



PHASE FIELD METHODS II
Hackathon \ \ Workshop

NORTHWESTERN UNIVERSITY

CHIMAD.NORTHWESTERN.EDU
OCTOBER 14-16, 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

AGENDA
PHASE FIELD METHODS II: HACKATHON
CHIMAD Headquarters

OCTOBER 14, 2015

9:00 am *A shuttle will be available to take attendees from Hilton Garden Inn to CHiMaD Headquarters*

9:00 am **Breakfast & Registration**
*A light lunch will be available
Please setup between 9.00-10.00am*

9:30 am **Welcome & Setup**
Begum Gulsoy (NU – CHiMaD)

9:40 am **An Introduction to the Benchmark Problems**
Olle Heinonen (ANL - NAISE)

10:00 am **Hackathon begins**

12:00 pm **Lunch**

3:00 pm **Coffee snacks!**

7:00 pm **Dinner**

OCTOBER 15, 2015

12:00 am **Midnight snacks!**

6:30 am **Breakfast sandwiches**

10:00 am **Hackathon ends**

10:15 am *A shuttle will be available to take attendees from CHiMaD Headquarters to Hilton Garden Inn*

5:50 pm *A shuttle will be available to take attendees from Hilton Garden Inn to CHiMaD Headquarters*

6:00 pm **Phase Field Methods II: Hackathon & Workshop Reception**

Coffee station will be available all day and night, along with soda, juice, cookies.

AGENDA
PHASE FIELD METHODS II: WORKSHOP
CHiMaD Headquarters

OCTOBER 15, 2015

11:30 am *A shuttle will be available to take attendees from Hilton Garden Inn to CHiMaD Headquarters*

11:45 am **Lunch**
A light lunch will be available

12:00 pm **Welcome**
Peter Voorhees (NU - CHiMaD)

Session One: Updates Since Phase Field Workshop I

12:15 pm **An Introduction to the Proposed Benchmark Problems and Updates from the Benchmark Questions Committee**
Olle Heinonen (ANL – NAISE/CHiMaD)

12:45 pm **Canadian Computational Network**
Nikolas Provatas (McGill)

1:15 pm **Updates on MOOSE Framework**
Larry Aagesen, Daniel Schwen (INL)

1:30 pm **Updates on PRISMS-PF**
Siva Rudraraju (U-M)

1:45 pm **Updates on FiPy**
Jonathan Guyer (NIST)

2:00 pm Coffee Break

Session Two: Discussion on Benchmark Questions & Implementation

2:15 pm **Discussion: Benchmark Questions, what to add, how to improve**
Olle Heinonen (ANL – NAISE/CHiMaD)

4:30 pm **Discussion: Logistics and Implementation**
James Warren (NIST)

6:00 pm **Phase Field Methods II: Hackathon & Workshop Reception**

7:15 pm *A shuttle will be available to take attendees back to the hotel*

OCTOBER 16, 2015

8:15 am *A shuttle will be available to take attendees from Hilton Garden Inn to CHiMaD Headquarters*

8:30 am **Breakfast**
A light breakfast will be available

9:00 am **Recap of Hackathon Questions**
Olle Heinonen (ANL – NAISE/CHiMaD)

Session One: Hackathon Results

9:10 am **Team 1, lead by Olle Heinonen**
John Mangeri (UConn), Narut Sereewattanawoot (NU)

9:30 am **Team 2, lead by Nikolas Provatas**
Gabriel Kocher (McGill), Matthew Seymour (McGill)

9:50 am **Team 3, lead by Peter Voorhees**
Kevin McReynolds (NU), Stefan Poulsen (NU)

10:10 am **Team 4**
Stephen Dewitt (U-M), Siva Rudraraju (U-M)

10:30 am **Team 5, lead by Daniel Schwen & Larry Aagesen**
Karim Ahmed (INL), Sudipta Biswas (Purdue)

10:50 am **Team 6, lead by Jon Guyer**
Trevor Keller (NIST), Linyun Liang (ANL)

11:10 am **Results to the Hackathon Questions using FIPy**
Jon Guyer (NIST) – these results were produced prior to the event

11:20 am Coffee Break

Session Two: Discussion

11:30 am **Discussion: Hackathon Results**
Lead by Marius Stan (ANL – NAISE/CHiMaD)

12:45 pm **Lunch**
Allen Center

2:00 pm **Discussion: Future Plan and Action Points**
Lead by Peter Voorhees (NU)

3:00 pm **Adjourn**
Cabs to the airport can be arranged upon request, please inquire with a CHiMaD representative.

