Simulations in Statistical Physics

Discrete element methods part 2.

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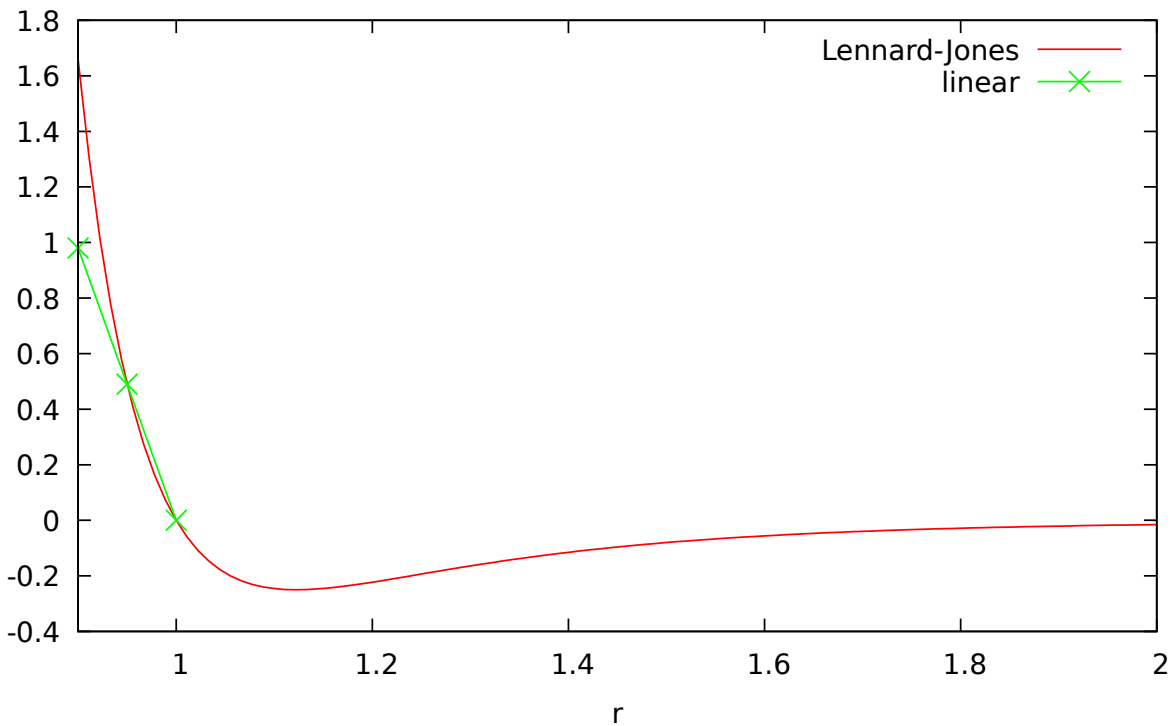
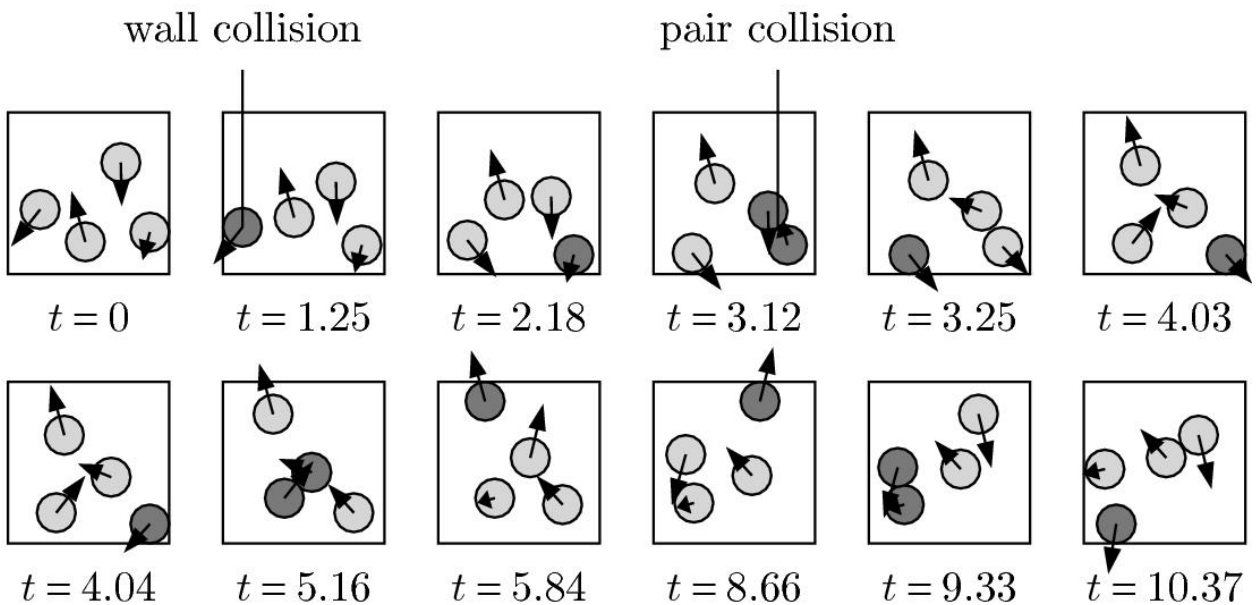
Problems with molecluar dynamics

