CHiMaD

Center for Hierarchical Materials Design

PHASE FIELD METHODS II
Hackathon \\ Workshop

NORTHWESTERN UNIVERSITY

CHIMAD.NORTHWESTERN.EDU
MAY 3-5, 2016

CHiMaD | Center for Hierarchical Materials Design

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 III
Hackathon \\\ Workshop
May 3-5, 2016
CHiMaD Headquarters

May 3, 2016

08.30 am   *Shuttle from Hilton Orrington to CHiMaD HQ*

08.45 am   Breakfast, Registration, Setup

09.00 am   **Welcome**
             Begum Gulsoy (NU/CHiMaD)

09.05 am   **Hackathon Benchmark Problems**
             Olle Heinonen (ANL/NAISE)

12.00 pm   **Lunch**

07.00 pm   **Deep Dish Pizza!**

May 4, 2016

6.30 am   Breakfast

8.00 am   **Hackathon Ends**
             All files must be uploaded to the Dropbox folders

8.15 am   *Shuttle from CHiMaD HQ to Hilton Orrington*

Coffee & soda & snacks will be available throughout the hackathon.

CHiMaD | Center for
Hierarchical
Materials Design

Agenda
Phase Field Methods III
Hackathon \\\ Workshop
May 4-5, 2016 | CHiMaD Headquarters

May 4, 2016

08.50 am   *Shuttle from Hilton Orrington to CHiMaD HQ*

09.00 am   Breakfast, Registration, Setup

09.20 am   **Welcome**
            Peter Voorhees (NU/CHiMaD)

09:30 am   **DUNE project**
            Oliver Sander (Techniche Universitat Dresden)

10.00 am   **Updates on MOOSE Framework**
            Daniel Schwen (INL)

10:15 am   **Updates on PRISMS-PF**
            Shiva Rudraraju (U-M)

10:30 am   Coffee Break

10:45 am   **Updates on FiPy**
            Jonathan Guyer (NIST)

11.00 am   **Phase Field Website**
            Daniel Wheeler (NIST)

11.30 am   **Updated Benchmark Problems from Hackathon I**
            Olle Heinonen (ANL/NAISE), Andrea Jokisaari (NU/ANL)

12.00 am   **Benchmark Problems of Hackathon II**
            Olle Heinonen (ANL/NAISE)

12.30 pm   **Lunch**

1.00 pm   **Discussion**

5:00 pm   **Workshop Reception**

CHiMaD | Center for Hierarchical Materials Design

Agenda
Phase Field Methods III
Hackathon \\\ Workshop
May 4-5, 2016 | CHiMaD Headquarters

May 5, 2016

08:30 am   *Shuttle from Hilton Orrington to CHiMaD HQ*

08:45 am   Breakfast

09:00 am   **Recap of Hackathon Questions**
                  Olle Heinonen (ANL - NAISE)

Session One: Hackathon Results

9:10 am   **Team 1, lead by Olle Heinonen**
                  John Mangeri (UConn), Krishna Pitike (UConn)

9:30 am   **Team 2, lead by Tatu Pinomaa**
                  Kaushik Shampur (McGill), Nathan Smith (McGill)

9:50 am   **Team 3, lead by Michael Tonks**
                  Kasra Momeni (Penn State), Ian Greenquist (Penn State)

10:10 am   **Team 4, lead by Shiva Rudraraju and Stephen Dewitt**
                  Beck Andrews (U-M), Jason Luce (U-M)

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

10:50 am   **Team 6, lead by Trevor Keller**
                  Trevor Keller (NIST), Daniel Wheeler (NIST)

11:10 am   Coffee Break

Session Two: Discussion

11:25 am   **Discussion: Hackathon Results**

12:30 pm   **Lunch**

2:00 pm   **Discussion: Future Plan and Action Points**

3:00 pm   **Adjourn**

CH¡MaD | Center for Hierarchical Materials Design

Attendee List
CHiMaD Phase Field Methods Workshop III & Hackathon
May 3-5, 2016

Larry Aagesen, *Idaho National Laboratory, USA*
Larry.Aagesen@inl.gov

Karim Ahmed, *Idaho National Laboratory, USA*
karim.ahmed@inl.gov

W. Beck Andrews, *University of Michigan, USA*
wband@umich.edu

James Belak, *Lawrence Livermore National Laboratory, USA*
belak1@llnl.gov

Sudipta Biswas, *Purdue University, USA*
Biswas7@purdue.edu

David Chopp, *Northwestern University, USA*
chopp@northwestern.edu

Stephen Dewitt, *University of Michigan, USA*
stvdwtt@umich.edu

Ian Greenquist, *Penn State University, USA*
itgreenquist@gmail.com

Jonathan Guyer, *National Institute of Standards and Technology, USA*
jonathan.guyer@nist.gov

Olle Heinonen (Co-Organizer), *Argonne National Laboratory, USA*
heinonen@anl.gov

Andrea Jokisaari, *Northwestern University, USA*
Andrea.jokisaari@northwestern.edu

Trevor Keller, *National Institute of Standards and Technology, USA*
Trevor.keller@nist.gov

