Simulations in Statistical Physics

Course for MSc physics students

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November 3, 2015

Név:	Homework
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Gáldi Ádám György	4
Gróf Gábor	3
Janecska Máté István	2
Seress Mátyás	3
Rudas Csilla	2
Böröczki Zoltán István	2
Kovács Péter	4
Boldoczki Fanni	1
Molnár Zsanett	1
Takács Hajna Eszter	4
Nagy Dániel Bálint	4
Szegedi Domonkos	2
Orosz István	1
Pölöskei Péter Zsolt	3

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Lucsányi Dávid	2
Galambos Tamás	3
Pázmán Koppány	2
Vécsi István Áron	2
Kátai András	1
Szekér Péter	3
Pető János	1
Bagaméry Gergő	3
Hügelné Imecs Gabriella	4
Szendi Zsuzsanna	3
Sarah Thieme	4

Homework 1

Daemon with bag with tolerance. Responsible: András Lászlóffy

Consider an $N \times N$ square lattice with periodic boundary conditions and the Ising-model: $H = -\sum_{ij} J_{ij}\sigma_i\sigma_j$. Calculate the average magnetization for different system sizes (5×5, 10×10) and energies in the microcanonical ensemble. Calculate the probability of move denial as function of the energy.

Use the following parameters:

- J_{ij} are random constants between 0 and 1.
- Energy fluctuation must be smaller than E_0/N, where E_0 is the initial energy of the system

Homework 2

Kinetic Monte Carlo simulation

Investige polimer chains with Monte Carlo method on a 2d square lattice. Take a chain of N atoms, which can bend at every single atomic position, and so change the shape of the polimer. The probability of bending depends on the distance from the end (l) in the following way:

$$P_l = e^{-2\beta l/L}.$$

Every 3 possible position has the same probability, but if the chosen direction is occupied, the step will be denied. Measure the average length of the chain at different temperature values
$\beta = 0,\ 0.5,\ 1,\ 2,\ 5$ for chains of length $N = 20,\ 40,\ 80$.

Homework 3

Event-driven simulation

Consider a two-dimensional gas of rigid disks (mass: m, radius: R)! Put the disks in a square box with a size of $L \times L$. All the collisions are elastic, and the friction is neglible. Write an **event driven simulation** that simulates the dynamics of the gas. The main goal of the simulation is to describe the effect of opening a small hole on the box through which the disks can leak out.

- Run the simulation with $N = 100$ particles
- Wait until the gas thermalizes! (Simulate $\sim 10N$ collisions!)
- Now open a small hole on one of the walls.
- The hole size should be small, eg. define a $R/2$ length segment on one of the walls and if a prarticle touches it the particle is removed.
- Measure the kinetic energy per particle/disk in the box as a function of the remaining particle number! Try to explain the result!

Homework 4

Modularity of a network

Write an algorith which reads in a network file and then partitions it with the modularity community detection algorithm into two parts. Use simulated annealing to determine the optimal partition. Using an ensemble average of 100 samples determine the probability of links belonging to the same cluster. Measure the average of this value for the three supplied networks.

Optional:

Try to plot the networks using gephi, try also to plot the resulting network with gephi using link weights proportional to the probability of belonging to the same cluster.

Program

- Have an algorithm to calculate forces
- Get list of interacting particles
- Determine accelerations and velocities; step particles
- (Set temperature)

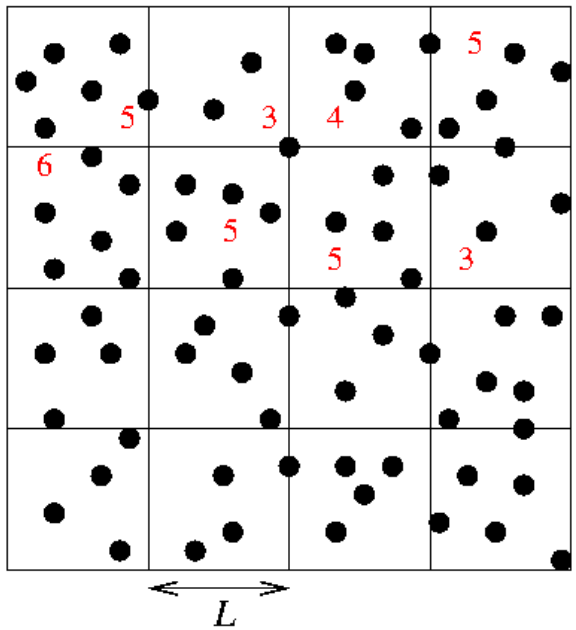
Find pairs

Now we know how to calculate forces. How to get pairs?

