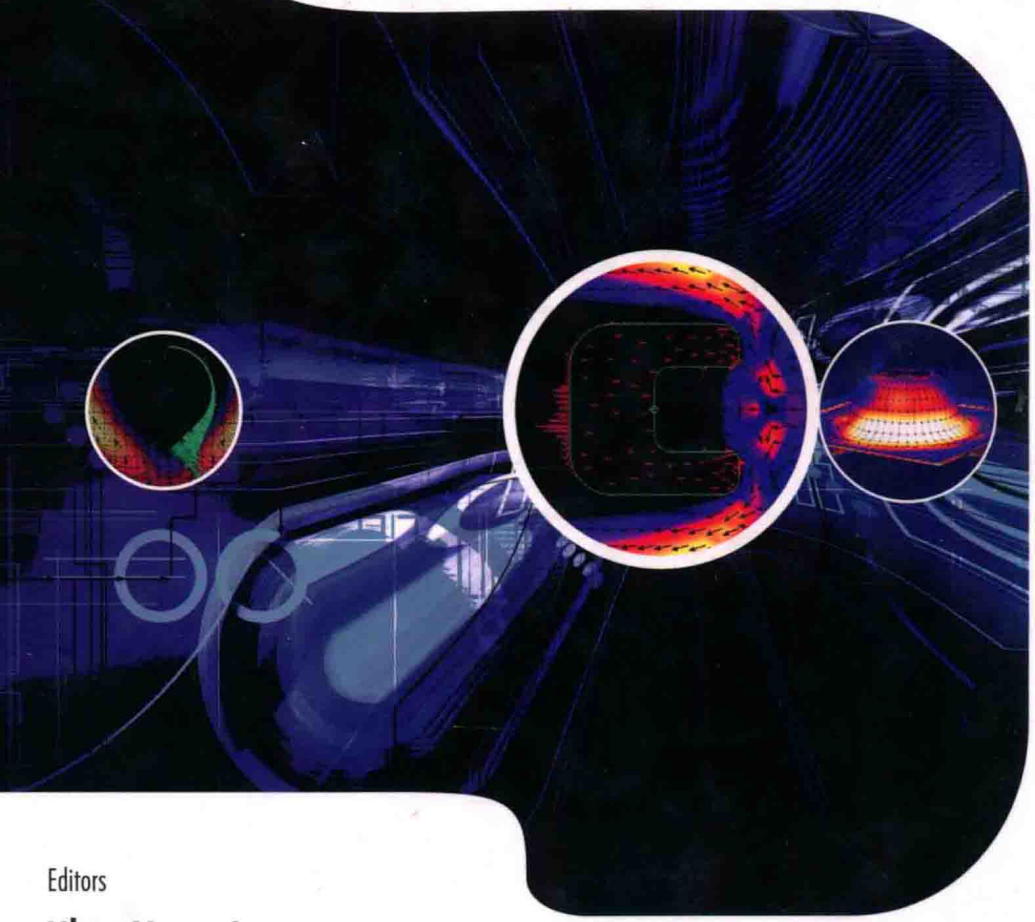
Lecture Notes Series, Institute for Mathematical Sciences,
National University of Singapore
Vol. 6



Editors
Khin-Yong Lam
Heow-Pueh Lee

# COMPUTATIONAL METHODS IN LARGE SCALE SIMULATION

Lecture Notes Series, Institute for Mathematical Sciences,
National University of Singapore
Vol. 6

# COMPUTATIONAL METHODS IN LARGE SCALE SIMULATION

Editors
Khin-Yong Lam
Heow-Pueh Lee
Institute of High Performance Computing, Singapore


World Scientific
NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI

*Published by*

World Scientific Publishing Co. Pte. Ltd.

5 Toh Tuck Link, Singapore 596224

*USA office:* 27 Warren Street, Suite 401-402, Hackensack, NJ 07601

*UK office:* 57 Shelton Street, Covent Garden, London WC2H 9HE

**British Library Cataloguing-in-Publication Data**

A catalogue record for this book is available from the British Library.

