CHEN, MICHAEL. Electromagnetic Energy Localization in Random Mediums. (Under the direction of Michael Steer.)

This dissertation investigates the electromagnetic (EM) scattering of microwave excitations in energetic composites, specifically RDX (cyclotrimethylene trinitramine). Of interest is the presence of electric field peaks in these mediums with insight into the potential of a microwave neutralization system for explosives. Such mediums are characterized by large numbers of crystals with sizes on the scale of hundreds of microns, a small fraction of the wavelength of the incident microwave excitation, and an explosive device comprised of many millions of crystals. Furthermore, the critical features in the initiation process are electric field peaks that have a size that is a further fraction of that of the crystals, and durations which are picoseconds long. The number and size of crystals, and the required time and space resolutions make exhaustive re-creation and EM simulation of these mediums extremely time-consuming and infeasible without abstraction. This work develops new, efficient and accurate methods to reduce the time required to perform EM simulation of large volumes of energetic composites.

The crystals are subwavelength in size, suggesting a description of the structure using an effective permittivity, thus characterizing the complex scattering medium with a single parameter. This permittivity is determined for a variety of structures varying in crystal number and complexity. It is found that more detailed investigations via full-wave EM simulations do not yield significantly improved results over well-known analytic models. In addition, very little variation of the effective permittivity is found between different arrangements and types of crystals, in contrast to previous studies.

In efforts to improve simulation efficiency while maintaining accurate prediction of peak
field behavior, a range of abstractions of crystals is considered to determine the minimum complexity which correctly models field peaking. These abstractions are compared to the more realistic structure of non-uniform crystals placed using a physics based script. It is determined that a medium of randomly rotated and positioned cubes is the best model, offering improved speeds while maintaining the majority of the field localization phenomenon. The presence of hotspots is seen to be heavily influenced by local geometry, with the presence of multiple corners and edges resulting in the highest fields. Peak fields eight times that of the incident excitation are observed.

Finally, a coupling of the electric field behavior into thermal heating is performed via a simulation of dielectric heating and thermal conduction. Locations of high temperature in an RDX-estane composite are tracked over 20 ms for a 1 MV/m sinusoidal excitation, with peak temperature increases of over 75 K. It is observed that while locations of highest electric field do display higher than average temperatures, the higher dielectric loss of the estane binder results in the regions of highest temperature being locations where binder density is high. It is found that regions of high binder density have higher temperatures overall. Still, the highest field locations generally correspond to areas of high temperature. With the compounded effects of electric field and temperature, these locations will have a lower threshold for initiation than would be suggested by the separate effects.

The cubic crystal abstraction is shown to work well from the perspective of predicting high peak fields, as well as displaying thermal behavior in agreement with previous observations. The success of this abstraction offers significantly improved runtimes or expanded scope for future investigations of energetic materials and may be adapted to other methods of excitation, such as purely thermal, acoustic or mechanical stress, or a combination of coupled sources.
Electromagnetic Energy Localization in Random Mediums

by
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To my parents.
BIOGRAPHY

Michael Chen was born in Heidelberg, Germany. Until 2013, he worked towards the PhD degree under the guidance of Professor Michael Steer at North Carolina State University. He enjoys singing.
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Introduction

1.1 Overview

Energetic materials, which give explosive devices their destructive capabilities, release energy through the breaking of many chemical bonds in a chain reaction. In this way, they are inherently unstable. This instability can be undesirable, as in the case of an unexpected shock which causes accidental, unwanted initiation. They may also be advantageous, as in the remote, non-contacting initiation of explosive devices via a distant source. In particular, it is possible to control the chain-reaction, causing energy to release at a slower rate, which results in the deflagration of the material, instead of a more violent detonation [1]. This manifests as a slow burning of the material, effectively neutralizing the device. Deflagration is less common in acoustically or mechanically excited explosives, and believed to be due to the ability of EM and thermal excitations to introduce energy at a slower rate.

Various methods of neutralizing energetic materials have been studied for the better part of a century, gaining significant traction in the past three decades. Various methods of
acoustic, mechanical and thermal excitation have shown consistent, reproducible success in initiating energetic materials. However, deflagration via purely electromagnetic (EM) excitation is relatively inconsistent and/or inefficient, and poorly understood. In particular, EM excitation sources in the microwave regime have been shown to cause initiation, but detailed results have proven difficult to record [2].

A key factor in the neutralization of these materials is the creation of hotspots, areas of particularly high stress. This stress can be the result of mechanical and acoustic interactions or chemical processes. However, in the case of EM excitation, the two main quantities relevant to hotspot formation are the electric field itself (as the materials in question are typically non-magnetic), and the heat and temperature changes generated through losses in electric field energy. High electric field strengths and changes in temperature have both been shown to cause or facilitate the initiation of energetic material [3], [4]. Therefore, it is imperative that the generation of these hotspots is better understood.

The end goal of this line of research is the development of a microwave system which is capable of reliably causing initiation of energetic materials, without knowledge of the material’s exact geometry.

1.2 Motivation

The work described in this dissertation is expected to have practical relevance to improvised explosive device (IED) countermeasure development, specifically the neutralization of hidden explosives. It also develops concepts applicable to more general, cross disciplinary situations involving propagating waves and random mediums.
1.2.1 Standoff Excitation of Explosives

The primary motivation of this work is the standoff excitation of explosives, particularly homemade, sub-military grade explosives. The structures studied in this work will bear greater resemblance to these lower quality explosives than military grade explosives, which feature significantly less randomness in their geometry, while improvised explosives are commonly of this lower quality.

This work will also focus exclusively on microwave frequency sources in the range of 3 to 30 GHz. While high-frequency laser sources have shown a higher degree of reliability in reproducing initiation, microwave sources offer several distinct advantages. The microwave excitations in question are approximately 1000 times lower in frequency than the onset of the infrared portion of the frequency spectrum, allowing for larger areas of illumination. With beamwidth inversely related to the frequency of the source, Gaussian laser sources offer beamwidths in the micron range, while very high power microwave sources have been shown to possess much larger beam areas.

In addition, a wide variety of nonmetal substances are relatively transparent at microwave frequencies, while frequencies at infrared and above struggle to penetrate many common materials used in the covering or containment of explosives. This also allows microwaves to pass through these materials non-destructively, where high powered laser sources may cause heat damage and be unable to pass through coverings.

However, microwave sources are not without their drawbacks. In particular, their non-destructive interactions with and ability to pass through many materials without substantial loss comes at the cost of being an ineffective heating source. This further heightens the importance of generating the most intense hotspots possible in order to compensate for
the relatively ineffective conversion of energy, as nearly all studies suggest a correlation between source strength and the effectiveness of the excitation.

1.2.2 Creation of a Microwave System

To overcome these difficulties and fully exploit the possibility of the neutralization of energetic materials with a microwave excitation, it is necessary to gain a detailed insight into the behavior of microwaves in these mediums and their effects. Several specific challenges in understanding must be overcome to facilitate the development of a microwave neutralization system for these materials.

One challenge is the size of the inclusions in these materials relative to the wavelength of microwaves. Linear dimensions are typically on the scale of tens to hundreds of microns [5]–[8], which is far larger than wavelengths at laser frequencies, but at least an order of magnitude less than microwave wavelengths. In situations such as this, scattering effects of individual inclusions are sometimes considered negligible, and the medium as a whole defined as an effective permittivity.

The concept of effective permittivity is one possibility for characterization of a medium. However, as it has been shown that ignition locations of energetic materials is on the micron scale [5], and may be caused by behavior at even smaller scales [9], it may also be necessary to understand the behavior at the sub-inclusion level. Effective permittivity characterizations would be unable to describe behavior at these levels, as the onset of initiation is not a bulk effect. Rather, localized extremes in field and temperature over

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1In this work, the terms crystal and inclusion are used interchangeably, and refer to the pieces of higher permittivity material in our two phase composites. This is in contrast to other definitions of inclusion, which may refer to additions or impurities in a two-phase medium.
minute intervals of time and space are the triggering mechanism.

Successful development of the aforementioned microwave initiation system would augment countermeasure capabilities for IEDs. The capabilities of such a system include remote landmine disarmament and neutralization of suicide bombers. Many current methods typically require user input in close proximity of the explosive, an inherently dangerous proposition. Furthermore, a directed microwave excitation system would have little effect on non-explosive materials caught in its beam, limiting collateral damage. High strength fields may damage electronic systems, though this may have its own benefits for a neutralization system.

Application of directed energy weapons will almost certainly result in deflagration of an explosive and not in detonation, a preferable outcome. In addition, better understanding of the behavior of microwaves in these materials would assist in the study of complementary initiation mechanisms. This would benefit the development of systems which also utilize acoustic, shock, or thermal excitation systems.

1.2.3 Other Applications

At its core, this work relates to the behavior of waves in random mediums, particularly electromagnetic waves in crystalline composites. It looks at effective dielectric permittivity, electric field localization, and inducing thermal heating through EM excitation. However, the core concepts of the three investigations are effective material characterization, inclusion abstraction, and energy coupling as they relate to random mediums. These concepts also apply to similar situations where energy localization in random mediums is of interest. With the development of random or highly complex materials an active area of
research across many disciplines, application areas for these concepts is expected to greatly increase. Possible subjects include carbon fiber reinforced composites, which utilize random fibers, characterization of solid rocket fuel, buried structure demolition, as well EM characterization of nanomaterials (nanotubes, walls, stars, etc.).

1.3 Approach

In addition to being strictly regulated, experimental characterization of energetic materials is often impractical, with detailed in situ measurements usually impossible. In addition, successful initiation of the material can have destructive results. This work will focus on various simulation-based approaches capable of obtaining more detailed data. Simulation-driven methods grant the user the flexibility to define data resolutions in both space and time (within computing resource limitations). The disadvantage lies in the long runtimes required to run simulations in the detail required for the purposes of this work.

Three major investigations will be performed:

1. Characterization of effective permittivity

2. Abstraction of medium to generate EM hotspots

3. Analysis of EM-thermal coupling

For all cases, an EM representation of RDX (cyclotrimethylene trinitramine) will be used as the inclusion/energetic material of choice. When a binder is necessary, a generic form of estane will be used. Various physical properties of both these substances will be sourced from the literature.
EM simulations will be performed using Remcom’s xFDTD software, which uses the finite-difference time domain (FDTD) method [10]. FDTD has the advantage of scaling well with increased parallel computing resources relative to other methods. Thermal analysis is done via an in-house MATLAB script – developed specifically for this project – which combines the effects of dielectric heating with conductive diffusion. Structures for simulation are defined with the aid of the Bullet Physics software library [11], which is utilized in in-house C++ scripts to define the scattering structures. These structures are imported into the other programs for simulation.

1.4 Outline

The goal of this work is to determine the proper level of abstraction to capture energy localization in sub-millimeter scale granular composites, and apply those abstractions to test their validity.

Chapter 2 provides a literature review of topics indirectly related but relevant to the EM initiation of energetic materials, particularly the characterization of and various methods of simulation for EM waves in random mediums, as well as a summary of research in energetic material initiation across multiple disciplines. A brief overview of directly related topics is covered at the beginning of subsequent chapters.

Chapter 3 consists of an investigation on the effective permittivity behavior of crystalline composites that is an extension of the work of Dr. Austin Pickles [12][13]. This serves as the starting point for the abstraction of the complex scattering medium. This serves as the starting point in the search for a method of abstracting complex scattering mediums. It is widely understood that a composite mixture of inclusions with individual sizes of less
than one-twentieth of a wavelength of the EM excitation may be characterized with an effective permittivity. It is less clear whether this will allow for predictions concerning field peaking. In addition, there are many effective permittivity models. It is not clear which, if any, are adequate for the situation here. The purpose of this chapter is to first determine which effective permittivity model best applies to the composite granular structure and then to determine the peak fields that could be predicted using an effective permittivity model. The field peak fields predicted through this model may be compared to the peak fields determined from more detailed EM simulations in latter chapters. The benefits and drawbacks of the effective permittivity characterization are explored.

Several inadequacies are discovered with the effective permittivity method during the investigations performed in Chapter 3. Chapter 4 investigates the applicability of various lower level abstractions of the medium of energetic material (lower level in this case refers to a lower degree of abstraction, i.e. closer to the actual structure). The goal of this investigation is to determine the abstracted structure which provides significant advantages in setup and simulation runtimes, while maintaining the energy localization of interest. In doing so, the most effective abstraction is obtained, as is insight into the generation of hotspots.

While the abstractions of Chapter 4 appear adequate, it is necessary to test their effectiveness in the scope of a larger investigation. Chapter 5 leverages the reduced computational requirements obtained in Chapter 4 to extend the simulation. A new simulation which includes the dielectric heating of the medium is performed, in an effort to explore the coupling between multiple stress factors in the medium. This coupling requires the inclusion of a binder to allow for a reasonable degree of conduction between non-contacting inclusions. A detailed analysis of the development of thermal hotspots in the material is performed,
and possible features of interest noted.

The final Chapter ties the observations from the preceding chapters together, providing a summary and suggesting areas for improvement or further investigation.

This work establishes a method of abstraction offering substantial computational benefits while maintaining meaningful results. In addition, this method is applied to a simulation of practical value, demonstrating previously unrealized simulation capabilities.
Literature Review

2.1 Introduction

The overall goal of this work is the development of characterizations for crystalline composites and the examination of the formation of electric energy hotspots in energetic materials, towards the common goal of understanding the behavior of energetic materials under electromagnetic stress. The combination of these two pursuits is relatively uncommon. Individually however, both fields have been extensively researched. This chapter provides an overview of the progress to date in three loosely related fields: the first being the bulk electromagnetic characterization of random mediums, the second being the investigation of hotspots in random mediums, and the third being the response of energetic materials to electromagnetic (and other) stresses.
2.2 Bulk Characterization of Random Mediums

While sub-wavelength detail into the scattering of electromagnetic waves is an admirable goal for any electromagnetic simulation, it is for many applications sufficient to determine a single, or greatly reduced set of parameters which captures the behavior of interest. This is especially true in communications and sensing, where the overall power of the transmitted or reflected signal is of far greater importance than minute details of the signal's journey.

2.2.1 Effects on Communications

A significant portion of the studies of electromagnetic propagation in and through random mediums considers the degradation of radar and communications signals in a scattering medium such as the atmosphere or various forms of precipitation. Several factors make this situation relatively simple to analyze. In communications systems the desired metric is the received power at a point beyond the medium – the behavior of the wave within the medium itself is of little interest. Therefore, it is convenient to generate a bulk characterization of the medium focused solely on this metric. In addition, the majority of the mediums that hamper, but still allow the possibility for, radio communications are sparsely populated, reducing the overall complexity of the problem. Finally, the interfering medium is usually a small portion of the total channel, diminishing the impact of near-field effects.

The majority of these problems consider water as the scattering medium, the most common of which is rain or other forms of precipitation. These make for relatively sparse mediums with less than 10% fill factor even in the heaviest rainfall. These mediums also tend to be large, with a common metric being decibels of loss over a kilometer (dB/km). A
vast number of studies have been performed in this area, across a wide range of frequencies and types of precipitation. Several reviews provide a fairly comprehensive summary of the state of the field over the past half-century [14]–[16]. Most of the work has focused on statistical models which provide acceptable accuracy over a range of conditions. There has also been work performed for specific inclusion shapes, which may then be superimposed to generate results for a custom geometry [17], [18].

A second set of communications challenges in random mediums focuses on electromagnetic propagation through vegetation canopies. These have also seen analysis as a summation of discretized scatterers [19]. However, as the dominant constituent material in these mediums is water, they may be analyzed in a manner similar to the precipitation [20].

### 2.2.2 Sensing and Imaging

The study of EM propagation in random mediums also finds application in the field of remote sensing and imaging systems, which often encounter mediums with structures similar to the granular composites in this work. These include various types of soil and sand, as well as packed snow and ice. In these cases, the result of interest is the reflected or backscattered power, in order to determine the composition of the medium under investigation. It is often convenient to characterize the random medium with an effective permittivity. This may be done by Monte-Carlo simulation of many generated random mediums [21], [22], or experimental characterization[23].

Sensing with random mediums also finds application in the analysis of scatter from sea surfaces. These are often reduced to 2D problems of rough lines [24], [25] and analyze the scattering spectrum of varying levels of sea roughness in search of anomalies.
There have been some studies on the localization of EM energy in composite mediums with scales of size similar to this work [12], [26], [27]. These will be reviewed in Chapter 4. However, a larger number of investigations fall under the category of particle physics and quantum optics. Significant research has been performed in this area on the synthesis of inclusions capable of producing high levels of Surface Enhanced Raman Scattering (SERS). As the Raman scattering effect is generally weak, high field levels are required to create a detectable result. Certain geometries have long been known to produce enhanced field levels for this purpose [28], while noble metals have been shown to generate the highest level of SERS [29]. This finds application in biomedical imaging, where the effect can be incorporated into a process which greatly enhances the visibility of certain pathogens [30]. A variety of shapes have been synthesized from silver, gold and platinum which display greatly enhanced fields [31]–[35]. The most prominent among these is the hollow nanostar (HNS) [31], [35], illustrated in Figure 2.1. The combination of the geometry and material of these inclusions can result in a response many orders of magnitude greater than would be observed without their presence [30].

2.3 Excitation of Energetic Materials

Extensive work has been performed on the effects of various excitations on the initiation of energetic materials, especially impact and heat. Multiple cases of successful initiation via these sources have been documented [36], [37]. While electromagnetic have received significantly less attention, several cases of successful initiation by both microwave [2], [38] and laser sources have been recorded [3], [4].

The study of initiation mechanisms in energetic materials may be roughly categorized
Figure 2.1 Silver/Gold hollow nanostar. In medical applications, these are added to target areas to enhance response to imaging tools. From [31].
into the macroscopic (bulk), mesoscopic (inclusion), and microscopic (molecular) levels, with different effects dominating at each. Examples of the three levels of scale are presented in Figure 2.2, with the three panels showing a heating experiment for a packed sample of energetic material, an EM-thermal simulation of a collection of circular inclusions, and a molecular dynamics simulation of a single molecule of explosive material.

2.3.1 Macroscopic Investigations

At the macroscopic scale, energetic materials are often excited through heating, with the purpose of initiating explosion or deflagration. This heating can occur via conduction [39], [40], friction [41] or via an electromagnetic excitation [2], [38], [42]. Such investigations typically monitor temperatures at several points in the material. Initiation through thermal heating is typically consistent but the time to initiation is highly dependent on the heating rate, with studies having been performed for both slowly heated [40] and flash heated samples[42].

At this scale, experimental measurements are a possibility, although they are typically limited to examining the surface through thermal imaging [41], [43], or through various methods of observing the actual explosion [3], [38], [44]. Approaches using simulation may provide more details within the medium [42]. However, at this scale, simulations are inherently limited to bulk heating.

Microwave excitations have been studied at this scale, due to their ability to pass through most materials relatively unhindered, but these methods have proven to be slow [2] or unreliable [38].

Laser sources are a more popular method of excitation on account of their higher heating
Figure 2.2 Examples of structures used in previous investigations of initiation mechanisms at the macro, meso and micro-scale.
rate, as well as their interactions with individual molecules at the microscopic level. The main mechanism behind is the heating of the binder [1], as the actual energetic material itself is much more difficult to heat. Unfortunately, the low effective range and beamwidth and these lasers restricts their applicability for standoff excitation. Typical experiments are limited to ranges of a few centimeters or less [45], or requiring the use of systems of mirrors and lenses too focus the beam at the surface of the material [3], [4], [46], limiting their potential for use in real world applications.

2.3.2 Mesoscopic Investigations

Relative to the other scales, it is difficult to obtain a full picture of the situation from a mesoscopic investigation. A macroscopic perspective offers easy access to experimental results, and while these experiments may run over many periods at the excitation frequency, the duration in real time is short. At the opposite end of the spectrum, the very small scale of the microscopic study allows for an in-depth analysis of molecular dynamics or even quantum effects, with a wide range of commercial tools available. However, the mesoscopic situation may help develop understanding the interactions between inclusions, which is not possible at the other two scales.

Investigations at this scale have been limited to simulations. While measurements at this scale are more feasible than at the molecular level, performing them in an energetic material is less so. Brown et. al performed an extensive thermal analysis of the laser heating of RDX, including the effects of dielectric heating with other stress factors [47]. Among other things, it was determined that the consideration of smaller inclusions resulted in less uniform distributions of temperature and stress, as well as higher peak values of both.
Pickles et al. examined the structure from an effective permittivity perspective [12], [26]. However, they observed high levels of deep sub-wavelength field localizations in composite mediums. Localizations at a scale of one-hundredth the free space wavelength have been determined in simulation. Perry et al. also examined the EM induced thermal behavior in energetic composites, observing ignition points on the sub-inclusion scale[5].

2.3.3 Microscopic Investigations

Studies at the microscopic level are typically performed from a quantum chemistry perspective. Similar to the mesoscopic studies, microscopic investigations are entirely done in simulation. The main features of interest here are the covalent bonds between the molecules’ constituent atoms, which break to begin the initiation of the energetic material. Temperature and impact shock are essentially constant over these scales – variation exists in the electric potentials and chemical properties. A typical excitation mechanism is the dropping of the molecule from a height [48].

It may also be the case that multiple types of excitation are coupled, their compounded effects likelihood of initiation to a greater degree than the sum of the individuals. Multiple investigations have explored the relation between impact initiation and the temperature of the energetic material [49], [50]. The general consensus is that the stress from either the impact or thermal energy can increase the energetic materials sensitivity to another stressor. In short, the different excitations work together to induce activity in the material.

Work by Murray and Politzer has also raised the possibility of a relationship between electric potentials and the sensitivity of explosives to impact, noting that high potential differences corresponded to increased sensitivity, possibly through a weakening of bonds
Such investigations are performed from a chemistry perspective, focusing on inherent potential differences due to charge imbalances. However, it may be possible to induce similar charge balances through an external source.

Work by Wood et al. has investigated the increase in energy of energetic materials due to electromagnetic excitation. They found that frequencies corresponding to the resonant modes were the most efficient at initiating decomposition of the material, though the electromagnetic excitation has a positive effect on decomposition regardless of frequency.

An overarching theme among these microscopic level studies is the importance of hotspots in the initiation process. These various stresses (impact, heat, electric potentials, bond weakness) are not universally present or equal throughout the medium. For these effects to compound, their areas of influence need to overlap. The hotspot sizes of these stresses, can vary greatly, from the sub-molecular scale of the chemical bond to the much larger impact shock area caused by a drop.

2.4 Summary

A significant amount of investigation has been performed concerning electromagnetic waves in random mediums, as well as the excitation of energetic materials with external stimuli. Still, extensive opportunities for further investigation remain.

Investigations regarding the bulk characterization of electromagnetic fields in random mediums have generally focused on the backscattered or transmitted powers. In addition, the mediums under investigation typically are of extremely low (rain, foliage) or high (soil, snow, ice) filling factors.
The studies in electric field localization have focused on nanoscale particles and corresponding frequencies, searching for ways to maximize SERS. They are typically performed a semi-classical or quantum perspective, while the methods in this work operate from an entirely classical perspective. In addition, while these SERS studies seek to synthesize a structure to maximize fields, this work seeks to better abstract existing structures which display peak fields.

Regarding the excitation of energetic materials, there exist many studies at the macroscopic and microscopic scales. There is, however, a lack of studies at the mesoscopic levels, while those that exist employ significant simplifications or assumptions. While the smaller and larger scales have their merits, it is at this intermediate level where external microwave fields should localize, and therefore at this level which this work must operate.

Previous studies in this mesoscopic range display limitations when applied to the situation of interest – the mechanisms which cause microwaves to localize in energetic materials and the effects of these localizations. This work will seek to address some of these limitations. Pickles et al. were able to observe field localization within simulation, but did not perform any extensive analysis of the phenomenon, instead focusing on effective permittivity [12]. Brown et al. used high-frequency lasers, and limited the simulation to two-dimensions [47]. Perry et al. also limited their simulation to two-dimensional, and created a medium of circular inclusions in a configuration designed for periodicity [5]. Kort Kamp et al. created a detailed reproduction of an actual explosive sample through the use of CT scans, but this requires significant additional hardware and software, as well as an actual explosive sample for each simulation [27].

