ARMY RESEARCH LABORATORY

An Overview of Mesoscale Modeling Software For Energetic Materials Research

by James Larentzos, Jean Blaudeau, Anthony D. Rollett, Peter W. Chung

ARL-MR-0737 **March 2010**

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ARL-MR-0737 **March 2010**

An Overview of Mesoscale Modeling Software For Energetic Materials Research

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED (From - To)
March 2010	Final	July 2009-January 2010

4. TITLE AND SUBTITLE
An Overview of Mesoscale Modeling Software For Energetic Materials Research

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
James Larentzos, Jean Blaudeau, Anthony D. Rollett, Peter W. Chung

5d. PROJECT NUMBER
BW9825Z2

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
U.S. Army Research Laboratory
ATTN: RDRL-CIH-C
2800 Powder Mill Road
Adelphi, MD 20783-1197

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-MR-0737

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Engineering of novel energetic materials requires a thorough understanding of the phenomena that control chemistry, processing, structure, and performance over multiple length and time scales. While atomistic methods are typically limited in time and length scale, and continuum approaches tend to break down at microstructural scales, mesoscale modeling approaches are critical in bridging the gap between the modeling scales. This document serves as an overview of the current state-of-the-art mesoscale modeling software for energetic materials research that is available through commercial or general public licensing.

15. SUBJECT TERMS
Mesoscale, commercial software, overview

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE	UU	38	Peter Chung
Unclassified	Unclassified	Unclassified			19b. TELEPHONE NUMBER (*Include area code*) (410) 278-6027

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

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1. Summary

Multiscale modeling approaches are increasingly important as they complement experimental and theoretical Research and Development (R&D) of innovative materials. Engineering of novel materials requires a thorough understanding of the phenomena that control chemistry, processing, structure, and performance over multiple length and time scales. While atomistic methods are typically limited in time and length scale, and continuum approaches tend to break down at microstructural scales, mesoscale modeling approaches are critical in bridging the gap between the modeling scales.

This document serves as an overview of the current state-of-the-art mesoscale modeling software that is available through commercial or general public licensing. Depending on the system and properties of interest, there are significant implementational or fundamental variations among mesoscale modeling software. This overview is focused on three potential application areas of specific interest to the U.S. Army Research Laboratory (ARL).

The emphasis of this overview is on software or codes that are available at a specified cost or through free downloads (some by request). Thus, necessarily excluded are close-hold academic codes and one-off modifications to the software listed in this report. In some instances, distributable versions of academic codes are found to lack features and capabilities documented in open literature publications. Thus, a user's discretion is required before using software unconditionally.

The subject areas of primary interest with regard to mesoscale modeling software are:

- **Soft materials, such as polymers, melts, blends, surfactants, complex fluids and biological material applications:** It is important to understand the structure, molecular arrangement, self-assembly, rheology, phase morphology, and phase behavior of these materials. Some extensive reviews are available on multiscale modeling of soft materials (*4,75*).

- **Materials science applications**: Materials properties can evolve over longer length and time scales. Software capabilities are desired for such features as materials microstructure, the long range effects of voids and defects, grain boundary migration, crack propagation, and dislocation dynamics. Some extensive reviews, lectures and workshops are available on multiscale modeling of materials applications (*76-78*).

- **Multi-phase mixtures of materials:** Processing of materials requires an understanding of how polycrystalline materials interact with polymer binders. Mesoscale modeling capabilities are needed to handle mixed and multiphase solids.

Table 1 summarizes the software that is discussed hereafter. The listing provides condensed descriptions of ostensibly relevant software. Thereafter, in the remainder of the report, more detailed descriptions follow.

Table 1. Mesocale modeling software summary.

Software	Algorithms	Applications/Properties
MesoDyn	Dynamic Density Field	Soft matter, polymers, melts, blends, surfactants, composites, structured materials, nanoparticle-polymer systems, carbon nanotube dispersion in solvents/polymers, mesoscale structure, dynamics and equilibrium properties, microstructure, phase morphology, adsorption/adhesion phenomena of complex liquids
Mesocite	CGMD, DPD	
Mesoprop	Finite Element Analysis	
Mesotek	Density Self-consistent Field Model	
OCTA	Molecular Dynamics, Dynamic Density Field, DPD	
ESPResSO	DPD	
Q-DPD	Quaternion Dissipative Particle Dynamics	
Fluidix	DPD	
LAMMPS	Molecular Dynamics, BD, DPD, Peridynamics	Polymers, biomolecules, soft-materials, crystalline materials, equilibrium and transport properties, chemical reactions, grain boundaries, voids, defects, microstructure
Digital Material	Quasicontinuum method	Crystalline materials, crack propagation, nanoindentations, dislocation junctions, fracture process, material structure and evolution, grain boundaries, voids, defects, dislocations, microstructure
Quasicontinuum	Quasicontinuum method	
ParaDis	Dislocation Dynamics	Dislocation propagation, elastic properties, dislocation densities, microstructure, internal stresses, global mechanical response, energetics of the cross-slip mechanism
microMegas	Dislocation Dynamics	
PARANOID	Dislocation Dynamics	

