CHIMaD

Center for Hierarchical Materials Design

PHASE FIELD METHODS WORKSHOP

NORTHWESTERN UNIVERSITY

CHIMAD.NORTHWESTERN.EDU

JANUARY 9, 2015

Center for Hierarchical Materials Design (CHiMaD) is a NIST-sponsored center of excellence for advanced materials research focusing on developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry, one of the primary goals of the Obama administration's Materials Genome Initiative (MGI).

This Chicago-based consortium includes Northwestern University as the lead, University of Chicago, Northwestern-Argonne Institute for Science and Engineering, a partnership between Northwestern University and Argonne National Laboratory, and the Computational Institute, a partnership between University of Chicago and Argonne National Laboratory. The consortium is also partnered with Questek Innovations, a pioneering materials design company, ASM International and Fayetteville State University.

Designing novel materials of specific properties for a particular application requires simultaneously utilizing physical theory, advanced computational methods and models, materials properties databases and complex calculations. This approach stands in contrast to the traditional trial-and-error method of materials discovery. CHiMaD aims to focus this approach on the creation of novel hierarchical materials which exploit distinct structural details at various scales, from the atomic on up, to obtain enhanced properties. The center's research focuses on both organic and inorganic advanced materials in fields as diverse as self-assembled biomaterials, smart materials for self-assembled circuit designs, organic photovoltaic materials, advanced ceramics and metal alloys.

For more information, please visit ***chimad.northwestern.edu***

CHIMaD Center for Hierarchical Materials Design

Agenda
Phase Field Methods Workshop
Friday, January 9, 2015

8:00 am **Registration & Breakfast**

8.30 am **Welcome**
Peter Voorhees (NU)

8:40 am **Creating Community Codes:**
Past Experiences & Future Suggestions
James Belak (LLNL)

9:00 am **Discussion & Coffee**

Session 1: Current Codes & Capabilities

9.15 am **FiPy: A Finite Volume PDE Solver Using Python**
Jonathan Guyer & Daniel Wheeler (NIST)

9:35 am **Implementing Phase Field Models Using the MOOSE Framework**
Michael Tonks (INL)

9:55 am **PRISMS-PF: Massively Parallel Computational Framework for Phase Field Modeling**
Katsuyo Thornton & Siva Rudraraju (U-M)

10:15 am **Discussion & Coffee**

Session 2: Large Scale Computing

10:30 am **Scalable Libraries**
Barry Smith (ANL)

10:50 am **Scalable Solver Algorithms**
Dmitry Karpeev (ANL)

11:10 am **Hardware for Large Scale Computing**
James Belak (LNNL)

11:40 am **Discussion on Deliverables & Lunch**

Session 3: Potential Focus Areas

12:40 pm **Identifying Benchmark Problems**
Olle Heinonen (ANL)

1:00 pm **What Physics Should be Included?**
James Warren (NIST)

1:20 pm **Industrial Interest & Needs – Experiences from Hero-m**
Joakim Odqvist (Hero-m)

Session 4: Discussion

1.40 pm **What should a mesoscale community code be capable of solving (immediate community needs)?**
Lead by James Warren (NIST)

2.30 pm **Coffee Break**

2.40 pm **How do we structure a code so that it is extendable both in terms of capabilities (near-future needs) and high-performance scalability?**
Lead by James Belak (LLNL)

3.30 pm **What community standard problems should we formulate for testing and benchmarking?**
Lead by Olle Heinonen (ANL)

4.20 pm **How do we organize and maintain a community repository, and who should do that?**
Lead by Dmitry Karpeev (ANL)

5.10 pm **Final Remarks**
Peter Voorhees (NU)