This dissertation reports on research into the individual peak electric fields from mi-
crowave excitation using three dimensional full-wave electromagnetic simulations. The mediums will be generated with randomized, physics based procedures, limiting the level of bias possible in their structure. Finally, unlike all aforementioned studies, this work will perform a much higher number of simulations to generate statistics across many runs. This will be facilitated by the creation of abstraction levels which reduce computational complexity.
Effective Permittivity

3.1 Introduction

In Chapter 1, the problem of the excitation of a granular composite medium by an EM wave was introduced. The major complication in the analysis of this situation is the large number of inclusions, each with its own contribution to the scattering of the incident wave, making an exhaustive analysis extremely time-consuming. To conserve time, studies may be limited to few realizations of the random medium, limiting confidence in the results. The development of a simplified model of the structure which retains the relevant scattering behavior would greatly increase rate at which simulations may be performed, resulting in faster development of insight into the phenomenon.

This chapter explores the possible characterization of energetic materials via calculations of effective permittivity. Effective permittivity presents an appealing solution for the analysis of complex scattering mediums. The possibility of describing the entire medium with a single parameter greatly simplifies or even trivializes the calculations and simu-
lations required. While presenting clear drawbacks – this solitary value cannot possibly encapsulate all the information of value – effective permittivity methods have nonetheless remained popular since the first studies of EM propagation through random mediums.

To facilitate the characterization of scattering mediums with an effective permittivity, a variety of experimental, theoretical, and simulational investigations have been performed regarding the matter. Since the final result is to be condensed to a single value, abstracting the medium is a logical intermediary step. Many abstractions have been attempted, ranging from the relatively high–level models involving slabs [53] and cylinders, to relatively lower level attempts with spheres [54] and dipoles [55].

Another possible tradeoff that can be made regards the number of dimensions considered in the problem. The aforementioned slab and cylinder abstractions reduce the dimensionality of the problem to some degree, but still involve analysis in three dimensions. However, extensive analysis has been performed at the 2-dimensional level, with studies leveraging the simplicity offered by rough surfaces [56] and circles [57]. Even 1-dimensional analyses of certain surfaces have proven informative [58].

In this investigation, various abstractions will be investigated. Focus will mainly be placed on lower levels of abstractions, which retain details at the inclusion scale, such as collections of spheres and cubes. In addition, this portion of the investigation will prove useful as a comparison and generate motivation for the later sections. While the effective permittivity of the medium is incapable of providing details about positions of field localization, there may be some correlation between the effective permittivity predicted for a certain structure and its propensity for localizing electric fields.
3.2 Established Effective Medium Approximations

Among the many studies which utilize effective mediums, several effective medium theories or mixing models are commonly utilized. While not as well-suited for specific mediums as customized models, these general models often serve as an initial estimate, or a standard of comparison for a customized model. Whereas customized models often rely on numerical fitting of empirical data, these standard models are derived theoretically. The models in this section will prove valuable for comparison and validation of results.

3.2.1 Maxwell-Garnett Effective Medium Approximation

The Maxwell-Garnett approximation estimates the effective permittivity of a two-phase composite medium as

\[
\varepsilon_{\text{eff}} = \varepsilon_2 + \frac{3q_v \varepsilon_1 - \varepsilon_2}{\varepsilon_1 + 2\varepsilon_2 - q_v (\varepsilon_1 - \varepsilon_2)}
\]  

(3.1)

where \(\varepsilon_1\) is the permittivity of the inclusion material, \(\varepsilon_2\) is the permittivity of the surrounding matrix, \(q_v\) is the fill factor of the inclusions, and \(\varepsilon_{\text{eff}}\) is the approximated effective permittivity of the matrix. The Maxwell-Garnett approximation can be derived from a combination of the Clausius–Mossotti relation and the electrostatic analysis of a polarized sphere [60]. As such, it inherits the limitations of both. The Clausius–Mossotti relation limits the structure of the medium to one that is relatively sparse, such that the local-field effects from individual scatterers have little effect on other scatterers, while the spherical electrostatic analysis limits the inclusion shape to spheres. It is generally accepted that in the majority of naturally occurring mediums, the Maxwell-Garnett approximation remains reasonably accurate up
to a fill factor of approximately 35%, around the percolation threshold\(^1\) for a medium of spheres [61]. This upper bound of this range sits at approximately the fill factor of interest.

### 3.2.2 Bruggeman's Model

A second effective medium model is that of Bruggeman. In its two-phase form it is [62]

\[
q_1 \frac{\epsilon_1 - \epsilon_{\text{eff}}}{\epsilon_1 + 2\epsilon_{\text{eff}}} + q_2 \frac{\epsilon_2 - \epsilon_{\text{eff}}}{\epsilon_2 + 2\epsilon_{\text{eff}}} = 0
\]

(3.2)

In Equation (3.2), \(\epsilon_1\) and \(\epsilon_2\) are the permittivities of the medium's constituent materials, and \(q_1\) and \(q_2\) their respective fill factors. Unlike the Maxwell-Garnett approximation, Bruggeman's model does not require the identification of a specific material as the inclusion, and the other as the matrix. The matrix and inclusions are homogenized and treated as a whole in the derivation, making the Bruggeman model perhaps a better embodiment of the effective medium concept.

The Bruggeman model has the advantage of being extendable to mediums with more than two phases by appending additional terms, as well as being more accommodating of shapes. It has also been reported to remain accurate to slightly higher fill factors, up to 50%, comfortably above that of our structure of interest [62]. However, the homogenization technique used is still limited to ellipsoidal shapes.

---

\(^1\)Percolation refers to the tendency of long chains of connected inclusions to appear in a medium of randomly distributed inclusions as the filling factor is increased. Above the threshold, the presence of such chains is likely.
3.2.3 Wiener Bounds

The Wiener bounds set the upper and lower limit on the conductivity ($\sigma$) of a random composite medium. Perhaps not technically an effective medium theory, the bounds still provide a starting point and range for possible values of effective permittivity. Both bounding structures are composed of slabs of material rather than inclusions. The upper limit on conductivity is the case of slabs aligned parallel to the propagation direction of the wave, illustrated in Figure 3.1. At the opposing end of the spectrum, the case of slabs aligned perpendicular to the direction of propagation presents the lowest possible conductivity.

One analogy for this behavior is a comparison to a set of connected resistors. The slabs in the maximum conductivity configuration are analogous to a set of resistors in parallel, where all the excitation has a direct path via the material of greatest conductance (lowest value resistor). The overall conductivity is dominated by the most conductive element. Similarly the minimum conductivity configuration is analogous to a set of resistors in series. The excitation must always pass through the least conductive element (highest value resistor). The overall resistance is therefore dominated by the most resistive element.

The conductivity expressions for these bounds take a form similar to those of the resistive networks, and for a two-phase composite is given by [53]

$$\frac{1}{\sum_{n=1}^{2} \frac{q_n}{\sigma_n}} \leq \sigma_{\text{eff}} \leq \sum_{n=1}^{2} q_n \sigma_n$$  \hspace{1cm} (3.3)

It is apparent from the form of both bounds in Equation 3.3 that, as with Bruggeman’s model, it is not necessary to designate a material as the inclusion or as the binder. A conversion from conductivity to permittivity is relatively straightforward and results in [53]
Figure 3.1 Wiener Bounds, maximum and minimum conductivity examples, the direction of the arrow represents the direction of the propagation of the excitation wave, $+x$. 
\[
\epsilon_{\text{max}} = q_v \epsilon_1 + (1 - q_v) \epsilon_2 \geq \epsilon_{\text{eff}} \geq \epsilon_{\text{min}} = \frac{\epsilon_1 \epsilon_2}{q_v \epsilon_2 + (1 - q_v) \epsilon_1} \] (3.4)

Though these bounds are admittedly coarse, they provide a first step sanity check for any results produced.

### 3.2.4 Hashin-Shtrikman Bounds

A more comprehensive and relevant set of bounds can be found in the work of Hashin and Shtrikman [63]. These bounds are derived from a structure of tightly packed spherical inclusions of varying size, and always fall between the Wiener Bounds, that is, the minimum Hashin-Shtrikman (HS) bound is higher than the minimum Wiener Bound while the maximum HS bound is lower than the maximum Wiener Bound. The theory behind the HS bounds is not unique to the study of effective permittivity and is applicable to the characterization of any form of wave propagation through a composite medium. The derivation is significantly more involved than the models of previous sections – their final form with regard to effective permittivity is given by [63]

\[
\left[ \epsilon_{\text{min}} = \epsilon_1 + \frac{q_v}{\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2}} + \frac{1 - q_v}{3 \epsilon_1} \right] \leq \epsilon_{\text{eff}} \leq \left[ \epsilon_{\text{max}} = \epsilon_2 + \frac{1 - q_v}{\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1}} + \frac{q_v}{3 \epsilon_2} \right] \] (3.5)

It should be noted that unlike those of the Wiener bounds, the forms of the minimum and maximum HS bounds are symmetric. Which bounds are actually the minimum and maximum is determined by the relative permittivities of the materials. That is, the \( \epsilon_{\text{min}} \) of Equation 3.5 may actually be higher than \( \epsilon_{\text{max}} \) if \( \epsilon_1 \) is greater than \( \epsilon_2 \). In this case, it is assumed that the inclusion has the higher permittivity, as the binding matrix is taken as
vacuum for the first portion of this work.

In practice, these bounds are in fact the Maxwell-Garnett approximation and its complement (with the materials properties of the inclusion and matrix switched). However, the difference in their origin warrants the HS bounds their own mention. This also constrains the effectiveness of the HS bounds to the same range of filling factors as the Maxwell-Garnett approximation.

### 3.2.5 Section Summary

Several theories which predict the effective permittivity of a composite medium have been presented. These models share the advantage of generating a closed form solution with three known or easily determined input variables: the two constituent permittivities and the inclusion fill factor. However, each theory also makes assumptions which simplifies the problem to a certain degree. The use of approximations in these models, and the resulting simplicity of the formulas, limits their overall accuracy. The extent to which accuracy is compromised must be weighed against the savings in time when judging the efficacy of these models.

### 3.3 Preliminary Estimates

Before the simulation of any specific structures, it is informative to apply the models of Section 3.2 using the general properties of the energetic material of interest. Equations 3.2, 3.4 and 3.5 were evaluated for a medium of RDX inclusions \((\varepsilon_r = 3.5 + j0.003)\) [42]. Throughout this section, the binder will be simulated as vacuum \((\varepsilon_r = 1)\). The Maxwell-
Garnett approximation is omitted, as the inclusion of the HS Bounds makes it redundant. Fill factor ranges from 0% to 50%. The resulting plot is presented in Figure 3.2.

**Figure 3.2** Preliminary estimates of effective permittivity from various models and approximations over range of filling factors from 0 to 50%. The Bruggeman model is calculated from Eqn. 3.2, the Wiener Bounds calculated from Equation 3.4, and the HS Bounds from Equation 3.5.

The curves behave as expected, with the Wiener bounds forming the widest range, the HS bounds slightly more constrained, and the Bruggeman model estimating the effective
permittivity between the two sets of bounds. At the fill factor of interest, approximately 30%, the effective relative permittivity ($\epsilon_{r,\text{eff}}$) predicted by the models are, based on the order in Figure 3.2, 1.570, 1.840, 1.284, 1.684, and 1.508, for the Bruggeman, upper Wiener bound, lower Wiener bound, upper HS bound and lower HS bound, respectively. The Wiener bounds show a difference between the upper and lower bounds of up to over 40% for various structures with the same filling factor, while the HS bounds only vary by about 6.5%. However, as mentioned in Section 3.2, a 30% fill factor is at the upper end of the reliability range for the HS model. Using the quadratic relation between field magnitude and power, a first order analysis suggests that with field magnitudes over the Wiener bounds differing by 40%, the bound on the field power would differ by 100%. This is due to the fact that the slabs facing the direction of propagation reflect the incoming wave much more effectively, an intuitive result. However, neither of these cases are very representative of the granular composite being examined here. The most appropriate range would be between the Bruggeman model and the Maxwell-Garnett Approximation, as these models are meant to model mediums of many inclusions evenly dispersed and relatively similar in size. This range is much lower, at less than 5%.

### 3.4 Method

The permittivity of a material is typically determined through an evaluation of its interactions with electric fields. In an experimental process, it is conveniently evaluated using a “Capacitor Method”, where the random medium is used as the dielectric in a parallel plate capacitor between two conducting sheets. The capacitance of the system is evaluated and the effective dielectric constant determined. Useful for experimentation, this method
is unnecessarily tedious for use with simulations. Here, the effective permittivity will be
determined via a waveguide method, which considers the propagation characteristics of
an EM wave propagating through the medium to determine its properties.

### 3.4.1 Simulation Setup

The simulation setup is shown in Figure 3.3. The setup resembles a waveguide, with ports
(outlined in green) in the $x$ $y$ axes at $z=0$ (Port 1) and $z=1.1$ mm (Port 2). The waveguide
measures 1.05 mm in the $x$ direction and 1.13 mm in the $y$ direction. The body of the
waveguide is bounded by electric walls at the $y$ limits and magnetic walls at the $x$ limits.
This effectively mirrors the channel in the $x$ and $y$ directions. The scattering medium,
shown here in red, is replaced by various abstractions which will be described in Section
3.4.3. A sinusoidal EM excitation centered at 15 GHz is introduced at Port 1, with transmitted
power recorded at Port 2, in the form of the transmission scattering parameter $S_{21}$.

### 3.4.2 Computing Resources

All simulations described in this chapter are performed using the commercial finite differ-
ence time domain software xFDTD from Remcom Inc. The software runs on a Dell Precision
7810 with 16 physical cores and 172 GB of memory. The actual timestepping process is per-
formed on two Nvidia K20 Tesla GPUs each with 5 GB of memory, although only one of the
GPU accelerators at a time is utilized/necessary for any of the simulations in this chapter.
Codes for generating the simulation structures are written in JavaScript, see Appendix A.
Conversion of S-parameter data to effective permittivity values is performed in MATLAB,
see Appendix B.
3.4.3 Types of Composite Mediums Used

The types of inclusions used in the effective permittivity study to comprise the scattering medium are outlined in Figure 3.4. Cubes have been previously identified as displaying in higher levels of field localization [12], they are compared to a classical study which uses spherical inclusions as in [5]. While cubes in Figure 3.4(c) are aligned to the Cartesian axes, this is solely to maintain clarity in the image. The medium of cubic inclusions will primarily be simulated with the cubes rotated about their centerpoints. This process will be outlined later in this section. Mediums composed of evenly spaced slabs of material are included as part of the verification process, as these are the structures considered in developing the bounds with the strongest theoretical foundation. The effective permittivities extracted
from these structures are compared to the Wiener bound of Equation 3.4.

Several other structures are simulated in addition to the ones shown. The simulation of the slabs parallel to the direction of propagation, see Figure 3.4, is performed for both the case of slabs aligned with and perpendicular to the polarization of the excitation signal. In addition, the structure of cubes includes a modification where the cubes are rotated around their individual center points.

3.4.4 Generation of a Composite Medium

The graphical editing tools provided by Remcom in the xFDTD program focus on complex, single element geometries, and are inefficient at generating structures comprised of many inclusions such as the ones studied here. While the mediums comprised of slabs are handled in xFDTD, it is necessary to generate the structures with many inclusions separately, using Javascript codes, and then imported to xFDTD as a data file. The structures in this chapter are not as complex as those in later chapters, and are less difficult to generate, since the inclusions are placed on a regular grid. This is convenient for the purposes of the FDTD method; the only difficulty is the number of inclusions which needed to be created.

The process of placing the inclusions is straightforward. The inclusion centerpoints are spaced 160 µm apart. The geometry of the inclusion, which is uniform across the medium, is defined as the radius \( r \) for spheres, and the three orthogonal linear dimensions of \( l, w, h \) for cuboids. For each individual inclusion, an \( x y z \) origin was recorded. Finally, for inclusions which are rotated, a rotation matrix is randomly generated and recorded as well. These 3 data elements are read into xFDTD, and used to generate the inclusions to populate the medium.
Figure 3.4 Simulation structure examples.
<table>
<thead>
<tr>
<th>Fill Factor (%)</th>
<th>Cube Side Length (µm)</th>
<th>Sphere Radius (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4</td>
<td>58.94</td>
<td>73.15</td>
</tr>
<tr>
<td>6.8</td>
<td>74.27</td>
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</tr>
<tr>
<td>13.6</td>
<td>93.57</td>
<td>116.12</td>
</tr>
<tr>
<td>17.0</td>
<td>100.79</td>
<td>125.09</td>
</tr>
<tr>
<td>20.4</td>
<td>107.11</td>
<td>132.93</td>
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<td>152.17</td>
</tr>
<tr>
<td>34.0</td>
<td>126.99</td>
<td>157.61</td>
</tr>
</tbody>
</table>

**Figure 3.5** Inclusion dimensions for the medium of cubic inclusions and medium of spherical inclusions described in Figure 3.4 across range of fill factors from 0–34%

To modify the fill factor of the mediums, the size of the individual inclusions is scaled, rather than modifying the number of inclusions in the medium. For slabs, the thickness is scaled, while the radius is adjusted for spheres, and the edge length of the cubes is scaled by the same factor in all dimensions. The specific dimensions of the inclusions are outlined in Tables 3.5 and 3.6.

### 3.4.5 Extraction of Effective Permittivity from Scattering Parameters

Smith et al. created a method, derived from transmission line theory, for extracting the effective permittivity of a (composite) medium [64]. Similar methods have been developed and used by others [65]. These methods are extensions of solutions to boundary condition wave problems, with the added consideration of propagation loss. The function used to
<table>
<thead>
<tr>
<th>Fill Factor (%)</th>
<th>$x$–oriented ($\mu$m)</th>
<th>$y$–oriented ($\mu$m)</th>
<th>$z$–oriented ($\mu$m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
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<td>9.2</td>
<td>9.4</td>
</tr>
<tr>
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<td>26.25</td>
<td>27.5</td>
<td>28.3</td>
</tr>
<tr>
<td>20</td>
<td>35.0</td>
<td>36.7</td>
<td>37.7</td>
</tr>
<tr>
<td>25</td>
<td>43.75</td>
<td>45.8</td>
<td>47.1</td>
</tr>
<tr>
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<td>52.5</td>
<td>55.0</td>
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</tr>
<tr>
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<td>61.25</td>
<td>64.2</td>
<td>65.9</td>
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<td>82.5</td>
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<tr>
<td>50</td>
<td>87.5</td>
<td>91.7</td>
<td>94.2</td>
</tr>
</tbody>
</table>

**Figure 3.6** Slab thickness for the composite mediums of Figure 3.7. In all cases, six slabs in total are evenly spaced in the medium.

determine $\epsilon_{\text{eff}}$ from $S_{21}$ is given by Equation (3.6) as [65]

$$ F = S_{21} \ast (1 - R^2 e^{-2 j k d \sqrt{\epsilon_{\text{eff}}}}) - (1 - R^2) e^{-2 j k d \sqrt{\epsilon_{\text{eff}}}}; \quad (3.6) $$

where $F$ is the function to be minimized (ideally 0)

$$ R = \frac{Z - 1}{Z + 1}, \quad Z = \frac{1}{\sqrt{\epsilon_{\text{eff}}}} \quad (3.7) $$

$k$ is the wavenumber in free space and $d$ is the length of the medium in the direction of the propagation. Given $S_{21}$, the system can be solved iteratively for $\epsilon_{\text{eff}}$. In this case, a generic Newton's method solver is implemented in MATLAB, see Appendix B. The system is well-behaved and converges predictably, typically in around 7500 iterations for an absolute accuracy of $F \leq 10^{-8}$, with an initial guess of $\epsilon_{\text{eff}} = 1$. 
3.4.6 Section Summary

The methods described in this section may be summarized as follows:

1. A general framework shared by mediums of all inclusion types is generated. This includes the creation of a waveguide-like simulation structure in Xfdtd which measures the transmission scattering parameter $S_{21}$. An accompanying MATLAB script which extracts the effective permittivity from $S_{21}$ is also created.

2. Next, a set of scripts for generating the randomized inclusion positions and orientations within the waveguide is written in JavaScript, along with accompanying scripts for the export and generation of this structure in xfdtd.

3. Finally, various parameters are defined, which will be used in the random generation script to create the individual scattering mediums.

3.5 Results

Based on the methods outlined in Section 3.4, effective permittivity extractions are performed on the structures described in 3.4.3. Composite mediums of three types of inclusions will be simulated across a range of filling factors, those of aligned slabs, of spheres, and of randomly rotated cuboids. Several other mediums are simulated at the filling factor of interest, 30%. The estimations provided by the various structures are compared with each other and the values predicted by the models of Section 3.2.
3.5.1 Slabs

Three different structures comprised of RDX slabs are simulated. The first is the structure shown in Figure 3.4(a), where the slabs are in the $x$–$y$ plane. This will henceforth be referred to as $z$–oriented. The other 2 structures resemble that shown in Figure 3.4.(b). The structures with slabs in the $x$–$z$ plane and $y$–$z$ plane will be referred to as $y$–oriented and $x$–oriented, respectively. The $y$–oriented slabs align with the polarization of the waveport, while the $x$–oriented slabs are perpendicular to the polarization. Figure 3.7 shows the effective permittivity values extracted from the recorded values of $S_{21}$ for each of these 3 cases. The Wiener bounds which they should correspond to are shown for comparison.

The effective relative permittivity across the fill factor range extracted from the simulations increases from 1–1.89, 1–1.53 and 1–2.27 for the $x$–oriented, $y$–oriented, and $z$–oriented slabs, respectively. This is compared to maximum values of 1.583 and 2.40 for the analytical bounds. A good agreement is observed between the $z$–oriented slab structure and the upper Wiener bound, as well as between the $y$–oriented slabs and the lower Wiener bound. The $x$–oriented slabs fall in between, closer to the upper bound, although the 50% point drops closer to the middle of the bounds. Figure 3.8 shows a second order polynomial fit of the $y$– and $z$–oriented slabs, and relative error of these fits to the Wiener bounds. The agreement between the two is confirmed, with relative errors of less than 6% over the entire fill factor range for both fits. These small discrepancies may be attributed imperfect periodicity of the boundary conditions caused by cross polarization generated in the scattering process, limiting the effectiveness of the periodic boundary conditions at emulating an infinite space.

Overall, the excellent agreement between the simulation results and theoretical bounds
Figure 3.7 Extracted permittivities from simulation of slab structures with $x$, $y$ and $z$ orientation, as described in Section 3.5.1. Filling factor varied at 10 evenly spaced points between 0 and 50%. Maximum and minimum Wiener bounds from Eqn. 3.4 included for comparison.
Figure 3.8 Extracted permittivities: (a) Best fit lines for the extracted permittivities of the $y$– and $z$–oriented slabs plotted in Fig. 3.7. Wiener Bounds included for comparison (b) Relative error between the best fit lines and the Wiener Bounds. $z$–oriented slabs are compared to the maximum bound, while $y$–oriented slabs are compared to the minimum.
confers greater confidence in our simulation and parameter extraction process. The $x$ oriented slabs are of passing interest. The case is generally ignored, as the Wiener bounds were initially derived for two dimensional structures, and its addition in three dimensions contributes nothing to the bounds.

### 3.5.2 Spheres

The second structure considered is that of 3.4(c) where the composite medium is comprised of spherical inclusions. The calculated effective permittivities are plotted in Figure 3.9, with the HS-bounds included for comparison.

Figure 3.9 remains between the HS-Bounds for the of the duration, with the effective relativity permittivity increasing from 1.05–1.65 over a fill factor of 0–34%. The extracted permittivity at the low volume fractions closely follows the minimum HS-bound up until around 10%, where the simulated value gradually rise to a vary between the two bounds. By the final point at 34%, the extracted permittivity sits squarely between the maximum and minimum HS-bounds.