2. Mesoscale Modeling Software

2.1 MesoDyn

MesoDyn takes a coarse-grained description of a complex fluid and performs time-evolution dynamics of the density and potential fields of the system by seeking a free energy minimum. The coarse-graining of the system involves replacing polymer chains by a Gaussian representation with the same response functions and including non-ideality of the system via effective external potentials, the magnitude of which is determined by the Flory-Huggins interaction parameters of the various binary pairs in the system. Electrostatics may be included via the Flory-Huggins parameter, or they may be explicitly included for each bead in the system, (*1–6*).

2.1.1 Underlying Algorithm

The algorithms used in MesoDyn are the classical density functional theory (DFT) method, coarse-graining, generalized time-dependent Ginzburg-Landau (TDGL) theory for conserved order parameter and integration of functional Langevin equations.

Table 2. MesoDyn summary.

Company/Institution	Accelrys
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Composite materials a. Clay-Polymer systems b. Carbon nanotube dispersion in solvent or polymers
Properties	1. Mesoscale structure, dynamics and equilibrium properties 2. Microstructure, phase morphology a. Aggregation and coagulation b. Effect of shear on morphology c. Effect of confinement on miscibility d. Adsorption/Adhesion phenomena of complex liquids
Advantages	1. GUI a. interfaces with Accelrys visualization and analysis tools b. allows investigation of microstructure c. allows one to slice the system 2. Designed to run on HPC machines – parallelized 3. Good tool for modeling soft matter, polymers

Table 2. MesoDyn summary (continued).

Disadvantages	4. Commercial software a. Licensing fees b. Cannot modify the source code 5. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations 6. Does not handle reactive potentials within MesoDyn 7. The number of beads types (chemical species) is limited to 10. The number of mesoscale molecules is limited to 10 (single beads or chains of beads). 8. Neglects hydrodynamics effects and assumes incompressibility. Does not correctly reproduce hydrodynamics, thus cannot link to CFD or Lattice Boltzmann methods.

2.2 Mesocite

Mesocite uses coarse-grained particle simulations to access the mesoscopic time and length scales. The software incorporates two different simulation methods: dissipative particle dynamics (DPD) for soft interactions, and coarse-grained molecular dynamics (CGMD) for hard interactions, enabling simulations on a wide range of materials, such as cosmetics, nanocomposites, biomolecular systems, polymers, and other nano/meso-structured materials (*7–12*).

2.2.1 Underlying Algorithms

In CGMD, the elementary particle is a bead, which represents multiple atoms or even multiple molecules of a material. The interactions between each bead are described through a forcefield. Various functional forms are supported within Mesocite to describe bond stretches, angles bends, non-bonded and electrostatic interactions. CGMD can be simulated in the constant volume-energy, volume-temperature, or pressure temperature (constant Number of particles, Volume and Energy [NVE], constant Number of particles, Volume and Temperature [NVT] and constant Number of particles, Pressure and Temperature [NPT], respectively) ensembles.

DPD is also a particle-based method that is used to reproduce the Navier-Stokes hydrodynamics of the fluid. Small regions of fluid and complex material are represented by beads or chains of beads. Three types of forces describe the interactions between pairs of beads: (1) a harmonic conservative interaction (2) a dissipative force representing viscous drag between moving beads (i.e., fluid elements) and (3) a random force to maintain energy input into the system in opposition to dissipation. Interaction parameters between particles are typically mapped from a well-defined theory, such as Flory-Huggins for polymer systems. DPD is limited to short-ranged interactions within Mesocite (i.e., no electrostatic interactions) and also limited to the NVT ensemble.

Table 3. Mesocite summary.