- All particles are soft (force as function of overlap)
- Collision must be smooth ($\sim$ 50 timesteps), which sets dt
- Problem with gases, free path is 100$-$1000 times the particle radius
- Timescale problems with temporal fluctuations



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 (Can be also solved for gravity)
- Particles: $\mathrm{r}_i(t)$, $\mathrm{v}_i(t)$, $\boldsymbol{\omega}_i(t)$, R_i
- Calculate collision time: Let $\mathrm{d}_{ij} = |\mathrm{r}_i - \mathrm{r}_j| - R_i - R_j$, Then

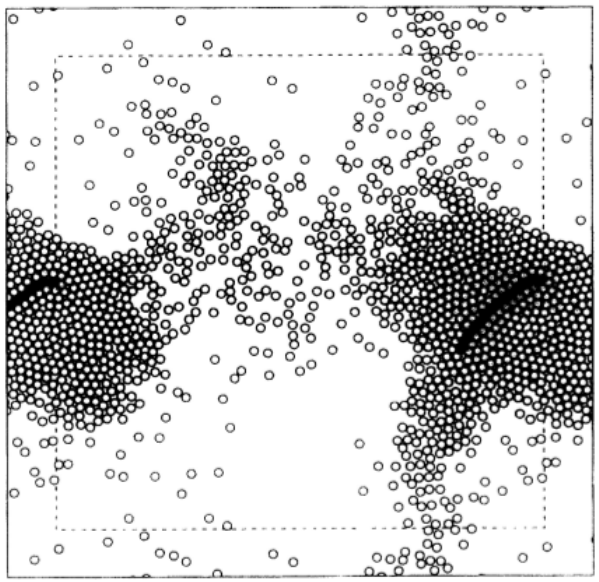
$$\tau_{ij} = \frac{|\mathrm{d}_{ij}|^2}{(\mathrm{v}_i - \mathrm{v}_j)\mathrm{d}_{ij}}$$

- Order collision times, get the smallest $\tau_c = \min_{ij}(\tau_{ij})$
- Go to time $t + \tau_c$ $\mathrm{r}_i(t + \tau_c)$
- Calculate velocities after collision $\mathrm{v}_i(t + \tau_c)$ (may be hard...)
- Restart loop

- Next time Calculate collision time only with i, j
- Dynamic list, change only newly calculate collision times