### 3.5.3 Randomly Rotated Cubes

The cubic structure of Figure 3.4(d) is modified by rotating the cubes around their origins. A random rotation between 0 and $2\pi$ rotation is performed around each of the $x, y$ and $z$–axes. The calculated effective permittivities are plotted in Figure 3.10, with each plot marker representing an averaged effective permittivity estimate over 5 individual random runs. The individual runs showed very little variation in the effective permittivity estimates, varying no more than .3% from the averaged value. The HS-bounds are once again plotted...
Figure 3.9 Extracted relative effective permittivity for a medium with inclusions comprised of randomly positioned spheres created with the method described in Section 3.4.4, with filling factors at 10 evenly spaced points between 0 and 34%. The HS bounds are plotted between 0 and 50% for comparison.
It is observed that the extracted effective permittivity of the rotated cubes closely resembles that of the lower HS-bound, or Maxwell-Garnett approximation. As is shown in Fig. 3.11, the difference between the cubic and the MGA is less than 1% across the filling factor range of 0 to 34%.

Comparing the simulated permittivities of the sphere in cube mediums in Figure 3.11, the cubic medium is within 1% of the Maxwell-Garnett approximation, while the spherical medium is within 4%. The cubic medium is consistently a few percent higher than the spherical medium. Based on the nature of the approximation, the spherical medium would be expected to have the better agreement. However, from an effective medium perspective, it appears that the rotated cubes follow the Maxwell-Garnett approximation better than do the spheres assumed in its derivation. This may be caused by geometry of the spheres forcing them closer together, reducing the validity of the local field analysis performed in the Maxwell-Garnett approximation. A sphere of diameter $d$ occupies approximately half the volume of a cube with the same side length. In addition, scattering from the spheres is more prone to generating cross-polarization, which the particular simulation structure used is ill-equipped to handle. Thus, while the spherical inclusions are the ones used in the derivation of the model, they may reach the percolation threshold, and inaccuracy associated with it, more quickly. The very good agreement shown by the cubic inclusions suggests that there may be little to no difference between the spheres and cubes from an effective permittivity standpoint, they simply push the limits of the model at different fill factors.
Figure 3.10 Extracted relative effective permittivity for a medium with inclusions comprised of randomly rotated cubes created with the method described in Section 3.4.4, with filling factors at 10 evenly spaced points between 0 and 34%. Individual plot points are average values from 5 separate random runs. The HS bounds are plotted between 0 and 50% for comparison.
Figure 3.11 Comparison of extracted permittivities of medium comprised of cubic inclusions from Fig. 3.10, medium comprised of spherical inclusions from Fig. 3.9, and Maxwell-Garnett approximation from Eqn. 3.1.
3.5.4 Overview of Other Structures

Although not simulated at the level of detail of the previous sections, several other cases are examined at a fill factor of 30%. These are the non-rotated cube structure of Figure 3.4d, as well as composites of one large spherical or cubical inclusion. The extracted effective permittivities of these cases, along with those already presented, are given in Table 3.1.

Table 3.1 Extracted effective permittivity values for expanded set of structures, simulated with a filling factor of 30%.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$\epsilon_{r,\text{eff}}$</th>
<th>Approximation</th>
<th>$\epsilon_{r,\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubes, regular</td>
<td>1.31</td>
<td>Slabs x</td>
<td>1.65</td>
</tr>
<tr>
<td>Cubes, rotated</td>
<td>1.50</td>
<td>Slabs y</td>
<td>1.27</td>
</tr>
<tr>
<td>Spheres</td>
<td>1.57</td>
<td>Slabs z</td>
<td>1.79</td>
</tr>
<tr>
<td>Single Cube</td>
<td>1.49</td>
<td>Maxwell-Garnett</td>
<td>1.51</td>
</tr>
<tr>
<td>Single Sphere</td>
<td>1.29</td>
<td>Bruggeman</td>
<td>1.57</td>
</tr>
</tbody>
</table>

It is apparent that the structures not comprised of slabs show similar effective permittivities. The regular cubes and single sphere show similar properties close to the lower bound, while rotated cubes, spheres, and single cube show properties close to that of the Maxwell-Garnett Approximation. The non-slab structures show permittivities in the lower half of the range predicted by the Wiener bounds ($\epsilon_r \leq 1.53$). The sole exception is the medium of spheres, with an relative effective permittivity of $\epsilon_r = 1.57$. There is more variation across the entire range of cases than between the cubes of Section 3.5.3 and the spheres of Section 3.5.2. However, this mostly caused by the overly simplistic cases (single sphere, regular cubes) displaying low effective permittivities. The case of the regular cubes in particular
may be thought of as analogous to the lower Wiener bound, as the path of least resistance always exists.

### 3.5.5 Section Summary

In this section, composite mediums of various inclusion types were used as a dielectric filling in a waveguide simulation. From the scattering parameters obtained in these simulations, the effective permittivities of these mediums was determined with an iterative method. The slab-like structures used in the derivation of the Wiener bounds showed good agreement with the theory, providing validation for the accuracy of the method used. Mediums of spheres and randomly rotated cubes were swept over a range of filling factors. Variations between the evaluated permittivities shown by these two types of mediums was small, with relative variations less than 5%. This is in contrast to previous investigations showing significant differences in their scattering behavior. A wider range of structures was simulated at a filling factor of 30%. Slightly more variation was observed. However, this variation was in the direction of lower effective permittivities, which goes against the objective of generating high peak field values in the simulation.

### 3.6 Chapter Summary

In this chapter, the effective permittivity properties of a composite medium of RDX and vacuum were examined. Multiple structures were simulated at a wide range of fill factors, while several additional structures were examined at the fill of factor of greatest interest (30%). A waveguide like simulation space was used to record transmitted power via the
scattering parameter $S_{21}$. A function derived from basic concepts of wave propagation and reflection at interfaces was then used to extract the effective permittivity from the recorded data.

An initial evaluation of several established effective permittivity approximations suggested potential permittivity/field variations greater than 40% over the range of possible structures of composite mediums. The more conservative Hashin-Shtrikman bounds placed the limit on permittivity variation at less than 7%.

In an effort to validate the simulation and parameter calculation methods proposed, the slab-like structures which defined the Wiener bounds were simulated. Excellent agreement was achieved between the theoretical bounds and the values extracted from the recorded data, increasing confidence to proceeding with the method.

Attention then shifted to structures comprised of individual inclusions. The first structure examined was one comprised of spherical inclusions. Ideally, this should closely follow the Maxwell-Garnett approximation. However, the simulated permittivities were consistently slightly higher than the approximation. This may be due to the percolation of the spheres, resulting in larger “clumping” of particles than the approximation expects.

The next structure simulated was comprised of cubes. It showed improved agreement with the Maxwell Garnett Approximation with permittivities slightly lower than that of the spherical case. Overall, it appears that the cubes behave similarly to the spheres at the medium level.

Simulations for several addition cases were performed at fill factor of 30%, the frequency of greatest interest in the study of homemade explosives. It was found that variation across the range of structures was small, and that all the mediums examined were much more
prone to follow the lower HS bound than any of the other models. The Maxwell-Garnett model, Bruggeman model and the structures of spheres and rotated cubes all predicted effective relative permittivities of around 1.5. Using 1.5 as the effective relative permittivity of the medium, a normally incident plane wave would transmit 80.8% of its power into the medium, resulting in a peak field within the medium of .899 that of the incident wave.

### 3.7 Conclusion

A comprehensive examination of various forms of composite mediums was performed. While effective permittivity varied substantially over various composite structures with the same fill factor, mediums comprised of many individual inclusions showed very little variation. None of the previously observed field localizations are explainable or suggested in any way through an examination of effective permittivity.

It appears that established models do a reasonable job of estimating the effective permittivity. However, the lack of discernible difference in the effective properties of spheres and cubes is surprising, given previous investigations into the subject. Due to their ability to maintain higher volume fractions while avoiding percolation, cubes may present a superior option for a generic inclusion shape, especially for any studies utilizing finite-difference simulation.

Further investigations at the inclusion are necessary and will be the focus of the following chapters. However, the work in this chapter does provide confidence in our simulation method, and also provides higher-level insight into the behavior of EM waves in various forms of composite mediums. Even if behavior at the inclusion scale is vastly different, this does not necessarily translate to large variations in total reflected or received power in a
channel.
Chapter 4

Abstraction of Inclusions

4.1 Introduction

In Chapter 3, the effective permittivities of mediums populated by various types of inclusions was examined. It does not appear that the characterization of the composite mediums of interest with an effective permittivity is adequate to describe the electromagnetic behavior within. The structures showed very little variation overall, in contrast to previous investigations \[12\].

The motivation behind the investigation into the use of an effective permittivity characterization was the potential reduction in the computational complexity required compared to the exhaustive simulation of a realistic granular structure, as well as circumvention of the difficulty of mapping an exact structure to a simulation environment. However, the effective permittivity concept does not provide an adequate characterization of field localization. A possible solution may lie somewhere between the two extremes. The effective permittivity method virtually erases the impact of any inclusion scale geometries, while an
exact recreation levies an exorbitant computational cost in maintaining every feature.

Field localization in a granular medium is the result of multiple scattering events and in particular scattering by sub-wavelength scale inclusions, and so at least some geometry at these scales must be preserved. A lower level abstraction of the medium would allow for reduced strain on computing resources, while selectively retaining certain characteristics of the medium which are expected to lead to high levels of energy localization. The purpose of this chapter is to explore various levels of abstraction to determine the optimal balance of accuracy and computing costs.

One of the most widely used methods of abstraction is the modeling of inclusions as spheres and cylinders. The Mie solution provides an exact analytical solution for scattering by a single sphere \[66\]. While there has been some success in extending this solution to systems of a few spherical inclusions, the effort required rapidly increases with the size of the structure, quickly rendering such methods ineffective. Numerical simulation is necessary for the large crystal structures of interest here.

In general, structures must be simplified in some way to ease demand on computing resources and limit what could otherwise be a virtually unbounded simulation space. There are some prior investigations of interest – analyses involving water or other liquid particulates reduce computational complexity by approximating individual scatters as spheres or ellipsoids \[5, 67\]. The spherical boundary conditions allow for greatly simplified discretization for certain EM solvers. In this investigation, the crystals of energetic materials feature many rough edges and corners. It has been shown that spherical approximations significantly underestimate the impact of such inclusions \[68\]. In addition, preliminary analyses have shown edges and corners to be the locations of interest for high energy
concentration [26]. This has been studied and remains an area of active research at the nano-scale and particle level in various fields of physics, but has received significantly less attention at the scale of the mediums here. This investigation will attempt to quantify these effects in terms of energy localization.

This chapter will seek to address areas not covered by previous inclusion studies. Pickles et al. investigated a similar, relatively large medium – however the results were limited to various comparisons of effective permittivity [12]. Perry et al. have performed heating analysis at the inclusion level [5], [6]. However, the authors admitted to using a large degree of simplification in their simulation space and rely on periodicity to extend the effective size of the space, eliminating the potential for stochastic extremes. Kort-Kamp et al. performed perhaps the most comprehensive of all investigations at this scale, with an exhaustively recreated medium [27]. The abstractions presented in this chapter seek to develop an acceptable balance between oversimplification and exhaustive reproduction.

### 4.2 Method of Simulation

Previous simulation based studies have shown that modeling an energetic material as a medium of regularly spaced, regularly oriented cubes does not produce the high electric field strength localization seen with more random arrangements [12]. This also suggests that a periodic structure, realized using electric and/or magnetic walls, cannot be relied upon to reduced the complexity of the structure. It was also observed in these simulations that more cubic inclusions resulted in disproportionately higher peak concentration of fields [12], [26]. However, availability of computing resources limited analyses to simulations with a few tens of inclusions. With increased computing capabilities available here, it is possible to
perform multiple simulations of greater complexity. Even so, abstraction of the inclusions is necessary to obtain manageable setup time, run time, and memory consumption. It will also enable many variations of larger structures consisting of some hundreds of inclusions to be studied.

All simulations described in this chapter are performed using the commercial finite difference time domain software xFDTD from Remcom Inc. The software runs on a Dell Precision 7810 with 16 physical cores and 64 GB (subsequently upgraded to 172 GB for Section 4.5.1 forward) of memory. The actual timestepping process is performed on two Nvidia K20 Tesla GPUs each with 5 GB of memory.

4.2.1 Simulation Details

The simulation structure is presented in Figure 4.1. For the characterization of the abstractions’ relative performance, the binding medium is determined to be unnecessary, and so the inclusions are suspended in vacuum, the difference from a binder of air is assumed to be negligible. This has the added benefit of eliminating boundary effects between the scattering medium and the observation/excitation medium, which is always vacuum (air).

A linearly-polarized plane wave is introduced into the simulation environment from the \(-x\) direction. The total electric field strength is periodically recorded at all mesh points within the medium. The excitation waveform is described in Figure 4.2. The frequency content is distributed from 3 to 30 GHz as shown, with a center frequency of 16 GHz, resulting in a pulse duration of approximately 180 ns. This frequency range is chosen to emulate the excitations have been shown to successfully cause ignition in explosives materials [2].
Figure 4.1 Simulation structure with excitation propagating from $-x$ to $+x$. The incident EM field has an E-field polarization in the $z$ direction. Scattering medium filling factor is reduced for clarity and not representative of actual packing density of simulation medium.
The scattering medium in Figure 4.1 is sparsely populated to enhance visualization. In the actual simulations, the medium consists of 500 packed inclusions forming a volume fraction of approximately 35%. All inclusions have a predetermined complex relative permittivity $\varepsilon_r = 3.5 + j0.003$ [42]. Once again, this value is chosen to mimic the physical properties of previously tested explosive materials, in this case RDX. The actual shape of the inclusions will vary for individual simulations. However, all inclusions have a ‘characteristic’ dimension of 100 $\mu$m. For a sphere this corresponds to its diameter, while for a cube it is the length of each edge. For the other shapes, the characteristic dimension will roughly correspond to their furthest vertex to vertex distance, though there will be some random variation. At the excitation pulse’s center frequency of 16 GHz, the free space wavelength is just under 2 cm, while in the medium, the wavelength would be approximately 1.1 cm. This puts the characteristic dimension of the inclusions at less than 1% of the wavelength within the inclusion material. Conventional mixing theories suggest that such a large difference should allow for the treatment of the composite as a homogeneous mixture, per Chapter 3. However, the quantities of interest are the individual points of high-field in both space and time, and an averaged value is unacceptable.

### 4.2.2 Meshing

One of the main concerns in a simulation-based investigation is the impact that the fineness of the structure’s meshing has on the accuracy of the results. Compared to other methods, such as finite element (FEM) or finite integral (FIM), the FDTD method has a straightforward approach to meshing, where mesh points are located on a Cartesian grid, and assigned to Yee cells [69]. While modern FDTD approaches have improved the accuracy of the method
Figure 4.2 Excitation pulse: (a) with a center frequency of 15 GHz and width of 180 ps; and (b) frequency content.
for geometries that do not readily conform to such a grid, the method in general has an easier
time meshing, and thus provides more accurate results for, Cartesian shapes compared to
spherical ones. Figure 4.3 compares the resultant 3D mesh for a cube of side length $d$ and a
sphere of diameter $d$ at a meshing density of $\frac{d}{30}$. It is apparent that even with the relatively
high density, the gridlike meshing attempts to recreate the cube results in a staircase effect
on the edge of the sphere, while the cube is faithfully recreated. As previous investigations
identified corners and edges – features prevalent in cube and prism-like shapes but absent
from spheres – as areas of interest in regard to the localization of electric fields\[12\], the FDTD
method is well suited for the purposes of this investigation. In addition, compared to the
other methods, the FDTD method scales relatively well with parallel computing capabilities,
an advantage in this case, as multiple simulations of large structures is required.

4.2.3 Choice of Abstraction

With the end goal of obtaining a satisfactory abstraction of the crystals of interest, it is
important to first obtain a general characterization of these crystals. A microscope image of
HMX is displayed in Figure 4.4\[70\]. Ignoring the much smaller inclusions present among
the larger crystals, we note that the crystals display relatively smooth faces and edges. In
general, they seem to have prism-like shapes. Similar features can be seen from other
sources. Previous investigations have shown that one particular feature of interest in the
formation of hotspots are the edges and corners of crystals\[12\], \[26\]. As such, it is preferable
that these features be preserved in the abstractions. Higher levels of energy localization
have also been observed with more "random" arrangements of crystals, suggesting that
the artificial enlargement of a simulation structure through the use of periodic boundary
Figure 4.3 Meshing comparison showing the difficulty the FDTD method encounters meshing spherical shapes, observable by the staircase effect on the sphere’s surface. Mesh only images included for improved visibility.
conditions is inadequate to generate the desired energy localization.

Figure 4.4 SEM image of RDX Crystals, showing edges and corners of inclusions. Crystals can be seen ranging from approximately 10 to over 50 microns in size. From [70].

The cube presents itself as a promising candidate. It possesses the edges and corners of interest, and is relatively simple to randomly generate and place through a script. By comparison, the commonly used sphere is expected to be a relatively poor abstraction,
possessing no corners or edges, though it is similarly straightforward to generate and place. However, it is necessary to compare multiple cases to gauge the relative performance of each case – the sphere will be used as a baseline. In addition, it is not sufficient to simulate an individual inclusion. Though this did not significantly change the results for extracted effective permittivity, it is expected to do so here. The inclusions will be arranged in various formations and results from each are compared. A visualization of the abstractions utilized is presented in Figure 4.5.

While it is possible to imagine many more abstractions than those shown, these five are expected to serve as an adequate starting point for the investigation. The five arrangements in Figure 4.5 will henceforth be referred to as Cases 1 through 5, in descending order of their individual level of abstraction. Case 1 of the single sphere will be used as a baseline for all other cases. Case 2 is of a single cube, randomly rotated around its center point, and will be used as a secondary baseline for the cubical inclusions, gauging the relative effectiveness of other cases consisting of cubical inclusions. Case 3 consists of regularly spaced cubes aligned to face the excitation wave. Case 4 consists of spheres randomly positioned within the medium and is expected to offer an improved result over the single sphere. Case 5 consists of cubes of random position and orientation, and is expected to display the highest degrees of energy localization.

Case 5 represents the most detailed, yet still computationally light abstraction explored in this work. Cases 1-4 offer multiple comparisons from what is expected to be a lower level of performance. However, it is beneficial to also have comparisons from a higher level of performance. Case 6, illustrated in Figure 4.6, is meant to fulfill this role. The inclusions of Case 6 are generated from randomly shaped and sized prisms, meant to more accurately
resemble those in Figure 4.4. These prisms are placed with a script generated using the Bullet Physics software library [11]. This "game" program utilizes simple mechanics to simulate the crystals being dropped into a bucket and shaken in various ways, in an attempt to mimic one method by which homemade explosives are made. The script will be referred to as the Bucket script, see Appendix C. Although this greatly increases setup and simulation time, as well as memory requirements, it is still computationally inexpensive relative to the recreation of an actual structure, and allows for the generation of subsequent structures for random runs.

The properties of all six cases are summarized in Table 4.1.

<table>
<thead>
<tr>
<th>Case</th>
<th>Inclusion Count</th>
<th>Position</th>
<th>Orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>Centered</td>
<td>N/A</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>Centered</td>
<td>Random</td>
</tr>
<tr>
<td>3</td>
<td>500</td>
<td>Regular Grid</td>
<td>Edges parallel to x y z axes</td>
</tr>
<tr>
<td>4</td>
<td>500</td>
<td>Random Offset from Grid</td>
<td>N/A</td>
</tr>
<tr>
<td>5</td>
<td>500</td>
<td>Random Offset from Grid</td>
<td>Random</td>
</tr>
<tr>
<td>6</td>
<td>700</td>
<td>Bucket script</td>
<td>Bucket script</td>
</tr>
</tbody>
</table>

### 4.2.4 Section Summary

A simulation-based method has been defined. The FDTD method will be used to analyze the EM response of a composite medium of RDX and vacuum to an incident microwave pulse. The data of interest are the peak electric field over extremely small spans of space and time, as these are likely to be the stresses which lead to initiation of the energetic material.
Figure 4.5 Various simulation structures Case 1 is a single sphere; Case 2 is a single randomly oriented cube; Case 3 is an array of cubes on a grid; Case 4 is an array of randomly arranged spheres; and Case 5 is an array of randomly arranged cubes.
Figure 4.6 Case 6, generated by the Bucket script of falling and shaken randomly generated crystals as described in Section 4.2.3, filling factor as simulated.
To adequately capture behavior at these resolutions, the meshing of the FDTD cells needs to be very fine, a maximum mesh density of 30 points per characteristic dimension is chosen.

A range of abstractions for the inclusions comprising the RDX structure have been defined. These include both spheres, which have been commonly used for their desirable meshing properties in non-FDTD methods, and cubes, which have been shown to generate increased field localization. Randomness is added to the abstractions via the rotation and translation of the individual inclusions. The most accurate abstraction is a structure of randomized crystals defined using the Bullet Physics library, the Bucket script.

4.3 Scaling of Peak Field Magnitude

The initial simulation setup used in this chapter utilizes a plane wave pulse with a peak field of 1 V/m as the excitation, per Figure 4.2. This value was initially chosen out of convenience, and its use continues to the end of this chapter to maintain consistency throughout. This is a very small field value, perhaps inconsequential in any real world applications. Modern microwave sources have been shown to be capable of generating field magnitudes close to the breakdown value in air (approximately 3 MV/m) [71]. While nonlinear EM responses of energetic materials has been explored, the effect has so far been limited to laser frequencies well beyond the microwave range, where resonances in molecular bonds may occur [72]. The permittivities used in this chapter were sourced from an investigation using high power excitations [42]. It is thus reasonable to linearly scale the peak fields observed in the simulations to the magnitude of a higher strength excitation.
4.4 Initial Results

The simulation method outlined in Section 4.2 is applied to the abstractions described in Section 4.2.3. Multiple random realizations of each of the abstracted structures will be simulated for peak electric field over a range of meshing densities. The goal is to determine the level of field localization generated by each method compared to its computing resource requirement, as well as to observe the tendency of the results to converge with increasing mesh density, providing increased confidence in the results.

4.4.1 Accuracy of Abstractions

As in situ measurement of electric field on such a scale is not feasible, the effectiveness and accuracy of our different cases will be assessed by comparisons with Case 6, the ‘best’ abstraction, and Case 1, the baseline. Figure 4.7 shows the values of the peak electric field over all time and space points at varying mesh densities for each case. Cases 1 and 3, those of the single sphere and the regularly spaced cubes were only simulated once per plot point, as there is no possible variation in individual realizations of the structure. For Cases 2, 4 and 5, 20 individual random arrangements were considered for each case at each mesh density. Case 6 was limited to 5 random arrangements, as the setup time and memory required for meshing these structures is extremely long relative to the other cases. Each plot point represents the average of the peak field values over the total number of arrangements for each setup. That is, the highest electric field recorded over the entire space and time of each individual simulation is average for each case. As it is believed that points of high electric field contribute to the initiation of energetic materials, these peak values are of significance.
when looking for possible activity. For this plot, the peak values are averaged over all runs to allow for an easier comparison between the fixed and randomizable cases.

The mesh densities of each case is varied from 1 to 30 points per characteristic dimension, or 0.1 to 0.0033 \( \mu \text{m} \) in meshpoint spacing. With runtime and memory requirements increasing with finer meshing, the scope of the simulations for Case 6 is once again necessarily limited, with the mesh density being varied from 1 to 20 points per characteristic dimension.

It is immediately observed that while the points follow a generally increasing pattern, the progression of the points is decidedly not monotonic. This is partly due to the mesh points being moved slightly off and back onto the hotspots as the meshing density is changed. This is particularly noticeable in Case 3, where the field value alternates between slightly increasing and slightly decreasing, yet maintains a very steady pattern. However, the increasing behavior for all 6 cases suggests an overall increase in accuracy as meshing is made finer. The simpler cases show asymptotic behavior rather quickly, while the more complex structures suggest field levels increasing with meshing beyond the scope of this analysis, raising the possibility that the actual field localization could be even greater than that shown. The increased peak fields observed for the cases with more “random” structure is seen as further evidence of the sensitivity of hotspot formation to randomness in these geometries.