Company/Institution	Accelrys
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Composite and structured materials a. Nanoparticle-Polymer systems b. Carbon nanotube dispersion in solvent or polymers
Properties	1. Phase formation, Phase morphology, time dependent morphology a. Effect of shear on morphology (within DPD) 2. Transport and dynamic properties
Advantages	1. GUI a. Interfaces with Accelrys visualization and analysis tools b. Allows investigation of microstructure c. Allows one to slice the system d. 3-D display of beads and polymers 2. CGMD within Mesocite a. Simulation of charged systems b. Supports the NVE, NVT and NPT ensembles. c. Variety of potentials: Buckingham, Morse, soft harmonic, Lennard-Jones 3. DPD within Mesocite: a. Lees-Edwards boundary conditions are implemented providing the ability to shear the system b. Incorporates Navier-Stokes hydrodynamics
Disadvantages	1. Commercial software a. Licensing fees b. Cannot modify the source code 2. Parallelization: The algorithms are not parallelized within Mesocite 3. Reactions: CGMD and DPD do not support reactive potentials a. Lisal, Brennan, and Smith developed reaction ensemble Monte Carlo combined with DPD (RxDPD), but it is not implemented within Mesocite. 4. Limited to soft matter simulations a. DPD can be extended to crystalline materials (energetic materials) interacting with a polymer binder. b. Crystalline systems (Energetic Materials) (1) Voids, Defects, Grain Boundaries, Dislocations 5. DPD limitations within Mesocite include a. DPD limited to 20 bead types and 100 molecule types b. Does not support electrostatics (charged systems) c. Limited to the NVT ensemble d. Limited to soft linear potential functional form

2.3 MesoProp

MesoProp uses finite element analysis to link the properties of pure components to complex blends. The phase morphologies are determined from MesoDyn and/or DPD software and are projected onto a finite element grid (*13–19*).

2.3.1 Underlying Algorithms

Bead positions are converted into concentration fields and mapped onto the finite element method (FEM) grid of homogeneous volume elements. Local properties are computed from the fraction of each component phase and its assigned pure component property value. Laplace's equation is solved to determine the predicted properties of interest.

Table 4. MesoProp summary.

Company/Institution	Accelrys
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Composite and structured materials a. Nanoparticle-Polymer systems b. Carbon nanotube dispersion in block copolymer melts
Properties	1. Bulk properties of multi-component nanostructured materials systems a. Elastic constants b. Thermal expansion coefficients c. Electrical and thermal conductivities d. Dielectric constants e. Gas diffusion constants 2. Interfaces with Synthia, enabling computation of the following properties a. Refractive Index b. Magnetic moments c. Swelling in solvents d. Liquid diffusion e. Liquid permeability
Advantages	1. GUI a. Interfaces with Accelrys visualization and analysis tools b. Allows investigation of microstructure c. Allows one to slice the system

Table 4. MesoProp summary (continued).

Disadvantages	1. Commercial Software a. Licensing fee b. Modification of source code 2. Limited to 10 chemical components 3. Reactions: Does not support reactive potentials 4. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations

2.4 Mesotek

Mesotek is a field-based simulation method for studying the behavior of complex fluid systems. The numerical methods enable the fast evaluation of mesophase free energies, giving the ability to generate phase diagrams of polymer systems (*20–21*).

2.4.1 Underlying Algorithm

Mesotek uses a pseudo-spectral method to solve a self-consistent field model of density fields, where the interactions among particles are replaced by the interaction of particles with one or more auxiliary fields. Coarse-graining of the system involves replacing polymer chains by a Gaussian representation with the same response functions and including non-ideality of the system via effective external potentials, the magnitude of which is determined by the Flory-Huggins interaction parameters of the various binary pairs in the system. The structure and free energy of the system relax to a saddle point due to a combination of a complex force and real Gaussian white noise. A modified diffusion equation is solved using Discrete Fourier transform. From these operators, the potential and pressure fields are evaluated for the cell, and the cell is updated to minimize the internal stress.

Table 5. Mesotek summary.