5:30 pm **Adjourn**

ABSTRACTS

9.35am

IMPLEMENTING PHASE FIELD MODELS USING THE MOOSE FRAMEWORK

Michael Tonks, Daniel Schwen, Idaho National Laboratory

The open source Multiphysics Object Oriented Simulation Environment (MOOSE) is a powerful toolset for implementing phase field models using the finite element method (FEM). MOOSE simplifies the development of advanced computational tools for solving partial differential equations with FEM. All tools implemented using MOOSE are dimension agnostic and work in 1D, 2D, or 3D, can run on a laptop or on a large super computer, employ the advanced solver technology available in PETSc, and have access to mesh and time step adaptivity (see mooseframework.org for more information). With MOOSE, users also get access to two physics modules that are specialized for mesoscale modeling. The phase field module provides all the necessary tools to quickly and easily implement phase field models in MOOSE. The module provides the tools to allow users to only implement information about the free energy functional (with all derivatives taken automatically, if desired) or use CALPHAD free energies, facilitating fast and easy development of a large range of models while retaining the flexibility to implement arbitrarily complex models, including multi-phase field models using the existing modular components. The tensor mechanics module provides the tools for small and finite strain mechanics at the mesoscale, ranging from linear elasticity to crystal plasticity, and the elastic constants and Eigenstrains can vary locally as a function of phase field variables. The phase field equations can easily be tightly coupled to the mechanics and solved together as a single nonlinear solve or loosely coupled and operator split. MOOSE provides a powerful, free, and open source option for implementing the phase field method.

9.55am

***PRISMS-PF*: MASSIVELY PARALLEL COMPUTATIONAL FRAMEWORK FOR PHASE FIELD MODELING**

Shiva Rudraraju, Katsuyo Thornton
PRedictive Integrated Structural Materials Science Center
University of Michigan, Ann Arbor

Phase Field Models have been central to computational modeling of complex morphological evolution in multiphase solids. Under the aegis of DOE's PRedictive Integrated Structural Materials Science (PRISMS) Center at the University of Michigan, a massively scalable framework *PRISMS-PF* is being developed. *PRISMS-PF* is a finite element method (FEM) code developed using the *deal.ii* open-source finite element library, which provides extensive support for various finite element constructs (higher-order classical and non-standard elements), peta-scale grid generation with adaptivity (p4est adaptive octree meshes), scalable data structures and solvers (e.g., internal hybrid-parallel, PETSc, and Trilinos). While the framework is expected to serve as a generic phase field library with coupled mechanics capability, the initial development focuses on modeling of precipitate evolution in binary and ternary alloys, as well as grain growth and recrystallization. Current code modules include matrix-free implementations of coupled Cahn-Hilliard, Allen-Cahn and Mechanics, with example demonstrations of spinodal decomposition, chemo-mechanical boundary value problems, and beta-prime precipitate evolution in magnesium/rare-earth binary alloys. The parallel performance and scaling has been demonstrated on terascale problems with billions of degrees of freedom running on thousands of processors. The code is currently under beta-testing phase and slated for first public release in Summer 2015, under a LGPL open source license.

10.50am
SCALABLE SOLVER ALGORITHMS
Dmitry Karpeev, Argonne National Laboratory

Phasefield models of materials frequently take on the form of coupled systems including elasticity, electrostatics, order parameter evolution and other types of physics. These can be "higher-order" equations such as Cahn-Hilliard and can involve interfaces and complex microstructure. As a result of this complexity the discretized equations can be difficult to converge, especially as the system gets large with the mesh refinement. I will discuss several of the difficulties behind the convergence issues and approaches to mitigating them (multiphysics preconditioners and multigrid, to name just a couple).

12.40PM
PHASE-FIELD STANDARD PROBLEMS
Olle Heinonen, Argonne National Laboratory

There exist many home-grown phase-field and mesoscale codes, and there are also emerging community codes, such as MOOSE and FEniCS. As we are undertaking efforts to discuss and propose standards for phase-field and mesoscale codes, it would be very useful to formulate and publish some small set of standard problems that developers and users can use to test and benchmark codes. This is something that the micromagnetics community did in the late 1990s as micromagnetic codes were being developed, and it was extremely useful to that community. In this talk I will suggest a few problems that may be suitable, but more importantly, I want to stimulate a discussion around this topic.