**COMPUTATIONAL METHODS IN LARGE SCALE SIMULATION**



ISBN 981-256-363-6

Printed by FuIsland Offset Printing (S) Pte Ltd, Singapore

# COMPUTATIONAL METHODS IN LARGE SCALE SIMULATION

**LECTURE NOTES SERIES**
**Institute for Mathematical Sciences, National University of Singapore**

Series Editors: Louis H. Y. Chen and Denny Leung
*Institute for Mathematical Sciences*
*National University of Singapore*

---

*Published*

Vol. 1 Coding Theory and Cryptology
*edited by Harald Niederreiter*

Vol. 2 Representations of Real and *p*-Adic Groups
*edited by Eng-Chye Tan & Chen-Bo Zhu*

Vol. 3 Selected Topics in Post-Genome Knowledge Discovery
*edited by Limsoon Wong & Louxin Zhang*

Vol. 4 An Introduction to Stein's Method
*edited by A. D. Barbour & Louis H. Y. Chen*

Vol. 5 Stein's Method and Applications
*edited by A. D. Barbour & Louis H. Y. Chen*

Vol. 6 Computational Methods in Large Scale Simulation
*edited by K.-Y. Lam & H.-P. Lee*

## Foreword

The Institute for Mathematical Sciences at the National University of Singapore was established on 1 July 2000 with funding from the Ministry of Education and the University. Its mission is to provide an international center of excellence in mathematical research and, in particular, to promote within Singapore and the region active research in the mathematical sciences and their applications. It seeks to serve as a focal point for scientists of diverse backgrounds to interact and collaborate in research through tutorials, workshops, seminars and informal discussions.

The Institute organizes thematic programs of duration ranging from one to six months. The theme or themes of each program will be in accordance with the developing trends of the mathematical sciences and the needs and interests of the local scientific community. Generally, for each program there will be tutorial lectures on background material followed by workshops at the research level.

As the tutorial lectures form a core component of a program, the lecture notes are usually made available to the participants for their immediate benefit during the period of the tutorial. The main objective of the Institute's Lecture Notes Series is to bring these lectures to a wider audience. Occasionally, the Series may also include the proceedings of workshops and expository lectures organized by the Institute. The World Scientific Publishing Company and the Singapore University Press have kindly agreed to publish jointly the Lecture Notes Series. This volume, "Computational Methods in Large Scale Simulation," is the sixth of this Series. We hope that through regular publication of lecture notes the Institute will achieve, in part, its objective of promoting research in the mathematical sciences and their applications.

January 2005

Louis H. Y. Chen
Denny Leung
*Series Editors*

## Preface

Due to major advances in basic and applied simulation sciences as well as the availability of large scale computational capability, high performance computing (HPC) has enabled engineers and scientists to solve complex, multi-disciplinary problems in which issues of scale are pervasive.

To further develop large scale simulation as a tool for the research community, the Institute for Mathematical Sciences (IMS) at the National University of Singapore and the Institute of High Performance Computing (IHPC) organized a program entitled "Advances and Mathematical Issues in Large Scale Simulation". The program, which commenced in October 2002, focused on two main themes: Multiscale Simulation and Fast Algorithms.

### Multiscale Simulation

The sub-program related to Multiscale Simulation was intended to provide a forum for the interdisciplinary blending of the different theoretical bases for describing physical phenomena at different length scales. In the process, an efficient coupling of the various disciplines for the modeling and direct simulation of various types of physical problems was created. In the different solutions developed, the systems to be investigated were divided into at least three sub-domains, namely the macro, micro and nano subsystems.

Although the multiscale simulation method was quite clearly defined conceptually inside each subsystem, the mathematical issues concerned the efficient and accurate transition, which involved the handshaking or transition, between the continuum and the molecular models, and between the molecular and quantum models. Attention was given to the description and mathematical modeling of the handshake or transition regions, as well as to the parallelization of the source codes for efficient multiscale computation.

## Fast Algorithms

For the sub-program on fast algorithms, focus was given to widely utilized methodologies in scientific and engineering computations such as Model Order Reduction, Fast Convergent Iterative schemes, Pre-corrected Fast Fourier Transform (FFT) methods, Fast Multipole Methods and the parallelization algorithm. Two major large scale engineering computation problems were highlighted: Computational Electromagnetics and Computational Acoustics.

The topic on computational electromagnetics involved the development of efficient techniques to simulate complicated, large scale electromagnetic problems. Efforts were devoted to effective model order reduction, fast convergent iterative schemes, pre-conditioning FFT methodology, fast multipole method and parallel computation.