Jason Luce, *University of Michigan, USA*
jpluce@umich.edu

John Mangeri, *University of Connecticut, USA*
john.magneri@uconn.edu

Kasra Momeni, *Penn State University, USA*
kzm5606@psu.edu

Tatu Pinomaa, *University of McGill, CANADA*
Tatu.pinomaa@mail.mcgill.ca

Krishna Pitike, *University of Connecticut, USA*
krishna.pitike@uconn.edu

Stefan Poulsen, *Northwestern University, USA*
Stefan.poulsen@northwestern.edu

Siva Shankar Rudraraju, *University of Michigan, USA*
rudraa@umich.edu

Oliver Sander, *Technische Universitat Dresden, GERMANY*
oliver.sander@tu-dresden.de

Daniel Schwen, *Idaho National Laboratory, USA*
Daniel.Schwen@inl.gov

Kaushnik Natarajan Shampur, *University of McGill, CANADA*
kshampur@gmail.com

Barry Smith, *Argonne National Laboratory, USA*
bsmith@mcs.anl.gov

Nathan Smith, *University of McGill, CANADA*
nathan.smith5@mail.mcgill.ca

Michael Tonks, *Penn State University, USA*
mrt5296@psu.edu

Peter Voorhees (Co-Organizer), *Northwestern University, USA*
p-voorhees@northwestern.edu (Co-Director CHiMaD)

James Warren, *National Institute of Standards and Technology, USA*
james.warren@nist.gov

Daniel Wheeler, *National Institute of Standards and Technology, USA*
daniel.wheeler2@gmail.com

Logistics
Phase Field Methods Workshop
May 3-5, 2016

Workshop Location

CHiMaD Headquarters
Northwestern University
2205 Tech Drive, Evanston, IL, 60208

Parking Information

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

If driving, please park at the North Garage and take a ticket as you enter. Validation tickets will be available at the CHiMaD headquarters.

