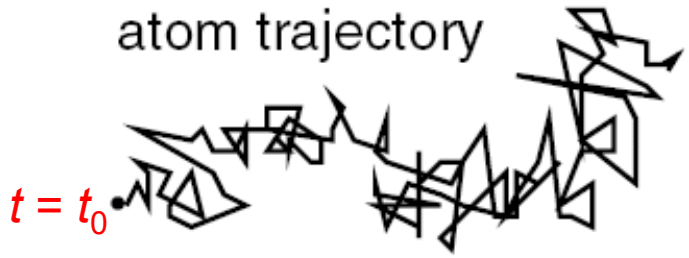
AtomEye （linux only）

原子可视化软件

Ovito （linux & windows）
http://ovito.org/

分子动力学软件 *LAMMPS*

积分算法（integrator）



积分算法用很短的时间步长（ Δt ）产生粒子长时间的运动轨迹。

$$\mathbf{x}^{3N}(t_0) \to \mathbf{x}^{3N}(t_0+\Delta t) \to \mathbf{x}^{3N}(t_0+2\Delta t) \to \ldots \to \mathbf{x}^{3N}(t_0+L\Delta t)$$

$\Delta t \sim 10^{-15}$ s, $L \sim 10^6$, 粒子运动时间 ~ 1 ns

(1) *Verlet* Algorithm

$$\mathbf{x}_i(t_0+\Delta t)+\mathbf{x}_i(t_0-\Delta t)=2\mathbf{x}_i(t_0)+\ddot{\mathbf{x}}_i(t_0)(\Delta t)^2+\mathrm{O}((\Delta t)^4)$$

加速度 $\ddot{\mathbf{x}}_i(t_0)=\mathbf{f}_i(t_0)/m_i$ （Taylor expansion with high order terms）

$$\mathbf{x}_i(t_0+\Delta t)=-\mathbf{x}_i(t_0-\Delta t)+2\mathbf{x}_i(t_0)+\left(\frac{\mathbf{f}_i(t_0)}{m_i}\right)(\Delta t)^2+\mathrm{O}((\Delta t)^4)$$

$$\mathbf{v}_i(t_0)\equiv\dot{\mathbf{x}}_i(t_0)=\frac{1}{2\Delta t}[\mathbf{x}_i(t_0+\Delta t)-\mathbf{x}_i(t_0-\Delta t)]+\mathrm{O}((\Delta t)^2)$$

(2) Velocity *Verlet* Algorithm

To advance one step from t_0 to $t_0+\Delta t$, $\mathbf{x}^{3N}(t_0+\Delta t)$ can be obtained via

$$\mathbf{x}_i(t_0+\Delta t)=\mathbf{x}_i(t_0)+\mathbf{v}_i(t_0)\Delta t+\frac{\mathbf{f}_i(t_0)}{2m_i}(\Delta t)^2$$

evaluate $\mathbf{f}^{3N}(t_0+\Delta t)$, and then calculate $\mathbf{v}^{3N}(t_0+\Delta t)$