Company/Institution	Accelrys
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Nanoparticle dispersions and nanocomposite materials a. Spherical nanoparticles in complex liquid matrices
Properties	1. Calculate phase diagrams and stress distributions of polymer systems mesophase free energies
Advantages	1. GUI a. Interfaces with template builder in Materials Studio b. Interfaces with Accelrys visualization and analysis tools c. Allows investigation of microstructure d. Allows one to slice the system 2. Parallelized using MPI 3. Cell optimization using fast explicit Euler and semi-implicit Seidel field relaxation methods for fast evaluation of mesophase energies 4. Variable cell shape during cell optimization 5. Evaluation of stress fields 6. Mobile solid inclusions: spherical inclusions, randomly distributed
Disadvantages	1. Commercial Software a. Licensing fee b. Modification of source code 2. Reactions: Does not support reactive potentials 3. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations

2.5 OCTA

OCTA is an integrated simulation system for soft materials. It consists of four simulation programs:

- COarse-Grained molecular dynamics program by NAgoya Cooperation (COGNAC)
- Polymer rheology Analyzer with Slip-link model of entanglement (PASTA)
- Simulation Utilities for Soft and Hard Interfaces (SUSHI)
- MUltiFarious FIeld simulator for Non-equilibrium system (MUFFIN)

OCTA also consists of one graphical user interface (GUI) program– Graphical Open UseR interface for Material design EnvironmenT (GOURMET) and an Input/Output (I/O) interface library (*22*).

2.5.1 Underlying Algorithms

The algorithms used for OCTA are CGMD, Dynamics DFT method, slip-link model, finite difference method (FDM), FEM, and self-consistent field method. Detailed descriptions of the four simulation programs are below:

- COGNAC—A molecular dynamics program that covers a large class of molecular models, ranging from full atomistic models to bead-spring models. Equilibrium or nonequilibrium simulations under constant temperature, pressure, shear and elongational deformation can be modeled. A special zooming function generates the equilibrium molecular configuration for given density profile of atoms. It can deal with both isotropic and anisotropic interactions between the non-bonded atomic units.
- Rheology simulator – PASTA—Calculates the rheological properties of polymeric liquids from knowledge of the molecular weight distribution and branching structure. It is based on the slip-link model, in which polymer molecules interact through the creation and release of binary entanglements. PASTA can handle polydisperse linear and star polymers, and it can predict various linear and nonlinear rheological properties.
- Interfacial dynamics simulator – SUSHI—Calculates the equilibrium and non-equilibrium structures in polymer blends and block copolymers by solving the self-consistent Edwards equation. SUSHI can deal with a variety of polymers: linear polymer, branched polymers with any topology, copolymers with any monomer sequences (block, random, tapered-random) and the polymers grafted on a solid surface. SUSHI can be used to study the surface modification caused by polymer grafting or polymer adsorption and the self-assembly of block polymers (micellar formation).
- Continuum dynamics simulator – MUFFIN—A general solver for the continuum models for the dynamics of soft materials based on FDM or FEM. MUFFIN includes six packages, Elastica, ElaDyna, GelDyna, Electrolyte, MEMFluid and PhaseSeparation and can deal with various problems in soft materials, such as the elasticity of multi-phase materials, swelling and deswelling of gels, ion transport in charged colloids, reaction and diffusion in narrow channels, phase separation and droplets deformation in shear and electric field.

Table 6. OCTA summary.

Company/Institution	Masao Doi (Nagoya University) and Japanese industries, government and academia.
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Nanoparticle dispersions and nanocomposite materials
Properties	1. Rheological properties 2. Multi-phase structures 3. Polymer grafting, adsorption 4. Self-assembly of block copolymers 5. Elasticity of multi-phase materials 6. Swelling and deswelling of gels 7. Ion transport in charged colloids 8. Reaction and diffusion in narrow channels 9. Phase separation 10. Droplet deformation in shear and electric field.
Advantages	1. Free and open source software a. Ability to modify source code 2. Available on Windows, Linux and MacOSX operating systems 3. Common GUI 4. COGNAC a. Density biased Monte Carlo and density biased potential methods are implemented (1) Compute equilibrium chain configurations from self-consistent field calculations b. New potential functions can be added to the list of existing potential functions by users. (1) Gay-Berne potential is implemented. c. Staggered reflective boundary conditions (1) Allows smaller systems sizes as compared to periodic boundary conditions
Disadvantages	1. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations 2. Website does not indicate that it is parallelized

2.6 ESPResSo-Extensible Simulation Package for RESearch on Soft Matter

ESPResSo is a software package for simulation and analysis of coarse-grained atomistic or bead-spring models used in soft matter research with an emphasis on charged systems. It also contains a DPD thermostat for hydrodynamics (*23–24*).

2.6.1 Underlying Algorithms

The algorithms for ESPResSo are:

- Equilibrium and non-equilibrium molecular dynamics of bead-spring models in various ensembles.
- DPD.
- Peridynamics.
- Lattice-Boltzmann (under development).

