the evolution of the density field as obtained from the temperature field
from the FG solutions of the LEM using equation (5.2). The equation depicts the density as being inversely proportional to the temperature by a factor of the heat release parameter. This is clearly conspicuous from figure 9.2. The regions with high temperature have lower density and vice versa. The fluctuations in the temperature field are also manifested in the density introducing random perturbations in the field. This random density is sampled by the LEM with ten points in each CG, to give out the average $\bar{\rho}_f$ per cell. These sampled densities become the observations for the state correction models. The broadening of low-density zones relative to the higher density zones also is a reflection of the ignition propagation mechanism discussed above. Another factor in the broadening and compression of the density profiles may be attributed to the role of large-scale advection as discussed below. This advection results in alternating regions of positive velocity gradients or expansion and regions of negative velocity gradients or compression.

Figure 9.2- Evolution of density field at 4 different time t=0, 500, 1500, 2500
9.2.2 Evolution of CG Fields

The velocity is set up on the CG as a three period sinusoidal function so that alternating regions have a transport in opposite directions with the mean velocity being zero. Figure 9.3 shows the evolution of the filtered velocity field corresponding to the solution of the Burgers’ equation for 4 different times corresponding to \( t = 0, 500, 1500 \) and 2500. The velocity decays with time primarily due to the attenuating role played by diffusion, while the periodic structure of the profiles is maintained. The nodes of the profile stay intact indicating that there is no material transport through the regions. The position of the peaks and the minima also remain the same. The velocity profiles are reasonably smooth further emphasizing the smoothing role of the Kalman filter.

![Figure 9.3- Evolution of Filtered velocity profiles at t=0, 500, 1500, 2500](image)
Figure 9.4 shows a comparison of different densities. Figure 9.4 shows the evolution of these profiles at three different times corresponding to \( t = 500, 1500 \) and \( 2500 \) and the three different filtered densities: 1) the solution with KF (solid lines) \( \bar{\rho} \), 2) the solution of the continuity equation (long dashes) \( \bar{\rho}_c \) and 3) the density obtained by filtering the FG density field (dot-dashed lines) \( \bar{\rho}_f \). There are some very distinguishable observations to these plots. With advancement in time \( \bar{\rho}_c \) keeps drifting away from the LEM and KF solutions. On comparing the values of \( \bar{\rho}_c \) at different time-steps there is very little discernable change since the CG is completely oblivious to the small-scale chemical interactions. Initially (not shown), the 3 density profiles are identical since the filtered density from the FG profiles is interpolated to initialize the density used in the continuity equation. However, a closer inspection of the plots shows that the peak values of \( \bar{\rho}_c \) increase beyond the corresponding peaks of the original profiles and the minima actually decrease. These trends are attributed to the shapes of the velocity profiles as shown in Figure 9.3 where velocity gradients are positive (resp. negative), expansion (resp. compression) occurs, and invariably a decrease (resp. increase) in the peak values of the density occurs. Meanwhile \( \bar{\rho}_f \) and \( \bar{\rho} \) decrease continuously because of the evolution of heat. The \( \bar{\rho}_f \) helps to drive back the corrupted density \( \bar{\rho}_c \) by providing an account of the chemical interactions. The density associated with FG, \( \bar{\rho}_f \), exhibits minor perturbations in its plots which can be convincingly attributed to the sampling errors in the LEM solution. In contrast, the KF density \( \bar{\rho} \) is fairly smooth and exhibits the desired features from the continuity equation, its smoothness, and the ability to track the heat release.
Figure 9.4- Evolution of filtered density profiles based on KF (solid), the solution of the continuity equation (long dashes) and the spatial filtering of the LEM density field (dot-dashes) at t=500, 1500 and 2500
To illustrate how the Kalman filter is able to smooth the filtered density profiles, the power-density spectra in Fourier domain of $\bar{\rho}_f$ (long dashes) and $\bar{\rho}$ (solid lines) are plotted and shown in Figure 9.5. The figure shows that the density after KF exhibits a single dominant wavenumber, which corresponds to the period of oscillations of the density field. In contrast, the density field $\bar{\rho}_f$ exhibit additional contributions from primarily higher wave. These contributions are reflected in the non-smoothness of this density profiles in the physical domain. Therefore, KF is able to preserve the dominant wave numbers inherent with the shapes of the profiles of the filtered quantities. The present results show the Kalman filtering

**Figure 9.5** - Comparison of the power density spectra of the filtered density fields. Solid: KF filtering; dashed: spatial filtering of LEM densities
can effectively couple the CG and FG solutions for the density resulting in a smoother density field.

9.3 Results and Discussions of Particle Filtering

9.3.1 Evolution of FG Fields

The application of Particle filter follows the same initialization steps as implemented for the Kalman filter. Consequently, the results obtained from the Particle filter follow virtually similar trends as those of the Kalman filter.