The average peak fields in Cases 1 to 5 are 2.00, 2.95, 2.63, 4.34 and 6.35 V/m for an incident peak field of 1 V/m. This is a significant range with the most realistic modeling indicating a factor of over six in the field localization, corresponding to an energy amplification of 16 dB. The single sphere approximation has the lowest degree of field localization,
Figure 4.7 Peak field values for the waveform in Figure 4.2, and the abstractions in Figures ?? and 4.6 for varying mesh density and a characteristic dimension of 100 $\mu \text{m}$. 
approximately twice the incident excitation level. It is also of interest that the single randomly oriented cube, Case 2, has energy localization that is slightly higher than that for the uniform array of cubes, consistent with the overall observation that corners and edges are critical factors in field localization. The highest levels of energy localization occur for the randomly positioned inclusions, Case 6 and the randomly arranged cubes, Case 5, where the greater than sixfold increase in peak field value is observed.

The peak field observed for Case 5 for each of 480 simulations for 16 structures are plotted as points in Figure 4.8 against varying mesh density. It is seen that there is considerable variation in peak field. However, it is the highest peak which is important – it is this highest peak field observed for multiple randomized structures that is representative of the strongest hotspot that will occur. Since initiation of deflagration or ignition occurs at just one point in space (as small as a molecule) and time (as small as the chemical reaction time of femtoseconds), this is the most significant factor in initiation of activity in these materials.

The solid line shown in Figure 4.8 is a least squares fit to the peak field points and shows the desirable asymptotic behavior with mesh density. If this fit is extended beyond the 30 points per characteristic dimension limit of our plot, convergence to within 0.1% of the asymptotic value of 7.11 occurs at 39 points per characteristic dimension. At the limit of our plot (30 points per characteristic dimension), our least squares fit is within 3% of this value. The higher mesh density corresponds to finer geometry and time resolution so that the asymptotic characteristic provides confidence that the peak field can be simulated using meshing of objects with sharp edges. Figure 4.8 illustrates that there is sensitivity of the peak field value to geometry. While here the field orientation was fixed and the geometry
Figure 4.8 Peak field values for the waveform in Figure 4.2, and the abstractions in Figure 4.7 and 4.6 for varying mesh density and a characteristic dimension of 100 µm. The markers correspond to the peak field values for each of the 16 randomly generated structures.
randomized, the same behavior would be observed with the direction of illumination changed (due to movement of the illumination source) and with a more realistic size of material many centimeters on a side, many hundreds of times larger than the size of the structures simulated here. Also, somewhat more pronounced asymptotic behavior is observed when only the highest peak fields are considered.

Overall, it is apparent from Figure 4.7 that the randomly oriented cubes are a satisfactory abstraction to use in simulating hotspot formation while Figure 4.8 indicates that the mesh density should correspond to less than 5 µm, i.e. 0.025% of a wavelength for a high degree of accuracy.

Figure 4.8, for each meshing resolution, shows a scatter of peak values. For each individual randomized structure, the peak E field anywhere in the structure is plotted – each scatter point is the peak field for a different randomized structure. Repeatedly simulating randomized structures provide a means to effectively look at larger, more realistic, structures of energetic material. In addition, very small changes to the beam, such as a movement of the microwave source, would result in different internal material scattering and hence peak field that differs in amplitude and location. Thus, the maximum of the peak fields in Figure 4.8 are representative of the peak field that would most likely initiate deflagration of explosion. From that perspective, i.e. considering the maximum peak field at each meshing density, the maximum peak field is also seen to be asymptotic.

### 4.4.2 Resource Efficiency of Abstractions

The runtimes and memory requirements for the simulations are presented in Table 4.2. Generally the run time and memory required increase with lower levels of abstraction
(i.e. greater fidelity). In particular, it is seen that Case 6, which most closely approximates a realistic material, requires a very long time commitment. A significant part of this is the time required to create and mesh the structure. Also, the meshing process for Case 6 at the low mesh dimension (the 3.3 \( \mu \text{m} \) mesh) requires memory significantly greater than the 64 GiB available (before the upgrade) and no results are reported. It should be noted that the simulation process utilizes memory on both the GPU and CPU. Thus, the overall memory used can be higher than the 10 GiB available on the GPU. The excessive memory requirements and runtimes render Case 6 impractical for large-scale repetition. The cases with the cubic inclusions are observed to have slightly higher memory and runtime requirements than the cases with spherical inclusions. It was previously noted that Case 3, with its regularly spaced cubes, shows very low levels of localization. Here it is observed that this is in spite of Case 3 requiring the second highest simulation runtime and memory. The random orientations and positions of inclusions in Case 5 results in a slightly higher computing overhead, but generates much improved results. An efficiency argument can be made for Case 4, that of the randomly positioned spheres, as it displays much lower computational cost than Case 5 while producing significantly better results than Case 3. However the runtime and memory usage of Case 5 are acceptable, and the field results make it the abstraction of choice.

4.4.3 Section Summary

The observed electric field localization is possibly the result of multiple scattering by many very small objects. The characteristic dimension of an inclusion is 100 \( \mu \text{m} \), which is 1/200\(^{th}\) the free-space wavelength at the incident pulse’s center frequency. The hotspot regions,
Table 4.2 Simulation runtimes and memory requirements for each level of abstraction or Case. The memory is the combined CPU (up to 64 GiB) and GPU (up to 10 GiB) memory used in the EM simulation. The memory required for mesh generation determines the maximum memory required.

<table>
<thead>
<tr>
<th>Case</th>
<th>5 µm mesh</th>
<th>3.3 µm mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runtime</td>
<td>Memory</td>
</tr>
<tr>
<td>1</td>
<td>1 m 10 s</td>
<td>146 MiB</td>
</tr>
<tr>
<td>2</td>
<td>1 m 20 s</td>
<td>172 MiB</td>
</tr>
<tr>
<td>3</td>
<td>18 m 4 s</td>
<td>3.6 GiB</td>
</tr>
<tr>
<td>4</td>
<td>14 m 32 s</td>
<td>2.8 GiB</td>
</tr>
<tr>
<td>5</td>
<td>21 m 6 s</td>
<td>4.0 GiB</td>
</tr>
<tr>
<td>6</td>
<td>223 m</td>
<td>7.6 GiB</td>
</tr>
</tbody>
</table>

defined as the half-peak power areas, are themselves a fraction of the size of the inclusions, about 10 µm, based on investigation of several randomly chosen runs. That is, critical hotspots can have a size one thousandth of a wavelength or less. Hence, the level of abstraction significantly affects the determination of the peak electric fields. We observe a ratio of 6.35/2.0 = 3.17 between the averaged peak fields obtained with the highest and lowest levels of abstraction. It is apparent that a high level of randomness is required to create high field localization.

Case 5 results in similar hotspot formations as Case 6, but its inclusion structure affords a much lower computational complexity. This results from the uniformity of the shapes, as well as the ability to generate the structure without the need for physics emulation. The results for the model in Case 5 indicate that it is sufficient to use a model in which the cubes are on a regular three-dimensional grid, and in contrast to Case 3, it is necessary to randomly offset the cubes from the grid as well as randomly orient them, the latter is a conclusion from simulating many variations of Case 5. The script used to generate Case 5
requires only random variables for each cube's offset and orientation, with checks to ensure that inclusions do not overlap. In contrast, Case 6 requires a much more complex simulation. While it was always possible to simulate many Case 5 variations, Case 6 was not as well-behaved, with some (random) configurations resulting in excessively large computation times due to meshing complexity or failure to mesh due to memory limitations. Thus, Case 5 offers a more robust option, while retaining the features of interest.

Cases 1, 2 and 3 are high levels of abstraction, and compared to the more realistic model in Case 6, are not acceptable models, even though their computational advantages are attractive. Cases 4 and 5 are lower levels of abstraction and show the peak field behavior of Case 6, the reference structure. Case 4 is the structure with randomly arranged spheres, a situation that does not have the sharp edges that are thought to be critical to hotspot formation. Still, the randomness in the positions of the inclusions has somewhat increased field peaking. As well as supporting multiple sub wavelength scattering, Case 5 also has the additional field localization due to the sharp edges and corners. It is apparent that the randomly arranged cubes, Case 5, come closer to a realistic material than any of the other approximations.

The near-asymptotic behavior shown in Figure 4.8 provides further confidence in the validity of the simulation accuracy, particularly in regards to the accuracy of the meshing. Besides this, the spread of the peak values of the individual runs displays some interesting behavior, and will be one of the focuses of the next section.
4.5 Extension of Case 5

Case 5 presents the best abstraction for the purpose of investigating hotspot formation, and warrants further investigation. The other four abstractions have all proven inadequate in terms of their ability to maintain the field localization. The following section will introduce modifications to the setup of Case 5 to gain greater insight into its behavior.

4.5.1 Decomposition of Case 5

From Section 4.4.1, it was observed that the transition from spheres to cubes results in an approximately 50% increase in peak electric field. However, an even greater increase was observed by randomizing the position and orientation of the cubes (Case 3 versus Case 5). The random positioning of the cubes in Case 5 is comprised of 2 elements — a random rotation from 0–2\(\pi\) around each of the \(x\), \(y\), \(z\) axes, followed by a random displacement in the \(x\), \(y\) and \(z\) directions of up to 30\(\mu\)m. It is of interest to determine the individual contributions to localization from these 2 elements.

Case 5 is separated into Case 5R (for rotation only) and Case 5T (translation only), to isolate the effects. Henceforth, Case 5 may also be referred to as Case 5RT for convenience. This is illustrated in Figure 4.9. Simulations for these two new cases are performed, repeating the procedure outlined in Section 4.2. 5 additional runs were performed for Case 5, bringing the total number of simulations to 25. Both Case 5R and 5T require fewer simulations to reach asymptotic maximum peak values of the E field. 10 runs are performed for Case 5T and 15 for Case 5R. The scatter plots and best fit lines for all 3 cases are presented in Figure 4.10.
Figure 4.9 Visualization of (a) Case 5R (b) Case 5T (c) Case 5 or 5RT.
Figure 4.10 Peak field values for the waveform in Figure 4.2 for Cases 5R, 5T and 5RT in Figure 4.9 for varying mesh density and a characteristic dimension of 100 µm.
The best fit line of Case 5RT with the additional simulations reaches 0.1% of its asymptotic value by 39 grid points per characteristic dimension, the same value observed in section 4.4.1 – The additional 9 runs did not significantly change the results’ asymptotic behavior. However, the best fit lines for both Cases 5R and 5T have reached 0.1% of their respective asymptotic values of 4.97 and 2.89 V/m by 30 points per characteristic dimension. This agrees with the findings in Section 4.4.2 that adding the random elements increases the strain on computing resources. However, it is also observed that the spread of the peak fields increases dramatically from the cases with a single element of randomness to the cases with the combination of the two. This is visible in Figure 4.10, and further illustrated by the addition of scattering bounds in Figure 4.11.

All three of the cases in Figure 4.11 show scattering bounds which initially widen as the meshing density is increased. This is expected, as the goal of increasing the meshing is to be able to resolve the field spikes at the hotspots. It is unsurprising that some structures will require greater meshing due to either smaller hotspots or simply pure chance. The scattering range of both Cases 5T and 5R stabilize to a value lower than the peak by the end of our independent range, suggesting that the meshing density of 0.0033 mm is sufficient to capture all of the hotspot behavior. The scattering range of Case 5 shows signs of stabilizing at this point, but is still varying. This is consistent with the behavior of our best fit lines, where Cases 5T and 5R have reached their asymptotic values, whereas Case 5 is still a ways off. To better quantify this behavior, Figure 4.12 fits the size of the scattering ranges in Figure 4.11 to a polynomial using a least-squares method. We see that Cases 5R and 5T have reached stable values of 0.38 and 0.11 V/m, respectively, in their scattering range. However, the scattering range of Case 5RT has surpassed 1.00 V/m and continues to increase. An
Figure 4.11 95% scattering bounds of the scatter plot of 4.10 for varying mesh density and a characteristic dimension of 100 μm, center point defined by best fit line.
extension of the fit curve reaches a peak value of 1.05 V/m between 38 and 39 points per characteristic dimension. This aligns well with the fit of the overall scatter plot, suggesting that the field values and precision of the results should stabilize by that point. It is apparent that the results of Cases 5R and 5T have already reached a stable level of precision.

The higher mesh density required to reach a stabilization in both peak field magnitude and its scattering range for Case 5RT suggests that the size of the hotspots decreases with increasing randomness. Since the ignition points of are on the sub-micron scale [73], any effects on initiation should not be negatively impacted by the smaller size. Though a complete investigation into the changes in hotspot size is not performed, preliminary analysis of arbitrarily chosen cases shows that Case 5R displayed hotspot regions of 15–20 µm across, while Case 5T showed regions of up to 50 µm across. Further analysis of this behavior is a candidate for continued investigation.

It was already established in Section 4.4.1 that the higher degree of randomness for Case 5RT yields a significantly higher degree of field localization than Case 3. However, due to the lack of intermediary cases, it was not possible to determine the individual contribution from the addition of randomness in either rotation or translation. In Figure 4.10, it is clear that the addition of rotation randomization increases the level of field localization by a greater degree than the addition of translation randomization. Figure 4.13 compares the relative increase in peak field for each case. At the highest meshing density, the relative field increases are 1.90, 1.11, and 2.61 times for Cases 5R, 5T and 5RT, respectively. A simple addition of the relative increases from Cases 5T and 5R yields a value of 2.01, while their product yields a value of 2.10. In addition, while it is difficult to make a comparison to Case 3 due to its single element realization, it is apparent from Figure 4.11 that the standard
Figure 4.12 Fit lines of the range of the scattering bounds of Figure 4.11 for Case 5R, 5T and 5RT. Individual points represent the magnitude of the single sided 95% scattering bound at the points mesh densities in Figure 4.11. One very high peak field scattering range is recorded at the lowest meshing density for the Case 5RT simulations. This is an anomaly due to low mesh resolution.
deviation (confidence range) of Case 5RT is disproportionately large relative to those of Case 5R and Case 5T. These observations suggest that the increase in field localization in Case 5, or 5RT, cannot be described as simply the combination of its two constituent cases: the random rotation of Case 5R and the random translation of Case 5T.

Figure 4.13 Relative increases in peak field of Cases 5R, 5T and 5RT from Figure 4.9, defined as the increase in peak field values at each mesh density relative to the peak field strength for Case of the regular cubes, Case 3. The product of the increases of Case 5R and Case 5T is also included.
4.5.2 Intersection of Inclusions

A second extension to Case 5 is proposed to gain better understanding of the effect of inclusion shape. In this case, the cubic inclusions of Case 5 are allowed to intersect, resulting in the modified Case 5I. This is accomplished by relaxing checks in the generation script which prevented this geometry in the original Case 5RT structure. Figure 4.14 illustrates the difference between Case 5RT and Case 5I.

From a geometric perspective, this results in the nonphysical case of multiple inclusions occupying the same physical space. However, from an EM standpoint, the case of overlapping inclusions is correctly accommodated. This structure allows for more exotic inclusion shapes, as well as higher packing densities. In this case, however, the filling factor is maintained to be between 30–35%, as this is representative of improvised explosives.

![Figure 4.14 Illustration of randomly generated cubes (a) allowed to intersect and (b) reoriented to avoid intersection](image)

The excitation, boundaries and data recording followed the same procedure outlined...
in Section 4.2.3. Without the need to simulate Cases 1–4, the number of realizations can be increased. A total of 25 randomized structure realizations of Case 5I were simulated, and the number of realizations for Case 6 is increased by 5. That is, the 5 realizations from Section 4.2.3 are supplemented with 5 new realizations.

Figure 4.15 shows the run-averaged peak field localization over 25 simulations of Case 5, and 10 simulations of Case 6. When compared with the plot of Case 6 in Figure 4.7, we see that the increased number of runs has resulted in substantial improvement in the smoothness of the progression of data points of Case 6. In addition, the peak field localization for Case 5I displays smoother behavior than that of Case 5, as well as showing better agreement with Case 6. To better understand this, Figure 4.16 compares the hotspot geometry for Case 5 and Case 5I at 0.004 mm mesh density. While these images represent 2 specific runs, they are typical of the general behavior across all runs.

While the hotspot occurs at a point of overlap in Case 5I, the geometries leading to field localization in the two cases are similar. The original goal of preventing intersection among inclusions was to avoid situations illustrated in Figure 4.14, but those geometries do not appear to lead to extraordinary levels of peak field. Rather, the areas of interest appear to be locations where multiple corners exist in close proximity. Thus, while preventing large overlaps, the exclusion of intersection also limited the number of situations in Figure 4.16, where small overlaps in geometry allow for the existence of what are essentially “double corners”. Both Case 5 and Case 5I show a high field localization at one of these double corners. The difference lies in the structure of Case 5I being connected by a thin region of energetic material, while the structure of Case 5 is connected through a thin region of air. Case 5 eliminates the possibility of the former structure. This helps explain the
Figure 4.15 Comparison of peak field values of Case 5I, the modified version of Case 5 with intersection allowed with those of Case 6, from Figure 4.6 over varying mesh density. The results are the average of 25 random realizations of Case 5I and 10 random realizations of Case 6. The peak incident E-field is 1 V/m, as shown in Figure 4.2.
Figure 4.16 Field cross section comparing peak field geometries of Case 5 and Case 5I. The color-bar for both figures represents the electric field strength in V/m

more consistent behavior of Case 5I in Figure 4.15 relative that of Case 5 in Figure 4.7. The features which result in the highest levels of energy localization are more likely to “survive” the structure generation process.

It appears that of the edges and corners, corners produce the greatest degree of field localization. To further illustrate this, hotspot formation for Cases 3, 5R and 5T is displayed in Figure 4.17. The edges of Case 3 and Case 5T show decidedly lower levels of energy localization than the corners in the remaining cases. The close proximity of the edges in Case 5T (there is no overlap allowed in this Case) results in higher fields, while the increased proximity from Case 5R to Case 5 to Case 5I shows a similar effect.

This double-corner feature provides a better explanation for the results in Figure 4.13. If the double corner feature is considered as an imperfect superposition of two corners, the increase in fields for the double corner (Case 5RT) should be slightly less than that of a single corner (Case 5R). This is indeed the case, with the values being 2.61 and 2.82 times,
Figure 4.17 Field cross section comparing peak field geometries of Case 3, Case 5R, and Case 5T
respectively. The high fields seen in structures with many corners are commonly exploited through the use of star like shapes of nanomaterials to generate high field localizations [31]. Due to the physical bulk of the inclusions in this situation, geometries such as those used to enhance fields at the nanometer level are not possible [31]. The voluminous shape of the energetic crystals preclude the presence of many corners.

It is also apparent that one of the shortcomings of the non-rotated cases is the alignment of the cube edges with the wave polarization, presenting an edge as opposed to a corner. It is therefore important the inclusions not be aligned to the polarization or with each other.

### 4.5.3 Section Summary

The most promising of the initial cases of Figure 4.7, Case 5, has been examined in further detail. First, the two random factors in the generation of the cubic inclusions, their rotation and translation, were separated. This resulted in the creation of two new Cases, 5R and 5T, with Case 5 being referred to as Case5RT for clarity.

It was determined that though both the random rotation and translation of the cubes increased the degree of field localization, the increase caused by the rotation was much greater. In addition, the expansion in the scattering bounds was much greater for the rotation. However, the peak field level and confidence range for Case 5RT was greater than the combined effects of both Case 5R and Case 5T.

The second extension allowed for the intersection of individual inclusions – Case 5I – a non-physical situation that nonetheless allowed for interesting geometries. It was observed that the peak field localization was more reliably observed with this allowance. Upon further examination of the local geometries at the peak fields of both Case 5RT and Case 5I, it was
Table 4.3 Inclusion properties for the variations of Case 5 described and simulated in Section 4.5

<table>
<thead>
<tr>
<th>Case</th>
<th>5</th>
<th>5R</th>
<th>5T</th>
<th>5RT</th>
<th>5I</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inclusion</td>
<td>Cube</td>
<td>Cube</td>
<td>Cube</td>
<td>Cube</td>
<td>Cube</td>
</tr>
<tr>
<td>Rotation</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Translation</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Intersection</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>

determined that the peak field localizations were caused by “double corners”, which were more likely to be present in Case 5I due to the allowance of intersections. Case 5 and all of its variations are outlined in Table 4.3.

4.6 Limitations

While the results presented thus far seem promising, certain liberties were taken to facilitate and expedite their collection. This section will look to address potential concerns raised by these cutbacks.

4.6.1 Excitation

The excitation used for all simulations in this section is a uniform plane wave. In a real world application, the excitation waveform would be comprised of spherical wavefronts, resulting in phase discrepancies across the medium. However, taking into account the relative size of the sample (less than 2 mm across), it is safe to assume the wavefront as planar. At a distance of 5 m, this corresponds to an angle of less than .01°. While a medium of IED scale size might experience phase variations across its surface, portions of the device
with scales similar to those in this work would not.

In addition, the excitation in this section is always linearly polarized in the $y$-direction. While the use of a different polarization will impact the location and magnitude of field localizations, the setup of the scattering medium is random, suggesting that a comprehensive set of data can be acquired by simply increasing the number of simulations performed with different randomized structures.

Finally, this study neglects any possible nonlinear effects. Recent studies have suggested the possibility of nonlinear EM responses in similar materials \cite{72}. However, this effect has been shown to be relatively weak, and is likely to be due to interactions with molecular bonds, putting the onset of these effects at the lower end in the THz region, well beyond the excitation frequency here. Previous studies with scales similar to this one have neglected any nonlinear effects \cite{27}.

### 4.6.2 Sample Sizes

The size of the simulation structure is still small, which limits the scope of the investigation. It would, for example, be desirable to compare the behavior of fields deeper within the medium, if for no motivation other than thoroughness. However, with the inclusion of a relatively high loss binder in a real world application, it is likely that the field strength would weaken further into the medium. Therefore, for the purposes of results relevant to the causes of initiation, a study of the material closest to the surface is sufficient. In addition, given the scope of other investigations at the inclusion scale \cite{5}, \cite{6}, \cite{26}, the simulation space in this work is of adequate size.

Another possible concern in regards to sample size is the number of runs performed.
Monte-Carlo simulations often iterate many thousands of times to produce confidence in the result. This would entail an infeasible time requirement for simulations of the length described in Section 4.4.2, and is unnecessary for a study of this nature. Due to the random nature of our structures, it is inevitable that fluctuations arise in the observed fields. The goal in this case is not precision of the numbers, but whether the general trends from the real-world situation are reflected in our data. From Figures 4.7 and 4.15, this appears to be the case. In addition, with multiple trials across 15 cases and 30 meshing densities, there is an enormous amount of data on which to build confidence in our conclusions.

4.6.3 Accuracy of Method

Results in Sections 4.4.1 and 4.5.1 suggest that for optimal accuracy, the meshing of the simulation space for Case 5RT (and 5I) needs to extend to 40 points per characteristic dimension for optimal confirmation of accuracy. As stated in Section 4.4.1, the fit curve of Case 5 reaches 3% of its asymptotic value by the highest degree of mesh density in this work. Combined with the asymptotic results of both the fir and confidence ranges for Case 5R and Case 5T, this gives confidence in the accuracy of the result. In addition, it is visible in Figure 4.10 that the absolute maximum of the field peaks across all runs of Case RT displays further pronounced asymptotic behavior.

It may be argued that even the most accurate abstraction in this work, Case 6, is a poor recreation of the real-world situation displayed in Figure 4.4. However, while more exhaustive reproductions of energetic materials in EM simulations have been performed [27], they require time, materials, capabilities beyond the scope of this work, while producing incremental improvements. Relative to the majority of the literature, the abstractions in
this work operate at a comparable or more complex level [5], [7], [12]. In particular, Case 6 generates shapes using a random number generator, while accurately emulating gravity and collision effects. Whereas, other studies have relied on completely user-defined inclusion geometries and positions. While the method in this work may not be 100% representative of real-world processes, it effectively eliminates the possibility of degenerate, unrepresentative structures dominating the randomized pool.

4.7 Validation

Validation for this portion of this work is difficult. The greatest confidence in the accuracy of the results stems from the asymptotic results presented in many of the figures. The validations presented in Chapter 3 and Chapter 5 will better develop confidence in the overall validity of this work.

4.8 Chapter Summary

The investigations performed in this chapter explored the possibilities of abstracting the inclusion shapes and medium structure into a form that was simpler to simulate, but which still generated the high levels of electric field localization. Whereas Chapter 3 attempted to, and was ultimately unsuccessful in, describing the medium without any mention of geometry, Chapter 4 sought to determine how much geometry needed to be retained to produce adequate results.