- All pairs: $\sim N^2$ calculations. *Only* if there is no other way!
- Short range interactions: box method
- Long range interactions: k-space

Bucketing algorithm

Finite interaction length L



b[0,0]={1,7,9,147,8};
b[0,1]={12,8,99};

- Grid with size L
- Grid of array with particle indexes in box
- Maximum number of neighbors or dynamic array
- If there is $v_{\max}$ then $L' = L + v_{\max}\Delta t$, then reset array every Δt timesteps

k-space solution

- Long reange interactions (e.g. Coulomb) cannot be cut off
- Often more periodic images are needed
- k-space (Fourier-transformation in 3d!)

$$V(\mathbf{k}) = g^2 \frac{4\pi}{k^2 + m^2}$$

  - Solution of linear problems by Green's-function
  - Coulomb problem: in Fouier space $\rightarrow$ multiplication!
- Ewald summation:
  - Handle short range in real and long range in k-space

Program

- Have an algorithm to calculate forces
- Get list of interacting particles
- Determine accelerations and velocities; step particles
- (Set temperature)

Euler method

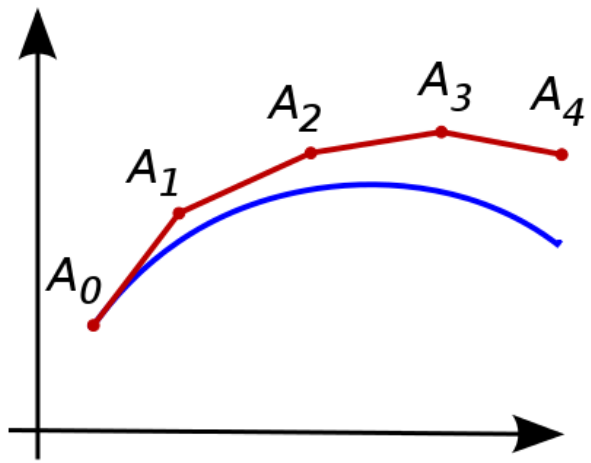
- Velocity:

$$\frac{\Delta v}{\Delta t} = F/m$$

$$\Delta v = F/m\Delta t$$

- Displacement

$$\Delta x = v\Delta t$$



Too bad!

Runge-Kutta method

$$\dot{y} = f(t, y), \quad y(t_0) = y_0.$$

$$y_{n+1} = y_n + \frac{1}{6}h\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$t_{n+1} = t_n + h$$

$$k_1 = f(t_n, y_n),$$

$$k_2 = f(t_n + \frac{1}{2}h, y_n + \frac{h}{2}k_1),$$

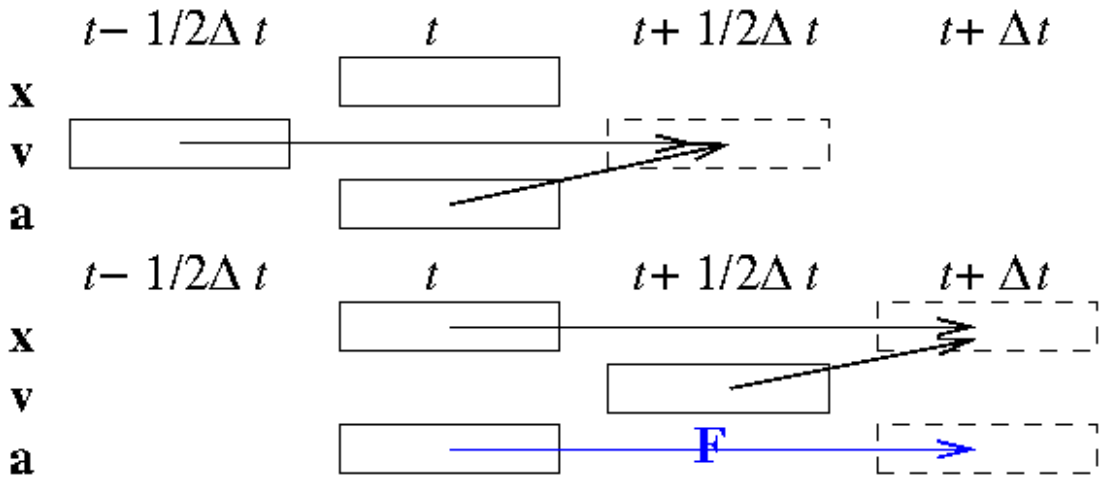
$$k_3 = f(t_n + \frac{1}{2}h, y_n + \frac{h}{2}k_2),$$

$$k_4 = f(t_n + h, y_n + hk_3).$$

- Fourth order method
- Very precise but
  - Four times force calculation
  - No energy conservation (non-sympletic)