For computational acoustics, the problems investigated included the prediction of the effectiveness of sound protection shields in environment problems and noise reduction in both the automotive industry and in households. Some issues that were considered included infinite elements, wave-envelope elements, effective iterative solvers, local/global FE acoustical solutions, conjugated infinite elements for transient problems and parallel computation.

This volume of the Lecture Notes Series is dedicated to the "Advances and Mathematical Issues in Large Scale Simulation". The articles in the book document the research undertaken by various Principal Investigators in the field of large scale simulations and illustrate the manner which computational methodology can be utilized to solve highly complex problems. Their efforts in writing the articles are deeply appreciated.

We would like to express our gratitude to the Science and Engineering Research Council (SERC) of the Agency for Science, Technology and Research (A*STAR) for supporting the program. A special thanks to Professor Louis Chen for his foresight in forging this collaboration to initiate the creation of new knowledge in the field of modeling and simulation.

Last but not least, we would like to thank all researchers from both IHPC and NUS who participated in the program. Their collective contributions have given the program a huge diversity that clearly demonstrates the great versatility of large scale simulations.

January 2005

Khin Yong Lam and Heow Pueh Lee
Institute of High Performance Computing,
Singapore

## Contents

Foreword vii

Preface ix

Methods of Multiscale Modeling in Mechanics
*W. A. Curtin* 1

Efficient and Accurate Boundary Methods for Computational Optics
*Christian Hafner and J. Smajic* 57

Finite Element Modeling of Periodic Structures
*Zheng Lou and Jian-Ming Jin* 129

Factorization of Potential and Field Distributions without Utilizing the Addition Theorem
*Ali-Reza Baghai-Wadji and Erping Li* 169

Virtualization-Aware Application Framework for Hierarchical Multiscale Simulations on a Grid
*Aiichiro Nakano, Rajiv K. Kalia, Ashish Sharma, Priya Vashishta, Shuji Ogata and Fuyuki Shimojo* 229

Molecular Dynamics Simulation and Local Quantities
*Tamio Ikeshoji* 245

Recent Advances in Modeling and Simulation of High-Speed Interconnects
*Michel Nakhla and Ram Achar* 269

Multiscale Modeling of Degradation and Failure of Interconnect Lines Driven by Electromigration and Stress Gradients
*Robert Atkinson and Alberto Cuitiño* 335

# METHODS OF MULTISCALE MODELING IN MECHANICS

W. A. Curtin

*Division of Engineering, Brown University*
*Box D, Providence, RI 02912*
*E-mail: curtin@engin.brown.edu*

Multiscale modeling can be accomplished by either information passing across scales, using appropriate methods at each individual scale, or by coupled modeling wherein several scales are handled simultaneously in different regions of space. This chapter reviews some of the basic methods at each scale and some approaches to atomistic/continuum coupling in solid mechanics.

## 1. Introduction

The mechanical behavior of materials involves processes over a wide range of length and time scales. Electron and ion interactions dictate all behavior, but it is not feasible to describe macroscopic behavior at this fundamental level. Hence, quantum methods are useful for determining crystal structure and elastic constants, for instance, as well as capturing the chemistry of alloying and some details of individual defects such as vacancies and dislocations. Atomistic mechanics, wherein the electronic interactions are replaced by effective classical interatomic potentials, more readily permits the study of material defects, and the interactions between defects such as cracks and dislocations, or dislocations and impurities. Computational power limits such studies to millions of atoms, typically, corresponding to submicron volumes of material. In materials that deform plastically and/or undergo fatigue degradation, the collective behavior of defects, and especially dislocations, occurs on

much larger scales of microns to millimeters. Descriptions of such phenomena thus rely on simplified models of the defects, where atomistic details such as the core structure of a dislocation are neglected while the long-range fields and interactions among separated defects are captured accurately. At the largest scales, corresponding to phenomena occurring in structural components, continuum methods are employed, wherein the defect behaviors are subsumed into effective constitutive laws for the material deformation, and the macroscopic continuum field quantities (displacement, stress) are calculated from appropriate partial differential equations. Multiscale modeling is aimed at connecting these different scales of phenomena.

