FYS2160 2025, Lecture 6

Dag Kristian Dysthe

Molecular dynamics

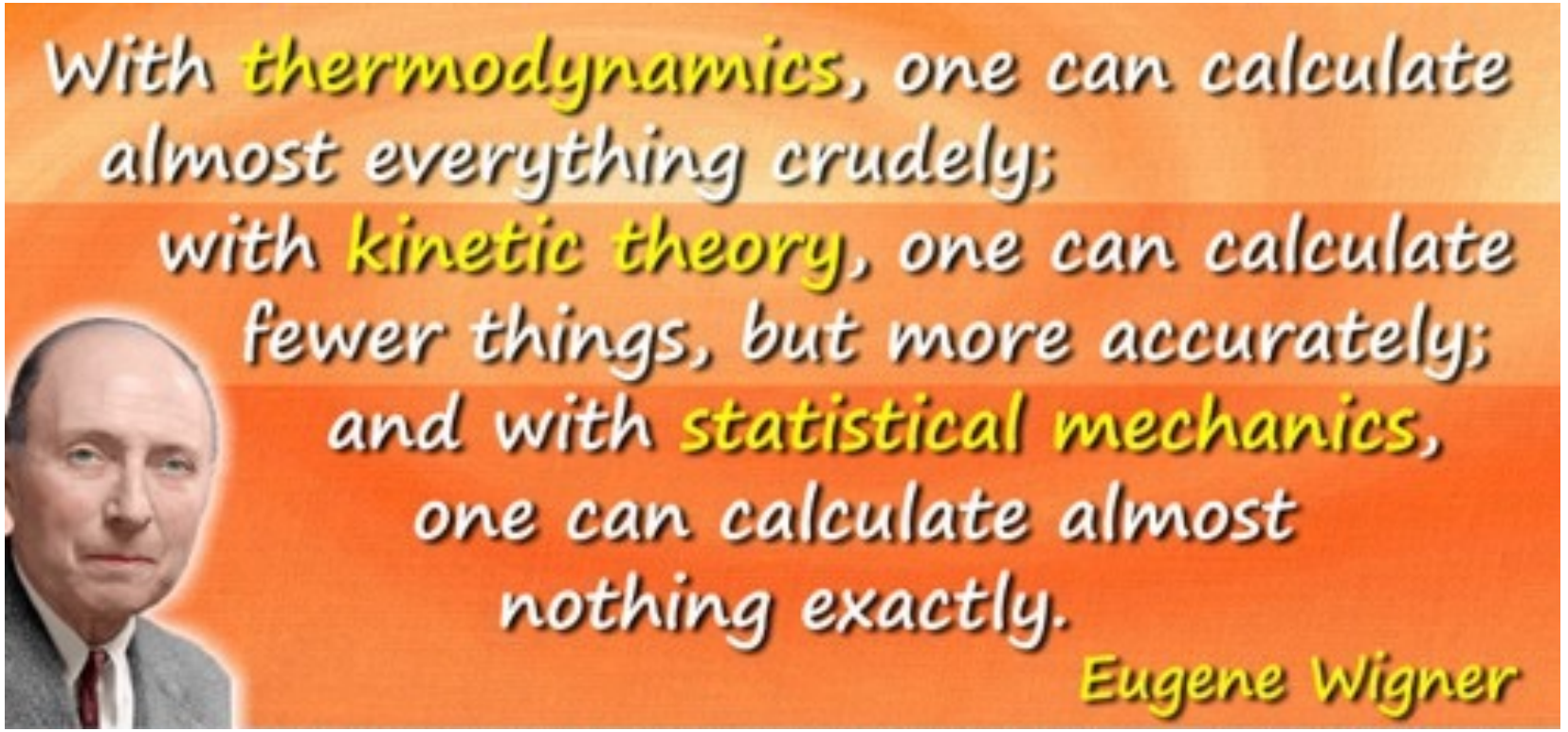
09.09.2025

Oracle sessions

Trial period: Sessions Thursday 14:15-16:00

Those who have student union meetings in this period:

Thursday 12:15-14:00 at Silja’s office, room FV 427



- But statistical mechanics defines how to calculate thermodynamic properties from simulation of model systems.
- This makes stat. mech. even more important in the era of computers!
- This is why computation should be part of your thermydyn. & stat. mech. curriculum!