Table 7. ESPResSo summary.

Company/Institution	Max Planck Institute for Polymer Research
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc.
Properties	—
Advantages	1. Free and Open Source under GPL. a. Ability to modify source code. 2. Parallelized 3. Molecular dynamics in various ensembles (NVE, NVT, NPT) 4. DPD thermostat 5. Charged systems – electrostatics implemented 6. Periodic and non-periodic boundary conditions
Disadvantages	1. No GUI 2. Reactions: Does not support reactive potentials 3. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations

2.7 Q-DPD

Quaternion-based Dissipative Particle Dynamics (Q-DPD) includes a modification of DPD that uses a velocity-Verlet algorithm. This allows solid inclusion motion that can be determined from a quaternion-based scheme (*25–28*).

2.7.1 Underlying Algorithm

The algorithm for Q-DPD is Quaternion Dissipative Particle Dynamics. The National Institute of Standards and Technology (NIST) Q-DPD is a modification to DPD where there are two types of particles: "free" particles and ellipsoidal particles that allow for solid inclusion motion.

Table 8. Q-DPD summary.

Company/Institution	NIST – Mathematical and Computational Sciences Division
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Complex fluids – suspensions (colloids, ceramic slurries, concrete) 3. Concrete flow 4. Fluid/Fluid and Fluid/Solid phases
Properties	1. Flow properties of complex fluids like suspensions 2. Steady-shear viscosity of suspension of solid inclusion (ellipsoids)
Advantages	1. Parallelized a. Shared and distributed memory versions 2. Sheared systems
Disadvantages	1. SOFTWARE IS NOT ADVERTISED TO BE AVAILABLE! 2. No GUI 3. Reactions: Does not support reactive potentials 4. Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations

2.8 Fluidix

The Fluidix modeling software can model the fluid dynamics and coarse-grained physics simulations of soft matter. Flowing liquids, deformable and interactive surfaces, polymer-based and solid structures, and custom particle interactions can be evolved through time and space using a parallel computation engine. Sandbox is 2-D interactive implementation of DPD. It is possible to model fluid flow around complex shapes and boundaries and include particles, polymers, and shapes with simplicity. A mean field theory, which removes the need for explicitly treating water particles is implemented (*29–32*).

2.8.1 Underlying Algorithm

The algorithm for Fluidix is the DPD technique.

Table 9. Fluidix summary.

Company/Institution	OneZero Software
Applications	1. Soft matter, complex fluids, polymer melts and blends, surfactants, etc. 2. Static and flowing liquids 3. physics: crystal structure, atomic behavior, diffusion, nanoscale flow 4. biology: bacterial surfaces, cell growth, membrane dynamics 5. health science: drug release mechanisms, blood flow and bypasses 6. fluids: oil pipelines, oceanography, microfluidics, chemical flow 7. traffic flow: air, vehicle, pedestrians, flow of people within a building
Properties	1. Flow properties 2. Shear forces
Advantages	1. GUI, 3-D visualization 2. Can customize code through plug-ins. 3. Parallelized 4. Electrostatics–Debye screening 5. Water can be modeled as a continuum
Disadvantages	Commercial Software a. Licensing fee b. Modification of source code Reactions: Does not support reactive potentials Limited to soft matter simulations a. Crystalline systems (Energetic Materials) b. Voids, Defects, Grain Boundaries, Dislocations

2.9 Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

LAMMPS is a parallel particle simulator designed to run efficiently on parallel computers. It has the ability to model systems at the atomic, meso, or continuum scale. The systems include atomic (Lennard-Jones), molecular, bead-spring systems, soft materials, metals, granular materials, coarse-grained mesoscale models, ellipsoidal particles, and point dipolar particles. Common interaction potentials for soft materials, solid-state materials, coarse-grained or mesoscopic systems are implemented (*33–41*).

2.9.1 Underlying Algorithm

The algorithms for LAMMPS are molecular dynamics in various ensembles, non-equilibrium molecular dynamics, Brownian dynamics, CGMD, DPD, and reactive dynamics

LAMMPS is geared around molecular dynamics simulations, where it integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long-range forces with a variety of initial and/or boundary conditions.

Table 10. LAMMPS summary.