Multiscale modeling can be divided into two basic approaches. The first is "information passing", in which information from smaller scale models is distilled into appropriate use within larger scale models (Figure 1). For instance, quantum mechanical calculations of elastic constants can be directly used in continuum elasticity calculations. More subtly, quantum calculations can be used to design effective interatomic potentials for atomistic scale modeling[1-2]. Another example is the use of quantum or atomistic models to determine effective material separation laws (cohesive zones) for mesoscale modeling of crack nucleation and growth[3-4]. In all cases, in the appropriate distillation of the smaller scale information, the retention of key physical details must be retained while secondary details such as fluctuations are neglected.

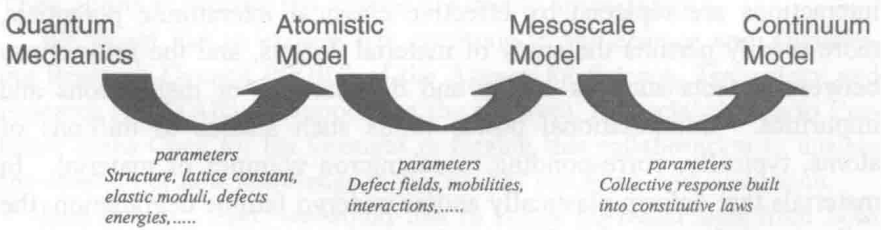



Figure 1. Schematic of the "information passing" mode of multiscale modeling.

The second approach to multiscale modeling is "direct coupling", wherein methods from several scales are used simultaneously within a single computational framework (Figure 2). Such an approach retains the small scale details in spatial regions where such details are absolutely

necessary, often because the behavior has no clear accurate representation in a larger-length scale description. Examples are chemical reactions at a crack tip, which require quantum mechanics for accurate rates, solute/dislocation-core interactions, which require atomistic or quantum studies to elucidate the complex interactions in the non-linear core region, and local amorphization at a crack tip, which requires atomistics. Outside of such critical regions, a larger-scale description can be perfectly acceptable, serving the purpose of providing the smaller-scale region with the appropriate boundary conditions (e.g. stress intensity factor or dislocation driving force). In general, the overall strategy of this type of modeling is to eliminate degrees of freedom where they are not necessary. As increasing scales are bridged, quantum electronic degrees of freedom give way to atomistic degrees of freedom, which give way to mesoscale degrees of freedom characterizing only the defects, which are then subsumed into constitutive laws for macroscopic behavior where the degrees of freedom are the field quantities of interest.

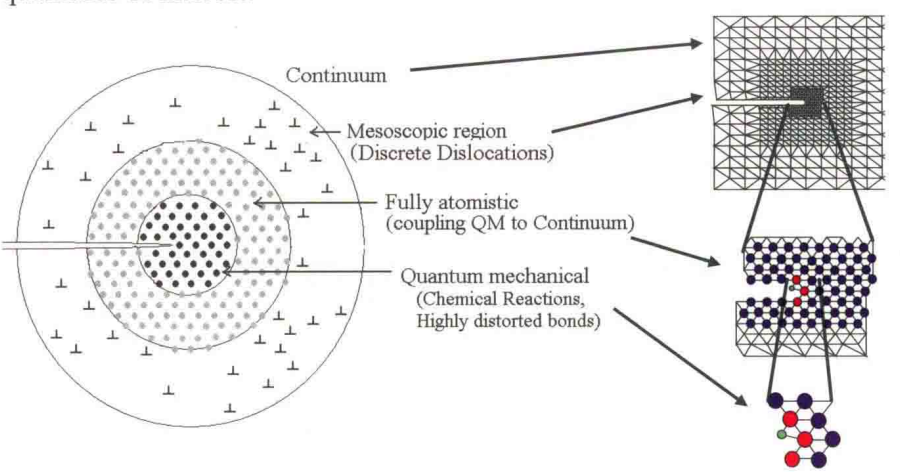



Figure 2. Schematic of "direct coupling" or hierarchical multiscale modeling for predicting stress corrosion cracking in a plastically-deforming metal.

There are two key issues in the "direct coupling" approach. The first issue is the treatment of the interfaces between regions treated by different methods, for which it is desired to avoid any artifacts due to the merging of two physically different descriptions of the material. The

second issue is the transfer of defects among the regions, where the defect has a fundamentally different character in each regime. A pertinent example is the transfer of an atomistic dislocation into a continuum dislocation, wherein the details of the dislocation core are lost, and the subsequent transfer of a continuum dislocation into a continuum plastic strain field, wherein the dislocation as a separate entity disappears entirely.