Inelastic collapse

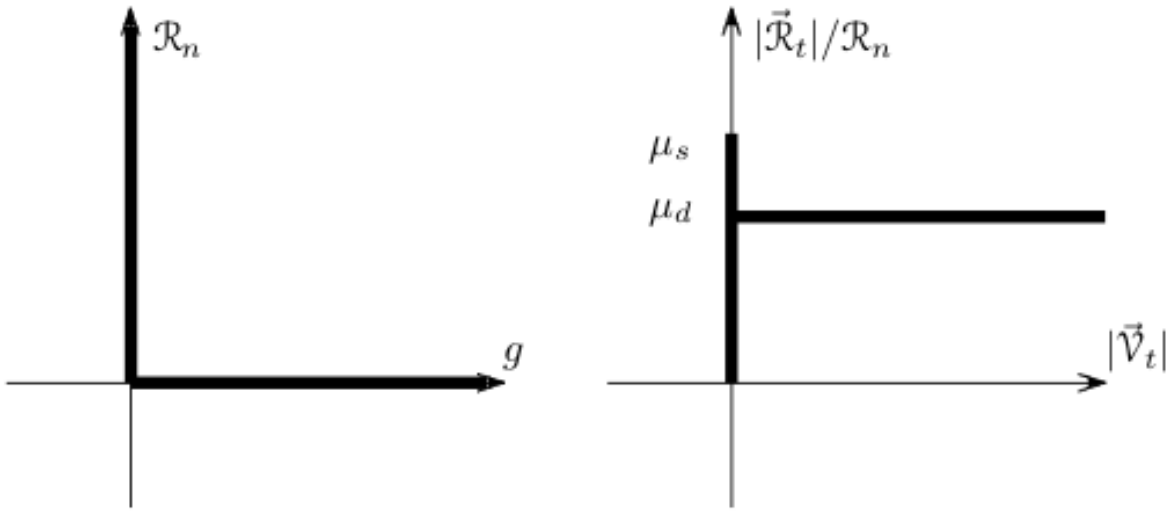
- Coefficient of restitution $r = v_n(t_c+)/v_n(t_c-)$
- Energy is lost in an exponential way (Ping Pong)
- Infinite collisions in finite time
- Solution $\rightarrow$ $r = 1$ if collisions occur more frequently than a parameter t_{cont}, the contact duration
- Contact $\rightarrow$ small vibration :-(well...)



MOVIE

Contact dynamics

- Perfectly rigid particles
- Non-smooth dynamics
- Constraints



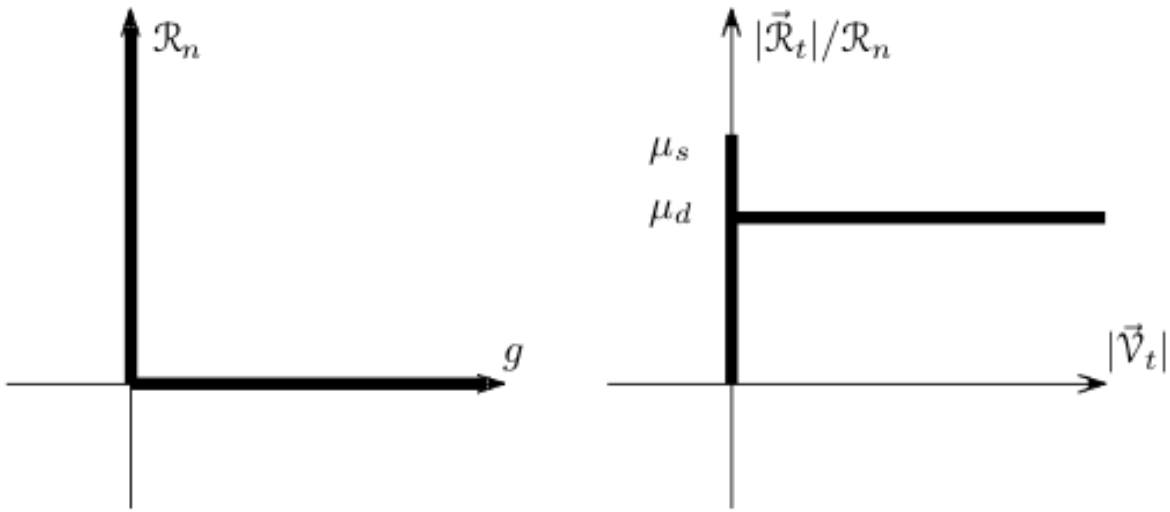
- Molecular dynamics
  - Normal force: overlap (smooth)
  - Shear force: history

Contact dynamics

- Implicit forces

$$v_i(t + \Delta t) = v_i(t) + \frac{1}{m_i} F_i(t + \Delta t)\Delta t$$
$$x_i(t + \Delta t) = x_i(t) + v_i(t + \Delta t)\Delta t$$

such as constraints are fulfilled



Contact dynamics

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$$v_i(t + \Delta t) = v_i(t) + \frac{1}{m_i} F_i(t + \Delta t)\Delta t$$
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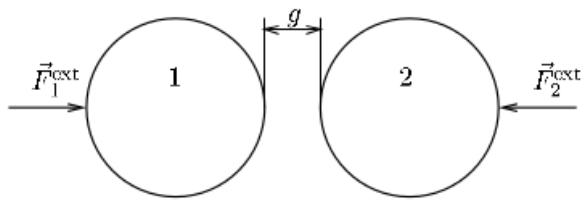
such as constraints are fulfilled