my-first-md-simulation.in

```
# Move camera to a nice position
#/camera position 15 15 40
#/camera target 15 15 0

# Set atom size and color
units lj
boundary p p p
atom_style atomic

# Define the space and put atoms in
dimension 2
region simbox block 0 30 0 30 -0.1 0.1
create_box 1 simbox
lattice hex 0.45
create_atoms 1 box

# Define properties of the atoms
mass 1 1.0
velocity all create 0.65 87287
pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5

# Speed up simulation with neighbour lists
neighbor 0.3 bin
neigh_modify every 20 delay 0 check yes

# Define thermodynamic ensemble
#fix 1 all nvt temp 0.3 0.3 0.3
fix 1 all nve

# Define trajectory file name and content...
dump 1 all custom 10 dump.lammpstrj id type x y vx vy

# Define thermodynamic data file (log.lammps)
thermo_style custom time pe ke temp press
thermo 100

# run simulation + number of steps
timestep 0.003
run 10000
```

www.uio.no/studier/emner/matnat/fys/FYS2160/h25/lectures/lecture6/index.html

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← Studier ← Emner ← Matematikk og naturvitenskap ← Fysikk ← FYS2160 ← Høst 2025 ← Lectures

Lecture1
Lecture10
Lecture11
Lecture12
Lecture13
Lecture14
Lecture15
Lecture16
Lecture17
Lecture18

FYS2160 - Termodynamikk og statistisk fysikk

Lecture notes

Lecture notes

Your first Atomify Lammps simulation

Open your First simulation using Atomify Lammps

My first MD simulation

Click on the example entitled: **My first MD simulation**

Follow the instructions on that web page!