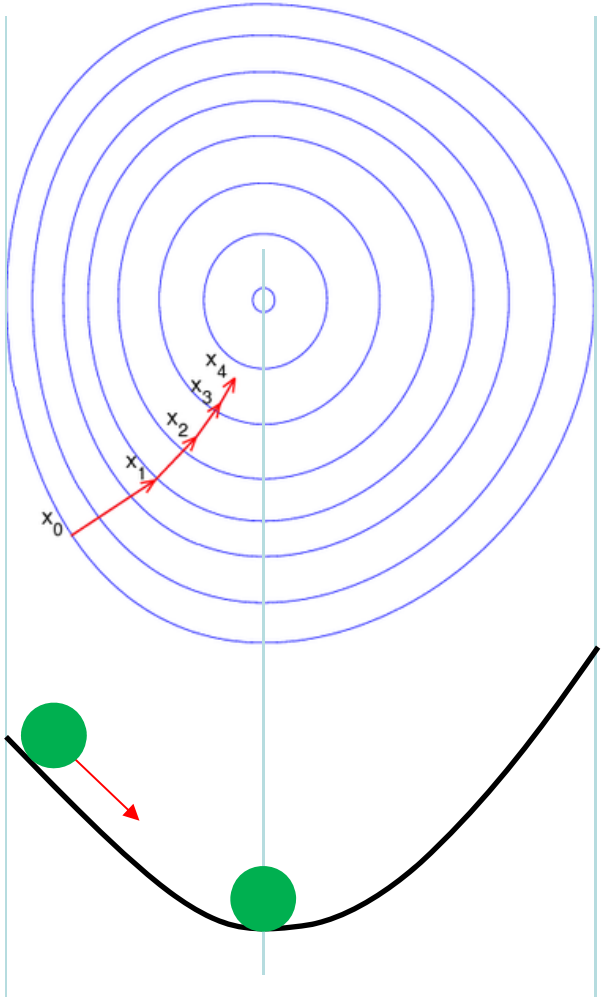
$$\mathbf{v}_i(t_0+\Delta t)=\mathbf{v}_i(t_0)+\frac{1}{2}[\frac{\mathbf{f}_i(t_0)}{m_i}+\frac{\mathbf{f}_i(t_0+\Delta t)}{m_i}]\Delta t$$

such that one can have $\mathbf{x}^{3N}(t_0+\Delta t)$ and $\mathbf{v}^{3N}(t_0+\Delta t)$ simultaneously

(3) Predictor-corrector Algorithm
(4) …

能量最小化

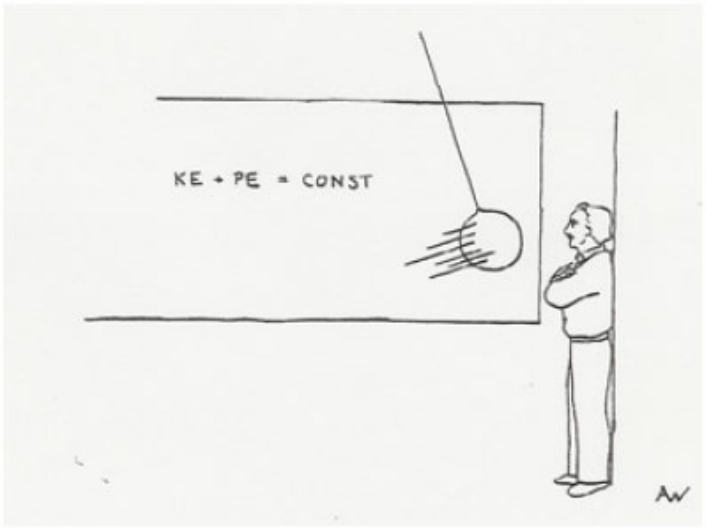
When atoms move they most likely approach to a local **state** of minimum energy, step by step