Attendee List
Phase Field Methods II: Workshop
October 15-16, 2015

Larry Aagesen

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Attendee List
Phase Field Methods II: Hackathon
October 14-15, 2015

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Matthew Seymour

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Logistics
Phase Field Methods II: Hackathon & Workshop
Friday, January 9, 2015

Workshop Location

CHiMaD Headquarters

Northwestern University
O.T. Hogan Biological Sciences Building
2205 Tech Drive, Evanston, IL, 60208

Parking Information

Please use the [North Campus Parking Garage](#) for parking on campus.

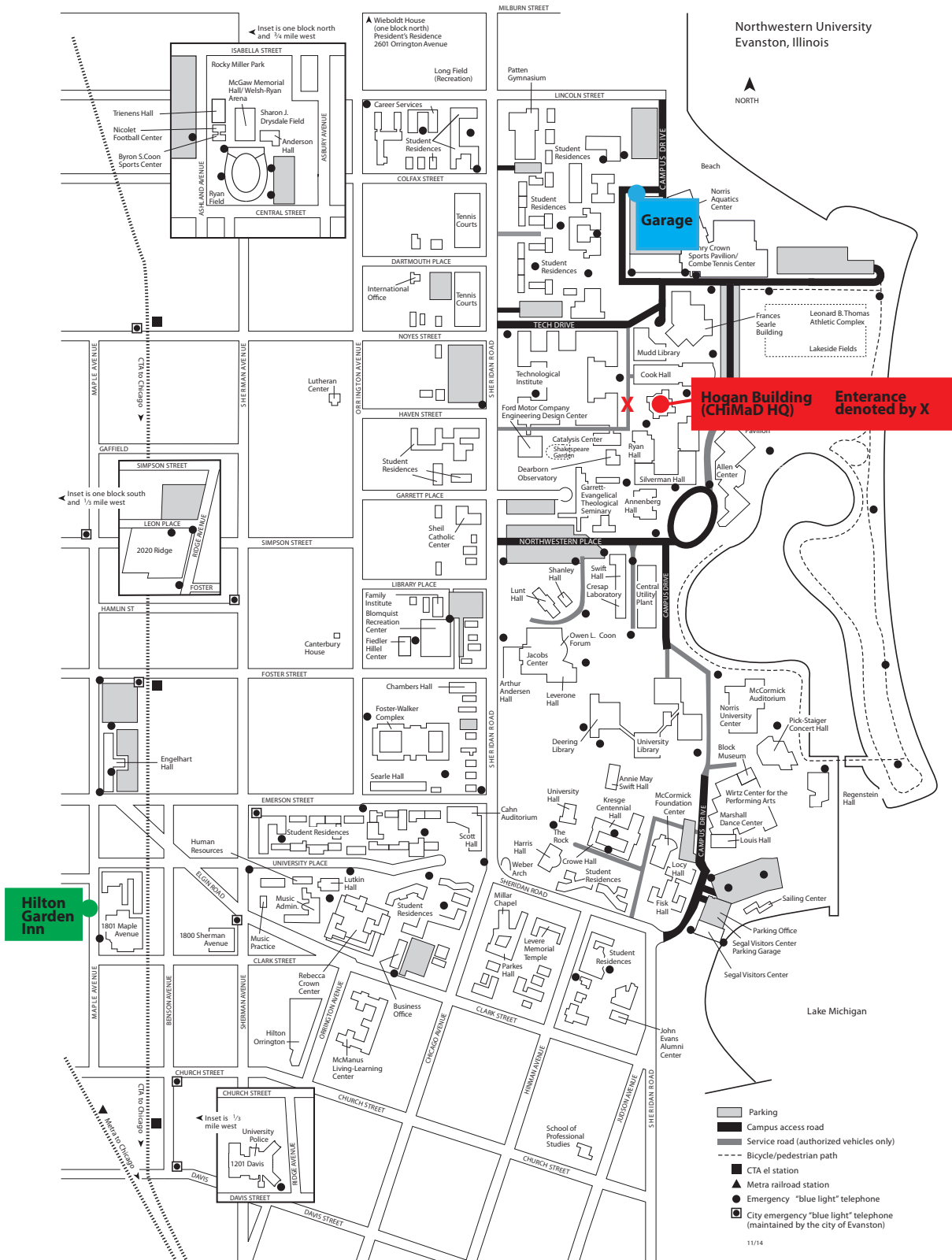
Visitor Parking Passes will be available for pick-up in the morning of the workshop at CHiMaD Headquarters.

Hotel & Shuttle Information

Hilton Garden Inn

1818 Maple Ave, Evanston, IL, 60201

Please see the map on the next page for locations.



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 Juliet Ludwig at juliet.ludwig@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 juliet.ludwig@northwestern.edu for further processing.
3. Reimbursement will be made via check and mailed to the traveler.

If you have any questions contact Juliet Ludwig at (847)467-NAIS(E) or by e-mail at juliet.ludwig@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.