Previous knowledge suggested that shapes which retained corners and edges displayed higher levels of localization, and that the overall randomness of the inclusions’ orientation
played a factor in the degree of localization as well. The initial choice of abstractions sought to confirm and quantify this behavior, by observing the localization generated in mediums of cubes and spheres, while varying the inclusion structure from a single inclusion to collections of regular and randomly positioned and oriented inclusions. These results were compared to a medium of randomly shaped crystals placed with our bucket-shaking program, which was taken as the most accurate representation of the medium in this investigation.

Results showed that both randomness of the geometry and the inclusion shape played a substantial role in field localization. In comparisons of like inter-inclusion geometries, that is Case 2 versus Case 1 and Case 5 versus Case 4, cubes produced approximately 50% higher peak field levels than spheres, 2.95 versus 2.00 V/m and 6.35 versus 4.24 V/m respectively. The peak field value in Case 5, 6.35 V/m, correspond to a peak electric energy density more than 10 times greater than the baseline of the single sphere in Case 1, and over 100 times greater than that of the incident field in air.

While an exhaustively accurate simulation of a random structure of energetic material was not attempted, and its computational requirements are thus unknown, all five of the attempted abstractions showed substantial memory and time improvements over the Bullet Physics generated, most accurate model of Case 6. Even the most complex of the abstracted cases offers a substantial reduction in both runtime and memory requirement, allowing for more detailed meshing or simulation of larger structures.

It was decided that Case 5 was the most promising abstraction for further study. Case 5 displayed field levels comparable to Case 6, while also requiring significantly reducing runtime and memory requirements. The high levels of field localization observed set it
apart from the remaining cases.

The first extension of the Case 5 model was the decomposition of the randomness of the inclusions into a translation and a rotational component, Cases 5R and 5T. After an analysis of the fit curves and confidence intervals of the 3 cases, it was determined that while both Cases 5R and 5T offered an improvement over the multi-cube baseline of Case 3, a simple combination of the two elements of randomness did not amount to the total increase offered by Case 5RT.

The second extension of Case 5 was to allow the individual cubes to intersect showed that allowing the cubes to intersect resulted in higher levels of energy localization, as well more consistent generation of these high field values. It also suggested that the idea of multiple corners results in higher degrees of energy localization. However, higher order corners are uncommon due to the shape of the inclusions.

Finally, it is recognized that limitations and approximations inherent to the nature of the work which limit its resemblance to the real world situation of interest. These were acknowledged, with explanations and possible areas for future improvement suggested.

4.9 Conclusion

It has been determined that the cubic abstraction of Case 5RT and Case 5I display high levels of peak field localization, and it has been confirmed that multiple edges and corners are crucial to the generation of peak field localization. These field levels cannot be predicted using effective permittivity models, even though the use of an effective permittivity would seem justified for such inclusions of such small size. The commonly used spherical approximation for inclusions generates significantly lower localization, with peak fields
over one third lower, equating to less than half of the electric field energy density.

As numerous investigations have shown that these effects impact the rate and/or probability of detonation or deflagration super-linearly and potentially exponentially [9], [37], [51], [52], [74], the difference in the fields generated by these abstractions could offer drastically different results in energetic materials. The total runtime improvement over the Bucket script of Case 6 is over 10x, without the increased hardware and software costs necessary for an exhaustive reproduction.

With linear scaling for an excitation of 2 MV/m, Case 5I shows peak fields of over 13 MV/m. As the breakdown field strength in plastics tends to be around 20 MV/m. Real-world samples often contain defects which reduce this threshold [75], it is conceivable that initiation could be caused by the breakdown of the energetic material itself.

The high peak fields observed with these abstractions, and particularly the large variation between abstractions, is in stark contrast to the results of the effective permittivity study of Chapter 3. At the maximum meshing density simulated, the peak fields observed for Case 4, see Figure 4.7, average out to 4.35 V/m, while Case 5I is observed to have peak fields to average at 6.7 V/m, see Fig. 4.15, an increase of 55% in field strength or 140% in energy density. The highest peak fields observed over the course of Case 5I is 8.2 V/m, an increase of 89% in field strength and 255% in energy density over 65 times the incident energy density. For cubical and spherical structures, the effective permittivity is observed to vary by less than 5%, see Fig. 3.11. The effective relative permittivity of the cubical abstractions at 35% is 1.6. A solid block of this permittivity would expect to have a field with an instantaneous peak strength of .88 V/m, less than 10% of the peak value observed in the time-domain simulation. The effective permittivity therefore vastly underestimates both
parameters of interest, the maximum peak field anywhere in the medium, as well as the variation between different abstractions.

Both Cases 5 and 6 are characterized by a general absence of uniformity throughout the medium. Both structures possess many sharp edges and corners while displaying similar peak field localization results. This suggests that non-uniformity and overall randomness are important considerations when investigating field localization. It is also important to consider multiple randomized structures to find the maximum peak field. This supports the idea that there are multiple sub wavelength scattering events and scattering paths collectively generating a much stronger peak field, extant over a period and space much smaller than that of the excitation wave. To enable the multiple scattering events, it is preferable to simulate a large structure. Smaller structures, 2D structures and structures artificially enlarged through periodicity all decrease the impact of these events.

Overall, the abstraction of the inclusions offered significant insight into the behavior of EM waves in granular composites. Electric field hotspots are observable with significantly reduced effort in computing. It was determined that the rotation and translation of the cubes combine to generate an effect on the field localization greater than either of the individual components. In particular, the multiple corner observation should be able to significantly refine the scope of any future extensions of this research.

Despite some limitations, the results presented in this chapter should be of benefit to the broader field of energetic material neutralization research. The acquisition of precise field values at very fine time and space resolutions in three dimensions also allows for a full three-dimensional coupling of electromagnetic and thermal effects in the microwave excitation of energetic materials. To the best of the author’s knowledge, such an investigation has yet
to be performed, and will be the focus of the next chapter.
Microwave-Induced Thermal Behavior

5.1 Introduction

The chemical processes which lead to detonation or deflagration of energetic materials are induced or aggravated by a variety of stress factors. Among these, it has been suggested that initiation by EM excitation is due to the localized shifting of electric charges by an electric field, which weakens chemical bonds within the material at the molecular level and facilitates their breakage [9], [51]. This effect is augmented by the heating of the material due to the dielectric loss of an EM wave [47], [52]. Increased levels of both temperature and charge gradients in the materials have also been shown to reduce initiation thresholds for excitation via shock or acoustic sources [39], [51]. Thus, it is important that any potential EM or EM-hybrid initiation/neutralization system seeks to maximize peak electric field and temperature rise by EM-induced heating.

Experimental investigations of EM standoff initiation generally involve the use of laser sources [1], [3], [4], [46]. Lasers, known for their high intensities, are an attractive choice to
maximize charge gradients and heating. However, these laser beams are typically highly focused, with sub-millimeter beamwidths – over distance, beam spreading rapidly reduces the observed power density. Thus, the effective range demonstrated in experiments is often very low [45] or requires a laboratory environment with a focusing system of mirrors and lenses [4], which limits their applicability in real world situations. In addition, EM waves at laser frequencies (750 nm to 10 µm) have poor penetrative capabilities and are also easily blocked, most noticeably by the ground, limiting their efficacy against buried devices.

In contrast to lasers, microwaves are known for their ability to penetrate many common mediums relatively unimpeded, including soil types from around the world [76], [77]. Though most effective below 10 GHz, attenuation rates remain reasonable up to 100 GHz. Recent developments have demonstrated gigawatt power pulsed microwave sources in the 10 GHz range with ranges of several meters [71]. With increases in range and penetration, directed microwave beams could have a distinct advantage in the neutralization of buried and hidden explosives.

The penetrative properties of microwaves come with drawbacks. In particular, the relatively low loss of microwaves in most mediums limits the volumetric power density transferred to the medium as heat. Previous investigations using microwaves have demonstrated substantially lower heating rates than those with lasers [2], [42], [57], resulting in reduced reliability of initiation. To ensure the viability of a microwave excitation system, the reliability and time to event should both be improved. To more effectively exploit the microwave excitation of energetic materials, the precise behavior of the EM fields within the scattering medium and the thermal changes induced by these fields must be understood.

The objective of this chapter is to determine the peak electric field and maximum heating
that occurs in the material for an incident electric field with magnitude an approaching the breakdown condition in air, which is approximately 3 MV/m, representing the some of the highest fields that can be transmitted in a directed beam. This provides information to gauge the feasibility of a standoff microwave neutralization system. Using the abstractions of Chapter 4, field simulations are performed for a composite medium of RDX and estane binder. The resulting temperature changes caused by these fields are obtained using a thermal simulator. This approach offers insight into the temperature behavior within the medium, as well as the ability to analyze temperature changes over time in very small timesteps, two capabilities lacking in experimental studies.

5.2 Approach

Ideally, physical insights into the behavior of energetic systems would be obtained through experimentation and accompanying measurements, which are respectively inherently dangerous and difficult to record. To minimize this danger, experiments often use small samples of material, which generally burn rather than violently explode [2], [39]. Indirect forms of measurement may also be employed, as in situ electric field measurements within an exploding energetic material are infeasible. Such indirect data may range from surface temperature measurements using infrared cameras [2], [27], [45], to the analysis of acoustic data recorded during the explosion event [38].

However, such system-level measurements can not describe the mechanisms behind detonation and deflagration, which requires very fine resolutions in both space and time. Thus, it is important that highly localized effects in both field and temperature are recorded, as changes that occur in very small windows of space and time can incite initiation in
energetic materials. Previous investigations have shown field power densities up to 50 times higher than the incident wave [47], [78]. Proper modeling of field extrema caused by sub-wavelength scattering and geometries are therefore crucial to (understanding) these events.

There have been previous investigations which have utilized simulations to study temperature and field behavior in these materials in high resolution. Brown and Zikry performed an extensive analysis to examine the temperature change caused by an array of coupled stress factors, including EM excitation [47]. Pickles et al. examined effective permittivity properties to determine the potential of composite energetic materials to absorb and retain energy [12], [26].

Due to the complicated nature of these mediums – inclusions may be on the scale of microns, while the composite structure may have a volume of cubic centimeters – all investigations must compromise on their thoroughness. This may manifest as a reduction to two-dimensions [5], [47], significant simplification in the shape of the inclusions [5], or the de-emphasis of inclusion-scale scattering in favor of a bulk analysis [12], [26].

This work performs full 3D EM simulations while maintaining the contribution of sub-inclusion scale field variations. The time resolution is on the scale of picoseconds. Abstraction of the inclusions is still necessary, though the abstraction level is somewhat lower than those of some previous investigations, and has proven to be effective in maintaining electric field localization at the desired scale [78]. In addition, the dielectric heating of the system will be modeled at the same space scale. Both the EM and thermal simulations will be performed in the time domain, allowing for peak field values to be recorded in time. This allows for an instantaneous peak value to be recorded rather than a value average over
a time window, reducing the possibility that critical peaks are not captured due to lack of time resolution.

5.3 Methods

To complete the desired thermal analysis of the RDX-estane composite, a process is necessary which couples the EM and thermal effects. Commercial solutions which analyze coupled EM, thermal and additional effects exist [79]. However, the level of detail at which the methods are implemented results in runtimes unacceptable for this work. It is necessary to devise a more streamlined process which maintains acceptable levels of accuracy and precision.

5.3.1 Methods-Medium

The simulation medium used throughout this investigation is illustrated in Figure 5.1. The medium is modeled as a cubical block populated with cubical inclusions. The block measures 1.3 mm by 1.1 mm by 1.05 mm, and the cubes vary in side length from 0.7 to 1.3 mm. The structure is generated by a C++ script using the Bullet physics library, as described in [78], see Appendix C. Such a structure of cubes has been shown to display comparable levels of field localization to that of more complex structures, substantially improving upon a commonly used abstraction with a spherical inclusion model. Cubical crystals of randomly chosen size are dropped into a box similar to that shown in Figure 5.1, and the entire system is shaken to distribute the crystals throughout. Each crystal is given a randomly defined collision box which extends up to 0.02 mm beyond its physical
Table 5.1 Physical parameters of RDX and estane binder.

<table>
<thead>
<tr>
<th></th>
<th>RDX [42], [47]</th>
<th>Estane [47]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1820</td>
<td>1190</td>
</tr>
<tr>
<td>Specific Heat (J/kg-K)</td>
<td>1190</td>
<td>1500</td>
</tr>
<tr>
<td>Thermal Conductivity (W/m-K)</td>
<td>0.29</td>
<td>0.14</td>
</tr>
<tr>
<td>Relative Permittivity, Real</td>
<td>2.54</td>
<td>1.13</td>
</tr>
<tr>
<td>Relative Permittivity, Imaginary</td>
<td>0.003</td>
<td>0.0117</td>
</tr>
</tbody>
</table>

dimensions to prevent an orderly structure. The material chosen for the inclusions is RDX and the binder an estane polymer, the EM and thermal material properties of which are presented in Table 5.1. It should be noted that the values used for RDX are from a different source than those in Chapter 4, which did not contain thermal properties. The overall volume fraction of the RDX inclusions is approximately 37%, slightly higher than those of the mediums of Chapter 4, though still in the range typical of homemade explosives. The simulation process is divided into two separate portions, an EM simulation of a microwave excitation, and a thermal simulation of the medium’s thermal response to the EM behavior.

5.3.2 Methods-Electromagnetics

The EM and thermal portions of the simulation are separated, with the EM analysis performed first. These simulations are performed in Remcom’s xFDTD tool [10]. The software runs on a Dell Precision 7810 with 172 GB of memory, with certain simulations accelerated using two Nvidia K20 Tesla GPU accelerators. The generation and meshing of the structure does not utilize the GPUs.

As shown in Figure 5.1, an EM plane wave is applied from the \(-x\) direction. The waveform of the excitation signal is a 16.5 GHz sinusoid. This microwave frequency is chosen
Figure 5.1 Simulation structure (shown here in xFDTD).
based on previous investigations which displayed successful initiation of energetic materials with EM excitation. The magnitude of the electric field is 1 MV/m, a relatively high value, but significantly less than the breakdown field strength in air of approximately 3 MV/m. Neither the RDX inclusions nor the estane binder displays a significant magnetic response. In addition, there is to date no evidence to suggest that magnetic fields influence initiation. The recorded data is therefore limited to the electrical field response of the system. The excitation is run over four periods of the sinusoid, and the electric field is recorded at all points on the mesh at a polling interval of 1/120th the period of the excitation, approximately 8.3 ps.

The simulation space is terminated with absorbing boundary conditions implemented using the perfectly matched layer (PML) method, at a distance from the scattering medium equal to the medium’s size.

### 5.3.3 Methods-Thermal

The thermal simulation is performed separately from the EM simulation. A uniform initial temperature of 300 K is assumed throughout the medium. The field values recorded from the EM simulation are used to determine the electric heating response of the medium through the dielectric heating equation (assuming magnetic effects are negligible):

\[
\frac{dQ}{dt} = \omega \cdot \varepsilon_0 \cdot \varepsilon_{r,\text{imag}} \cdot E^2
\]  

(5.1)

where \( \frac{dQ}{dt} \) is the rate of heating, \( \omega \) is the angular frequency of the EM wave, \( \varepsilon_{r,\text{imag}} \) is the imaginary relative permittivity of the material, \( \varepsilon_0 \) is the free-space permittivity, and \( E \)
is the electric field magnitude. In addition to the dielectric heating, thermal diffusion is incorporated using the heat conduction equation:

\[ \rho c_p \frac{dT}{dt} = \kappa \nabla^2 T \]  

(5.2)

where \( T \) is the Temperature, \( \rho \) is the material density, \( c_p \) is the specific heat of the material, and \( \kappa \) its thermal conductivity. To accommodate the grid-like meshing structure utilized by the FDTD method in the EM simulator, the Laplacian in Equation 5.1 is realized in its three-dimensional finite difference form, as

\[ \nabla^2 (f(x, y, z)) = \sum_{i=1,2,3} f((x, y, z) + e_i \cdot (\Delta x, \Delta y, \Delta z)) - 2f(x, y, z) + f((x, y, z) - e_i \cdot (\Delta x, \Delta y, \Delta z)) \]  

\[ \frac{\Delta x^2}{\Delta x^2} \]  

(5.3)

As the material outside the scattering medium is treated as vacuum, there is no conduction of heat, and the conduction equation is disregarded. At the edges of the medium, the Laplacian is terminated with a single-sided differential in the direction of the border. This termination method is chosen to avoid the temperature gradients that would occur if heat were allowed to dissipate into the vacuum, which would be unrepresentative of the structure, as it is part of a larger block of material.

This portion of the simulation is implemented in MATLAB, see Appendix D.

### 5.3.4 Methods-EM Thermal Coupling

The total duration of the electromagnetic simulation is only four cycles (0.4 ns), too short to generate a significant change in temperature. This limitation is due to the fineness of the EM mesh required to achieve the necessary spatial and temporal resolution, it is necessary
to limit the timeframe – spatial and temporal resolutions are directly linked in the FDTD method – because of the very large data sets produced. The response during the time of the first cycle is ignored due to startup effects. Also, the excitation must be windowed to be physically realizable, as illustrated in Figure 5.2. The response of the last cycle is ignored as well, leaving 122 ps of electric field data in between. To couple this into a significant thermal response, this electrical response is repeated for a duration of 4 ms. This is justified as previous results have shown the field response to remain stable after the initial buildup [78]. It also assumes that the permittivity of the medium remains constant as the temperature increases, while permittivity is well known to vary with temperature. This assumption is commonly used [5], [42]. More recent investigations have shown dielectric properties of HMX (a similar energetic material), to remain relatively constant. The real permittivity, which is several orders of magnitude higher than the imaginary component, is shown to vary less than 1% between temperatures of 300 K and 400 K [27].

The EM simulation timescale is much finer than is necessary to accurately model thermal conductivity. In addition, attempting to perform the thermal simulation at the time resolution of the EM process would result in exorbitant runtimes. Therefore, to perform the simulation within a reasonable timeframe and maintain accuracy, the thermal conduction simulation is slowed down. This is accomplished by not updating the conduction behavior as often as the dielectric heating. While the dielectric heating is updated every period, the thermal conduction is only updated every 2000 RF cycles.

In the simulations reported here, peak memory usage is 150 GB during meshing, and virtual disk during post-processing of results. Typical runtimes for the EM simulation is 70 minutes and 18 hours for the thermal simulation.
Figure 5.2 Windowed sinewave showing the first two cycles of the excitation.

5.3.5 Section Summary

It was necessary to create a more efficient, faster simulation method to suit the goals of this investigation. This began with the generation of the composite medium, a carryover from the method of Chapter 4 using the Bucket script, with the important distinction of an added estane binder. The EM simulation was also similar to that of Chapter 4, performed in xFDTD with the Bucket generated medium and a 10 GHz sinusoidal excitation. A method for simulating dielectric heating and thermal conduction from the field data using finite-difference equations was also developed.

The difficulty arose in the simulation of the EM-induced thermal activity. Due to orders of magnitude in difference between the time constants of the electric field and temperature change, it was necessary to effectively slow down the EM data to be relevant on the temperature timescale. To this end, the dielectric heating due to the microwave excitation was
analyzed in periods of 2000 cycles, rather than the 250 timesteps per RF cycle with which
the EM simulation is considered. It was also assumed that the induced fields and dielectric
heating rate did not change with time.

5.4 Results

Per the methods of the previous section, the EM and thermal results are coupled, but
generated separately. As the features and potential impacts of EM results have been covered
extensively, the majority of the focus will be placed on the thermal results.

5.4.1 EM Results

Figure 5.3 illustrates the peak electric field data recorded in the EM simulation. To represent
the entire 3D medium in a two-dimensional image, the values on the color plot represent the
maximum instantaneous electric field over the $x$ dimension (direction of wave propagation),
and the time period of the recording (122 ps). The maximum peak value of the electric
field magnitude at any location is 2.910 MV/m, with a mean value of 0.880 MV/m. The
maximum field magnitudes are recorded in the RDX crystal, where the mean peak field is
0.730 MV/m. In the binder, the maximum peak field magnitude is 2.235 MV/m, with a mean
value of 0.968 MV/m. The discrepancy between the relative maximum and mean values
is attributed to fields which may be very high at the surface of inclusions, but decrease
substantially into the material. The peak fields occur at the edges of individual inclusions,
and the area of localization spreads over the RDX-binder interface. That is, the maximum
fields in both the RDX and binder are observed at these corners and edges of inclusions.
Figure 5.3 Cross section of peak electric field strength in MV/m, maximum value over $x$ projected onto $y$-$z$ plane.
It bears repeating that in addition to the role the electric field plays in the dielectric heating process, it is also relevant in its ability to incite instability in chemical bonds. This has been shown to combine with thermal, acoustic and mechanical stresses to lower the overall threshold for initiation [1], [4], [9]. Such bond weakening could intensify the impact of the increased temperatures caused by dielectric heating relative to similar changes in temperature caused by non-EM sources - the contribution of the electric field goes beyond simply that of its induced heating.

5.4.2 Dielectric Heating per Cycle

The dielectric heating density from Equation 5.1 is integrated over the 122 ps duration of the EM simulation to obtain the total change in heat due to dielectric loss over two periods of sinusoidal excitation. This is illustrated in the color plot in Figure 5.4. Similar to Figure 5.3, the values on the color plot represent the maximum heat change over the \( x \) dimension (direction of wave propagation):

A maximum heat change of 18.52 J/m\(^3\) is observed, with a mean value of 2.695 J/m\(^3\). The maximum heat change occurs in the binder, where the mean value is 3.94 J/m\(^3\). In the RDX crystal, the maximum is 7.724 J/m\(^3\), while the mean is only 0.558 J/m\(^3\). For comparison, a 1 MV/m plane wave orthogonally incident on an infinite medium of RDX or binder would transmit a field of magnitude .771 MV/m into the RDX or .9694 MV/m into the binder. This would correspond to dielectric heating of .7986 J/m\(^3\) and 4.9234 J/m\(^3\) in the binder over the same two cycle period. The peak heating in the RDX is nearly 10 times higher, while the peak heating in the binder is approximately 3.8 times higher.

Despite the high field values in the crystal, the relatively small loss coefficient results
Figure 5.4 Cross section of heat transfer density over two periods of excitation sinusoid in J/m$^3$, maximum value over $x$ projected onto $y$-$z$ plane.
in substantially less heating. It is apparent through examination of Figures 2 and 3 that the electric field hotspots and heat transfer hotspots mostly align, due to the presence of relatively high fields in the binder near the electric field peaks just inside the crystal inclusions. It is apparent that the locations of maximum heat generations are on the edges of crystals near the electric field peaks, and would presumably not be present in their absence.

5.4.3 Conduction Heat Transfer over Time

The thermal simulator is run for 30,000 thermal cycles or 60 million RF cycles (3.7 ms) and implemented Equations 5.1 and 5.2, with Equation 5.1 updating on each period and 5.2 updating every 1000 periods. Over the duration of the simulation, there are five locations within the medium which displayed significantly higher than average temperatures. These five spots are circled in Figure 5.5. Figs. 5.5–5.8 were developed using the same method as Figs. 5.3 and 5.4, where the color represents the maximum temperature over the $x$ dimension (projected in the $y$-$z$ plane).

After 500 cycles it is observed that the electric field localizations in Figure 5.3(a) align with the temperature peaks in Figure 5.5(a). Locations 1 and 2 show the highest temperature, with increases of 2–3 degrees over the initial 300 K, with locations 3 and 5 showing only a slightly lower temperature. Location 4 at this point shows very mild and unfocused heating. Examining the conduction heat transfer map in Figure 5.5(b), the locations with the highest conducted heat influx are in the proximity of the temperature peaks. This, along with the clear delineation between the crystal and the binder and the observation that the heat transfer on the crystal side is much higher, reinforces the suggested behavior that the highest
Figure 5.5 Thermal status at 1 million cycles (60.6 µs) projected in the $y$-$z$ plane: (a) temperature in kelvin; and (b) temperature change due to conduction in K/µs. The circles in (a) identify five locations of interest over the course of the simulation.
temperatures are occurring in the binder in the proximity of the electric field hotspots.