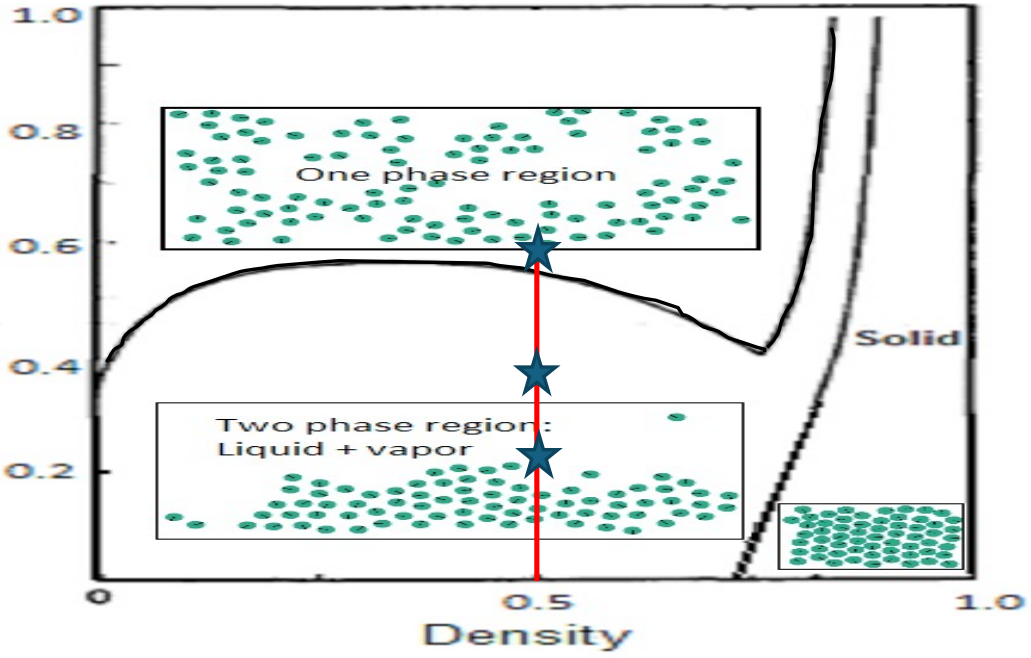
First simulation, run and visualize

https://tinyurl.com/2rmxz838

Change parameters and rerun

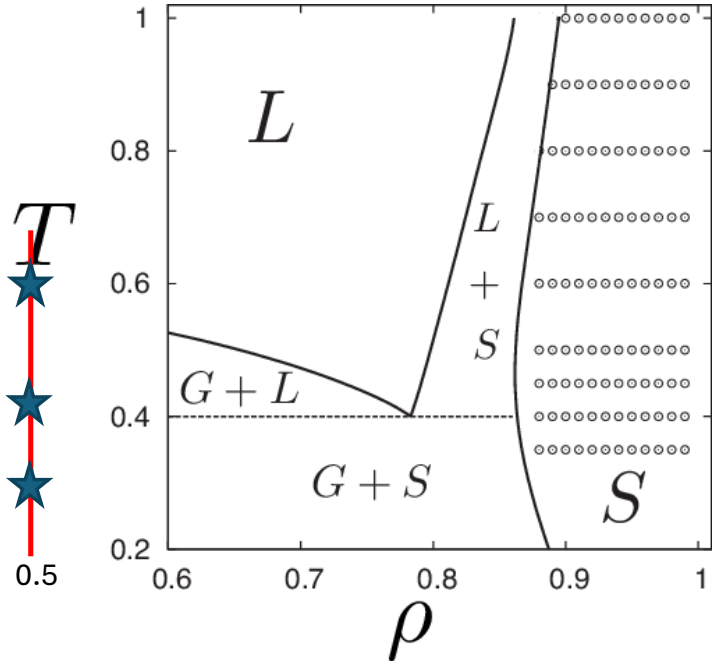
- open **my-first-md-simulation.in**
- run, view visualization, analyze with Notebook
- change temperatures in line «**fix 1 all nvt temp 0.3 0.3 0.3**» 0.3 -> 0.4 and 0.6
- rerun simulation

My first MD simulation



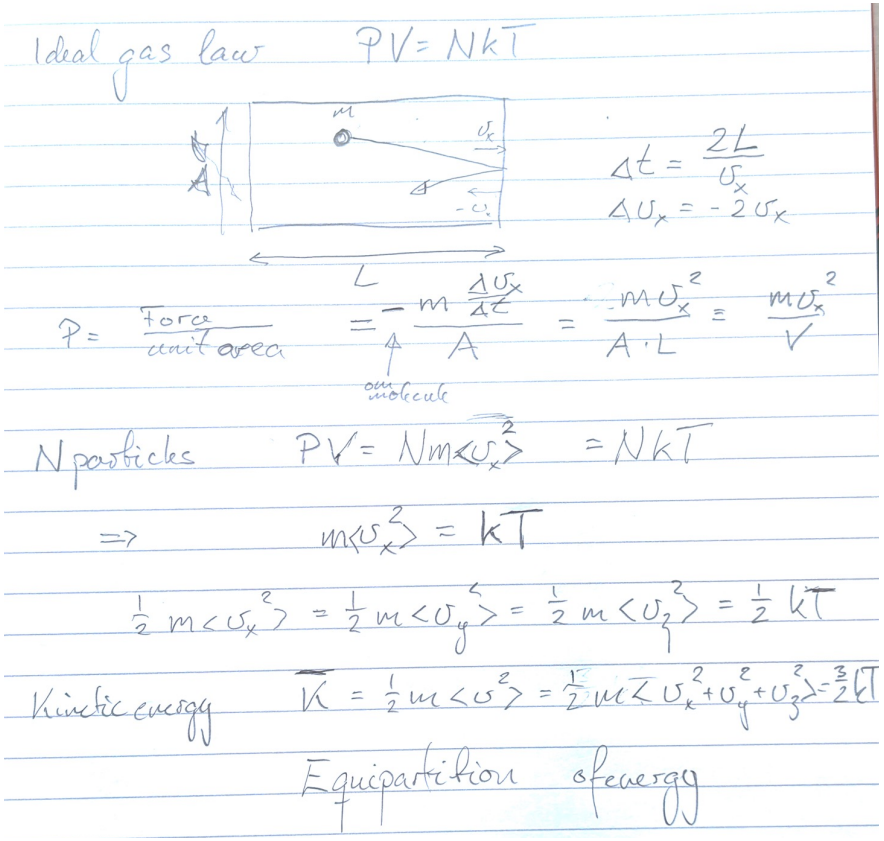
2D Lennard-Jones

velocity all create 0.5 87287



Ideal gas model

- Point particles
- Non-interacting
- Newtonian particles: $m\frac{d\vec{v}}{dt} = \vec{F}$
- Kinetic energy: $K = \frac{1}{2}mv^2 = \frac{3}{2}kT$
- Pressure: $P = \frac{mv^2}{V}$
- Ideal gas law: $PV = NkT$