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

Contact dynamics, force calculation

- Two particles with gap g



$$\text{if} \quad {\mathcal{V}^{\text{free}}}_n \Delta t + g^{\text{pos}} > 0$$

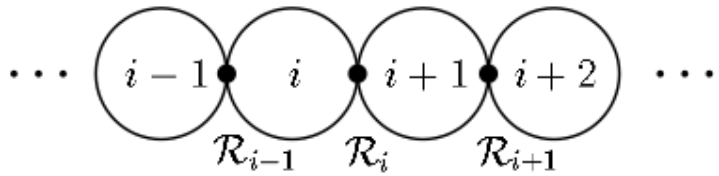
$$\text{then} \quad \left\{ \vec{\mathcal{R}}^{\text{new}} = 0 \right. \qquad \text{(no contact)}$$

$$\text{else} \quad \begin{cases} \mathcal{R}_n^{\text{new}} = -\dfrac{1}{\Delta t} m_n \left(\dfrac{g^{\text{pos}}}{\Delta t} + \mathcal{V}_n^{\text{free}} \right) \\ \vec{\mathcal{R}}_t^{\text{new}} = -\dfrac{1}{\Delta t} m_t \vec{\mathcal{V}}_t^{\text{free}} \end{cases} \qquad \text{(sticking contact)}$$

$$\text{if} \quad \left| \vec{\mathcal{R}}_t^{\text{new}} \right| > \mu \mathcal{R}_n^{\text{new}}$$

$$\text{then} \quad \left\{ \vec{\mathcal{R}}_t^{\text{new}} = \mu \mathcal{R}_n^{\text{new}} \frac{\vec{\mathcal{R}}_t^{\text{new}}}{\left| \vec{\mathcal{R}}_t^{\text{new}} \right|} \right. \qquad \text{(sliding contact)}$$

Particle chain



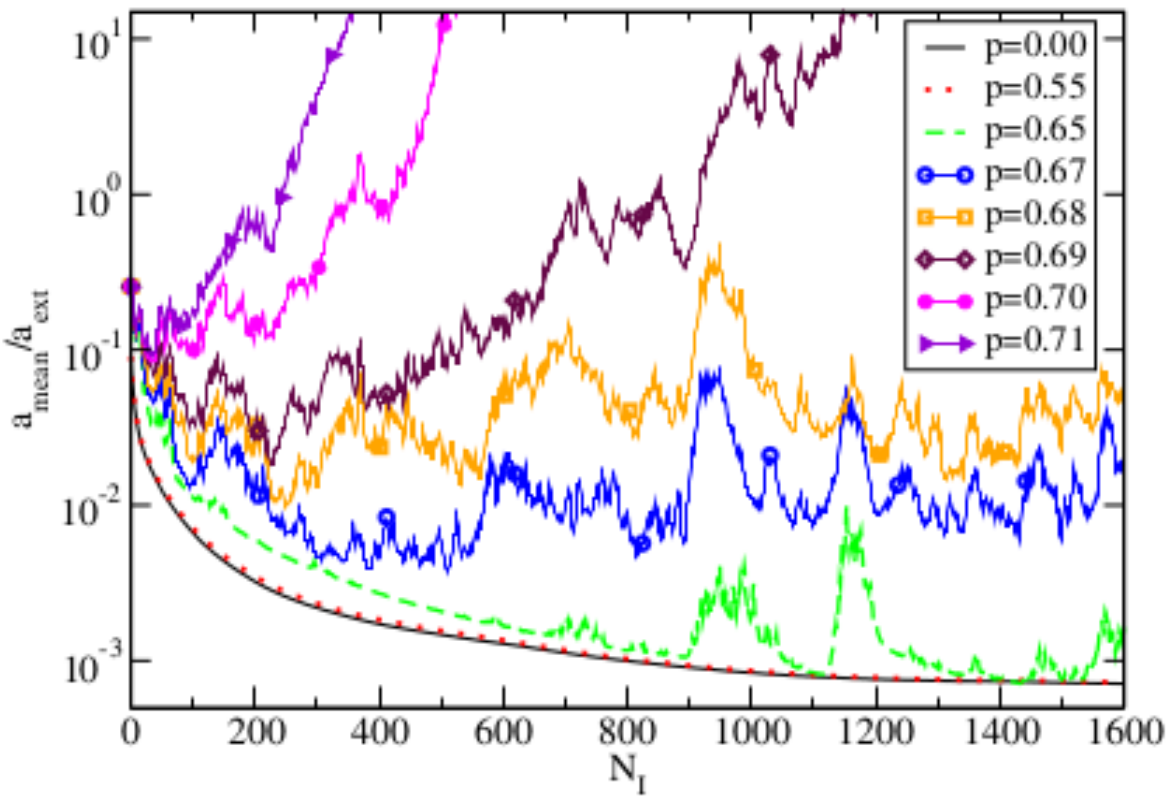
- One iteration step:

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

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

Iterative solver

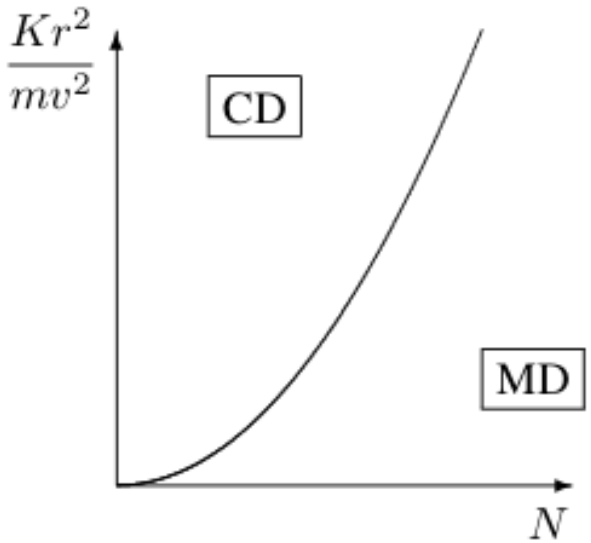
- Updates:
  - Parallel: calculate all contacts with old values then change to new at once $\rightarrow$ serious instabilities
  - Serial: update contacts one-by-one in random order