After 5000 cycles, the dominance of locations 1 and 2 has faded, and location 5 has taken over as the area of highest temperature. Location 4 still displays relatively measured temperature change. The conduction map still shows similar behavior to the Figure 5.5, though with significantly greater magnitudes as temperature gradients have become more pronounced. One noticeable change is a blurring of lines over the whole structure, suggesting that the conduction is taking effect, even though the plot of conduction heat flow looks relatively unchanged.

After 15,000 cycles, locations 1 and 2 are severely diminished and the peaks at the two locations are no longer discernible from each other, forming a small pocket of slightly above average heating. Conduction heating in the inclusions towards the bottom of the Figure is beginning to increase. This conduction is spread over a larger area with temperatures that, though higher than the average across the medium, are not among the highest in the medium.

After 30,000 cycles, it is apparent that the high binder areas near location 4 dominate with a large area of high heating, with Locations 3 and 5 still having the highest overall temperatures. By comparison, locations 1 and 2 are much further down in temperature. The areas of highest conduction heat transfer are focused towards the bottom of the cross section, where the material is more loosely packed.
Figure 5.6 Thermal status at 10 million cycles (606 µs) projected in the $y$-$z$ plane: (a) temperature in kelvin; and (b) temperature change due to conduction in K/µs. The circles in (a) identify five locations of interest over the course of the simulation.
Figure 5.7 Thermal status at 30 million RF cycles (1.82 ms) projected in the $y$-$z$ plane: (a) temperature in kelvin; and (b) temperature change due to conduction in K/µs. The circles in (a) identify five locations of interest over the course of the simulation.
Figure 5.8 Thermal status at 60 million RF cycles (3.64 ms) projected in the $y$-$z$ plane: (a) temperature in kelvin; and (b) temperature change due to conduction in $K/\mu s$. The circles in (a) identify five locations of interest over the course of the simulation.
5.4.4 Behavior within Inclusions

While Figures 5.5–5.8 were chosen to best display the gradual change of temperature throughout the medium, they are unable to show behavior within the individual inclusions. Specifically, taking the maximum temperature in the x direction obscures lower temperatures within the inclusions. Figure 5.9 takes a cross section at a single value of $x$ rather than a maximum over the whole range, taken from the temperature data at the end of the simulation (30,000 cycles). The location in the $x$ dimension corresponds to that of location 3 in Figures 5.5–5.8. It is observed that there is a consistent decrease in temperature below the surface of the inclusions. Larger inclusions have the largest temperature ranges, and the centers of these inclusions show temperatures which are the lowest in the entire medium. The dielectric heating here is expected to be low, as the results of Section 5.4.1 suggest low field strengths in these regions. The conduction heating which should be occurring, given their relative proximity to the high temperatures is unable to penetrate very far into the medium. This is observable in Figure 5.10, where very small portions of binder are responsible for the large conduction heat transfer to the edges and corners of inclusions, while the relatively higher volume of the inclusion interiors relative to the corners results in lower heating rates in these areas.

5.4.5 Section Summary

Thermal progression of the RDX-estane composite was analyzed via the temperature tracking of five locations of interest within the material. While binder material in the immediate vicinity of areas of high field localization (corners and edges of the RDX crystal) initially
Figure 5.9 Single dx cross section, chosen at 30000 cycles, showing cold interior of inclusions, temperature in Kelvin
Figure 5.10 Single dx cross section, chosen at 30000 cycles, showing conduction heat transfer within inclusions. Heat transfer in mJ/m³.
displayed the highest temperatures, the advantage steadily shifted to areas with higher concentrations of the estane binder material. The higher dielectric heating rate of the binder resulted in large pockets of binder with high temperature, the centers of which were shielded from conduction loss. Meanwhile, the relatively isolated binder at the corners of crystals lost large amounts of heat due to conduction to the neighboring RDX, which lagged behind in temperature due to low dielectric heating.

The temperature of the RDX below the surface of individual inclusions was shown to be particularly low. This is partially due to very low fields in the inclusion interiors resulting in weak dielectric heating, and exacerbated by the high ratio of cold to hot material of the interior relative to the corners, resulting in diluted conduction heat transfer per unit volume.

### 5.5 Graphical Analysis of Thermal Progression

The previous section tracked the temperature profile of the system with color contour plots, other behavior is better represented in the forms of Figure 5.11, which shows the temperature progression of five locations of interest within the medium. These were the five locations which displayed temperatures at or near the maximum within the medium for a significant portion of the simulation, as shown in Figure 5.5. The mean temperature of the entire system, henceforth referred to as the bulk temperature, is included for comparison:

The geometries of these hotspots are shown in Figure 5.12, where the yellow shading represents RDX and blue represents the binding polymer. Hotspots 1 and 2 are close in proximity, with being of 2 inclusions coming in close contact at an angle. These 2 locations also correspond to the areas of highest field localization shown in Figure 5.3. Hotspots 3
Figure 5.11 Absolute temperature (a) across entire medium (b) of five locations of interest, average temperature across structure for comparison, recorded over entire simulation.
and 5 are areas where inclusions are relatively close to each other, but not to the degree of
the first 2. Hotspot 4 is in a relatively loosely packed area consisting mostly of binder.

At the beginning, the areas of with inclusions in close proximity, hotspots 1 and 2, exhibit
high rates of heating, as shown in Figure 5.13. These rates drop off extremely quickly, to the
point where the show rates very similar to that of the bulk heating rate. Locations 3 and 5,
which contain a relatively lower density of crystal, show a much more gradual slowdown
of temperature, falling to half their initial rate after approximately 1.22 ms, compared to
approximately 0.78 ms for location 1 and 0.49 ms for location 2. Meanwhile location 4, which
is has the highest concentration of binder, shows the most constant rate of temperature
increase, and is the only location to show an increase in the rate of temperature change at
any point. It should be noted that although the temperatures of the locations diverge over
the duration of the simulation, they all remain above the bulk temperature for the duration
of the recorded period.

The differing behavior of these hotspots may be further explained by examining the rela-
tive change in the heating rates via dielectric heating and heat transfer through conduction,
ilustrated in Figure 5.14. Because the dielectric heating is constant over the simulation, this
comparison effectively realizes as a scaled version of Figure 5.13. It should be noted that the
Bulk heating rate is not perfectly flat, due to the boundary conditions imposed. Towards
the end of the simulation period, the bulk heating rate has surpassed that of locations 1
and 2, which continue to decrease. This suggests that while the bulk temperature has not
yet caught up in the scope of Fig 5, it would do so were the simulation period extended.

Examining the heating rates of the locations of interest, it is apparent that conduction
in all cases except location 4 works very quickly to counteract the effects of the dielectric
Figure 5.12 Local geometries of locations of interest
Figure 5.13 Total heating rate at each location of interest over entire simulation, bulk for comparison
heating. This effect is exaggerated in locations 1 and 2, with high local volume fraction of RDX behavior which suggests an overall flow of heat from the binder into the crystal.

This is confirmed in Figure 5.15, which shows the overall flow of heat due to conduction in both the RDX and binder. Presented as the total change in temperature, it is apparent that energy is consistently moving from the Binder into the RDX. This is partially due to the lower specific heat of the RDX relative to the binder material, but the major driving mechanism for this behavior appears to be the disproportionately high at which the binder is heated in comparison to the RDX.

**Figure 5.14** Conduction heating rate at each location of interest, the bulk response is shown for comparison
Figure 5.15 Total heating rate of RDX and binder due to conduction over entire simulation

5.5.1 Distribution

Figure 5.16 shows a histogram of the final distribution (after 30000 cycles) of temperatures within the medium, separated into individual plots for the distribution in the RDX and binder. The histogram edges are placed at each whole Kelvin. Overall, the Binder temperatures are substantially higher than that of the RDX crystals, even factoring in the higher volume fraction. The RDX temperatures follow a relatively smooth distribution, while the binder contains groups of aberrant temperatures. This is due to the behavior shown in Figure 5.9, where the majority of the volume of each individual crystal is held at a significantly lower temperature than the maximums which occur on the surface, and a gradual temperature gradient is observed with increasing depth into the inclusion.
Figure 5.16 Histograms of temperature distribution in: (a) RDX and; (b) binder at end of simulation, each division in the $x$–axis is 1 Kelvin
5.6 Chapter Summary/Discussion

Based on these predictions, a working hypothesis is that the highest electric fields occur in regions where there is high packing density of inclusions, resulting in a large number of corners and edges. This has been demonstrated before [12], [78]. However, the heating is much more efficient in the binder, and as such the location of the highest temperature gradually shifts to regions with the highest density of binding material. Between the two fill factor extremes, there is a balance of binder and field-localization inducing features. The highest temperatures of the RDX inclusions are at the surfaces.

Final peak temperatures in the RDX and Binder are 371 K and 378 K, respectively. In comparison, a 1 MV/m wave orthogonally incident on a solid block of material would generate a bulk temperature increase of 10.3 K for RDX and 81.4 K for the binder. The field peaking and conduction of the random structure has very little impact on binder temperatures, but results in an almost sevenfold increase in temperature rise in the RDX crystals. As the regions near RDX crystals are the most significant for the purposes of initiation, this peak temperature increase is directly correlated to the success of a neutralization system utilizing dielectric heating as the main stress mechanism.

Figure 5.9 shows that the inner portions of the RDX inclusions remain at relatively low temperatures, even though the high temperature difference compared to the surface should cause high levels of heat flow towards the interior due to conduction. This shows that the conduction moves very slowly relative to the dielectric heating. High temperature gradients are possible, although the areas of low temperature must be relatively far from the binder, where the heating is relatively efficient.
The positive heat transfer into location 4 is curious, in that it necessitates a neighboring location of higher temperature. As can be seen in Figures 5.5–5.8, location 4 resides between several local hotspots. Thus, its progression towards the highest temperature in the medium benefits from the field localizations in its vicinity, at least initially. This suggests that even though the highest temperature in the structure was at a location of moderate field strength, the presence of electric field peaks in surrounding areas contributes to these more moderate areas.

For relatively loosely packed explosives, such as the one considered here, the presence of binder results in relatively quick bulk heating. The relatively high level of binder present in these mixtures would allow for relatively straightforward heating of the binder. If the excitation does not cause the energetic material to explode, it may be possible to raise the temperature of the binder sufficiently to deform and neutralize the material. For highly packed energetic materials with binder volume fractions below 10%, bulk heating would be less prevalent. The results here suggest that ‘voids’ of binder in between crystals would be areas of interest in generating high heat at the surface of crystals, presenting an area of weakness. Eliminating these voids would increase the materials resistance to electromagnetic initiation.

This investigation focused solely on cubical inclusions. This results in a very predictable temperature profile within the individual inclusions, as shown in Figure 5.9. Different inclusion shapes may display different conduction properties, though it seems unlikely that this increase could overcome the heating efficiency. However, combined with findings that certain shapes are highly effective at creating field localizations [31] this may result in different heating behavior in mediums comprised of such inclusions. This is not particularly
useful for the neutralization of hostile devices, as such shapes are synthesized through a separate process, and unlikely to be naturally present in existing energetic materials. It may find application in the modification of friendly explosives.

### 5.7 Comparison to Previous Studies

In general, it is difficult to make a one to one comparison of studies involving electro-magnetic energetic materials. There exists a wide range of setup conditions valid for their individual purposes, varying across factors such as choice of explosive/binder material or excitation frequency and power. In addition, the inherently randomized nature of these composite structures renders direct comparison insignificant and possibly invalid.

Nonetheless, it may be informative to compare results with closely related investigations, focusing on more general trends rather than specifics. The range of studies is kept small, limited to those with conditions relatively similar to this work – limited to RDX or HMX (a similar energetic material) composites under microwave (1 to 30 GHz) excitation. These are summarized in Table 5.2. The important distinctions separating this work from all the others are the use of the cubic abstractions and the FDTD method, both of which allow for substantial gains in computing efficiency.

Details of the field and temperature results will now be discussed. These may be found in the source material [5], [27], [42].

The works of Perry et al. [5] and Daily et al. [42] both use high fill factors and substantially abstracted structures. The bulk analysis and lack of binder in Daily’s work result in an extremely slow and even heating process. Perry’s simulations display the closest peak field values to this work. However, the extremely high concentration of energetic material
substantially limits the heating rate and displays temperature surfaces which lack inclusion
level details. Still, it is apparent that locations of interest are dominantly within the binder,
particularly at the inclusion interfaces.

The most relevant work is by Kort-Kamp et al. [27], which utilizes a plane wave excita-
tion of similar frequency and duration, as well as similar values for the material thermal
properties, the thermal conductivity of the binder a notable exception. However, relative
permittivity values of the crystal and binder in [27] are much closer than those of this work.
This may be a contributing factor of the significantly reduced peak fields relative to the
excitation, hardly any increase is observed.

However, the distribution of the fields show similar properties to that of Section 5.4.1 –
with field peaks near the surface of inclusions and substantially lower levels throughout
the bulk. In both cases, the interiors of crystals displayed significantly lower temperatures,
barely increasing from the initial temperature. These agreements give increased in the
cubic abstractions and the FDTD method.

5.8 Conclusion

The cubic abstractions and Bucket script of Chapter 4 have been incorporated into a
simulation process which couples the dielectric heating from the electric fields with heat
transfer within the medium due to thermal conduction. Compared to previous studies,
this process offers significant advantages in ease and time of setup, as well as its use of the
FDTD method and its superior scaling with increased computing resources. It also served
as a further test of validity for our abstractions.

From a results perspective, the highest temperatures were observed in the binder. The
Table 5.2 Comparison of this work with similar studies

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fill Factor</td>
<td>95%</td>
<td>100%</td>
<td>≤15%⁴</td>
<td>37%</td>
</tr>
<tr>
<td><strong>Energetic Material</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>–</td>
<td>1900</td>
<td>1910</td>
<td>1820</td>
</tr>
<tr>
<td>Spec. Heat (J/kg-K)</td>
<td>–</td>
<td>1013</td>
<td>1165³</td>
<td>1190</td>
</tr>
<tr>
<td>Therm. Cond. (W/m-K)</td>
<td>–</td>
<td>.503</td>
<td>.2814³</td>
<td>.29</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>4.8 + j0.01</td>
<td>3.48 + j0.0026</td>
<td>5.0 + j0.007³</td>
<td>2.54 + j0.003</td>
</tr>
<tr>
<td><strong>Binder Material</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>–</td>
<td>–</td>
<td>1200</td>
<td>1190</td>
</tr>
<tr>
<td>Spec. Heat (J/kg-K)</td>
<td>–</td>
<td>–</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>Therm. Cond. (W/m-K)</td>
<td>–</td>
<td>–</td>
<td>.25</td>
<td>.14</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>2.3 + j0.02</td>
<td>–</td>
<td>4 + j0.38</td>
<td>1.13 + j0.012</td>
</tr>
<tr>
<td><strong>Simulation Details</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Simulation Type</td>
<td>FEM</td>
<td>FEM</td>
<td>FEM</td>
<td>FDTD</td>
</tr>
<tr>
<td>Crystal Abstraction</td>
<td>Circles (2D)</td>
<td>Bulk</td>
<td>None⁴</td>
<td>Cubes</td>
</tr>
<tr>
<td>Frequency (GHz)</td>
<td>2.45</td>
<td>10</td>
<td>13.3</td>
<td>16.5</td>
</tr>
<tr>
<td>$</td>
<td>E</td>
<td>_{\text{incident}}$ (MV/m)</td>
<td>1</td>
<td>.412</td>
</tr>
<tr>
<td>$</td>
<td>E</td>
<td>_{\text{peak}}$ (MV/m)</td>
<td>2.47</td>
<td>–</td>
</tr>
<tr>
<td>Duration (ms)</td>
<td>154</td>
<td>400</td>
<td>20</td>
<td>3.7</td>
</tr>
<tr>
<td>$T_{\text{initial}}$</td>
<td>300</td>
<td>273</td>
<td>293</td>
<td>300</td>
</tr>
<tr>
<td>$T_{\text{max}}$ (K)</td>
<td>347</td>
<td>550²</td>
<td>420²</td>
<td>378</td>
</tr>
</tbody>
</table>

¹ Perry et al. did not report thermal material properties
² Estimated from source figures
³ Varied over temperature, listed value at 350 K
⁴ Scan of HMX composite sample
binder also displayed a substantially higher mean temperature than the crystals, with
distribution of high temperatures throughout the structure. On the other hand, the RDX
crystals were observed with very low fields and temperatures in the crystal interiors, which
constitute the majority of the material's volume, though the RDX does display a combina-
tion of very high fields and relatively high temperatures at the surface of crystals. These
temperature increases are over seven times that predicted by a bulk heating of the binder.
Since the binder is generally inert, these locations present a likely possibility for an initiation
point due to a microwave source.

More importantly, from a process perspective, the successful implementation of the
methods of Section 5.3 holds great promise for future studies of electromagnetic propa-
gation in complex composite mediums. The in-house methods utilized in both the C++
based Bucket script and MATLAB-based thermal simulator allow incredible flexibility in
both the generation of the medium and the processing of results, while the FDTD method
offers simple meshing and significant gains with parallel computing. The combination
of these factors offers unmatched flexibility in defining, solving and analyzing complex
scattering mediums.
Chapter 6

Conclusion

6.1 Summary of Chapters

This dissertation investigated the behavior of microwave EM radiation in composite mediums, specifically those of the energetic material RDX. Particular emphasis was placed on mediums with an inclusion density of approximately 30%, typical of an improvised explosive device. The overall goal of this research is determining the potential of a standoff microwave neutralization system for these explosives comprised of RDX or similar materials, and to suggest relevant considerations for the implementation of such a system. Progress in this endeavor is limited by the difficulty of conducting experimental studies, as well as the long runtime and high computing requirements of simulations. To that end, this work explored the viability of various forms of abstractions meant to ease computing requirements and speed up simulations capable of capturing peak fields, and the induced heating, with extremely high resolution in time and space. The work began with an investigation in the use of an effective permittivity to characterize the composite mediums of
interest, see Chapter 3. More detailed abstractions at the inclusion level were explored in Chapter 4. Finally, Chapter 5 performed an EM-thermal coupling using the abstractions of Chapter 4, generating an overall picture of both electric field and temperature behavior throughout the medium.

### 6.1.1 Effective Permittivity

Chapter 3 investigated the use of effective permittivity as a characterizing metric for RDX composite mediums. Such a characterization was attractive for its potential to reduce a complex scattering problem to a single parameter. The effective permittivity estimated the effective permittivity of composite structures to determine whether variation among the type of inclusion considered significantly impacted this metric.

To develop a baseline for comparison, several established effective permittivity models were introduced. These included the Wiener bounds, the theoretical limit on the effective permittivity, the Hashin-Shtrikman bounds, a more stringent set of bounds, and the Maxwell-Garnett approximation and Bruggeman model, two methods of estimating the effective permittivity of inclusion based composites with low filling factor. These baselines were determined via calculation from the models’ defining equations.

To determine the effective permittivity of a specific structure, a waveguide like simulation setup was designed in xFDTD. A two-port rectangular waveguide was created, with electric conductors perpendicular to the direction of polarization and magnetic conductors parallel to the direction of polarization, designed to create periodicity and reduce the limitations of a restricted simulation space. The effective permittivity was extracted via an evaluation of the transmission scattering parameter, $S_{21}$, of the two-port system.
A variety of inclusion types was examined, ranging over single, few and many-element structures of slabs, spheres and cubes. While all of these structures were considered for a fill factor of 30%, several received increased attention. The structures comprised of slabs were simulated for fill factors from 0 to 50% at intervals of 5%, while structures of regularly placed spheres and regularly placed but randomly rotated cubes were simulated at 10 fill factors between 0 and 34%.

The calculated effective permittivities of the slabs were in good agreement with the Wiener bounds, a promising result. Effective permittivities of the structures of cubes and spheres at identical fill factors showed almost indiscernible differences from each other over the range, and were close to that of the Maxwell-Garnett approximation. The same held true for the wider variety of structures simulated with 30% fill factors.

With the completion of Chapter 4, it became clear that there was far greater variation in the local electric field behavior, particularly the small-scale peak field, than was suggested by any differences observed in the effective permittivity of various structures in Chapter 3. These fine resolution peaks also possessed far higher magnitudes than suggested by the effective permittivity. This lack of variation in effective permittivity over different inclusion types relative to the wide range of observed field localization using the abstractions of Chapter 4, and the overall weaker field results predicted, led to the conclusion that effective permittivity is an ineffective characterization of the crystalline composites of interest.

6.1.2 Abstraction of Inclusions

Chapter 4 explored a variety of inclusion abstraction levels meant to simplify the simulation process. These abstractions included single and multiple element structures of cubes
and spheres, with a range of randomness in the placement of the inclusions. An initial analysis of six cases was performed, with the objective of determining the peak field localization generated at any point in space and time for each case. The first five cases were the single sphere (Case 1), the single randomly rotated cube (Case 2), the multiple cubes with matching alignment on a regular grid (Case 3), the multiple spheres with positions randomly offset from a regular grid (Case 4), and the multiple cubes with random rotation and randomly offset positions (Case 5). The final case utilized a script, based on a compute game physics engine, to generate randomly sized and positioned inclusions (Case 6). All inclusions possessed a characteristic dimension of 100 \( \mu m \). The structures utilized RDX for the inclusions with no binder (vacuum). A plane-wave microwave pulse centered at 16 GHz, with a spectrum from 3 to 30 GHz, was used as the excitation.

The initial analysis revealed good agreement between peak fields observed in Case 6, the most physically realistic abstraction, and Case 5. This agreement progressively weakened for Cases 4 through 1. Case 5 recorded peak fields over six times that of the incident value, and over three times that seen in Case 1. These peak fields occurred over spaces of tens of microns, a fraction of the size of the inclusions and close to \( \frac{1}{200} \)th that of the free-space wavelength of the excitation. Although an asymptotic result with respect to increased meshing was not definitively reached for Case 5, which is estimated to occur at a meshing resolution of 2.5 microns, the peak field values at the maximum resolution of 3.3 microns comes within 3% of the projected asymptotic value at 2.5 microns. While computational improvements for Cases 1 through 4 were greater than that for Case 5 (which still displayed impressive gains), greatly improved accuracy elevated the abstraction of Case 5 above the others when all factors were considered in determining the optimal abstraction.
As Case 5 displayed the greatest promise for future use as an abstraction of energetic composites, further investigation was performed on it and its constituent elements of randomness. Case 5 was separated into Case 5R, where only random rotation of the cubes was performed with each cube centered on a regular grid, and Case 5T, where only random offset or translation from the regular grid was performed. The original Case 5 was renamed as Case 5RT, as it contained both elements of randomness. Separate field simulations for the three cases were performed, with additional runs of Case 5RT added, supplementing those already performed. It was observed that while the use of both rotation and translation individually resulted in increased peak fields levels, the combination of both had a significantly greater impact than compounding of the effects would suggest. Also, Case 5RT displayed a much wider spread in the distribution of peak fields, suggesting the exact combination of the rotation and translation resulting in the highest fields was relatively rare, and not present in every randomly generated structure.

The final modification to Case 5 resulted in Case 5I, where the individual inclusions were both rotated and translated, with inclusions allowed to intersect. The peak fields for Case 5I were in even better agreement with those found in Case 6. Examination of the resulting field distributions suggested the importance of local geometries, particularly the presence of multiple corners and edges in close proximity. The highest fields observed in this Chapter were 8.2 V/m, over eight times the incident field strength and over 65 times the incident field energy density. These peaks were observed over resolutions of less than 10 µm and 20 ps, a fraction that of the incident wavelength and period.

Overall, it was determined that a cubic abstraction with multiple elements of randomness created the best abstraction when considering both accuracy and improvements in
computational efficiency. The computational gains are impressive, while the accuracy is close to that of the realistic Case 6 model. The randomly oriented cube abstraction was over 10 times faster than the much more complex Case 6 model. Moreover, it was not possible to simulate Case 6 under all conditions because of computational requirements, as the placement and meshing of the inclusions led to excessive memory use.