My first MD simulation: pressure

- Pressure = Force / Area
  - *[P]= [F]/[A]=N/m²*
- Newtonian mechanics
  - $\vec{F} = m\vec{a} = \frac{d\vec{p}}{dt}$
  - Used this to calculate pressure of ideal gas:

$$P_x = \frac{1}{A}\sum_i \frac{\Delta p_{x,i}}{\Delta t} = \frac{1}{A} N \frac{m\bar{v}_x^2}{2L} = \frac{Nk_BT}{V} = \rho k_B T$$

- When forces at distance:
  - $P = \rho k_B T + \frac{1}{3V}\sum_{i<j} \vec{f}(\vec{r}_{ij}) \cdot \vec{r}_{ij}$
  - second term: virial

- **compute pressure** command
  - Syntax: compute ID group-ID pressure temp-ID keyword
  - Example: compute 1 all pressure thermo_temp
  - Define a computation that calculates the pressure of the entire system of atoms.

Documentation: https://docs.lammps.org/

3d-msd-diffusion.in

```
units lj
atom_style atomic
lattice fcc 0.3
variable T equal 1.4

# Geometry
...
# Set atom masses
mass 1 1.0
mass 2 100.0
# Set atom sizes and well depths
# Choose LJ with 2.5sigma cutoff
pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0 2.5

#pair_coeff 1 1 1.0 1.0 2.5
#pair_coeff 2 2 1.0 2.0 5.0
#pair_coeff 1 2 1.0 1.5 3.8

# Create two groups for computing diffusion coefficients
group light type 1
group heavy type 2
compute msd_light light msd com yes
variable diffusion_coeff_light equal c_msd_light[4]/6/(step*dt+1.0e-6)
compute msd_heavy heavy msd com yes
variable diffusion_coeff_heavy equal c_msd_heavy[4]/6/(step*dt+1.0e-6)

thermo_style custom time temp atoms vol press c_msd_light[4] c_msd_heavy[4]
thermo 100
dump 1 all custom 100 diffusion.lammpstrj id type x y z vx vy vz

fix 1 all nvt temp $T $T 1
run 10000
```

3D diffusion MSD

- What is the ratio of diffusion coefficients of the two atom types in this simulation?
- Look in the input file 3D-msd-diffusion.in and see if you can determine why one atom type diffuses much faster than the other.
- Try to change the parameter you think is responsible for the difference in diffusion coefficient and see if you can make them equal

```
units lj

variable Tstart equal 0.1
variable Tstop equal 0.6
variable Tdamp equal 1
variable rho equal 0.5

dimension 2
boundary p p p
atom_style atomic
lattice hex $(v_rho)
region simbox block 0 40 0 20 -0.1 0.1
create_box 1 simbox
create_atoms 1 box
mass 1 1.0

velocity all create ${Tstart} 87287
pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5

compute mymsd all msd com yes
variable mymsdv equal c_mymsd[4]
thermo_style custom time temp pe ke press c_mymsd[4]

fix 1 all nvt temp ${Tstart} ${Tstop} ${Tdamp}
thermo 100
run 100000
```

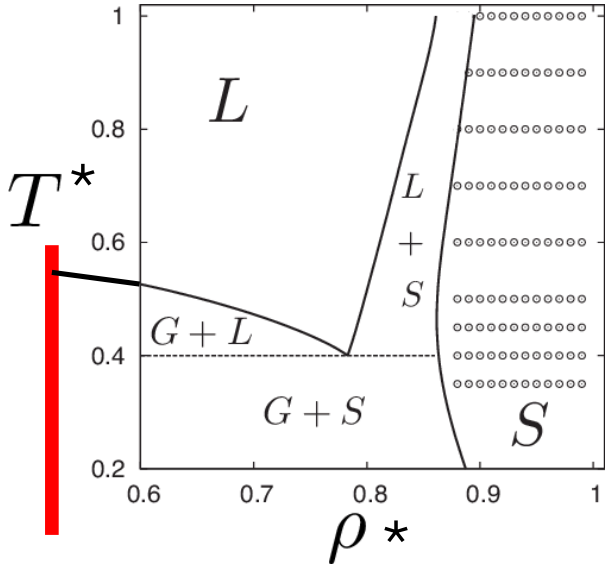
Melting of a 2D solid

- Observe the phases during the simulation. Which phases do you see?
- Does this correspond to what you expect from the phase diagram?
- How does the slope of the mean square displacement change for the different phases?