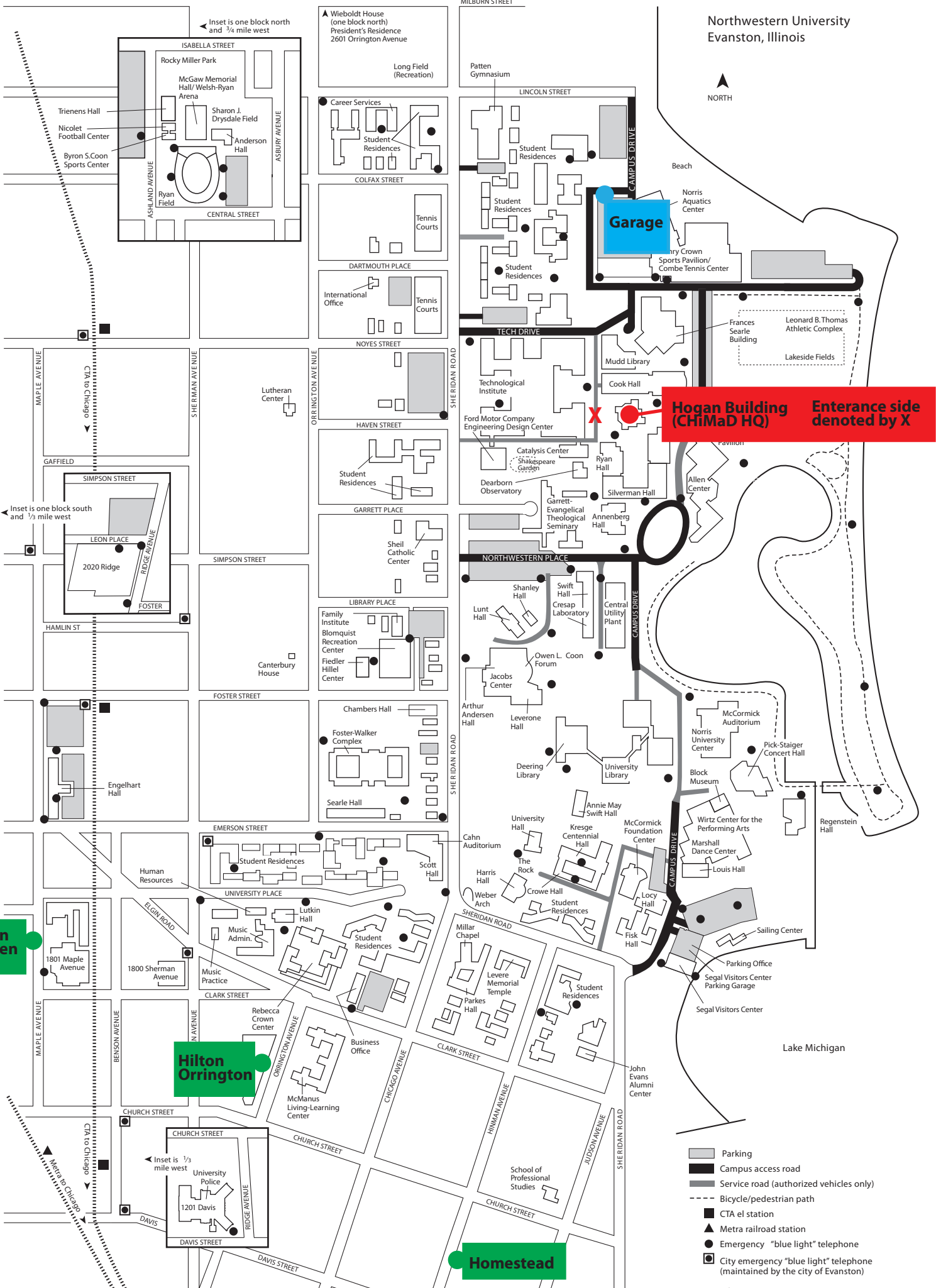---

Hotel & Shuttle Information

Hilton Orrington
1710 Orrington Ave, Evanston, IL, 60201

A shuttle is available to take the attendees from the hotel to workshop/hackathon and back.

Please see the map on the next page for locations.

Reimbursements

Please contact *Kathleen Bennett*, Kathleen.bennett@northwestern.edu.

Northwestern University
Evanston, Illinois

NORTH

Garage

Hogan Building (CHiMaD HQ)

Enterance side denoted by X

MILBURN STREET

Wieboldt House
(one block north)
President's Residence
2601 Orrington Avenue

ISABELLA STREET

Rocky Miller Park

McGaw Memorial Hall/ Welsh-Ryan Arena

Sharon J. Drysdale Field

Trienens Hall

Nicolet Football Center

Anderson Hall

Byron S. Coon Sports Center

Ryan Field

ASHLAND AVENUE

ASBURY AVENUE

CENTRAL STREET

Long Field (Recreation)

Patten Gymnasium

LINCOLN STREET

Career Services

Student Residences

COLFAX STREET

Student Residences

Student Residences

Student Residences

Beach

CAMPUS DRIVE

Norris Aquatics Center

Henry Crown Sports Pavilion/ Combe Tennis Center

Tennis Courts

DARTMOUTH PLACE

International Office

Tennis Courts

Leonard B. Thomas Athletic Complex

Lakeside Fields

Frances Searle Building

TECH DRIVE

Mudd Library

NOYES STREET

Lutheran Center

Technological Institute

Cook Hall

Ford Motor Company Engineering Design Center

ORRINGTON AVENUE

SHERMAN AVENUE

MAPLE AVENUE

CTA to Chicago

GAFFIELD

HAVEN STREET

Catalysis Center

Shakespeare Garden

Dearborn Observatory

Ryan Hall

Silverman Hall

Pavilion

Allen Center

Student Residences

GARRETT PLACE

Garrett-Evangelical Theological Seminary

Annenberg Hall

Inset is one block south and ⅓ mile west

SIMPSON STREET

2020 Ridge

LEON PLACE

RIDGE AVENUE

FOSTER

Sheil Catholic Center

NORTHWESTERN PLACE

Shanley Hall

Swift Hall

Central Utility Plant

CAMPUS DRIVE

SIMPSON STREET

HAMLIN ST

LIBRARY PLACE

Family Institute

Blomquist Recreation Center

Fiedler Hillel Center

Lunt Hall

Cresap Laboratory

Canterbury House

Owen L. Coon Forum

FOSTER STREET

Chambers Hall

Jacobs Center

Foster-Walker Complex

Arthur Andersen Hall

Leverone Hall

McCormick Auditorium

Norris University Center

Pick-Staiger Concert Hall

Engelhart Hall

SHERIDAN ROAD

Searle Hall

Deering Library

University Library

Block Museum

Regenstein Hall

EMERSON STREET

Student Residences

Human Resources

Cahn Auditorium

Scott Hall

University Hall

Kresge Centennial Hall

McCormick Foundation Center

Annie May Swift Hall

Wirtz Center for the Performing Arts

Marshall Dance Center

Louis Hall

ELGIN ROAD

UNIVERSITY PLACE

Lutkin Hall

Harris Hall

The Rock

Crowe Hall

Weber Arch

Student Residences

Locy Hall

Hilton Garden Inn

1801 Maple Avenue

Music Admin.

1800 Sherman Avenue

Music Practice

Student Residences

SHERIDAN ROAD

Millar Chapel

Fisk Hall

CAMPUS DRIVE

Sailing Center

Parking Office

MAPLE AVENUE

BENSON AVENUE

N AVENUE

CLARK STREET

Rebecca Crown Center

ORRINGTON AVENUE

Business Office

CHICAGO AVENUE

Levere Memorial Temple

Parkes Hall

CLARK STREET

Student Residences

Segal Visitors Center Parking Garage

Segal Visitors Center

Hilton Orrington

McManus Living-Learning Center

HINMAN AVENUE

John Evans Alumni Center

Lake Michigan

CHURCH STREET

CHURCH STREET

University Police

1201 Davis

School of Professional Studies

JUDSON AVENUE

SHERIDAN ROAD

Inset is ⅓ mile west

DAVIS

RIDGE AVENUE

DAVIS STREET

CHURCH STREET

Homestead

Metra to Chicago

CTA to Chicago

Inset is one block north and ¾ mile west

Legend

- 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