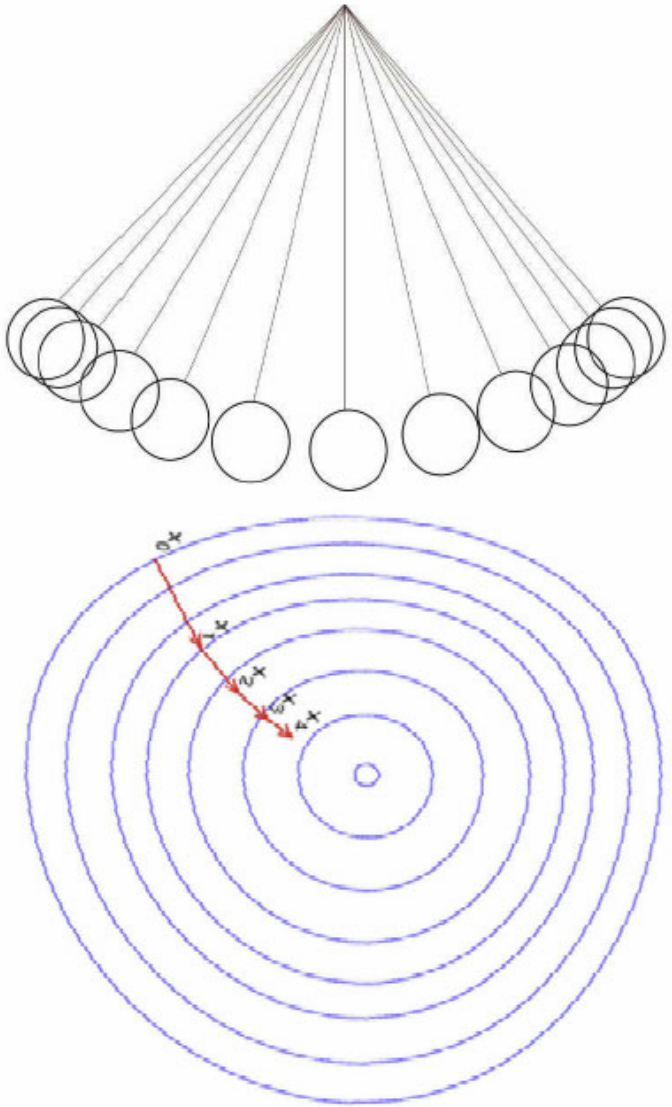


$$\begin{cases} \text{if } \mathbf{f}_i \cdot \dot{\mathbf{x}}_i > 0 & \dot{\mathbf{x}}_i(t) = \dot{\mathbf{x}}_i \\ \text{else} & \dot{\mathbf{x}}_i(t) = 0 \end{cases}$$

t is measured by time step, Δt

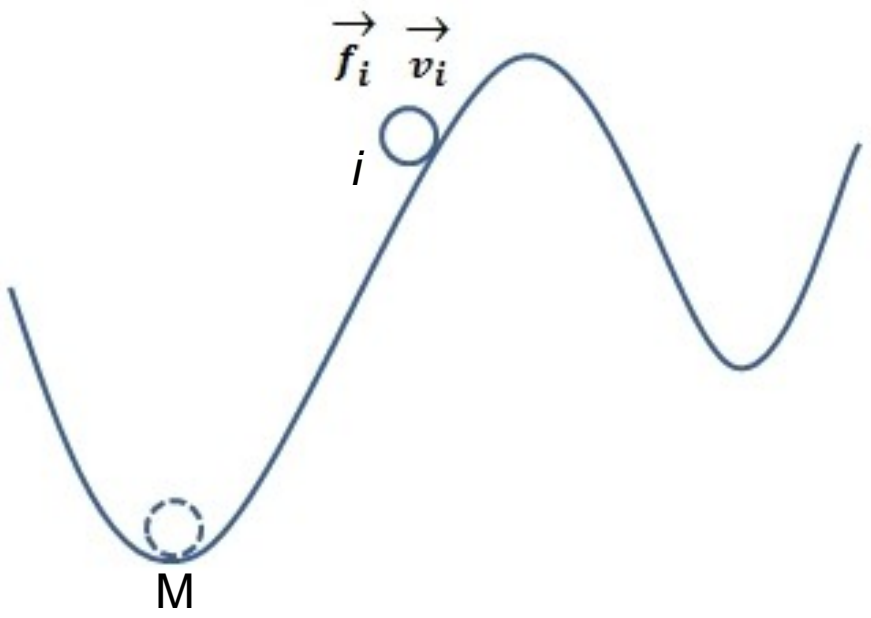
How to quickly minimize the energy of a pendulum?





