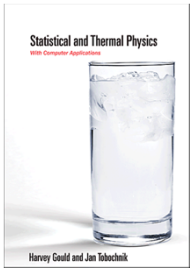
PHY 341/641 Thermodynamics and Statistical Mechanics
10-10:50 AM MWF Olin 107

Instructor: Natalie Holzwarth (Olin 300)
Course Webpage: http://www.wfu.edu/~natalie/s12phy341



Supplemental webpage:
http://www.compadre.org/STP/

PHY 341/641 Thermodynamics and Statistical Mechanics

MWF 10:00-10:50 AM | OPL 107 | http://www.wfu.edu/~natalie/s12phy341/

Instructor: Natalie Holzwarth | Phone:758-5510 | Office:300 OPL | e-mail:natalie@wfu.edu

- General information
- Syllabus and homework assignments
- Class notes

HOME | HELP | SEARCH | CONTENTS | CALENDAR | DIRECTORY

Last modified: Saturday, 07-Jan-12 12:15:59

Textbook: ("**STP**")
Statistical and Thermal Physics With Computer Applications by Harvey Gould and Jan Tobochnik, Princeton University Press, 2010

Supplemental materials provided by authors: http://www.compadre.org/stp/

This course integrates macroscopic and microscopic viewpoints of thermodynamics -- the study of energy and energy transfer, with a focus on equilibrium processes.

It is likely that your grade for the course will depend upon the following factors:

Problem sets*	40%
Take-home exams (2)	30%
Presentation	10%
Final exam	20%

*In general, there will a new assignment after each lecture, so that for optimal learning, it would be best to complete each assignment before the the next scheduled lecture. According to the honor system, all work submitted for grading purposes should represent the student's own best efforts. This means that students who work together on homework assignments should all contribute roughly equally and independently verify all derivations and results. Homeworks may be turned in 1 lecture past their due date without grade penalty. After that, the homework grade will be reduced by 10% for each succeeding late date.

Schedule and assignments

Note: This schedule may need to be modified -- please check for changes and additions frequently.

No.	Lecture Date	Topic	Text Sections	Problem Assignments	Assignment Due Date
1	1/18/2012	Introductory concepts	1.1-1.5	HW 1	1/20/2012
2	1/20/2012	Introductory concepts	1.6-1.12	HW 2	1/23/2012
	1/23/2012				
	1/25/2012				
	1/27/2012				
	1/30/2012				
	2/01/2012				
	2/03/2012				
	2/06/2012				
	2/08/2012				
	2/10/2012				

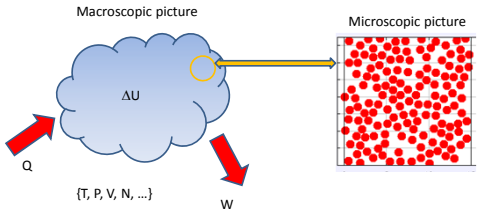
Spring 2012 Schedule
for N. A. W. Holzwarth

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00-10:00	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours
10:00-11:00	Thermo PHY341/641		Thermo PHY341/641		Thermo PHY341/641
11:00-12:30	Physics Research	General Physics II PHY114	Physics Research	General Physics II PHY114	Physics Research
12:30-2:00	Condensed Mater Theory Journal Club	Physics Research		Physics Research	
2:00-3:30	Physics Research				
3:30-5:00			Physics Colloquium		CEES - Renewable Energy Research

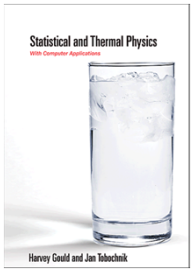
Travel dates:
- **Feb. 27 - Mar. 2, 2012** (March APS meeting -- Boston, MA.)

What will you learn?

Energy Analysis



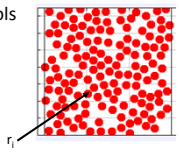
Chapter 1 – From Microscopic to Macrosopic Behavior



Assignment: Read Chapter 1 (quickly) during this week and checkout some of the corresponding simulations (HW 1 and HW 2).