Melting of a 2D solid

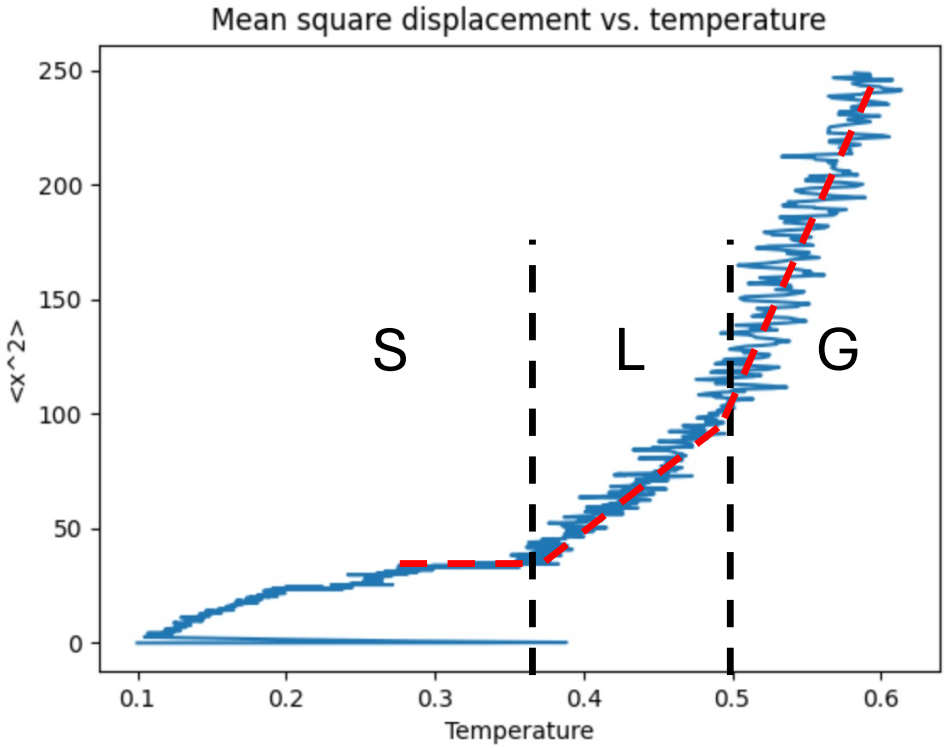
```
variable Tstart equal 0.1
variable Tstop equal 0.6
variable Tdamp equal 1
variable rho equal 0.5
fix 1 all nvt temp ${Tstart} ${Tstop} ${Tdamp}
```

