

06-640: Molecular Simulations

Final Project

Preliminary report due: Thursday 4/21

Final reports due: Friday 4/29

Peer Reviews due: Friday 5/6

One of the primary aims of this course has been to give you a broad enough introduction to the field of molecular simulations that you can successfully read papers in the literature that use these simulations. Although we cannot possibly cover every simulation technique in one semester, you should now know enough to understand and critically assess almost any simulation method you come across. This project gives you a chance to apply this knowledge by selecting some papers that use molecular simulations to examine a topic that interests you and writing a literature review of those papers.

Project Description

You should select a set of topically related papers to review. The topic that connects the papers may either be a physical system you are interested in (e.g., crack propagation in solids) or a simulation technique that we have not covered in class (e.g., semigrand ensemble MC). You will write a review paper that summarizes and synthesizes the contents of the papers you select. You should aim your review paper at readers with the same knowledge as other students in our class. To reinforce this fact, a portion of the total grade for this project will be assigned by your classmates (see below for more details). This means that you must motivate why the physical problem being studied is interesting. You must also explain the details of any simulation techniques we didn't cover in class in enough detail that an informed reader can understand how the techniques work. It is also important to put the papers you review within a larger context. This means that you should not only talk about simulations, but you should also say something about experimental approaches or other theoretical approaches to your topic.

Below is a list of the rules and regulations that will govern this project.

1. You must review at least 3 papers. You may of course review more, but note that padding the bibliography with dozens of references that you scarcely mention in your paper will not gain you any credit.
2. Your review should synthesize the results and methods of the various papers you read. Disconnected summaries of individual papers are not acceptable.
3. Your paper should be written in a form that makes sense when read aloud. For example, summarizing papers using itemized lists is unacceptable.
4. Your paper must include a bibliography with the full citation of any source you discuss in the text of your paper.
5. The paper must be typed with single-spacing. Grammar and spelling will be included in grading the paper.
6. *Do not plagiarize your sources.* This means that any wording taken directly from your sources must be attributed as a direct quote. Note that in general scientific writing, the use of direct quotes is extremely uncommon, so it is better to rewrite all information from your sources in your own words. You may include figures directly from your sources provided you indicate where they come from.

7. There is no maximum or minimum length. Despite this freedom, it is unlikely that any well written paper will be shorter than 10 pages or longer than 20 pages.
8. No extensions of the due date will be given.
9. Graduate students who are working on theoretical thesis projects may not choose their thesis topic as the topic for their paper. These students *are* strongly encouraged to choose a topic relevant to their research. If this applies to you, please discuss your choice of topic with Prof. Sholl before starting work.
10. Check the guidelines for written assignments on our class web-page for more general information.

Project Timeline

There are four important dates associated with this project.

Thursday April 21 – Preliminary Report due

By this date you should give Prof. Sholl a single page summary of the topic you will be covering in your report and the papers you have identified. Each paper should be summarized with 2 or 3 sentences indicating what it is about and why it is relevant to your chosen topic. 10% of the total grade for this project is allotted to turning in this report on time – to receive the full 10% you only have to turn in an acceptable report on time. The purpose of this preliminary report is to give Prof. Sholl a chance to suggest any important references that you may not be aware of.

Friday April 29 – Final Report due

Your final report should be in Prof. Sholl's mailbox in Doherty Hall by 5 pm on 5/11. **Make sure you provide 3 copies of your report (one for Prof. Sholl and two for your peer reviewers).**

Monday May 2– Papers Distributed for Peer Review

You will be responsible for reading two of your classmate's papers (see "Grading" below). The papers you will read will be available from Linda Dorsey in DH3114 after 9 am on Monday May 2.

Friday May 6 – Peer Reviews Due

Your reviews of the two papers you read must be in Prof. Sholl's mailbox by 5 pm on Friday May 6. If you do not return your reviews on time, the peer review grade for your own paper will be set to zero.

Grading

The total grade for this project will be split into 3 portions:

Preliminary report (10%)

Peer reviews of final report (25%)

Prof. Sholl's review of final report (65%)

Peer Reviews

Your final report will be read by two of your classmates, who will assign it a numerical grade in several specified criteria (e.g. clarity of presentation). The peer reviewers of each paper will be assigned randomly. The intent of this process is to provide a strong incentive for you to write your paper at a level that is informative and clear to your peers. As noted above, papers will be distributed for peer review one day after the papers are

due. Peer reviews must be returned to Prof. Sholl by Monday May 13. The review forms that will be used are attached as the last two pages of this document.

Possible Topics

You are free to choose any topic for your literature review. You will get the most out of this exercise if you choose a topic that you are genuinely interested in! Please feel free to discuss your ideas with Prof. Sholl. If you do not have a specific topic in mind that you would like to explore, you may consider the list of topics below. For each topic, two references that will provide a good starting point for your reading are suggested.

Phase equilibria of chemical mixtures using Gibbs Ensemble MC

J. G. Amar, *Mol. Phys.* **4** (1989) 739

R. D. Mountain and A. H. Harvey, *J. Chem. Phys.* **94** (1991) 2238

Large scale simulation of crack propagation

F. F. Abraham, *Phys. Rev. Lett.* **77** (1996) 869

J. Q. Broughton et al., *Phys. Rev. B* **60** (1999) 2391

Simulations of dense polymer systems

L. R. Dodd, T. D. Boone, and D. N. Theodorou, *Mol. Phys.* **78** (1993) 961

J. J. de Pablo et al, *J. Chem. Phys.* **96** (1992) 2395

Intermolecular potentials for water

M. Sprik and M. Klein, *J. Chem. Phys.* **89** (1988) 7556

E. R. Batista et al., *J. Chem. Phys.* **109** (1998) 4546

Properties of polar fluids

M. E. van Leeuwen and B. Smit, *Phys. Rev. Lett.* **71** (1993) 3991

J. J. Weis et al., *Phys. Rev. Lett.* **71** (1993) 2729

GCMC and Gibbs Ensemble Simulations for Dense Systems

G. L. Detrick, L. E. Scriven, and H. T. Davis, *J. Chem. Phys.* **90** (1989) 2370

M. R. Stapleton and A. Z. Panagiotopoulos, *J. Chem. Phys.* **92** (1990) 1285

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Peer Review of Final Project

Project Author: _____

Reviewer #: _____

Reviewer Name: _____

Reviewer Signature: _____

After carefully reading your classmate's final paper, give the paper a numerical grade in each of the categories listed on the following page. There is also space for you to provide written comments about the paper. Please include comments about both the strengths and weaknesses of the paper. As mentioned in class, reviewing these papers is not intended to take an excessive amount of time. If the paper takes a long time to read because it is difficult to follow, the responsibility lies with the author, not the reviewer.

This review must be placed in Prof. Sholl's mailbox (on the ground floor of Doherty Hall) by 5pm on Friday May 6.

This sheet will be returned to the paper's author

Author of paper: _____

Reviewer Number: _____

Numerical Grade (total possible grade is 10)

Clarity of presentation and writing ___ / 3

Description of background material
(e.g. motivation of physical problem) ___ / 3

Description of technical content ___ / 2

Ability to synthesize multiple sources
Into a coherent report ___ / 2

TOTAL: ___ / 10

Written Comments (attach extra sheet if necessary):