1.20PM

INDUSTRIAL INTERESTS AND NEEDS – EXPERIENCES FROM Hero-m

Joakim Odqvist, Hierarchic Engineering of Industrial Materials

Hero-m (Hierarchical Engineering of Industrial Materials) is a ten year venture between KTH Royal Institute of Technology, VINNOVA and Swedish Industry. The phase-field method (PFM) has been an important tool for study of microstructure evolution already from the start of Hero-m. However, it soon became clear that it often took a very long time for new users to learn the various PFM codes we were using, and sometimes even to install and get them running. At the same time, several of our industrial partners requested an easy to install and user-friendly tool for phase-field simulations. In this presentation I will talk about our work on developing such a tool.

Center for
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Materials Design

Attendee List
Phase Field Methods Workshop
Friday, January 9, 2015

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Center for Hierarchical Materials Design

Logistics
Phase Field Methods Workshop
Friday, January 9, 2015

Workshop Location

Allen Center, Room 222
Northwestern University
2169 Campus Drive, Evanston, IL, 60208

Parking Information

Please use the *North Campus Parking Garage* for parking on campus.

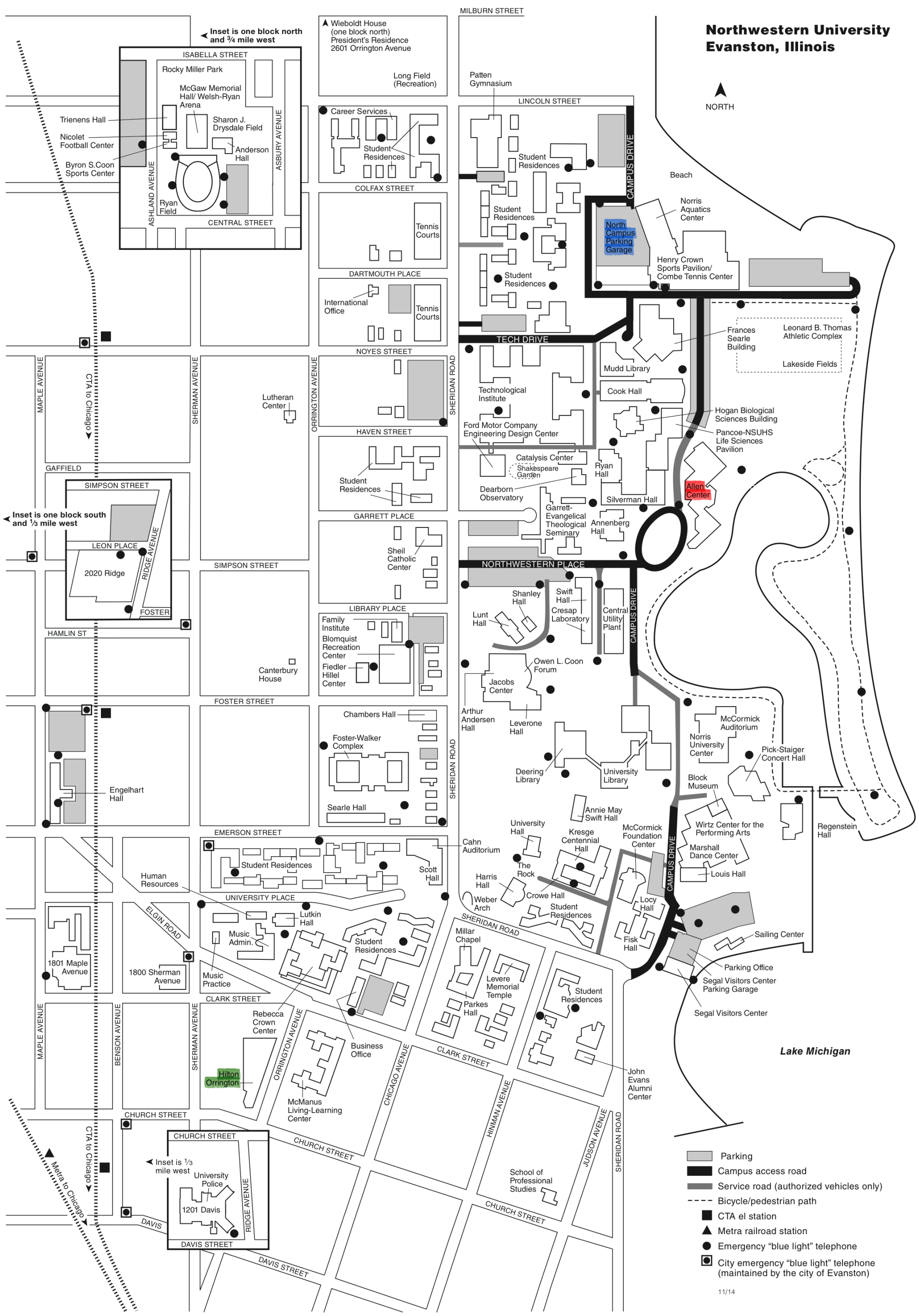
Visitor Parking Passes will be available for pick-up in the morning of the workshop at the lobby of The Allen Center.

