

Simulations in Statistical Physics

Course for MSc physics students

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November 10, 2015

Molecular dynamics

Program:

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

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:

$$\xi = \dot{s}/s = p_s/Q$$

$$\dot{\mathbf{q}}' = \frac{\mathbf{p}'}{m}$$

$$\dot{\mathbf{p}}'_i = -\frac{\partial U}{\partial \mathbf{q}'_i} - \xi \mathbf{p}'_i$$

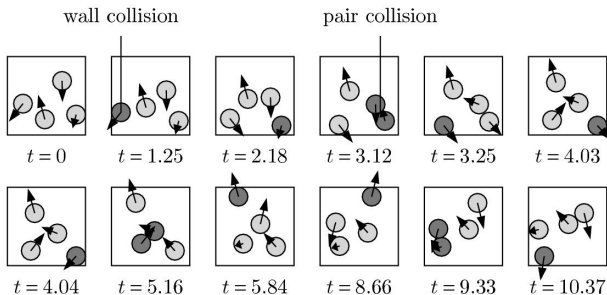
$$\dot{\xi} = \frac{1}{Q} \left(\sum_i \frac{\mathbf{p}'_i{}^2}{m_i} - g k_B T \right)$$

Alternatives

- ▶ Event Driven Dynamics
- ▶ Contact Dynamics
- ▶ Kinetic Monte Carlo

Event driven dynamics

- ▶ Hard core interactions
- ▶ Interactions short in time compared to flight
- ▶ (MD needs $\sim 20 - 50$ timesteps per collision, overlap of $10^{-3}d$)
- ▶ Integrable path \rightarrow do it



Event driven algorithm

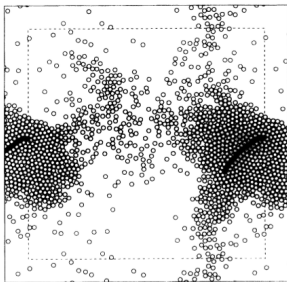
- ▶ No gravity
- ▶ Particles: $\mathbf{r}_i(t)$, $\mathbf{v}_i(t)$, $\omega_i(t)$, R_i
- ▶ Calculate collision time: Let $\mathbf{d}_{ij} = |\mathbf{r}_i - \mathbf{r}_j| - R_i - R_j$, Then

$$\tau_{ij} = \frac{|\mathbf{d}_{ij}|^2}{(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{d}_{ij}}$$

- ▶ Order collision times, get the smallest $\tau_c = \min_{ij}(\tau_{ij})$
- ▶ Go to time $t + \tau_c$ $\mathbf{r}_i(t + \tau_c)$
- ▶ Calculate velocities after collision $\mathbf{v}_i(t + \tau_c)$ (may be hard...)
- ▶ Restart loop
- ▶ Next time Calculate collision time only with i, j
- ▶ Dynamic list, change only newly calculate collision times

Inelastic collapse

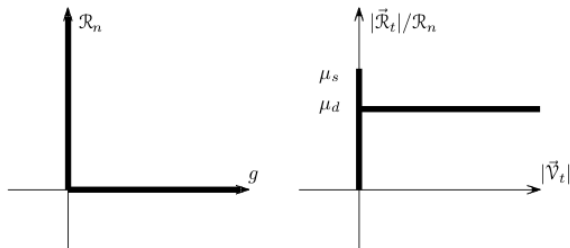
- ▶ Coefficient of restitution $r = v_n(t_c+)/v_n(t_c-)$
- ▶ Energy is lost in an exponential way (Ping Pong)
- ▶ Infinite collisions in finite time
- ▶ Solution $\rightarrow r = 1$ if collisions occur more frequently than a parameter t_{cont} , the contact duration
- ▶ Contact \rightarrow small vibration :-(well...)



MOVIE

Contact dynamics

- ▶ Perfectly rigid particles
- ▶ Non-smooth dynamics
- ▶ Constraints



- ▶ Molecular dynamics
 - ▶ Normal force: overlap (smooth)
 - ▶ Shear force: history

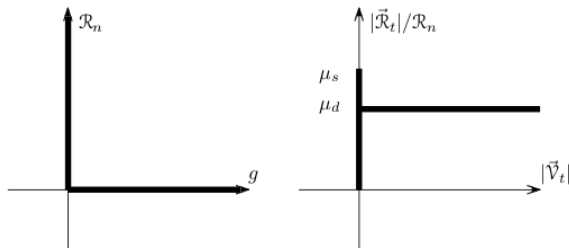
Contact dynamics

- Implicit forces

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + \frac{1}{m_i} \mathbf{F}_i(t + \Delta t) \Delta t$$

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t + \Delta t) \Delta t$$

such as constraints are fulfilled



Contact dynamics

- ▶ Implicit forces

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + \frac{1}{m_i} \mathbf{F}_i(t + \Delta t) \Delta t$$

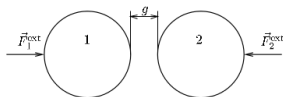
$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t + \Delta t) \Delta t$$

such as constraints are fulfilled

- ▶ if gap would be negative increase force
- ▶ if there would be a shear displacement increase shear force
- ▶ if shear force is larger than allowed restrict it to that value

