



## Welcome

On behalf of myself, and my co-organizer Olaf Wiest, I'd like to welcome you to Notre Dame for the Heidelberg@ND summer school. Some of you may remember the inaugural event held last summer in Heidelberg at the IWR. The summer schools have two goals: to provide a useful pedagogical experience and to foster collaborations between our campuses. We hope that besides learning something about computation, that students will take the opportunity to share their research, and of course that everyone has a good time. This document explains some of the simple logistics. If you have questions or urgent issues arise don't hesitate to contact me.

Best Regards-  
John Parkhill & Olaf Weist  
617-642-3837

## What to Expect

The format mirrors last year's summer school. Breakfast is provided, and there are talks in the morning. Lectures are 2 hours but are interrupted by a 15 minute break, and usually end in 10-15 minutes of questions. Wear what you would normally wear to lab. Lunch is provided followed by tutorials, which will use the computers in the lab. Students are encouraged to bring their laptops to work on as well.

## Schedule

All lectures occur in DeBartolo 228, and allow for 10-15 minutes of discussion. The social activity on Monday is a dinner picnic at St. Patrick's park in the Berta Shelter. All participants and guests are welcome.

7:30 - 8:30 Breakfast	7:30 - 8:30 Breakfast	7:30 - 8:30 Breakfast	7:30 - 8:30 Breakfast	7:30 - 8:30 Breakfast
8:30 - 10:30 Ed Maginn - Basic Statistical Mechanics	8:30 - 10:30 FG - Protein Structure as it pertains to Simulation	8:30 - 10:30 Shariar Mobashery & Kiran Mattasenan - Computation And Experiment	8:30 - 10:30 Steve Corcelli - Force fields in liquids	8:30 - 10:30 Bodo Martin - Specialized Forcefields for Inorganic Compounds - Potentials
10:30 - Coffee	10:30 - Coffee	10:30 - Coffee	10:30 - Coffee	10:30 - Coffee
11 - 1p Jon Whitmer - Basic Molecular Dynamics	11 - 1p Frauke Gräter - Non-Equilibrium MD, Course Grading	11 - 1p Olaf Wiest - Computer Aided Design	11 - 1p Case Studies: Drug Design (OW)	11 - 1p Tengfei Luo - Transport in Molecular Dynamics Molecular Dynamics
1p - 2p Lunch	1p - 2p Lunch	1p - 2p Lunch	1p - 2p Lunch	1p - 2p Lunch
2p - 4p Hands On Intro - Basics of Computation (JP)	2p - 7p Tutorial Problems - Haiming	2p - 7p Student Projects	2p - 4:30p John Parkhill - QM techniques and QM/MM	2p - 7p Student Projects
4p - 7p Social Activities			4:30p - 7p Case Studies: Materials (JP)	

## Tutorial Groups

When you arrive Monday, please find your group so that you can sit near them in the room. Simply sit in the Nth row of the room (left to right).

- 1- Patrick Louden, Eric Hansen, Xingfei Wei, Dieter Faltermeier
- 2- Wenqi Liu, Laura Nkulu, Michael Humbert, Marko Hermsen
- 3- Joong Hoon Koh, Neil Berkel, Yunsong Pang, Michael Gast
- 4- Kyle Conner, Vatsal Purohit, Francisco Herrera, Michael Quevillon, Tanju Eliguzel
- 5- Farbod Salahi, Trung T. Nguyen, Jarrod Schiffbauer, Salvatore Buonocore, Alexander Jacob
- 6- John Herr, Taylor Quinn, Yushan Zhang, Christopher Zapp

7- Brandon Tutkowski, Zeyu Liu, Teng Zhang,  
Alexander Dimmling

## Accommodations

Visiting students have their own rooms at Duncan Hall (Notre Dame, IN 46556) on the south side of Notre Dame's campus. Visiting faculty are housed at the Fairfield inn, on the southern end of campus.

## Local Information

The key locations are:

Debartolo Hall (Red dot on map below) where the summer school will be held.

Duncan Hall (Western house with flag) where visitors are housed.

Without a rental car the easiest way to get to/from Chicago ORD would be one of the bus services which stop at the Hesburg library. Another option is the South Shore line, which travels to/from South Bend Airport for about 10\$. This train terminates in the center of Chicago, to continue to ORD, board the CTA blue line to the airport.

A Google map annotated with points of local interest has been prepared.

<https://www.google.com/maps/d/edit?hl=en&hl=en&cauthuser=0&cauthuser=0&mid=1hjRHu-shAGODBVPnXa6fKZUMA2I>