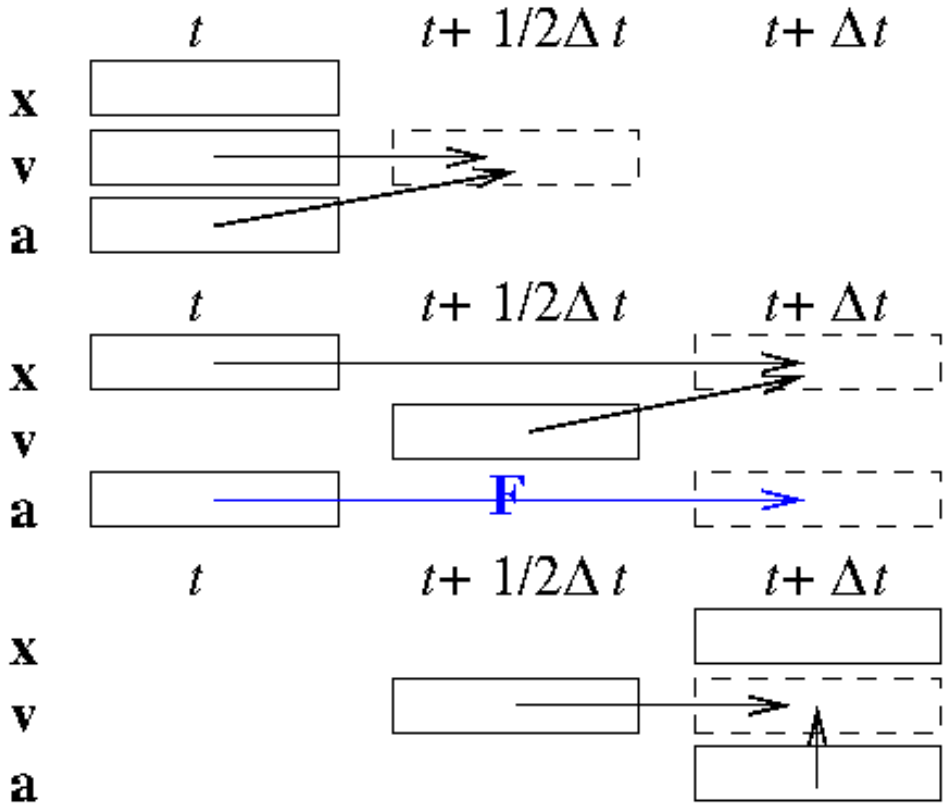
Leapforg method

- Calculate $\mathbf{v}(t + \frac{1}{2}\Delta t) = \mathbf{v}(t - \frac{1}{2}\Delta t) + \mathbf{a}(t)\Delta t$
- Calculate $\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \mathbf{v}(t + \frac{1}{2}\Delta t)\Delta t$



Verlet method

- Calculate $\mathbf{v}(t + \frac{1}{2}\Delta t) = \mathbf{v}(t) + \frac{1}{2}\mathbf{a}(t)\Delta t$
- Calculate $\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \mathbf{v}(t + \frac{1}{2}\Delta t)\Delta t$
- Derive $\mathbf{a}(t + \Delta t)$ from the forces
- Calculate $\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \frac{1}{2}\Delta t) + \frac{1}{2}\mathbf{a}(t + \Delta t)\Delta t$



Sympletic integrator

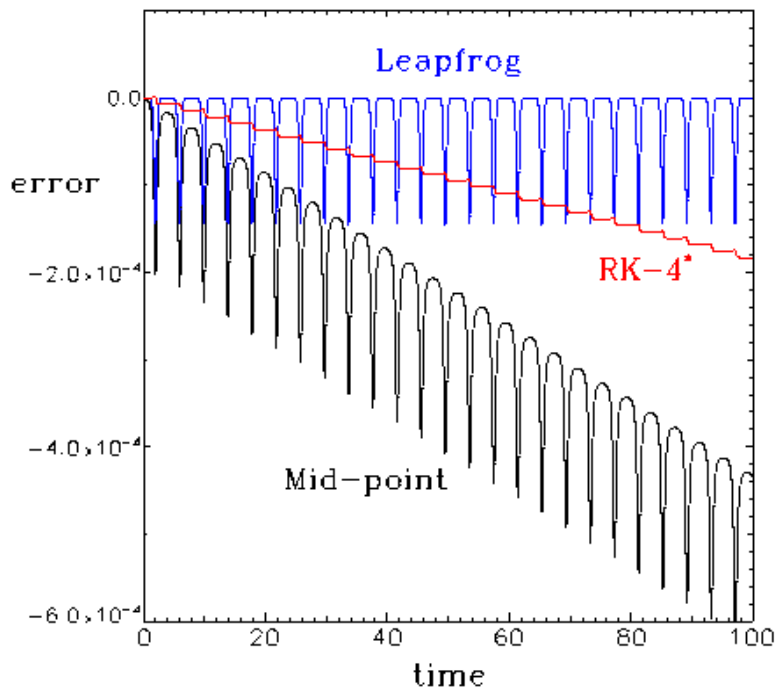
- Energy (slightly modified) is conserved
- Time reversibility
  - Verlet
  - Leapfrog
- Most molecular dynamics methods use Verlet!
  - Forces are calculated once per turn
  - Microcanonical (NVE) modelling can be only done with these