The purpose of this chapter is two-fold. We first present some of the basic underlying methods relevant at each scale of computation. These methods are the basis for the "information passing" approach. We then discuss some methods for "direct coupling" of the atomistic and continuum methods, and highlight some of the advantages and pitfalls of such coupled approaches. Along the way, we present some examples of these modes of multiscale modeling, drawn from the admittedly narrow scope of work by the author and collaborators. A number of reviews have been written recently on various aspects of multiscale modeling, and we urge readers to study these works and the references therein[5-7].

## 2. Methods of Modeling at Various Scales

### 2.1. Quantum Mechanics

The behavior of matter is controlled by the interactions of electrons and nuclei, which are governed by Schrodinger's equation. Within the Born-Oppenheimer approximation, wherein the nuclear motions $\{r_i^{(n)}\}$ are slow relative to those of the electrons $\{r_i^{(e)}\}$, Schrodinger's equation for the electrons with fixed nuclear coordinates is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(\{r_i^{(e)}\},\{r_i^{(n)}\})\Psi = E\Psi \qquad (1)$$

where $\Psi$ is the multi-electron wavefunction and $V$ is the total Coulomb potential function for the charge interactions. The necessity of antisymmetry of $\Psi$ under exchange of any two electronic coordinates makes this equation extremely difficult to solve, and so approximate methods are needed particularly for many-atom systems such as solids.

A useful approximation is based on the density functional theorem of Hohenberg and Kohn, who showed that the total energy is a unique functional of the electronic density $\rho$, and that the groundstate of the system is the minimum of the energy with respect to the density[8]. Formally, the energy is thus

$$E[\rho] = T[\rho] + \int dr \rho(r) V_{ps}(r) + \int dr \frac{\rho(r)\rho(r')}{|r-r'|} + E_{xc}[\rho] \tag{2}$$

where $T$ is the kinetic energy, $V_{ps}$ is the electron/ion interaction with core electrons lumped into a pseudopotential (this approximation is not necessary), and $E_{xc}$ is the exchange/correlation energy functional. Given an approximation for the unknown functional $E_{xc}$, the groundstate density and energy are often obtained as follows. Introduce a pseudo single-electron wavefunction $\psi_i$ for each electron and construct the density as

$$\rho(r) = \sum_i \left| \psi_i(r) \psi_i^*(r) \right| \tag{3}$$

with the sum over occupied electron states. Use this to create a new set of coupled effective Schrodinger equation for each electron wavefunction as

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ps}(r) + \int dr \frac{\rho(r')}{|r-r'|} + \varepsilon_{xc}[\rho] + \rho(r) \varepsilon'_{xc}[\rho] \right] \psi_i = \varepsilon_i \psi_i \tag{4}$$

and solve this coupled set of equations self-consistently, using a expansion of the individual $\psi_i$ in an appropriate basis set of orthogonal functions. The total energy of the system is then calculated as

$$E = \sum_i \varepsilon_i - \tfrac{1}{2} \int dr \frac{\rho(r)\rho(r')}{|r-r'|} + E_{xc}[\rho] - \int dr \rho(r) \varepsilon'_{xc}[\rho] \tag{5}$$

where we have used

$$E_{xc} = \int dr \rho(r) \varepsilon_{xc}(r) \; ; \; \varepsilon'_{xc} = \partial \varepsilon_{xc} / \partial \rho \tag{6}$$

With the energy above obtained for ions in some initial fixed positions, an equilibrium state is then found by moving the ions to minimize the total energy with respect to the ion coordinates. This is achieved by calculating the ion forces from the Hellman-Feynmann theorem as

$$f_{ion\,j} = -\frac{\partial E}{\partial r_{ion\,j}} \tag{7}$$

and using standard conjugate gradient or other numerical methods to move the ions toward the positions of zero force[8].