6.1.3 Microwave-Induced Thermal Behavior

The cubic abstractions of Case 5 in Chapter 4 were used in Chapter 5 to perform simulations combining the electric field behavior along with thermal conduction. This was accomplished by simulating the electric field response in xFDTD, while using an in-house script to model the thermal dynamics in MATLAB. The simulation setup was similar to that of Chapter 4, with the notable inclusion of an estane binder to promote heat diffusion, as well as a change in the excitation to a 16.5 GHz sinusoid. The inclusions were generated with a combination of random factors from Cases 5 and 6: specifically using cubic inclusions but maintaining the randomized script-based inclusion placement. Due to a difference of many orders of magnitude between the time constants of the electric field and thermal conduction responses, the thermal response is far slower, it was necessary to perform the two with different timesteps to have a feasible runtime. As xFDTD already operates at the largest timestep allowed by the FDTD method, the cumulative dielectric heating over 2000 periods of the excitation is used when considering heat transfer.

Results were presented in the form of both color contour plots showing the distribution of temperatures throughout the medium at select time points, as well graphs tracking specific locations of interest over the duration of the simulation. Initially, temperatures
rose quickly at the corners of high field localization, with lower temperatures in the binder. However, the more effective heat absorption of the binder gradually overcomes this, as areas with high presence of energetic material drains the initial hotspots of heat through conduction. The locations of highest temperature transition to areas with ever-increasing binder concentrations, until the highest temperature is observed in an area of almost entirely binder. After 3.6 ms, the highest temperature in the composite medium is observed at 378 K in the binder and 371 K in the RDX, with an overall mean temperature of 340 K. The majority of the RDX volume, that beneath the immediate surface region, show low temperatures over the course of the simulation, with average temperatures over the entire RDX regions 30 K lower than the peak of 371 K after 3.6 ms. In comparison, the same incident field on a solid block of material would result in a 10.3 K increase in RDX; the randomized composite displays a nearly sevenfold gain in peak temperature increase in the RDX.

The higher absorption efficiency of the binder ultimately leads binder heavy areas to dominate the upper end of the temperature distribution. However, regions of high fields correspond to the highest temperature regions in the immediate vicinity of inclusions, and thus remain promising as possible locations of initiation. While the interiors of the RDX inclusions remain relatively cold, this is of less concern, as activity is typically found to begin at the surface of inclusions. The peak temperature increases at the surface are what may be directed related to the likelihood of deflagration.
6.2 Overall Conclusions

The results of this work, particularly those of Chapter 5, reveal several considerations which must be taken into account in order to maximize the potential of a standoff microwave neutralization system. The heating rates observed are reasonably quick, with peak temperatures after 3.6 ms reaching 375 K from an initial uniform temperature 300 K, and suggest that the material should reach critical temperatures in under 100 ms. However, such heating rates require a massive sustained excitation field with a magnitude (1 M\textbf{V}) close to one third the breakdown field strength in air. It was also seen that random scattering effects cause peak fields within the medium approaching 8 MV/m, approximately half the estimated breakdown value of pure RDX (between 15 and 20 MV/m). The effective permittivity study of Chapter 3 indicated that for a filling factor of 30% the effective relative permittivity is approximately 1.5. The power transmitted into such an effective medium is 80.8% of that of the incident wave, indicating a peak field of .899 MV/m for an incident field of 1 MV/m. This is considerably less when scattering was considered in the medium. Real world samples would potentially display lower thresholds, particularly at the surface of inclusions where fields are highest, where half-molecules, dangling bonds, and mobile charges which may cause intrinsic gradients.

Characterization via an effective permittivity was shown to be ineffective for identifying localized behavior. In contrast, the abstractions used in this work are capable of capturing highly localized behavior in crystalline composite mediums. The aforementioned field peaks are over eight times the incident value across spaces of less than 10 \(\mu\text{m}\), while the peak temperature increases in the RDX are nearly seven times that predicted by a bulk
analysis, while spanning spaces of less than 30 µm. This localized behavior is seen using abstractions with features on the scale of 100 µm with an incident wavelength several orders of magnitude higher, while also reducing simulation times by an order of magnitude and memory consumption by half.

6.2.1 Potential of a Microwave System

Devices capable of generating such fields would appear to approach the territory of destructive directed energy weapons, going against one of the main motivations for a microwave neutralization system: the promise of a system with more finesse and subtlety. While sources capable of generating these fields at reasonable ranges exist, their use is not widespread, and significant advances are necessary to make their implementation practical. Under such a combination of high excitation fields, which require a more focused beam, and relatively long exposure times, the prospect of a wide area microwave scanning neutralization system seems impractical.

At present, it appears that the heating generated exclusively by EM excitation is not quite sufficient to reliably cause deflagration without these extremely high fields. Perhaps more promising is utilizing coupled excitations of different types. To this end, substantial value lies in the abstractions used, and the advantages conferred relative to an exhaustive recreation. At a minor cost in accuracy, these abstractions offer greatly increased simulation efficiency, allowing for greatly increased simulation speed, higher resolutions in time and space, or the flexibility to define some combination of both. This is accomplished while maintaining the behavior of interest, the existence of extremely high field strengths relative to the input excitation, highly localized in both space and time.
It is therefore recommended that further study focus on initiation of energetic materials through small-scale electric field peaking rather than temperature increases due to dielectric heating. The high power requirement and extended duration required would render a system reliant on dielectric heating extremely inefficient and unwieldy for sweeping over large areas. Sweeping cross-sectional area of several square meters would consume terajoules of energy, as well as potentially cause heat damage to the entire area.

Although the mechanisms behind the initiation of energetic materials through strong electric field or charge gradients are not as well understood, it is known that fields existing over extremely short periods in time and over very small dimensions in space are capable of triggering such processes. As the field behavior varies very little over the excitation duration, a small (<10) number of RF cycles would be sufficient, resulting in less time spent in simulation, as well as less energy consumed in real world applications. In addition, studies at the molecular level often couple many stresses, allowing for the methods of Chapters 4 and 5 to have their maximum possible utility.

Initiation by small-scale electric field stresses appears to the most promising path forward for any potential microwave neutralization system, requiring greatly reduced energy, time to event, and offering a greater coverage area. Continued pursuit of a system reliant on heating and temperature gradients, and may only be feasible for small areas at reduced range, reducing the field loss over distance due to wave spreading. It would also possible to apply the potential electric field stress neutralization system at close ranges for increased effects.
6.3 Future Work

6.3.1 Extensions of this Work

To give better perspective on the strength of the abstractions used in Chapter 4, it may be beneficial to determine the maximum field possible given the materials and geometries presented. While the present comparison with Case 6 is informative, comparisons with an irrefutable reference field strength would provide greater confidence. For instance, the fields near inclusion corners of a small set of dielectric crystals. Such a set of calculations or simulations would be time-consuming but relatively straightforward.

A degree of variation in the system not investigated is that of the input excitation. The excitation frequencies were chosen to mirror previously successful demonstrations of initiation, and also correspond to a range of the EM spectrum with particularly strong penetration capabilities. As such, future studies considering a large variation in excitation frequency are not recommended. It is, however, possible that the study of different waveforms in the same frequency leads to greater insight. This work considered sinusoidal excitations in Chapters 3 and 5, and a broadband pulse in Chapter 4. More complex waveforms such a time-varying sinusoid, random or pseudo-randomly generated waveforms could exhibit different behavior than observed here. The methods in this work are readily applicable to such a study with the exception of the dielectric heating equation, which would need to be adapted for varying frequencies.
6.3.2 System Level Considerations

The primary difficulty confronting future studies in this field remains the necessity of simulation structures which are severely limited in size. This is especially true for studies of many coupled effects, such as EM, thermal, mechanical and chemical. Any such simulations would place far greater strains on computing than the ones in this dissertation, which are by no means insignificant. While chemical processes may be faster, EM responses at microwave frequencies have time constants far shorter than most thermal and mechanical processes. Thus, gains made in the EM domain have great impact on the speed of the overall study. The advantages offered by the methods in this dissertation could substantially increase the breadth and depth of any such multi-excitation studies.

A system exploiting coupled excitations may deviate from the original vision of a stand-off microwave microwave system. Direct thermal and mechanical excitations may be limited in their effective range. A possible solution utilizing a remotely controlled robot may be able to safely apply multiple excitation types at a close distance. Such a system would also ease requirements of the EM source, allowing for the use of close-range, high power devices. Regardless of the excitation types used, the methods in this work would retain their utility.

While two different excitation waveforms, a pulse and a sinusoid, were used over the course of this work, there remains substantial room for variation. For example, excitations with time-varying, perhaps randomized, frequency content may prove beneficial in generating the highest fields possible, as peak field location and magnitude has been seen to vary with excitation frequency, as well as the direction of incidence and polarization. A system swept over all such variables would present the greatest likelihood of generating the highest possible fields.


FDTD Structure Generation

The following scripts allow for procedural generation of Cases 1–5 in Chapter 4, and may also be used for the cubic and spherical cases of Chapter 3. The scripts run in xFDTD’s scripting environment. The main input variables are as follows:

- $a, b, c$: These three variables define the number of inclusions on the grid in the $x$, $y$ and $z$ directions, respectively.
- $blocksize$: Length of an individual cubic inclusion in millimeters.
- $inc$: separation between
- $add"$: This boolean value determines whether or not to queue the simulation after generating the structure. Recommended off, memory intensive.
- $matlimit, Material1, Material2$: For multiphase composites, Material1 and Material2 may be defined as different materials, while matlimit is the ratio, from 1 to 100, used to randomly determine the material for each inclusion.
A.1 Cubical Inclusions

```javascript
var add = false;
var numRuns = 1;
var initialRun = 1;
var addSensors = true;
var k = 1/10000; //inches (2.54/100), cm (1/100), or mm (1/1000)
var a = 6;
var b = a;
var c = a

function RandomRun(limit,matLimit,blockSize)
{
    var cellmm = blockSize/17;
    var cellSize = "\" + cellmm + "\"mm";
    k = blockSize/1000;
    var project = App.getActiveProject();
    var Material2 = project.getMaterialList().getMaterial("Al");
    var Material1 = project.getMaterialList().getMaterial("nonmetal");
    var pi= Math.acos(0);
    var inc = 1.6;
    ;
    var index = 0;
    for(N=1;N<inc*a;N=N+inc)
```
index = index + 1;
//n = k*(N+Math.random()/4);
var r = new Recipe();
for(O=1;O<inc*b;O=O+inc)
{
//o = k*(O+Math.random()/3 + (index%2)/2*inc);
for(Z=0;Z<inc*c;Z=Z+inc)
{
  o = k*(O+Math.random()/3 + (index%2)/2*inc);
n = k*(N+Math.random()/4);
z = k*(Z+Math.random()/3+(index%2)/2*inc);
var ran1 = 2*pi*Math.random();
var ran2 = 2*pi*Math.random();
var ran3 = 2*pi*Math.random();
sin1 = Math.sin(ran1);
sin2 = Math.sin(ran2);
sin3 = Math.sin(ran3);
cos1 = Math.cos(ran1);
cos2 = Math.cos(ran2);
cos3 = Math.cos(ran3);
A11 = cos2*cos3;
A12 = -cos2*sin3;
A13 = sin2;
A21 = sin1*sin2*cos3 + cos1*sin3;
A22 = -sin1*sin2*sin3 + cos1*cos3;
A23 = -sin1*cos2;
A31 = -cos1*sin2*cos3+sin1*sin3;
A32 = cos1*sin2*sin3 + sin1*cos3;
A33 = cos1*cos2;

xp = -k/2;
d = k;

//Rotation Transforms
n1 = n + A11*xp+A12*xp+A13*xp;
o1 = o + A21*xp+A22*xp+A23*xp;
z1 = z + A31*xp+A32*xp+A33*xp;
n2 = n + A11*(xp+d)+A12*xp+A13*xp;
o2 = o + A21*(xp+d)+A22*xp+A23*xp;
z2 = z + A31*(xp+d)+A32*xp+A33*xp;
n3 = n + A11*(xp+d)+A12*(xp+d)+A13*xp;
o3 = o + A21*(xp+d)+A22*(xp+d)+A23*xp;
z3 = z + A31*(xp+d)+A32*(xp+d)+A33*xp;
n4 = n + A11*xp+A12*(xp+d)+A13*xp;
o4 = o + A21*xp+A22*(xp+d)+A23*xp;
z4 = z + A31*xp+A32*(xp+d)+A33*xp;
n5 = n + A11*xp+A12*xp+A13*(xp+d);
\[ o_5 = o + A_{21}x_p + A_{22}x_p + A_{23}(x_p + d) \]
\[ z_5 = z + A_{31}x_p + A_{32}x_p + A_{33}(x_p + d) \]

var add = Math.random();
if (add < limit)
{
  var sketch = new Sketch();
sketch.addEdge(new Line( new Cartesian3D(n1,o1,z1), new Cartesian3D(n2,o2,z2) ) );
sketch.addEdge(new Line( new Cartesian3D(n2,o2,z2), new Cartesian3D(n3,o3,z3) ) );
sketch.addEdge(new Line( new Cartesian3D(n3,o3,z3), new Cartesian3D(n4,o4,z4) ) );
sketch.addEdge(new Line( new Cartesian3D(n4,o4,z4), new Cartesian3D(n1,o1,z1) ) );
  var path = new Sketch();
path.addEdge( new Line( new Cartesian3D(n1,o1,z1), new Cartesian3D(n5,o5,z5) ) );
var sweep = new SweepPath(sketch, path);
r.append(sweep);
var mat = Math.random();
}
}
View.zoomToExtents();
//var project = App.getActiveProject();
//var part = project.getGeometryAssembly().at(0);
//var meshParams = project.getMeshParameters(part);
//meshParams.enableXACT(true);
m = new Model(r);
if (mat>matLimit)
{
  project.setMaterial(m, Material1);
}
if (mat <= matLimit)
{
  project.setMaterial(m, Material2);
}
}
m.name = "M"+index+"";
project.getGeometryAssembly().append(m);
}
}
function AddSensors()
{
var loops = App.getActiveProject().getGeometryAssembly().size();
//App.getActiveProject().getNearFieldSensorList().clear();
for (n =0;n<a;n=n+1)
{ 
    m = n+1;
    var nearFieldSensorList = App.getActiveProject().getNearFieldSensorList();
    var sensor = new SolidSensor();
    sensor.name = "P"+m+"";
    var geo = new SolidPartSensorGeometry();
    var geopart = App.getActiveProject().getGeometryAssembly().at(n+1);
    geo.setPart(geopart);
    sensor.setGeometry(geo);
    var sensorDataDefinitionList = App.getActiveProject().getSensorDataDefinitionList();
    var solidDef = sensorDataDefinitionList.at(0);
    sensor.setDataDefinition(solidDef);
    nearFieldSensorList.replaceNearFieldSensor(sensor.name,sensor);
}
}

function Add2Queue()
{
    // Create and start the simulation.
    var simulation = App.getActiveProject().createSimulation( true );
    Output.println( "Successfully created the simulation." );
}
Output.println( "Simulation\Path_=/" + simulation.
    → getSimulationPath() );
}
for( runs = initialRun; runs<=numRuns; runs = runs+1)
{
    //App.getActiveProject().getGeometryAssembly().clear();
    RandomRun(1,0,.1);
    numParts = App.getActiveProject().getGeometryAssembly().size();
    for(p = 0; p<numParts; p = p+1)
    {
        var project = App.getActiveProject();
        var part = project.getGeometryAssembly().at(p);
        var meshParams = project.getMeshParameters(part);
        meshParams.enableXACT(true);
    }
    if(addSensors == true)
    {
        AddSensors();
    }
    if(add == true)
    {
        Add2Queue();
    }
A.2  Spherical Inclusions

var add = false;
var numRuns = 1;
var initialRun = 1;
var clear = false;
var addSensors = false;
var k = 1/10000; //inches (2.54/100), cm (1/100), or mm (1/1000)

function RandomRun(limit,matLimit,blockSize)
{
    var cellSize = "a" + "\_mm";
    App.getActiveProject().getGrid().getCellSizesSpecification().
        setTargetSizes(new Cartesian3D(cellSize,cellSize,cellSize));
    var project = App.getActiveProject();
    var Material2 = project.getMaterialList().getMaterial("Al");
    var Material1 = project.getMaterialList().getMaterial("nonmetal");
    var pi= 2*Math.acos(0);
    var inc = 1.4;
    var a = 1;
    var b = 9;
    var c = 9;
    var index = 0;
    var zprev = 0;
var aaa = 7*inc;

//for(N=1;N<inc*a;N=N+inc)
for(N=aaa;N<aaa+inc;N=N+inc)
{
    index = index + 1;
    n = k*(N+(Math.random()- .5)/4);
    for(O=1;O<inc*b;O=O+inc)
    {
        o = k*(O+(Math.random()- .5)/4 + (index%2)/2*inc);
        for(Z=0;Z<inc*c;Z=Z+inc)
        {
            var r = new Recipe();
            z = k*(Z+(Math.random())-.5)/4;
            var cub = new Sphere(.5*k)
            r.append(cub);
            oD = k*(Math.random())-.5)/7*inc;
            nD = k*(Math.random())-.5)/7*inc;
            zD = k*(Math.random())-.5)/7*inc;
            var tz = new Translate(new Cartesian3D(nD,oD,
                zD));
            r.append(tz);
            var txyz = new Translate(new Cartesian3D(n,o,z
                ));
        }
    }
}
r.append(txyz);

m = new Model(r)
m.name = "M"+index+"";

project.getGeometryAssembly().append(m);
}

function AddSensors()
{

var loops = App.getActiveProject().getGeometryAssembly().size();
App.getActiveProject().getNearFieldSensorList().clear();
for (n =0;n<1;n=n+1)
{

m = n+1;

m = 1;

n = 0;

var sensor = new SolidSensor();
sensor.name = "SensorM"+m+"";
var geo = new SolidPartSensorGeometry();
var geopart = App.getActiveProject().getGeometryAssembly().at(n);
geo.setPart(geopart);
sensor.setGeometry(geo);
var sensorDataDefinitionList = App.getActiveProject().getSensorDataDefinitionList();
var solidDef = sensorDataDefinitionList.at(n);
sensor.setDataDefinition(solidDef);
var nearFieldSensorList = App.getActiveProject().getNearFieldSensorList();
nearFieldSensorList.addNearFieldSensor( sensor );
}
}

function Add2Queue()
{
    // Create and start the simulation.
    var simulation = App.getActiveProject().createSimulation( true );
    Output.println( "Successfully created the simulation." );
    Output.println( "Simulation Path = " + simulation.getSimulationPath() );
}

for( runs = initialRun; runs<=numRuns; runs = runs+1 )
{
    if(clear)
    {
        App.getActiveProject().getGeometryAssembly().clear();
    }
RandomRun(1,0,1);

numParts = App.getActiveProject().getGeometryAssembly().size();
    for(p = 0; p<numParts; p = p+1)
    {
        var project = App.getActiveProject();
        var part = project.getGeometryAssembly().at(p);
        var meshParams = project.getMeshParameters(part);
        meshParams.enableXACT(true);
    }

if(addSensors == true)
{
    AddSensors();
}

if(add == true)
{
    Add2Queue();
}
MATLAB Effective Permittivity Calculator

The following script estimates the effective permittivity of a medium from the scattering parameter $S_{21}$ via an iterative Newton method. The real and imaginary values of $S_{21}$ are entered as ordered pairs. The other inputs are the excitation frequency $f$, in Hz, and the length of the structure in the direction of propagation $d$, in meters. The script runs in MATLAB.

```matlab
f = ;
k = 2 *pi*f/3e8;
%S21 separate real, imag
S21 = [

]
S21(:,2) = S21(:,2)*-1i;
S21 = sum(S21,2);

d = 1.1/1000;
```
eff = 1.2;
for N=1:size(S21)
    while true
        Z = (1/eff)^.5;
        R = (Z-1)/(Z+1);
        n = eff^.5;
        dn = 1/2/eff^.5;
        dZ = -Z/2/eff;
        dR = 2*dZ/(Z+1)^2;
        S = S21(N);
        F = S * (1-R^2*exp(-2*i*k*d*n))-(1-R^2)*exp(-i*k*d*n);
        if abs(F)<1e-8
            break
        end
        dF = -2*S*exp(-2*i*k*d*n)*R*(dR-i*k*R*dn)+exp(-i*k*d*n)*((1-R)
        eff = eff - F/dF;
    end
    eperm(N) = eff;
end
Bucket Script

The following script is used to generate a composite random medium via the Bucket game. A graphical representation of the medium is not generated by this script and must be created separately. Options within the script allow for the use prisms, cubes or spheres of various size. The structure is exportable as a list of vertices for cubes and prisms, or a list of centerpoints and radii for spheres. The script provides a menu interface with a list of input options. Before running the script, cubes, prisms or spheres must be selected by modifying the function genDelCrystals function to only include one of the following functions (comment out the others):

- **genCube**: Generates cubical inclusions. The function variables crysRadius and randMargin define the cube size and expanded collision box, respectively. These include random elements by default.

- **genSphere**: Generates spherical inclusions. The function variables randRadius and randMargin define the cube size and expanded collision box, respectively. These
include random elements by default.

• genPrismRead: Generates prism inclusions. Requires a txt file which includes the vertices of a pool of prism shapes, one random shape per row. The file must be defined in the call to readCrystalGeometry() in the main function.

// CrystalDrop.cpp : Defines the entry point for the console application.