Hotel & Shuttle Information

Hilton Orrington
1710 Orrington Ave, Evanston, IL, 60201

A shuttle is available to take the attendees from the hotel to The Allen Center on Friday. The shuttle will depart at 7.45am from the hotel.

Please see the map on the next page for locations.


Northwestern University
Evanston, Illinois
NORTH
Inset is one block north and ¾ mile west
Inset is one block south and ⅓ mile west
Inset is ⅓ mile west
MILBURN STREET
ISABELLA STREET
LINCOLN STREET
COLFAX STREET
CENTRAL STREET
DARTMOUTH PLACE
NOYES STREET
HAVEN STREET
GARRETT PLACE
SIMPSON STREET
LIBRARY PLACE
FOSTER STREET
EMERSON STREET
UNIVERSITY PLACE
CLARK STREET
CHURCH STREET
DAVIS STREET
GAFFIELD
HAMLIN ST
LEON PLACE
FOSTER
TECH DRIVE
NORTHWESTERN PLACE
CAMPUS DRIVE
SHERIDAN ROAD
MAPLE AVENUE
SHERMAN AVENUE
ORRINGTON AVENUE
ASHLAND AVENUE
ASBURY AVENUE
RIDGE AVENUE
BENSON AVENUE
ELGIN ROAD
CHICAGO AVENUE
HINMAN AVENUE
JUDSON AVENUE
CTA to Chicago
Metra to Chicago
Wieboldt House (one block north) President's Residence 2601 Orrington Avenue
Long Field (Recreation)
Patten Gymnasium
Rocky Miller Park
McGaw Memorial Hall/ Welsh-Ryan Arena
Trienens Hall
Sharon J. Drysdale Field
Nicolet Football Center
Anderson Hall
Byron S.Coon Sports Center
Ryan Field
Career Services
Student Residences
Tennis Courts
International Office
Beach
Norris Aquatics Center
North Campus Parking Garage
Henry Crown Sports Pavilion/ Combe Tennis Center
Frances Searle Building
Leonard B. Thomas Athletic Complex
Lakeside Fields
Mudd Library
Cook Hall
Technological Institute
Hogan Biological Sciences Building
Pancoe-NSUHS Life Sciences Pavilion
Ford Motor Company Engineering Design Center
Catalysis Center
Shakespeare Garden
Ryan Hall
Dearborn Observatory
Allen Center
Silverman Hall
Garrett-Evangelical Theological Seminary
Annenberg Hall
Lutheran Center
Sheil Catholic Center
Family Institute
Blomquist Recreation Center
Fiedler Hillel Center
Canterbury House
2020 Ridge
Shanley Hall
Swift Hall
Lunt Hall
Cresap Laboratory
Central Utility Plant
Owen L. Coon Forum
Jacobs Center
Arthur Andersen Hall
Leverone Hall
Chambers Hall
Foster-Walker Complex
Searle Hall
Engelhart Hall
McCormick Auditorium
Norris University Center
Pick-Staiger Concert Hall
Deering Library
University Library
Block Museum
Annie May Swift Hall
University Hall
Kresge Centennial Hall
McCormick Foundation Center
Wirtz Center for the Performing Arts
Marshall Dance Center
Regenstein Hall
Louis Hall
Cahn Auditorium
Scott Hall
Human Resources
Harris Hall
The Rock
Crowe Hall
Weber Arch
Lutkin Hall
Music Admin.
Music Practice
1801 Maple Avenue
1800 Sherman Avenue
Millar Chapel
Levere Memorial Temple
Parkes Hall
Lucy Hall
Fisk Hall
Sailing Center
Parking Office
Segal Visitors Center Parking Garage
Segal Visitors Center
Rebecca Crown Center
Hilton Orrington
Business Office
McManus Living-Learning Center
John Evans Alumni Center
Lake Michigan
University Police
1201 Davis
School of Professional Studies
Parking
Campus access road
Service road (authorized vehicles only)
Bicycle/pedestrian path
CTA el station
Metra railroad station
Emergency "blue light" telephone
City emergency "blue light" telephone (maintained by the city of Evanston)
11/14