Contact dynamics, force calculation

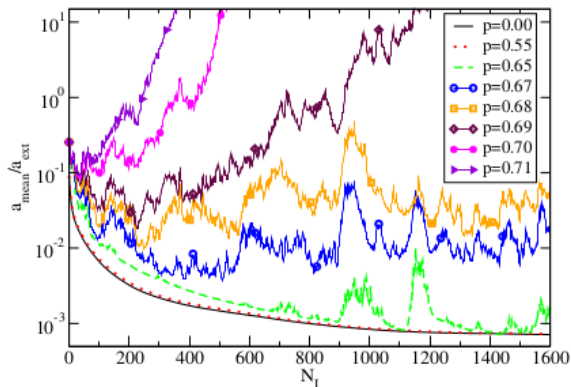
- Two particles with gap g



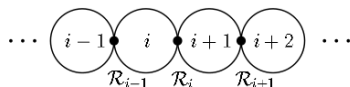
$$\begin{aligned} &\text{if } \mathcal{V}_n^{\text{free}} \Delta t + g^{\text{pos}} > 0 \\ &\quad \text{then } \begin{cases} \vec{\mathcal{R}}^{\text{new}} = 0 \end{cases} && \text{(no contact)} \\ &\quad \text{else } \begin{cases} \mathcal{R}_n^{\text{new}} = -\frac{1}{\Delta t} m_n \left(\frac{g^{\text{pos}}}{\Delta t} + \mathcal{V}_n^{\text{free}} \right) \\ \vec{\mathcal{R}}_t^{\text{new}} = -\frac{1}{\Delta t} m_t \vec{\mathcal{V}}_t^{\text{free}} \end{cases} && \text{(sticking contact)} \\ &\text{if } \left| \vec{\mathcal{R}}_t^{\text{new}} \right| > \mu \mathcal{R}_n^{\text{new}} \\ &\quad \text{then } \begin{cases} \vec{\mathcal{R}}_t^{\text{new}} = \mu \mathcal{R}_n^{\text{new}} \frac{\vec{\mathcal{R}}_t^{\text{new}}}{\left| \vec{\mathcal{R}}_t^{\text{new}} \right|} \end{cases} && \text{(sliding contact)} \end{aligned}$$

Iterative solver

- Updates:
 - Parallel: calculate all contacts with old values then change to new at once → serious instabilities
 - Serial: update contacts one-by-one in random order



Particle chain



- ▶ One iteration step:

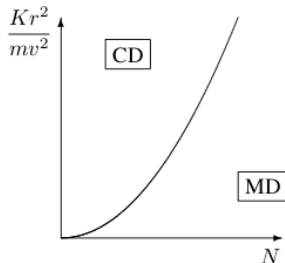
$$\mathcal{R}_i^{\text{new}} = \frac{1}{2} (\mathcal{R}_{i-1}^{\text{new}} + \mathcal{R}_{i+1}^{\text{new}}),$$

- ▶ Discretized one-dimensional diffusion equation
- ▶ Model of rigid particles \rightarrow elastic
- ▶ Elasticity depends on the number of iterations

Molecular versus Contact dynamics

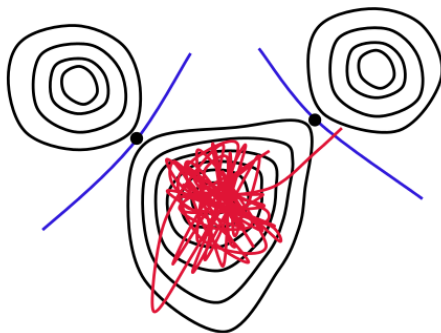
Limit

$$\frac{Kr^2}{mv^2} = N^{4/d}$$



Kinetic Monte Carlo

- ▶ Particle sits in a potential well for ages ...
- ▶ What to do?

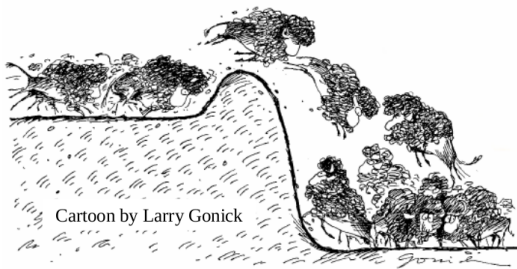


Kinetic Monte Carlo

- ▶ Long lasting steady state positions
- ▶ Slow thermally activated processes
- ▶ Infrequent-event system

Solution:

- ▶ Consider only jumps between neighboring energy wells
- ▶ Probability of jump $P \sim \exp(-\beta E_b)$
- ▶ Rate of jump $i \rightarrow j$, $k_{ij} = E_b$.