//
#include "stdafx.h"
#include <iostream>
using namespace std;
#include <btBulletDynamicsCommon.h>
#include <LinearMath\btIDebugDraw.h>
#include "GLDebugDrawer.h"
#include <GL/glew.h>
#include <vector>
#include <string>
#include <time.h>
#include <fstream>
#define PI atan(1) * 4
static string outputDir = ""
static int numCrystals = 0;
static bool pyramid = true;
static int addCrystals = 0;
static float localTime = 0.0;
static char menu;
static float dBox;
static int hack = 0;
static float hBox = 10.0;
static btCollisionShape* boxShape[6];
static btRigidBody* boxRigidBody[6];
static btDiscreteDynamicsWorld* simWorld;
static std::vector<btDefaultMotionState*> crysMotionState;
static std::vector<btCollisionShape*> crysShape;
static std::vector<btRigidBody*> crysRigidBody;
static btSequentialImpulseConstraintSolver* solver;
static btCollisionDispatcher* dispatcher;
static btBroadphaseInterface* broadphase;
static btDefaultCollisionConfiguration* collisionConfiguration;
static std::vector<std::vector<std::vector<float>>> crysVerticesRead;
static int currentNumCrystals = 0;
static int steps = 0;
static int sheetWidth = .01;
static bool isShaking = false;
static int shakeStep = 0;
static bool topOn = 0;
static double crysDepth;
static double crysRadius;
static clock_t startTime; //Start timer
static clock_t testTime;
static clock_t timePassed;
static double secondsPassed;
static void throwFit(void)
{
    cout << "Error";
}
static void activateAll(void)
{
    for (int n = 0; n < numCrystals; n++)
    {
        crysRigidBody[n]->activate(1);
    }
}
static bool checkMovement(void)
{
    int nState;
    for (int n = 0; n < numCrystals; n++)
    {
        nState = crysRigidBody[n]->getActivationState();
    }
if (nState == 1) return true;
}
return false;
}
static void initWorld(void)
{
  GLDebugDrawer* debugDrawer = new GLDebugDrawer();
debugDrawer->setDebugMode(1);
broadphase = new btDbvtBroadphase();
collisionConfiguration = new btDefaultCollisionConfiguration
  ();
dispatcher = new btCollisionDispatcher(collisionConfiguration
  );
solver = new btSequentialImpulseConstraintSolver;
simWorld = new btDiscreteDynamicsWorld(dispatcher, broadphase
  , solver, collisionConfiguration);
simWorld->setDebugDrawer(debugDrawer);
simWorld->setGravity(btVector3(0, -10, 0));
}
static void deleteAllOthers(void)
{
  /* Cleanup
   */
delete simWorld;
delete solver;
delete collisionConfiguration;
delete dispatcher;
delete broadphase;
}
static void addTop(void)
{
    btVector3 trans = btVector3(0, hBox, 0);
    btDefaultMotionState* groundMotionState = new btDefaultMotionState(btTransform(btQuaternion(0, 0, 0, 1), trans));
    pyramid = false;
    if (pyramid)
    {
        btVector3 points[9] = {
            btVector3(dBox, hBox, dBox),
            btVector3(dBox, hBox, -dBox),
            btVector3(-dBox, hBox, -dBox),
            btVector3(-dBox, hBox, dBox),
            btVector3(dBox, 2 * hBox, dBox),
            btVector3(dBox, 2 * hBox, -dBox),
            btVector3(-dBox, 2 * hBox, -dBox),
            btVector3(-dBox, 2 * hBox, -dBox),
        };
    }
btVector3(-dBox, 2 * hBox, dBox),
btVector3(0, 2*hBox, 0)
};
for (int n = 0; n < 3; n++)
{
    btConvexHullShape* prismShape = new
        btConvexHullShape();
    switch (n)
    {
    case 0:
        prismShape->addPoint(points[0], false);
        prismShape->addPoint(points[1], false);
        prismShape->addPoint(points[8], false);
        break;
    case 1:
        prismShape->addPoint(points[1], false);
        prismShape->addPoint(points[2], false);
        prismShape->addPoint(points[8], false);
        break;
    case 2:
        prismShape->addPoint(points[2], false);
        prismShape->addPoint(points[3], false);
        prismShape->addPoint(points[8], false);
break;

case 3:
    prismShape->addPoint(points[3], false);
    prismShape->addPoint(points[0], false);
    prismShape->addPoint(points[8], false);
    break;
}
prismShape->recalcLocalAabb();
btRigidBody::btRigidBodyConstructionInfo
   groundRigidBodyCI(0, groundMotionState,
   prismShape, btVector3(0, 0, 0));
btRigidBody* top = new btRigidBody(
   groundRigidBodyCI);
simWorld->addRigidBody(top);
}
return;
}

btRigidBody::btRigidBodyConstructionInfo groundRigidBodyCI(0,
   groundMotionState, boxShape[0], btVector3(0, 0, 0));
boxRigidBody[5] = new btRigidBody(groundRigidBodyCI);
simWorld->addRigidBody(boxRigidBody[5]);
}

static void genDelBox(bool genDel)
btVector3 trans = btVector3(0, 0, 0);
btDefaultMotionState* groundMotionState = new btDefaultMotionState(btTransform(btQuaternion(0, 0, 0, 1), trans));
if (genDel)
{
    boxShape[0] = new btBoxShape(btVector3(dBox, sheetWidth, dBox));
    boxShape[1] = new btBoxShape(btVector3(sheetWidth, hBox/2, dBox));
    boxShape[2] = new btBoxShape(btVector3(sheetWidth, hBox/2, dBox));
    boxShape[3] = new btBoxShape(btVector3(dBox, hBox/2, sheetWidth));
    boxShape[4] = new btBoxShape(btVector3(dBox, hBox/2, sheetWidth));
    btVector3 trans;
    for (int n = 0; n < 5; n++)
    {
        switch (n)
        {
        case 0:
trans = btVector3(0, 0, 0);
break;

case 1:
    trans = btVector3(-dBox, hBox/2, 0);
    break;

case 2:
    trans = btVector3(dBox, hBox/2, 0);
    break;

case 3:
    trans = btVector3(0, hBox/2, -dBox);
    break;

case 4:
    trans = btVector3(0, hBox/2, dBox);
    break;
}

btDefaultMotionState* groundMotionState = new
    btDefaultMotionState(btTransform(
        btQuaternion(0, 0, 0, 1), trans));
btRigidBody::btRigidBodyConstructionInfo
groundRigidBodyCI(0, groundMotionState, 
    boxShape[n], btVector3(0, 0, 0));
boxRigidBody[n] = new btRigidBody(
    groundRigidBodyCI);
simWorld->addRigidBody(boxRigidBody[n]);
}
}
else
{
    for (int n = 0; n < 6; n++)
    {
        simWorld->removeRigidBody(boxRigidBody[n]);
        delete boxRigidBody[n]->getMotionState();
    }
    delete boxRigidBody;
}
}

static std::vector<std::vector<float>> genCubeGeometry(double dR)
{
    cout << dR;
    int sides = 4;
    std::vector<std::vector<float>> singleCrystalVertices(sides * 2);
    float x, y, z, dx, dy, dz;
    float theta = 0;
    float phi = 0;
    dx = dR*cos(theta)*sin(phi);
dy = dR*sin(theta)*sin(phi);
dz = dR*cos(phi);
for (int n = 0; n < sides; n++)
{
    y = dR*(n % 2);
    x = dR * ((int)(n / 2));
    z = 0;
    std::vector<float> singleVertex, oppositeVertex;
    singleVertex.push_back(x);
    singleVertex.push_back(y);
    singleVertex.push_back(z);
    oppositeVertex.push_back(x + dx);
    oppositeVertex.push_back(y + dy);
    oppositeVertex.push_back(z + dz);
    singleCrystalVertices[n] = singleVertex;
    singleCrystalVertices[n + sides] = oppositeVertex;
}
return singleCrystalVertices;
}
static void genCube(int n)
{
    btScalar mass = 1;
    btVector3 crysInertia(0, 0, 0);
double randOffset = 0;
btConvexHullShape* prismShape = new btConvexHullShape();
btVector3 localInertia(0, 0, 0);
int randSides = 4;
crysRadius = (double)(rand() % 100) / 200 + .5;
crysRadius = crysRadius * 2;
std::vector<std::vector<float>> testCrystal = genCubeGeometry
    (crysRadius);
for (int i = 0; i < testCrystal.size(); i++)
{
    float x = testCrystal[i][0];
    float y = testCrystal[i][1];
    float z = testCrystal[i][2];
    prismShape->addPoint(btVector3(x, y, z), false);
}
prismShape->recalcLocalAabb();
float randMargin = (float)(rand() % 20) / 100;
prismShape->setMargin(randMargin);
crysShape.push_back(prismShape);
crysShape[n]->calculateLocalInertia(mass, crysInertia);
btQuaternion randomQ = btQuaternion(btVector3(rand(), rand(),
    rand()), rand());
btVector3 randomR = (btVector3(randOffset, 20, 0));
crysMotionState.push_back(new btDefaultMotionState(
    btTransform(randomQ, randomR));
crysRigidBody.push_back(new btRigidBody(mass, crysMotionState
    [n], crysShape[n], crysInertia));
}
static void genSphere(int n)
{
    btScalar mass = 1;
    btVector3 crysInertia(0, 0, 0);
    double randOffset = (double)(rand()%100)/100;
    double randRadius = 1;(double)((rand() % 1000) + 500) / 1000;
    float randMargin = (float)(rand() % 10) / 100;
    btSphereShape* sphere = new btSphereShape(randRadius);
    sphere->setMargin(randMargin);
    crysShape.push_back(sphere);
    btQuaternion randomQ = btQuaternion(0, 0, 0, 1);  //
    // btQuaternion(btVector3(rand(), rand(), rand()), rand())
    //;
    crysMotionState.push_back(new btDefaultMotionState(
        btTransform(randomQ, btVector3(randOffset, 20, 0))));
    crysShape[n]->calculateLocalInertia(mass, crysInertia);
    crysRigidBody.push_back(new btRigidBody(mass, crysMotionState
        [n], crysShape[n], crysInertia));
}
static void genPrismRead(int n)
{
        btScalar mass = 1;
        btVector3 crysInertia(0, 0, 0);
        double randOffset = 0;
        btConvexHullShape* prismShape = new btConvexHullShape();
        btVector3 localInertia(0, 0, 0);
        std::vector<std::vector<float>> testCrystal =
                crysVerticesRead[0];
        for (int i = 0; i < testCrystal.size(); i++)
        {
                float x = testCrystal[i][0];
                float y = testCrystal[i][1];
                float z = testCrystal[i][2];
                prismShape->addPoint(btVector3(x,y,z),false);
        }
        prismShape->reCalcLocalAabb();
        float randMargin = (float)(rand() % 1) / 100;
        prismShape->setMargin(randMargin);
        crysShape.push_back(prismShape);
        crysShape[n]->calculateLocalInertia(mass, crysInertia);
        btQuaternion randomQ = btQuaternion(btVector3(rand(), rand(),
        188
rand(), rand());
btVector3 randomR = (btVector3(randOffset, 20, 0));
crysMotionState.push_back(new btDefaultMotionState(
    btTransform(randomQ, randomR));
crysRigidBody.push_back(new btRigidBody(mass, crysMotionState
    [n], crysShape[n], crysInertia));
}
static void genDelCrystals(bool genDel)
{
    /*Generates and deletes the crystals to be dropped*/
    if (genDel)
    {
        int prevCrystals = numCrystals;
        numCrystals = numCrystals + addCrystals;
        for (int n = prevCrystals;n < numCrystals;n++)
        {
            //genPrismRead(n);
            //genPrismRand(n);
            //genSphere(n);
            genCube(n);
        }
    }
    else
for (int n = 0; n < numCrystals; n++)
{
    simWorld->removeRigidBody(crysRigidBody[n]);
    delete crysRigidBody[n]->getMotionState();
    delete crysRigidBody[n];
}

static void showMenu(void)
{
    cout << "\nmenu\ngoes\nhere";
    return;
}

static void gatherInput(void)
{
    cout << "Box\nSize:";
    cin >> dBox;
    hBox = dBox*2;
    printf("\nNumber\nof\nCrystals:");
    cin >> addCrystals;
}

static void readCrystalGeometry(string readFile)
{  
std::ifstream inFile(readFile);
float x, y, z;
std::vector<std::vector<float>> singleCrystalVertices;
int a = 0;
while (inFile >> x >> y >> z)
{
    a++;
    std::vector<float> singleVertex;
    singleVertex.push_back(x);
    singleVertex.push_back(y);
    singleVertex.push_back(z);
    singleCrystalVertices.push_back(singleVertex);
}
crysVerticesRead.push_back(singleCrystalVertices);
}
static void resetGravity(void)
{
for (int n = 0; n < numCrystals; n++)
{
    crysRigidBody[n]->setGravity(btVector3(0, -10, 0));
}
}
static void setGravity(int gX, int gY, int gZ)
{
    for (int n = 0; n < numCrystals; n++)
    {
        crysRigidBody[n]->setGravity(btVector3(gX, gY, gZ));
    }
}

static void exportVerticesC(string file) // atrocious hack
{
    ofstream outFile;
    outFile.open(""+file);
    int top = 0;
    if (topOn) top = 1;
    for (int n = 5; n < simWorld->getCollisionObjectArray().size
         - top; n++)
    {
        int M = 0;
        btRigidBody* body = static_cast<btRigidBody*>(
            simWorld->getCollisionObjectArray()[n]);
        btConvexHullShape *cs = (btConvexHullShape *)body->
            getCollisionShape();
        btMotionState *ms = body->getMotionState();
        btTransform ts;
ms->getWorldTransform(ts);
int numPoints = cs->getNumPoints();
cout << numPoints;
for (int i = 0; i < numPoints; i++)
{
    cout << i;
    btVector3 out = ts*cs->getScaledPoint(i);
    outFile << out.getX();
    outFile << ",/uni2423";
    outFile << out.getY();
    outFile << ",/uni2423";
    outFile << out.getZ();
    if (i!=numPoints) outFile << ",/uni2423";
}
outFile << "\n";
}
outFile.close();
}
static void exportVertices(string file) //atrocious hack
{
    ofstream outFile;
    outFile.open("" + file);
    int top = 0;
if (topOn) top = 1;
for (int n = 5; n < simWorld->getCollisionObjectArray().size
   - top; n++)
{
    btRigidBody* body = static_cast<btRigidBody*>(
        simWorld->getCollisionObjectArray()[n]);
    btSphereShape *cs = (btSphereShape *)body->
        getCollisionShape();
    btMotionState *ms = body->getMotionState();
    btTransform ts;
    ms->getWorldTransform(ts);
    btVector3 com = body->getCenterOfMassPosition();
    btScalar outR = cs->getRadius();
    outFile << outR;
    outFile << ",\u002C";
    btVector3 out = com;
    outFile << out.getX();
    outFile << ",\u002C";
    outFile << out.getY();
    outFile << ",\u002C";
    outFile << out.getZ();
    outFile << 
};
outFile.close();
}
static void updateInput(void)
{
    testTime = clock();
    timePassed = startTime - testTime;
    secondsPassed = -timePassed / (double)CLOCKS_PER_SEC;
    cout << "\n";
    cout << secondsPassed;
    cout << "\nAction_/to_/show_/menu:/";
    string writeTo;
    cin >> menu;
    switch (menu)
    {
        case 'm':
            showMenu();
            updateInput();
            break;
        case 'a':
            cout << "\nAdd_/how_/many?";
            cin >> addCrystals;
            genDelCrystals(true);
            break;
case 's':
    addTop();
    setGravity(0,10,0);
    activateAll();
    isShaking = true;
    topOn = true;
    break;

case 'e':
    cout << "\nOutput\nFile:";
    cin >> writeTo;
    exportVerticesC(writeTo);
    cout << "\nExport\ncomplete/\nto:/\n";
    cout << outputDir + writeTo;
    break;

default:
    cout << "\nInvalid\nInput,\nvalid\noptions\nlisted\n→\nbelow:\n\n";
    showMenu();
    updateInput();
    break;

}
static void draw(void)
{
    glClear(GL_COLOR_BUFFER_BIT | GL_DEPTH_BUFFER_BIT);
    simWorld->debugDrawWorld();
    glutSwapBuffers();
}
static void timer(void)
{
    float dtime = localTime;
    localTime = glutGet(GLUT_ELAPSED_TIME) / 100.0;
    dtime = localTime - dtime;
    if (simWorld)
    {
        simWorld->stepSimulation(dtime, 10);
        steps++;
        if (steps % 10 == 0 && currentNumCrystals<numCrystals)
        {
            cout << currentNumCrystals;
            cout << "\n";
            simWorld->addRigidBody(crysRigidBody[
                currentNumCrystals]);
            currentNumCrystals++;
        }
    }
}
if (steps%10 ==0 && currentNumCrystals == numCrystals)
{
    bool stillGoing = checkMovement();
hack = hack + 1;
if (!stillGoing)
{
    if (isShaking)
    {
        shakeStep++;
        cout << shakeStep;
        activateAll();
        switch (shakeStep)
        {
        case 1:
            setGravity(10, 0 ,0);
            break;
        case 2:
            setGravity(-10, 0, 0);
            break;
        case 3:
            setGravity(0, -10, 0);
break;

case 4:
    setGravity(0, 10, 0);
    break;

case 5:
    setGravity(0, -10, 0);
    break;

case 6:
    shakeStep = 0;
    isShaking = false;
    break;

default:
    break;

}

else updateInput();

}

if (hack == 100)
{
    hack = 0;
    updateInput();
}

}
```c
}

glutPostRedisplay();

}

static void initGlut(int argc, char** argv)
{
    glutInit(&argc, argv);
    glutInitDisplayMode(GLUT_RGB | GLUT_DOUBLE | GLUT_DEPTH);
    glutInitWindowSize(1024, 1024);
    glutCreateWindow("TEST");
    //*** init OpenGL
    glEnable(GL_CULL_FACE);
    glEnable(GL_DEPTH_TEST);
    glEnable(GL_LIGHT0);
    glEnable(GL_LIGHTING);
    glEnable(GL_COLOR_MATERIAL);
    glMatrixMode(GL_PROJECTION);
    gluPerspective(25, 1, 20.0, 100.0);
    glMatrixMode(GL_MODELVIEW);
    gluLookAt(45.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 0.0); //
        \vphantom{trimetric}
    //gluLookAt(45.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 0.0); //
        \vphantom{trimetric}
    glutDisplayFunc(draw);
```
glutIdleFunc(timer);
}

int main(int argc, char** argv)
{
    srand(time(NULL));
gatherInput();
initGlut(argc, argv);
readCrystalGeometry("");  
initWorld();
genDelBox(true);  
genDelCrystals(true);  
glutMainLoop();  
//Delete Everything  
genDelCrystals(false);  
genDelBox(false);  
deleteAllOthers();  
return 0;
}
MATLAB Thermal Scripts

The following is a pair of scripts to calculate dielectric heating levels from electric field data. The scripts run in MATLAB and requires a supplementary function which calculates the 3-dimensional discrete Laplacian. Minor customizations allow for data recording at individual time steps. The following input variables are required:

- \( c_R, c_B \): Specific Heat of the RDX and Binder.
- \( \rho_R, \rho_B \): Density of the RDX and Binder.
- \( k_R, k_B \): Thermal Conductivity of the RDX and Binder.
- \( T_0 \): Initial temperature, uniform across medium.
- \( \varepsilon_{Rim}, \varepsilon_{Bim} \): Imaginary relative permittivity component for the RDX and binder.
- \( h \): Mesh density, defined in xFDTD.
- \( dt \): Timestep in xFDTD.
• f: Frequency

• conductionFactor: Relative updating frequency of conduction relative to dielectric heating

### D.1 Dielectric Heating

```matlab
%clear;
Tmax = zeros(1,100000); TER = Tmax; TCR = Tmax; TCB = Tmax; TEB = Tmax;
baseDir = 'bullet/excitation/run5/10G/';
cR = 1260; cB = 1500; %Heat Capacity/Specific Heat in J/kg/K
rhoR = 1820; rhoB = 1190; %Density in kg/m3
kR = .29; kB = .14; %Thermal Conductivity in W/m/K
T0 = 300; %Starting Temperature
eps0 = 8.854e-12;
epsRre = 3.4; %Real Relative Permittivity
epsRim = .003; epsBim = .0117; %Fake Permittivity
expo = 100;
h = .1/40/1000; %Grid Separation
omega = 2*pi*10^9*10; %Frequency
tstep = 2.99e-12;
dt = tstep; % 5236227485288w4w848484
load(strcat(baseDir,'M1.mat')); %load part data
```
```matlab
Ex = TotalFieldE_X;
RDXpart = -1*(isnan(Ex)-1); %NaN = 0, Number = 1
RDXpart = RDXpart(:,:,1);
pZ = Z_Dimension_1;
pY = Y_Dimension_2;
pX = X_Dimension_3;
load(strcat(baseDir,'MaxDim.mat'));
sZ = zC;
sY = yC;
sX = xC;
RDXsolid = zeros(numel(zC),numel(yC),numel(xC));
RDXpart = p2sadapt(RDXpart,RDXsolid,pX,sX,pY,sY,pZ,sZ,h);
Bindpart = -1*(RDXpart-1);
[sX,sY,sZ] = size(RDXpart)
RDXpart = RDXpart(5:sX-5,5:sY-5,5:sZ-5,:);
Bindpart = Bindpart(5:sX-5,5:sY-5,5:sZ-5,:);
clearvars 'Ex' 'Ey' 'pX' 'pY' 'pZ' 'sX' 'sY' 'sZ' 'RDXSolid';
load(strcat(baseDir,'sC.mat'));
En = dataP;%(Ex.^2+Ey.^2+Ez.^2).^0.5; %|E|
En = En*2*10^6;
[sZ, sY, sX, sT] = size(En);
qdotR = zeros(sZ,sY,sX,sT);
qdotB = zeros(sZ,sY,sX,sT);
```
for t = 1:sT
    t
    qdotR(:,:,t) = omega*eps0*epsRim.*RDXpart.*En(:,:,t).^2/2;
    qdotB(:,:,t) = omega*eps0*epsBim.*Bindpart.*En(:,:,t).^2/2;
end
qdot = qdotR+qdotB;
QR = sum(qdotR,4)*dt;
QB = sum(qdotB,4)*dt;
save(strcat(baseDir,'cFMod/','Q.mat'),'QR','QB','sX','sT','sZ','sY',
     'Bindpart','RDXpart');
D.2 Conduction

%%
clearvars -except 'QB' 'QR' 'sX' 'sY' 'sZ' 'sT' 'h' 'RDXpart' 'Bindpart' 'T';
baseDir = 'bullet/excitation/run5/10G/';
start = 1;
if(start==1)
    Tmax = zeros(1,30000); TER = Tmax; TCR = Tmax; TCB = Tmax; TEB = Tmax;
    indmax = [Tmax;Tmax;Tmax]; Tmean = Tmax;
    Tmax = Tmax + 300;
    T = zeros(sZ,sY,sX)+300;
    time = zeros(1,30000);
end
% load(strcat(baseDir,'Temp5/','Tmax.mat'));
% load(strcat(baseDir,'Temp5/','T35.mat'));
% load(strcat(baseDir,'Temp5/','Q.mat'));
cR = 1260; cB = 1500; %Heat Capacity/Specific Heat in J/kg/K
rhoR = 1820; rhoB = 1190; %Density in kg/m3
kR = .29; kB = .14; %Thermal Conductivity in W/m/K
T0 = 300; %Starting Temperature
eps0 = 8.854e-12;
epsRre = 3.4; %Real Relative Permittivity
epsRim = .003; epsBim = .0117; %Fake Permittivity
h = .1/40/1000; %Grid Separation
omega = 2*pi*16.5^9*10; %Frequency
tstep = 2.99e-12;
dt = tstep; %
R = sum(sum(sum(RDXpart)));
B = sum(sum(sum(Bindpart)));
%T(:, :, :, 1) = T0;
conductionFactor = 1000;
cF = conductionFactor;
for cycle = start:30000
    A = T(:, :, :); %Current Temperature
    L = Laplacian_7(A, h); %Discrete Laplacian
    dTR = (1/rhoR/cR*(QR)).*RDXpart*cF;
    dTB = (1/rhoB/cB*(QB)).*Bindpart*cF;
    dTRC = (1/rhoR/cR*kB*L).*RDXpart*dt*sT*cF;
    dTBC = (1/rhoB/cR*kB*L).*Bindpart*dt*sT*cF;
    TER(cycle) = sum(sum(sum(dTR)))/R;
    TCR(cycle) = sum(sum(sum(dTRC)))/R;
    TEB(cycle) = sum(sum(sum(dTB)))/B;
    TCB(cycle) = sum(sum(sum(dTBC)))/B;
    dTC = dTRC+dTBC;
    dTE = dTR+dTB;
\[ T_{dotR} = \frac{1}{\rho_R/c_R} (QR) \cdot RDXpart; \]
\[ T_{dotRC} = \frac{1}{\rho_R/c_R/k_R*L} \cdot RDXpart; \]
\[ T_{dotB} = \frac{1}{\rho_B/c_B} (QB) \cdot Bindpart; \]
\[ T_{dotBC} = \frac{1}{\rho_R/c_R/k_B*L} \cdot Bindpart; \]
\[ TC = T_{dotRC} + T_{dotBC}; \]
\[ TE = T_{dotR} + T_{dotB}; \]
\[ TER(numel(Tmax)+1) = \text{mean} \left( \text{mean} \left( \text{mean}(T_{dotR}) \right) \right); \]
\[ TCR(numel(Tmax)+1) = \text{mean} \left( \text{mean} \left( \text{mean}(T_{dotRC}) \right) \right); \]
\[ TEB(numel(Tmax)+1) = \text{mean} \left( \text{mean} \left( \text{mean}(T_{dotB}) \right) \right); \]
\[ TCB(numel(Tmax)+1) = \text{mean} \left( \text{mean} \left( \text{mean}(T_{dotBC}) \right) \right); \]
\[ T(:,:,:) = T(:,:,:) + (dTC+dTE); \]
\[ Tmax(cycle) = \text{max}(\text{max}(\text{max}(T))); \]
\[ Tmean(cycle) = \text{mean}(\text{mean}(\text{mean}(T))); \]
\[ \text{save} \left( \text{strcat(baseDir,'l4max/','Tmax.mat')} \right) , 'Tmax', 'TCB', 'TCR', 'TEB', 'TER'; \]
\[ \text{save} \left( \text{strcat(baseDir,'l4max/','Tmean.mat')} \right) , 'Tmean'; \]
\[ \text{cycle} \]
\[ \text{if} \mod(cycle,500)==0 \]
\[ \text{save} \left( \text{strcat(baseDir,'l4max/','T',int2str(cycle),'.mat')} \right) , 'T', 'dTC', 'dTE'; \]
\[ \text{end} \]
\[ \text{if} \mod(cycle,10)==0 \]
\[ [\text{indmax}(cycle/10,:)] = \text{ind2sub(size(T)}, \text{find}(T==\text{Tmax}(cycle))); \]
save(strcat(baseDir,'l4max/','indMax',int2str(cycle),'.mat'),
       'indmax');
end
end
Tpart = T;