Molecular versus Contact dynamics

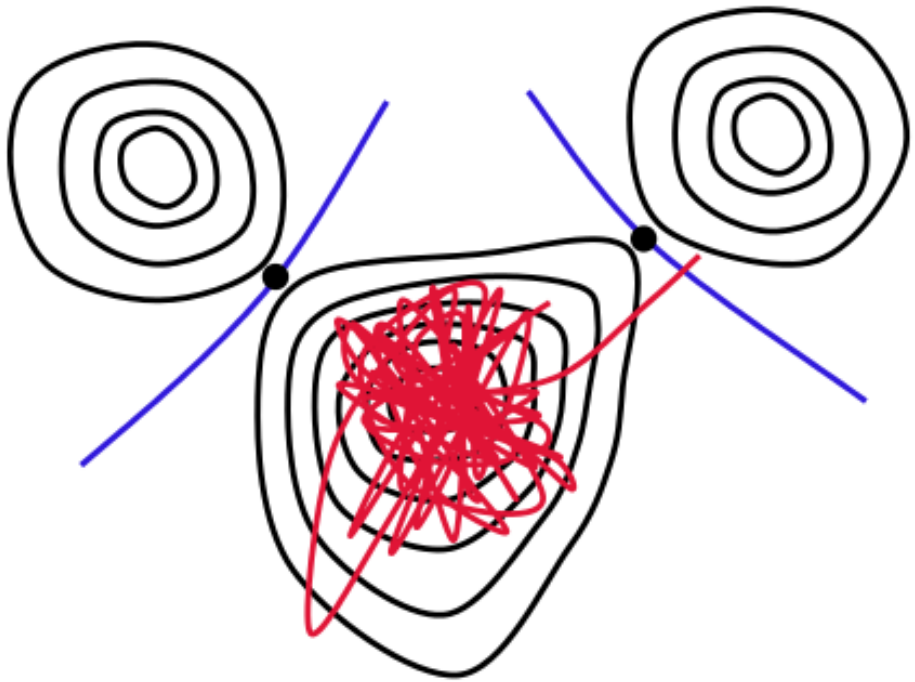
Limit

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



Kinetic Monte Carlo

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

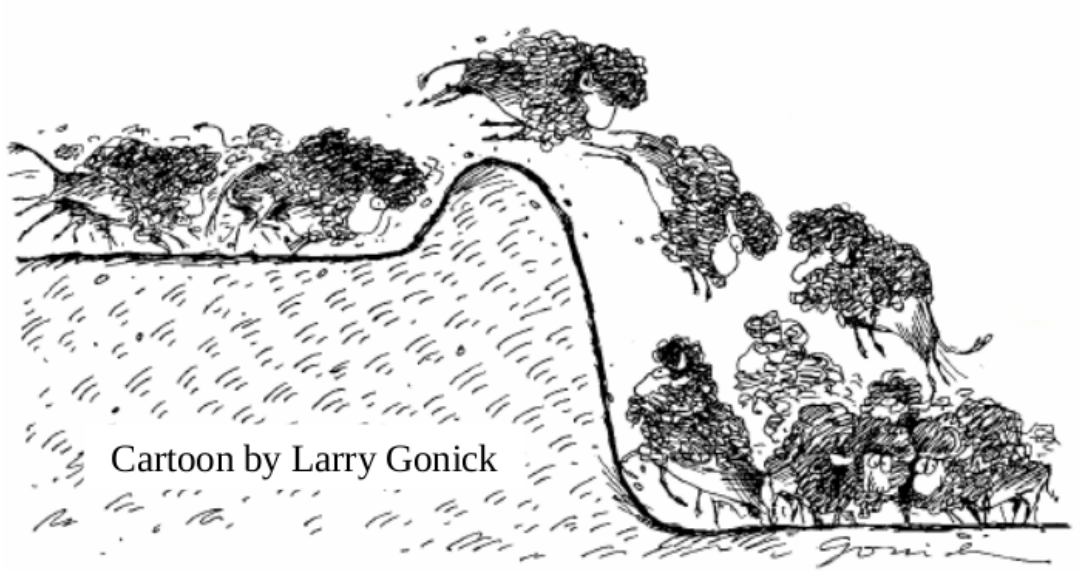


Kinetic Monte Carlo

- 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

- All possible moves i
- Rates for moves 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 $\sum_{j=1}^{i} k_j > uK > \sum_{j=1}^{i-1} k_j$
- 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

Kinetic Monte Carlo

- Rates
  - Physics
  - Molecular dynamics
- Must include all rates!
- Used for:
  - Surface diffusion
  - Surface growth
  - Syntering
  - 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