Kinetic Monte Carlo

- ▶ Get all possible rates k_i
- ▶ Calculate the cumulative function $K = \sum_i k_i$
- ▶ Get a uniform random number u (between 0 and 1)
- ▶ Execute the event i for which $\sum_{j=1}^i k_j > u > \sum_{j=1}^{i-1} k_j$
- ▶ Get new uniform random number u' (between 0 and 1)
- ▶ Update time to $t = t + \Delta t$, $\Delta t = -\log(u')/k_i$
- ▶ Recalculate rates, which have changed
- ▶ Restart loop

Monte Carlo

Why Monte Carlo? → Random numbers play big role!



Kinetic Monte Carlo

- ▶ Rates
 - ▶ Physics
 - ▶ Molecular dynamics
- ▶ Must include all rates!
- ▶ Used for:
 - ▶ Surface diffusion
 - ▶ Surface growth
 - ▶ Sintering
 - ▶ Domain evolution

Example....

Methods

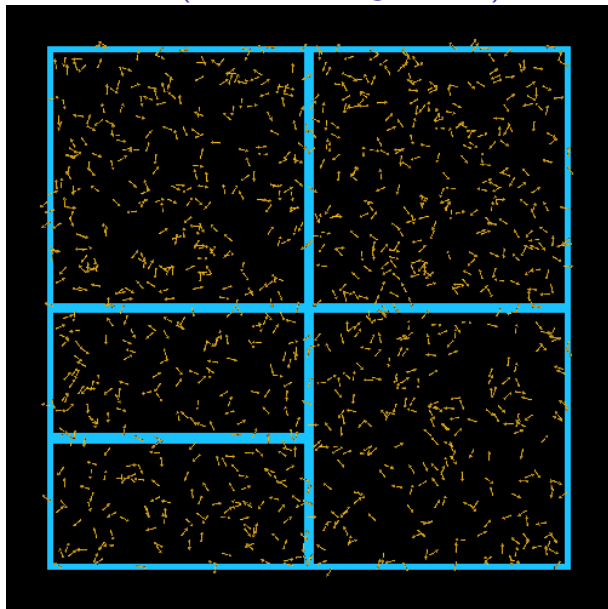
- ▶ Molecular Dynamics
 - ▶ General
- ▶ Event Driven Dynamics
 - ▶ Hard objects, at low density
- ▶ Contact Dynamics
 - ▶ Rigid particles
- ▶ Kinetic Monte Carlo
 - ▶ Infrequent events, bonded particles

Parallelization

- ▶ Why?
 - ▶ The speed of one core processor is limited
 - ▶ Larger system sizes
 - ▶ Multi-core processors
 - ▶ On multi-core system inter-processor data change is fast
- ▶ Why not?
 - ▶ Computing power is lost
 - ▶ **Much more code development**
 - ▶ Very often ensemble average is needed
 - ▶ Inter-computer communication is terribly slow

RAM \rightarrow $\sim 15\text{GB/s}$, Ethernet 125MB/s , Infiniband $\sim 1\text{GB/s}$

Parallelization (Bird flocking model)

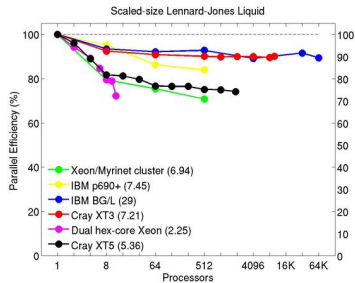
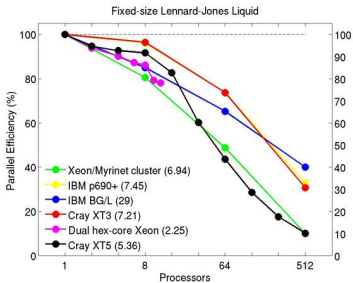


Parallelization

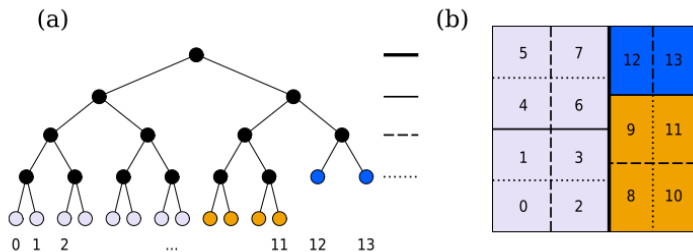
- ▶ Molecular dynamics
 - ▶ Short range interactions: Box must be duplicated, Verlet in parallel
 - ▶ Long range: Parallel fast Fourier transformation
- ▶ Contact dynamics
 - ▶ Short range interactions: Box must be duplicated, Iteration in parallel
- ▶ Event Driven Dynamics
 - ▶ List must be global, no way!
- ▶ Kinetic Monte Carlo
 - ▶ List must be global, no way!

Efficiency of parallelization

- ▶ Large systems are needed
- ▶ Boundary must be minimal



Efficiency of parallelization



- ▶ Calculate time spent in a branch
- ▶ Calculate $\sigma_T = \sqrt{\langle T^2 \rangle - \langle T \rangle^2} / \langle T \rangle$
- ▶ Move line if necessary ($\sigma_T > \sigma_T^*$)
- ▶ Lower in tree (up in Fig), larger the mass of the border
- ▶ Only rarely, data transfer is expensive