Company/Institution	Sandia National Labs
Applications	1. Polymers, biomolecules, soft-materials 2. Solid-state, crystalline materials
Properties	1. Equilibrium and transport 2. Reactions/Chemical 3. Grain boundaries, voids, defects, microstructure
Advantages	Free and open source software. Ability to modify source code Highly parallelized Ability to model reactions ReaxFF is implemented Charged systems Various mesoscale methods Brownian Dynamics DPD CGMD (1) Potentials include DPD, GayBerne, REsquared and colloidal (2) Implicit solvent potentials are implemented Peridynamics
Disadvantages	1. No GUI a. pizza.py is included–Python based codes used for pre- and post-processing the output from LAMMPS. b. Versatile in allowing user to specify common outputs transferable to many graphical packages.

2.10 Digital Material Software

Digital Material supports the simulation of material structure and evolution across multiple length and time scales. The quasicontinuum approach to materials simulation combines FEM with molecular dynamics in order to simulate only the relevant degrees of freedom (*42–49*).

2.10.1 Underlying Algorithm

The algorithms for Digital Material software are Molecular Dynamics and quasicontinuum.

Table 11. Digital Material Software summary.

Company/Institution	Cornell, James Sethna
Applications	1. Solid-state, crystalline materials 2. Surface deposition 3. Crack propagation and growth
Properties	1. Material structure and evolution 2. Grain boundaries, voids, defects, dislocations, microstructure
Advantages	1. Free and open source under GPL 2. Crystalline systems
Disadvantages	1. No GUI 2. Parallelization? 3. Modeling of crystalline systems with polymer binder? 4. Modeling of reactive materials?

2.11 Quasicontinuum

The quasicontinuum method is a mixed continuum and atomistic approach for simulating the mechanical response of polycrystalline materials at zero temperature (*50*). The method reproduces the results of standard Lattice Statics techniques at a fraction of the computational cost. The key idea is the selective representation of atomic degrees of freedom. Instead of treating all atoms making up the system, a small relevant subset of atoms is selected to represent, by appropriate weighting, the energetics of the system as a whole. Based on their kinematic environment, the energies of individual "representative atoms" are computed either in non-local fashion in correspondence with straightforward atomistic methodology or within a local approximation as befitting a continuum model. The representation is of varying density with more atoms sampled in highly deformed regions (such as near defect cores) and correspondingly fewer in the less deformed regions further away, and it is adaptively updated as the deformation evolves (*50–68*). Additional multiscale modeling groups are listed (*50*).

2.11.1 Underlying Algorithm

The MultiBench test suite is a unified implementation of 14 leading multiscale methods for static loading conditions. The implementation is based on quasicontinuum framework. The following 14 methods, with reference numbers, can be run using MultiBench:

1. Quasicontinuum – (*62, 66*)
2. Coupling of Length Scales (CLS) – (*61*)
3. Bridging Domain (BD) – (*68*)
4. Bridging Scale Method (BSM) – (*60, 67*)
5. Composite Grid Atomistic Continuum Method (CACM) – (*53*)

6. Cluster-Energy Quasicontinuum (CQC-E) – (*54*)
7. Ghost-force corrected Quasicontinuum (QC-GFC) – (*63*)
8. Ghost-force corrected Cluster-Energy QC (CQC-GFC) – (*54*)
9. Finite-Element/Atomistics Method (FEAt) – (*57*)
10. Coupled Atomistics and Discrete Dislocations (CADD) – (*64– 65*)
11. Hybrid Simulation Method (HSM) – (*58*)
12. Concurrent AtC Coupling – (*51–52*, *55*, *59*)
13. Ghost-force corrected Concurrent AtC Coupling (AtC-GFC) – (*62*)
14. Cluster-Force Quasicontinuum CQC-F – (*66*)

Table 12. Quasicontinuum summary.

Company/Institution	Ron Miller (Carleton University), Michael Ortiz (Cal. Tech.), Rob Phillips (Cal. Tech.), David Rodney (Institut National Polytechnique de Grenoble), Vijay Shenoy (Indian Institute of Science), Ellad Tadmor (Israel Institute of Technology)
Applications	1. Solid-state, crystalline materials 2. Crack propagation and growth 3. nanoindentations 4. dislocation junctions 5. fracture process
Properties	1. Material structure and evolution 2. Grain boundaries, voids, defects, dislocations, microstructure
Advantages	1. Free and open source software 2. Crystalline systems
Disadvantages	1. No GUI 2. Parallelization? 3. Modeling of reactive materials

2.12 ParaDis

ParaDiS is a large scale, massively parallel dislocation dynamics simulation code to study the fundamental mechanisms of plasticity. ParaDis introduces dislocation lines into a computational volume and allows them to interact and move in response to the forces imposed by external stress and inter-dislocation interactions (*69–70*).