Figure 9.6 shows the evolution of temperature fields on the FG scale. As seen in figure 9.1 as well there is higher increase in temperature in the zones that have a higher preheat. The temperature rises until the limiting value of 1 is reached. The random fluctuations observed in the fields are a consequence of the stochastic triplet maps representing diverse eddies following which the diffusion rarifies them.
The transient variations in temperature cause changes in density on the FG scale which have been shown in the figure 9.7. It is obtained from the relationship between temperature and density given by equation 5.2. and indicated by the figure as being in inverse relationship only shifted by the heat release parameter.

**Figure 9.6**- Evolution of the FG temperature field at 4 different times $t=0, 500, 1500, 2500$
Figure 9.7- Evolution of density field at 4 different time t=0, 500, 1500, 2500

9.3.2 Evolution of CG Fields

As initialized, the velocity field is a sinusoidal function of 3 periods. Figure 9.8 shows the changes reflected in the CG velocity field with time advancement. The magnitudes of the velocity decrease with time due to the effect of turbulent and, to a lesser extent molecular diffusion and the smoothness of the profile is maintained, further enforcing the smoothing role of Particle filter.
Figure 9.8- Evolution of Filtered velocity profiles at t=0, 500, 1500, 2500

Figure 9.9 shows a comparative picture of the various CG densities and how they react to the flow conditions. The plot shows three different densities: 1) the solution with PF (solid lines) $\bar{\rho}$, 2) the solution of the continuity equation (long dashes) $\rho_c$ and 3) the density obtained by filtering the FG density field (dot-dashed lines) $\bar{\rho}_f$. A worthy observation is the proximity of (solid lines) $\bar{\rho}$, with the (dot-dashed lines) $\bar{\rho}_f$ and the constant digression of $\rho_c$ from the solutions, thus emphasizing the rectifying role of the Particle filter to draw the solutions back on track. Temperature variations are observed by the LEM filtered density $\bar{\rho}_f$ and the information is provided to the Particle filter hence, the $\bar{\rho}_f$ and $\bar{\rho}$ continuously decrease with rise in temperature. Also, due to the smoothing role of Particle filter the unwanted fluctuations are removed and a smooth density profile is obtained.
Figure 9.9- Evolution of filtered density profiles based on PF (solid), the solution of the continuity equation (long dashes) and the spatial filtering of the LEM density field (dot-dashes) at $t=500$, $1500$ and $2500$
To further study the smoothing capability of the Particle filter power spectra of $\bar{\rho}$ and $\bar{\rho}_f$, are plotted as shown in figure 9.10. The plot of $\bar{\rho}$ (solid lines) demonstrates a single dominant wave number which corresponds to the one smooth frequency of the Particle filter solution. In contrast, the plot of $\bar{\rho}_f$ (long dashes) shows many more wave numbers which are representative of the additional oscillations in the LEM filtered density.

![Figure 9.10](image.png)

**Figure 9.10**- Comparison of power density spectra of the filtered density fields. Solid: density after Particle filtering; dashed: density from spatially filtering the density field in the FG solution
Chapter 10

Conclusions

A coupling algorithm of thermo-chemical scalars on the FG solutions and fluid mechanics on the CG solutions using the Kalman and Particle filters is presented and validated. The problem is relevant to the multiscale simulation of turbulent combustion flows using large-eddy simulation coupled with a low-dimensional stochastic model for subgrid-scale physics. Traditional LES targets the important role played by large-scale processes in the transport of momentum and scalars; however, in combustion important physics resides at the unresolved scales of LES. The scheme establishes the potential of Kalman and Particle filtering in coupling the densities from the FG and CG solutions resulting in smooth filtered densities that are also steered by the FG solutions where heat release is modeled.

The implementation of the Kalman filter exploits the inherent linearity of the continuity equation in density. Moreover, there is an explicit assumption about a Gaussian distribution of the density. This is a reasonable assumption for the present validation study. The results in chapter 8 convincingly establish the smoothing role of the Kalman filter and its ability to reduce statistical error in flow of information in a multi-scale simple combustion scenario. However, other scenarios of combustion may involve more complex non-Gaussian distributions, such as conditions sustaining both extinguished and burning conditions. For these conditions, more general recursive filter may be needed. In the present study, the Particle filter is implemented as well. The results shown in chapter 11 endorse the Particle filter as being a promising nonlinear filter algorithm for complex transport equations. Also an
important conclusion of this data assimilation task was the authenticity of the Weight function chosen in section 10.2.2.1 whose performance was consistent with that of the Particle filter.
REFERENCES


Welch G. and Bishop G. *An Introduction to the Kalman Filter*. Chapel Hill: Department of Computer Science, University of North Carolina at Chapel Hill, 2006.