The outcome of all of the above manipulations is a first-principles determination of the structure and energy of a system under some specified conditions. From the energy versus structure information, one can then investigate the possible existence of new phases of materials, the phase behavior itself, elastic constants, chemistry effects, surface energies, and defect structures, among other quantities. An example relevant to mechanical behavior is the influence of Hydrogen on the sliding behavior of blocks of Al along the (111) surface, which influences dislocation stability and structure[9]. Table I shows the energy of relevant stacking faults with and without H on the sliding (111) surface at the appropriate octahedral or tetrahedral sites.

| Energy ($J/m^2$) | Vector | Al | Al+H |
|---|---|---|---|
| Intrinsic (I) | $\frac{1}{6}[12\bar{1}]$ | 0.164 | 0.103 |
| Unstable (U1) | $\frac{1}{10}[12\bar{1}]$ | 0.224 | 0.126 |
| Unstable (U2) | $\frac{1}{4}[101]$ | 0.250 | 0.132 |
| Run-on (R) | $\frac{1}{3}[12\bar{1}]$ | 0.400 | 0.310 |

Table I. Energies of key stacking fault configurations in Al, with and without H on the sliding surface (after Ref. 9).

Quantum methods have severe computational limitations, however. While the cost of any particular calculation depends on many details, typical density functional calculations are performed on, at most, hundreds of atoms. Modeling of multiple defects, defects with long-range interactions, or situations with complex loading conditions, is prohibitive, warranting consideration of larger-scale methods.

## 2.2. Atomistic Mechanics

Atomistic methods eliminate the electronic degrees of freedom and follow the motions of the ions as atoms interacting via effective classical interatomic potentials[10]. There are a host of potentials in the literature that have been developed for various materials[11-20]. The energy of a collection of atoms is obtained by summing up the interactions among the individual atoms. A classic generic potential is the Lennard-Jones 6-12 potential, where

$$E = \tfrac{1}{2}\sum_{ij} V_{LJ}(r_{ij}) \;;\; V_{LJ}(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{8}$$

More-realistic potentials account for the multibody and environment-dependence of the energetics. A form in widespread use for metallic systems is the embedded-atom method (EAM) potential[11], where the energy for atom $i$ is

$$E_i(r) = F(\rho_i) + \sum_j V_{pair}(r_{ij}) \quad . \tag{9}$$

This form contains a pair potential such as the above Lennard-Jones potential plus an "embedding energy" $F$ that depends on the electron density at the atom i location due to the surrounding atoms,

$$\rho_i = \sum_{j\neq i} \rho^{(at)}(r_{ij}) \;;\; \rho^{(at)} \approx \text{Bare atom electron density} \tag{10}$$

In practice, parameters in the function $F$, the pair-potential, and the description of the bare electron density are varied to fit a wide range of material properties as obtained by either experiment or quantum

calculations. A typical set of properties used in the fit are equilibrium lattice structure and lattice constants, elastic moduli, surface energies, and vacancy formation energy.

A third class of potentials, typically used for covalently-bonded materials, are multibody potentials[13, 16-17]. These are typified by the Stillinger-Weber potential form[12]

$$E_i = \frac{1}{2}\sum_{j\neq i} V_{LJ}(r_{ij}) + \frac{1}{6}\sum_{j\neq i}\sum_{k\neq i,j} V^{(3)}_{ijk}(r_{ij}, r_{ik}) \tag{11}$$

used for Si. The three-body term in this type of potential permits the consideration of highly directional bonding.

With an appropriate potential in hand, the ionic force is given by

$$f_i = -\frac{\partial E}{\partial r_i} \tag{12}$$

where $E$ is the total system energy. Static equilibrium properties of a collection of atoms subject to desired boundary conditions are then obtained by solving for $f_i = 0$ using conjugate gradient or other numerical techniques. Dynamic behavior is obtained by Molecular Dynamics, i.e. solving Newton's equations of motion incrementally in time. To obtain static and dynamic properties at finite temperatures requires the use of a thermostat that monitors and adjusts the total kinetic energy of the system to simulate contact with an external heat bath and maintain the desired temperature[21]. With a thermostat, the equations of motion then generally include a viscous damping term.

Atomistic simulations are particularly useful for investigating the interactions of defects and structural evolution, such as during deposition of atoms onto a surface, including finite temperature behavior and motion of defects and atoms. Such simulations provide insight into the fundamental behavior and provide information that can be passed to larger-scale models. Figures 3-7 show various examples. Figure 3 shows crack growth in a nanolamellar Titanium-Aluminide, which exhibits dislocation emission from the crack tip and interaction of dislocations with the lamellar boundary[22]. From these simulations, one can extract fracture toughness as a function of nanolamellar thickness, for use in larger-scale cohesive zone models. Figure 4 shows the