Visitor Travel Reimbursement for Guests of the Northwestern Argonne Institute of Science and Engineering (NAISE)

General Process Description:
This process is to reimburse travel for those that are not Northwestern University Employees. The guest makes travel arrangements, saves the receipts, and completes the Visitor Expense Report. The entire document is scanned ensuring legibility and completeness. The scan is e-mailed to James.Soulikias@northwestern.edu for further processing. The reimbursement will be made via check to the traveler.

General Travel Requirements:

- Must travel on an American Carrier
- Alcohol cannot be reimbursed.
- Cannot mix receipts and per diems for reimbursement on same trip (i.e. all per diems or all receipts).
- Northwestern University Travel Policies & Procedures: http://www.northwestern.edu/financial-operations/policies-procedures/policies/travel.pdf

Required Documents:

- ❒ Visitors Expense Report. Available at this link: http://www.northwestern.edu/financial-operations/policies-procedures/forms/visitors_exp_rpt.pdf
- ❒ If submitting detailed receipts, affix to paper. If meal includes alcohol, make a note of the total without alcohol.
- ❒ If claiming per diem, include the page for city of travel found at U.S. Federal Government per diem rates by travel date/country/city http://aoprals.state.gov/web920/per_diem.asp
- ❒ If claiming online purchase (e.g. airfare, hotel, registration, etc.), include the online verification of cost and if possible boarding pass.
- ❒ If claiming mileage reimbursement include mileage documentation (use Mapquest, Google Maps, etc.)
- ❒ Agenda or program brochure.

1. Scan all items. (See scanning tips below)
2. Email scan(s) to James.Soulikias@northwestern.edu for further processing.
3. Reimbursement will be made via check and mailed to the traveler.

If you have any questions contact James Soulikias at (847)467-NAIS(E) or by e-mail at James.Soulikias@northwestern.edu

Note: some browsers require that you press the control button at the same time you click the link. You may also copy and paste the link into the browser.

Scanning Tips

- The recommended file format is .TIF and .PDF with a resolution of 200x200 DPI.
- You may attach one or more docs totaling no more than 1 MB file size.
- Manage scanned documentation for file size and legibility. Illegible files will be returned.
- Clear adhesive tape should not be placed on top of important information when prepping for sending or scanning. Scanners and fax machines do not read through clear adhesive tape, thus anything under the tape, while legible to the human eye, is not legible to the scanner/fax. (ex. do not tape over cash register receipts as the print disappears.)
- Receipts with faint print should be copied and darkened for scanning.
- Tape small receipts to an 8 ½ x 11 white sheet of paper.
- Be sure to tape all four sides to white paper.
- Do not use dark-colored highlighters to mark names, invoice numbers or important information. The highlights scan as blacked out.
- Do black out sensitive information such as Social Security Numbers.

Center for Hierarchical Materials Design

NOTES

Phase Field Methods Workshop

Friday, January 9, 2015