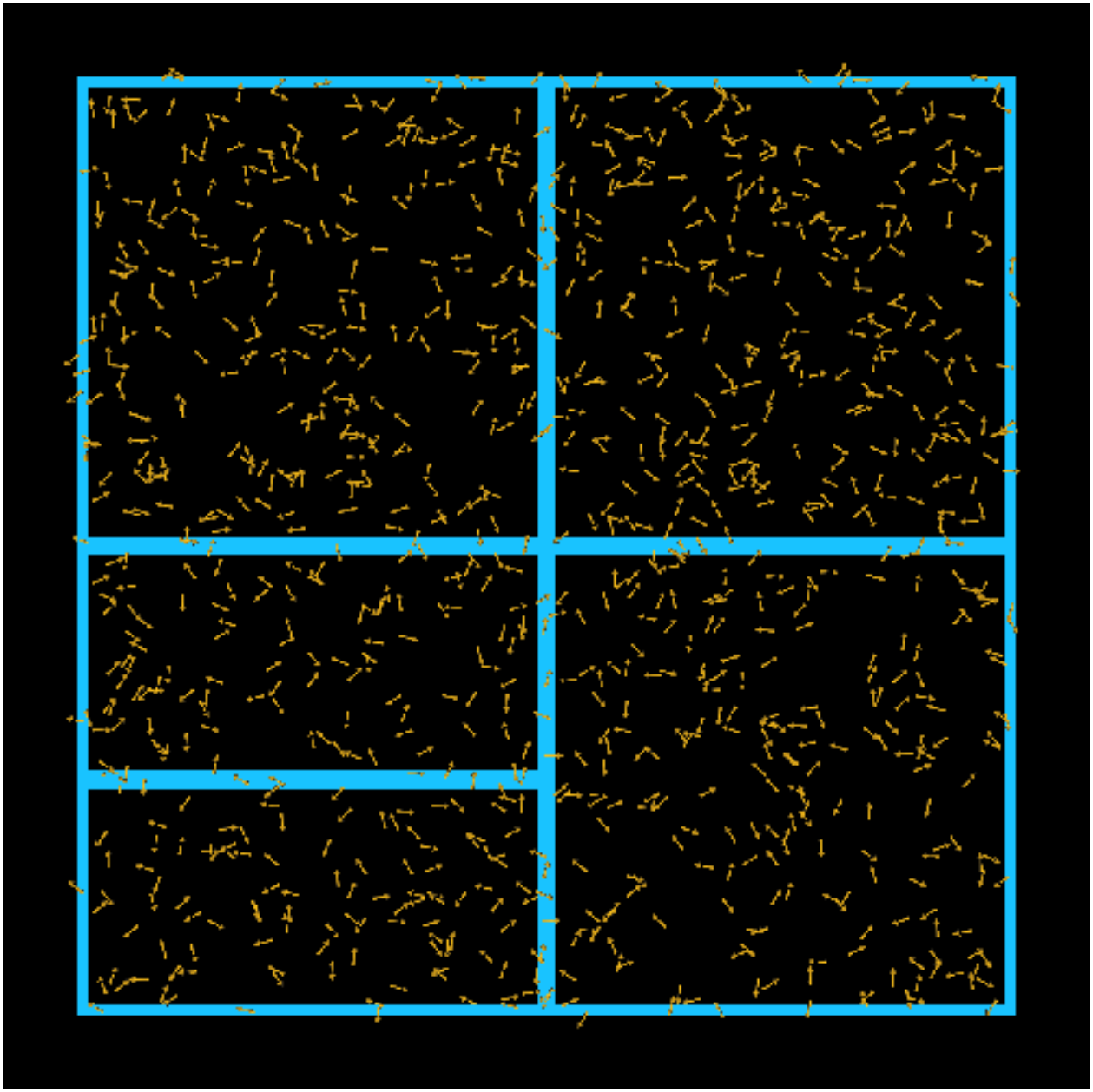
- Why?
  - The speed of one core processor is limited
  - Larger system sizes
  - Multi-core processors
  - On multi-core system inter-processor data change is fast
- Why not?
  - Computing power is lost
  - Much more code development
  - Very often ensemble average is needed
  - Inter-computer communication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

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

Parallelization: How?

- Code asks for more instances (e.g. run a loop in parallel)
  - Fork, multi-threading
  - Used in desktop applications
  - Punished on clusters
  - Shared memory
- Operating system (or even multiple machines) launches the code multiple times which can communicate
  - Now de facto standard: MPI (Message passing interface)
  - Communication is standardized, environment can be inhomogeneus
- GPU:
  - High number of cores
  - Non-standard processors
  - Non-standard libraries
  - Limited memory

Parallelization (Bird flocking model)