2.12.1 Underlying Algorithm

The algorithm used for ParaDis is Dislocation Dynamics.

Table 13. ParaDis summary.

Company/Institution	Lawrence Livermore National Laboratory
Applications	1. Dislocation propagation 2. Mass simulations on single crystals
Properties	1. Elastic properties of dislocations, Dislocation core properties, dislocation densities, tension, dislocation-dislocation interactions 2. Microstructure 3. Internal stresses 4. Slip systems activity 5. Global mechanical response 6. Stress vs. mobility 7. Energetics of the cross-slip mechanism
Advantages	1. Free and open source through Stanford 2. Highly Parallelized 3. Provides x-window display capability for visualization a. Visualization formats for TecPlot, GNUPlot, Povray, etc. 4. Utilities to create initial dislocations
Disadvantages	1. No GUI 2. Limited boundary conditions

2.13 mM

microMegas (mM) is a dislocation dynamics program intended for the modeling and visualization of dislocation-based plastic deformation in crystals. It is in the same spirit as molecular dynamics simulations, but instead of integrating the motion of atoms it considers properties of dislocation lines. It is mainly based on the elastic dislocation theory. The elementary objects treated by the code are discrete dislocation lines embedded into an elastic continuum. The dislocations move by discrete jumps on the underlying lattice, which allows including the slip geometry for a range of different crystallographic structures (fcc, bcc, dc, hcp) and cutting off very small length scales below, which elasticity theory breaks down (*71*).

2.13.1 Underlying Algorithm

The algorithm used for mM is Dislocation Dynamics. This algorithm is the same as molecular dynamics simulations, but instead of integrating the motion of atoms it considers properties of dislocation lines. It is mainly based on the elastic dislocation theory. The elementary objects treated by the code are discrete dislocation lines embedded into an elastic continuum. The dislocations move by discrete jumps on the underlying lattice, which allows the inclusion of slip geometry for a range of different crystallographic structures (fcc, bcc, dc, hcp) and cutting off very small length scales below which elasticity theory breaks down.

The elastic properties of dislocations (line tension, dislocation-dislocation interactions, etc ...) and the computation of the effective (net) force on each dislocation segment directly follow from

the classical theory of dislocations. The equation of motion of each segment is computed at its mid-point using classical methods similar to those employed in molecular dynamics simulations. Algorithmic parameters like the time step, the minimum length of the segments, and their maximum travel distance during a step are optimized in such a way as to reproduce known solutions for typical elastic problems like the critical stress for a Frank-Read source.

Table 14. mM summary.

Company/Institution	'Laboratoire d'Etude des Microstructures', CNRS-ONERA, France
Applications	1. Dislocation propagation 2. Mass simulations on single crystals
Properties	1. Elastic properties of dislocations, Dislocation core properties, dislocation densities, tension, dislocation-dislocation interactions 2. Microstructure 3. Internal stresses 4. Slip systems activity 5. Global mechanical response 6. Stress vs. mobility 7. Energetics of the cross-slip mechansim
Advantages	1. Open source under GNU General Public License 2. GUI 3. Parallelized 4. Ability to investigate complex materials and loading conditions when coupled to a finite element code, (not included in the standard distribution of ‘mM’)
Disadvantages	1. Very little documentation is available 2. The user’s manual is still in preparation

2.14 PARANOID

PARANOID is a highly parallelized code that has been developed to allow the realistic simulation of dislocation behavior. The code is based on elastic theory in the continuum limit, and should thus be applicable to situations in which the dislocation cores are more than a few nanometers apart. The stress tensor, which moves the dislocations, is calculated at every point by evaluating the full Peach-Koehler expression over all of the dislocations present. The self-interaction of the dislocations is regularized by the Brown method of splitting the dislocation in half, moving the two halves outward by some core parameter, and averaging the result. The code allows one to study the interactions between arbitrarily configured dislocations, located on any

allowed glide plane, passing from one glide plane to another, and having any allowed Burgers vector (*72*).

2.14.1 Underlying Algorithm

The algorithm used for PARANOID is Discrete Dislocation Dynamics.

Table 15. PARANOID summary.