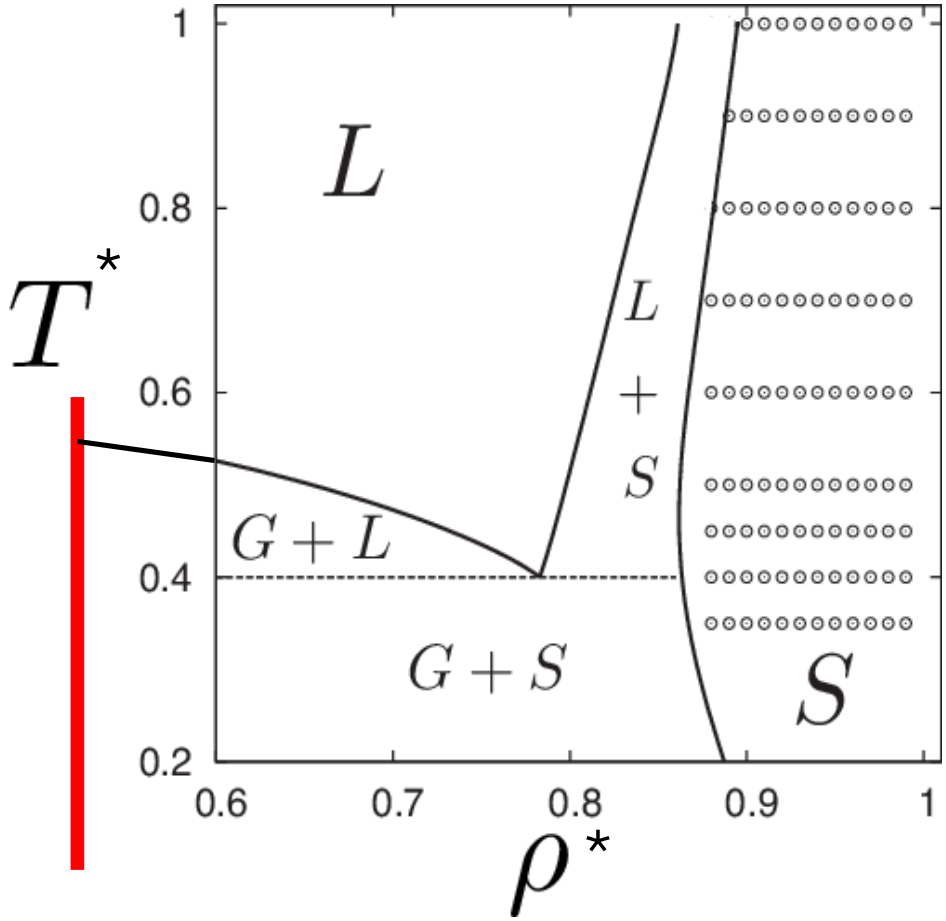
Atomify example **https://tinyurl.com/2rmxz838**




```
compute mymsd all msd com yes
variable mymsdv equal c_mymsd[4]
thermo_style custom time temp pe ke press c_mymsd[4]
```

Melting of a 2D solid





heat-capacity-lj.in

```
# Atomify commands start with #/

# Move camera to a nice position
#/camera position 20 85 55
#/camera viewcenter 20 20 10

# Set atom size and color
#/atom 1 2.0 #ffffff
#
# Define variables
##############################################
# dilute gas: rho = 0.005
# liquid:     rho = 0.85
# solid:      rho = 1.1
variable rho equal 0.005
##############################################
variable Tstart equal 0.7
variable Tstop equal 1.8
variable Tdamp equal 1
variable N equal 100
variable L equal ($N/${rho})^(1/3)

# Use Lennard-Jones units, periodic boundaries and
# atomic model
units lj
boundary p p p
atom_style atomic

# Define the space and put atoms in
dimension 3
region simbox block 0 $L 0 $L 0 $L
create_box 1 simbox

# Define properties of the atoms
create_atoms 1 random $N 12345 simbox
mass 1 1.0
velocity all create ${Tstart} 87287
pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5

# Define thermodynamic ensemble for thermalization
fix 1 all nvt temp ${Tstart} ${Tstop} ${Tdamp}
thermo_style custom time temp pe ke
thermo 100
run 50000
```

MD heat capacity experiment

Heat capacity calculation

- What is the heat capacity of the LJ fluid
  - In the dilute gas phase?
  - In the liquid phase?
  - In the solid phase?
- How does this fit with theory?