"The purpose of this introductory [material] is to whet your appetite… " The chapter introduces a lot of the concepts that we will use (more carefully) throughout the course.

Comment on simulation tools
Molecular dynamics



$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i$$

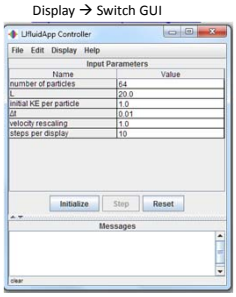
$$\mathbf{F}_i = -\nabla_i \sum_{j \neq i} u_{pair}(|\mathbf{r}_i - \mathbf{r}_j|)$$

Example model pair potential (Lennard-Jones):

$$u_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

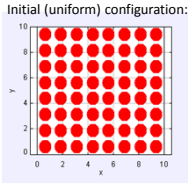
Simulation available from: http://www.compadre.org/STP/stp_LJ2DMD.jar

Note: in order to easily control the simulation, you need to use:
Display → Switch GUI

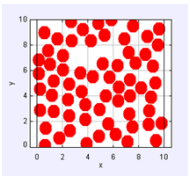


Results for N=64, L=10

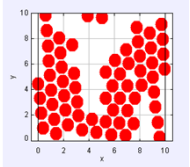
Initial (uniform) configuration:



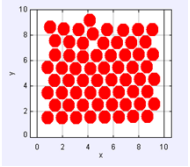
Thermalized (liquid-like) configuration:



Cooled (condensed) configuration:

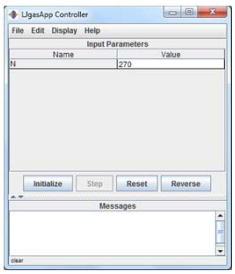


Cooled (condensed) configuration:



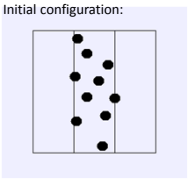
Simulation available from: http://www.compadre.org/STP/stp_MDApproachToEquilibriumThreePartitions.jar

Note: in order to easily control the simulation, you need to use:
Display → Switch GUI



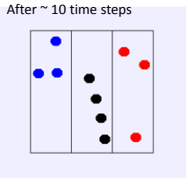
Results for N=10, t≈10 followed by reversal (v → -v)

Initial configuration:

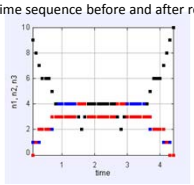


→

After ~ 10 time steps

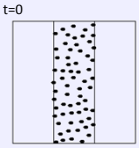


Plot of time sequence before and after reversal:

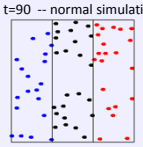


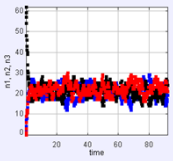
Results for N=64, t≈45-90, with and without reversal

t=0

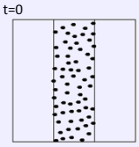


t=90 -- normal simulation

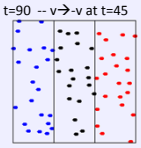


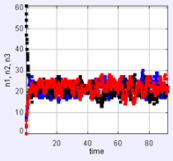


t=0



t=90 -- v→-v at t=45





Simulation available from: http://www.compadre.org/STP/stp_ApproachToEquilibrium.jar

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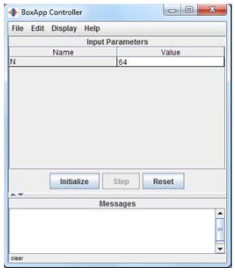
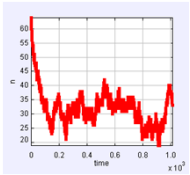


N=64, t≈1000 $\langle n \rangle = 32.08$, $\langle n^2 \rangle = 1{,}067.13$, $\sigma^2 = 38.12$, $\sigma/\langle n \rangle = 0.19$



N=64, t≈1000 $\langle n \rangle = 149.57$, $\langle n^2 \rangle = 23{,}086.17$, $\sigma^2 = 714.56$, $\sigma/\langle n \rangle = 0.18$