Company/Institution	IBM
Applications	1. Strain relaxation in thin heteroepitaxial films (SiGe) 2. Dislocation-blocking mechanism in thin films 3. Dislocation nucleation and patterning in the edge fields of a nitride pad on silicon (i.e., manufacture of semiconductor devices) 4. Modeling of work-hardening, dislocation patterning, metal fatigue, and related issues in metallurgy 5. Dislocation networks which are observed in relaxed quantum-dot structures
Properties	1. Elastic properties of dislocations, dislocation-dislocation interactions, dislocation nucleation 2. Microstructure 3. Internal stresses, strain relaxation
Advantages	Parallelized
Disadvantages	1. Not available for download a. No information provided on availability 2. No GUI

3. Additional Approaches to Mesoscale Modeling

Table 16 shows additional approaches to mesoscale modeling for which software may not be available.

Table 16. Additional approaches to mesoscale modeling.

Approach	Additional Information
1. Peierls-Nabarro Model	a. Continuum formulation for dislocation mechanics
2. MAAD	a. Fracture Dynamics b. Atomistic → classical molecular dynamics → Continuum Elasticity with Finite Element (1) Quantum Mechanics, Tight-binding
3. CGMD (Rudd)	—
4. Accelerated molecular dynamics techniques	a. Temperature accelerated dynamics (1) Time scales of seconds (2) Outstanding speedup for high barriers, modest for low barriers (3) Inefficient for systems larger than 1000 atoms b. Parallel-replica dynamics (1) Time is parallelized
5. ADESH	—
6. ParaDyn, Warp, GranFlow	a. Superseded by LAMMPS. Many features have been integrated into LAMMPS.
7. DPDmacs (*73*)	—
8. Mesoscopic Modeling (*74*)	Parallel DPD Parallel BD c. Parallel DDFT (aka MesoDyn) d. Parallel Hybrid engine (MBF)

4. Conclusions

A number of multiscale modeling approaches that have previously been applied to research topics ranging from soft matter, complex fluids, and polymer melts to crystalline microstructure, grain boundary propagation and dislocation dynamics have been reviewed. This report outlines the advantages and disadvantages of commonly-used software or codes that are available at a specified cost or through free downloads. The report assists the user in quickly determining the appropriate methods to use for a given problem and provides references to literature that describe the theoretical background of the methods. Depending upon the phenomena that control chemistry, structure, and performance, the choice of multiscale modeling approach is critical in the design of novel materials.

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List of Symbols, Abbreviations, and Acronyms

ADESH	Atomistic DEfect Simulation Handler
ARL	U.S. Army Research Laboratory
AtC-GFC	Ghost-force corrected Concurrent AtC Coupling
BD	Browian Dynamics, Bridging Domain
BSM	Bridging Scale Method
CACM	Composite Grid Atomistic Continuum Method
CADD	Coupled Atomistics and Discrete Dislocations
CFD	Computational Fluid Dynamics
CGMD	coarse-grained molecular dynamics
CLS	Coupling of length scales
COGNAC	COarse-Grained molecular dynamics program by NAgoya Cooperation
CQC-E	Cluster-energy Quasicontinuum
CQC-F	Cluster-Force Quasicontinuum
CQC-GFC	Ghost-force corrected Cluster-Energy
DDFT	Dynamic Density Field Method
DFT	density functional theory
DPD	dissipative particle dynamics
FDM	finite difference method
FEM	Finite Element Method
FEAt	Finite-Element/Atomistics Method
GPL	General Public License
GOURMET	Graphical Open UseR interface for Material design EnvironmenT
GUI	Graphical User Interface
HPC	High Performance Computing
HSM	Hybrid Simulation Method
I/O	Input/Output

LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
MAAD	Macroscopic Atomistic ab intio Dynamics
MBF	Mesoscopic Bead-Field
mM	microMegas
MPI	Message Passing Interface
MUFFIN	MUltiFarious FIeld simulator for Non-equilibrium system
NIST	National Institute of Standards and Technology
NPT	constant Number of particles, Pressure and Temperature
NVE	constant Number of particles, Volume and Energy
NVT	constant Number of particles, Volume and Temperature
PASTA	Polymer rheology Analyzer with Slip-link model of enTAnglement
Q-DPD	Quatemion Dissipative Particle Dynamics
QC-GFC	Ghost-force corrected Quasicontinuum
R&D	Research and Development
RxDPD	Reaction ensemble Monte Carlo combined with DPD
SUSHI	Simulation Utilities for Soft and Hard Interfaces
TDGL	time-dependent Ginzburg-Landau

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