Multiple time scale integration

- Different force range
  - Short range change fast
  - Long range change slowly
- Recalculate long range forces only in every *n*th times-step
  - Forces are calculated once per turn
- Typical examples:
  - Intramolecular forces: strong, high frequency
  - Intermolecular forces (e.g. Lennard-Jones, Coulomb) slow

Error

Method	Error	Cumulative error
Euler:	Δt^3	Δt
Runge-Kutta:	Δt^5	Δt^4
Verlet:	Δt^4	Δt^2
Leapfrog:	Δt^4	Δt^2



Molecular dynamics

Program:

- Have an algorithm to calculate forces
- Get list of interacting particles
- Determine accelerations and velocities; step particles
- Set temperature

Temperature

Definition:

- Encyclopedia Britannica, Wikipedia:
  "A temperature is a numerical measure of hot or cold."
- Thermodynamics:
  Second law of thermodynamics & Carnot engine

$$\delta Q = T dS$$

$$\eta_{\text{max}} = \eta_{\text{Carnot}} = 1 - T_C / T_H$$

- Statistical physics:

$$\beta \equiv \frac{1}{k_B} \left(\frac{\partial S}{\partial E} \right)_{V,N} = \frac{1}{k_B T}$$

Definition of temperature

Temperature is a measure of the random submicroscopic motions and vibrations of the particle constituents of matter.

The average kinetic energy per particle degrees of freedom is

$$\bar{E} = \frac{1}{2} k_B T$$

Molecular dynamics conserves only the *total* energy!

Task: Control kinetic energy!

Setting temperature

- Experiment
  - Environment
  - Mixing $\rightarrow$ uniform temperature
- Simulation
  - Control the kinetic energy (velocities)
  - Mixing $\rightarrow$ Maxwell-Boltzmann distribution

Nosé-Hoover thermostat

- Original Hamiltonian

$$H_0 = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + U(\mathbf{q})$$

- Heatbath in the Hamiltonian:

$$H_n = \sum_i \frac{\mathbf{p'}_i^2}{2m_i} + U(\mathbf{q'}) + \frac{p_s^2}{2Q} + gk_B T \log(s)$$

- Extra degree of freedom s.
- Q "mass" related to $s \rightarrow$ controls the speed of convergence
- $g = 3N$ the number degrees of freedom
- $\mathbf{p}'$ and $\mathbf{q}'$ are virtual coordinates

Nosé-Hoover thermostat

- Virtual coordinates, vs. original ones:

$$\mathbf{p} = \mathbf{p}'/s$$
$$\mathbf{q} = \mathbf{q}'$$
$$t = \int \frac{1}{s} dt'$$

- Solution of the new Hamiltonian:

$$\xi = \dot{s}/s = p_s/Q$$
$$\dot{\mathbf{q}}' = \frac{\mathbf{p}'}{m}$$
$$\dot{\mathbf{p}'}_i = -\frac{\partial U}{\partial q'_i} - \xi \mathbf{p}'_i$$
$$\dot{\xi} = \frac{1}{Q}\left(\sum_i \frac{\dot{\mathbf{p}'}_i^2}{m_i} - g k_B T\right)$$

Molecular dynamics

- Create sample
  - Crystal
  - Random deposition
  - Distorted crystal
  - Simulation
- Temperate sample
- Make test
- Collect data
  - Data size: e.g. $N = 10^4$, $t = 10^6$ small simulation:
  - 1 hour on 1 core PC
  - 3 doubles/atom $\rightarrow$ 24 bytes/atom/timesteps
  - Result 2.4 10^{11} bytes = 240 Gigabytes

Movie