Syntax

- fix heat command
  - Syntax: fix ID group-ID heat N eflux
  - Add non-translational kinetic energy (heat) to a group of atoms in a manner that conserves their aggregate momentum.

```
variable eFlux equal 0.01

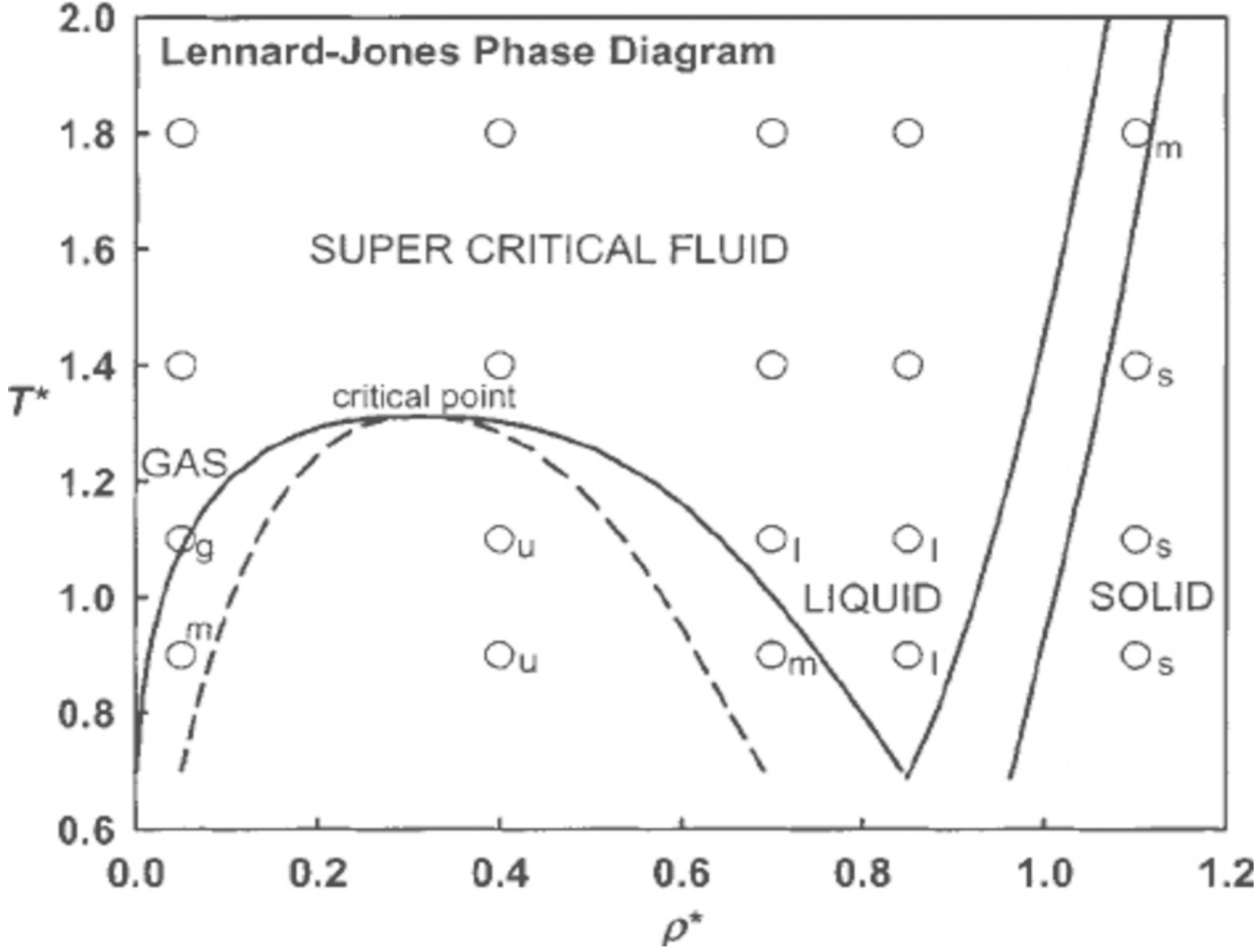
fix heat all heat 1 ${eFlux} region box
```

Heat capacity simulation

https://tinyurl.com/2rmxz838

- Definition?
  - $C = {}^{dQ}/_{dT}$
- Ideal gas energy?
  - $E = {}^{N}/_{2}\, m < v^2 >= {}^{3N}/_{2}\, kT$
- Heat capacity of ideal gas?
  - $C = {}^{dE}/_{dT} = {}^{3Nk}/_{2}$
- LJ units?
  - $C^* = {}^{C}/_{Nk} = {}^{3}/_{2}$
- Harmonic oscillator energy?
  - $E = {}^{N}/_{2}\, mv^2 + {}^{N}/_{2}\, kx^2 = 3NkT$
  - $C^* = 3$

3D


Lennard-Jones Phase Diagram
SUPER CRITICAL FLUID
critical point
GAS
LIQUID
SOLID
g
u
l
m
s
T*
ρ*
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.0
0.2
0.4
0.6
0.8
1.0
1.2