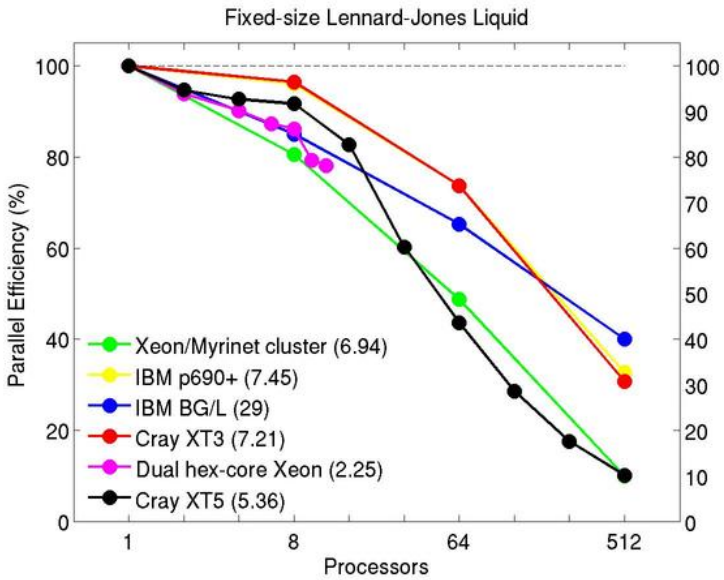
Parallelization

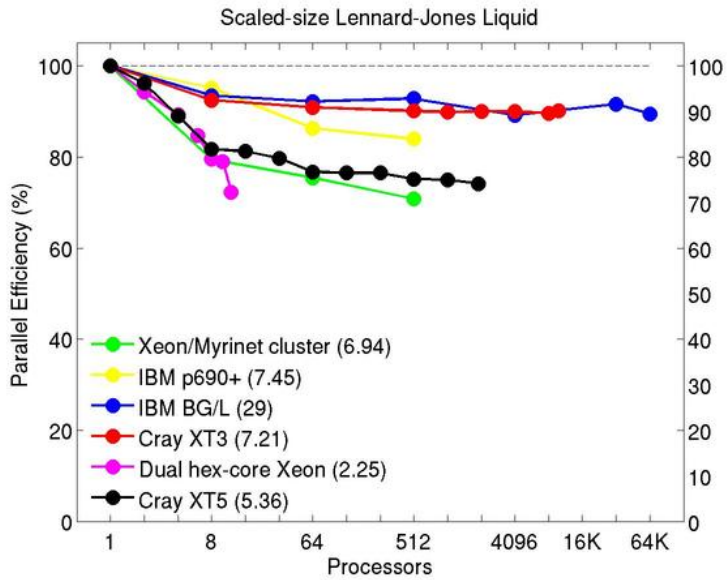
Extra steps needed:

- 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!

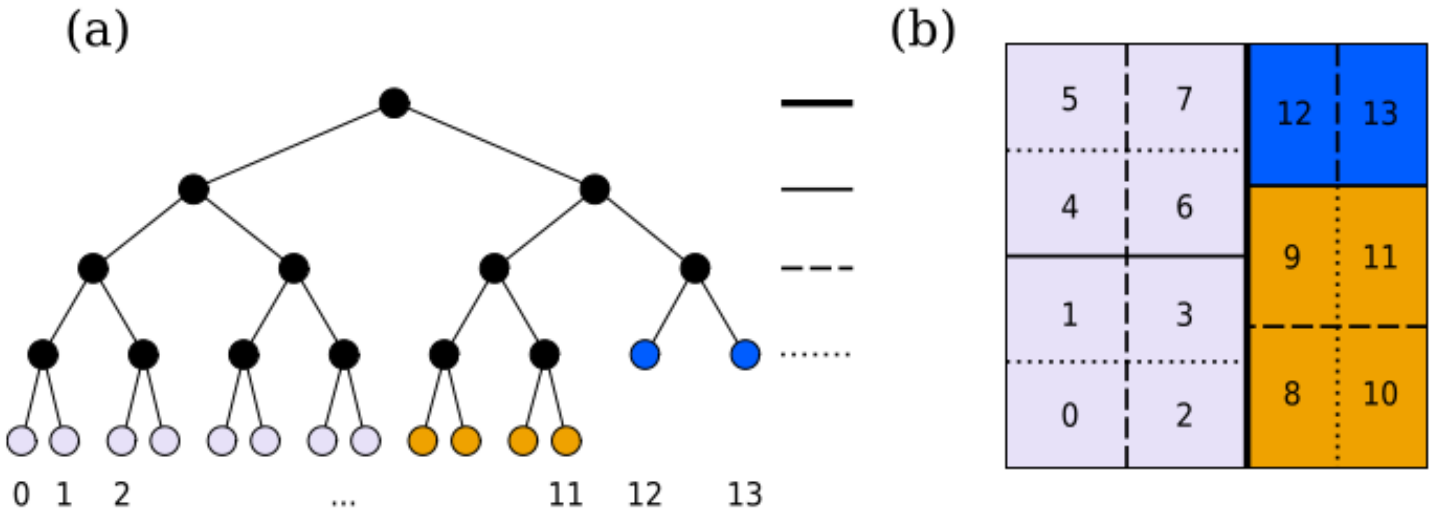
Efficiency of parallelization

- Large systems are needed
- Boundary must be minimal
- System size can be increased simulation time not really





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