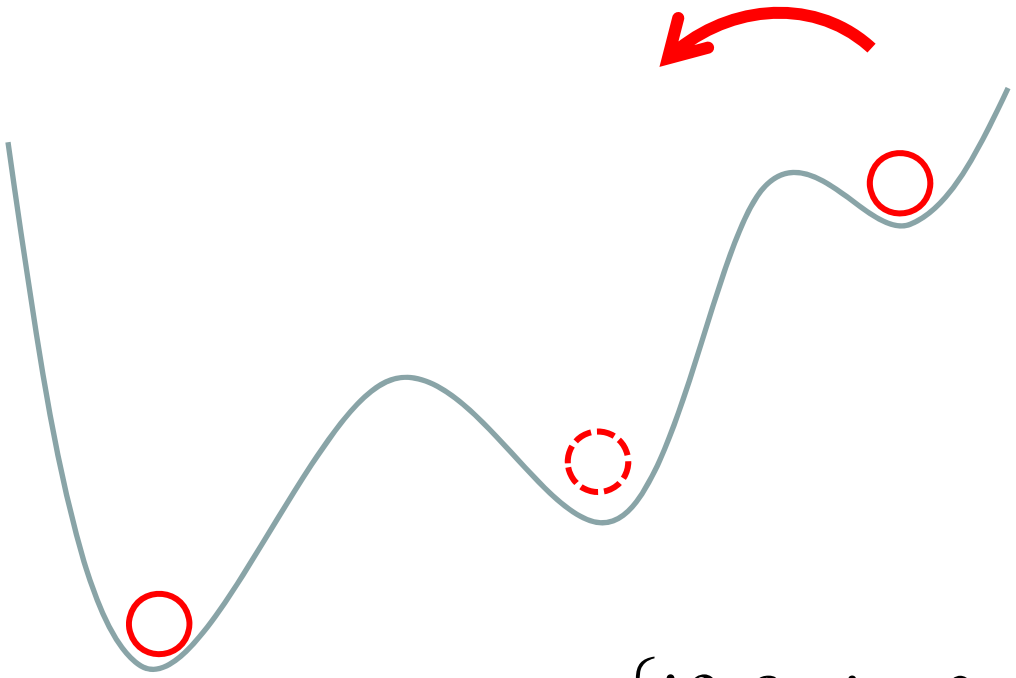
states

Energy surface



Energy surface

activation, e.g. thermally



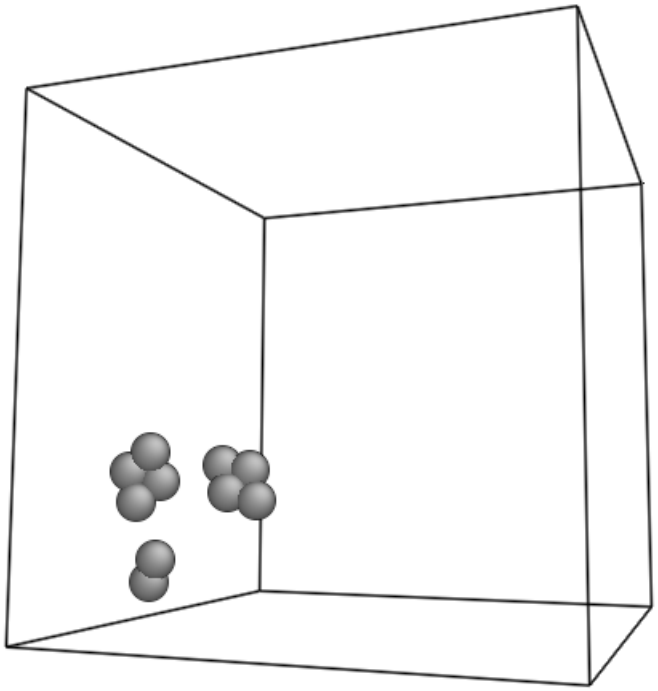
state of minimum energy

$$\begin{cases} \text{if } \mathbf{f}_i \cdot \dot{\mathbf{x}}_i > 0 & \dot{\mathbf{x}}_i(t) = \dot{\mathbf{x}}_i \\ \text{else} & \dot{\mathbf{x}}_i(t) = 0 \end{cases}$$

t is measured by time step, Δt

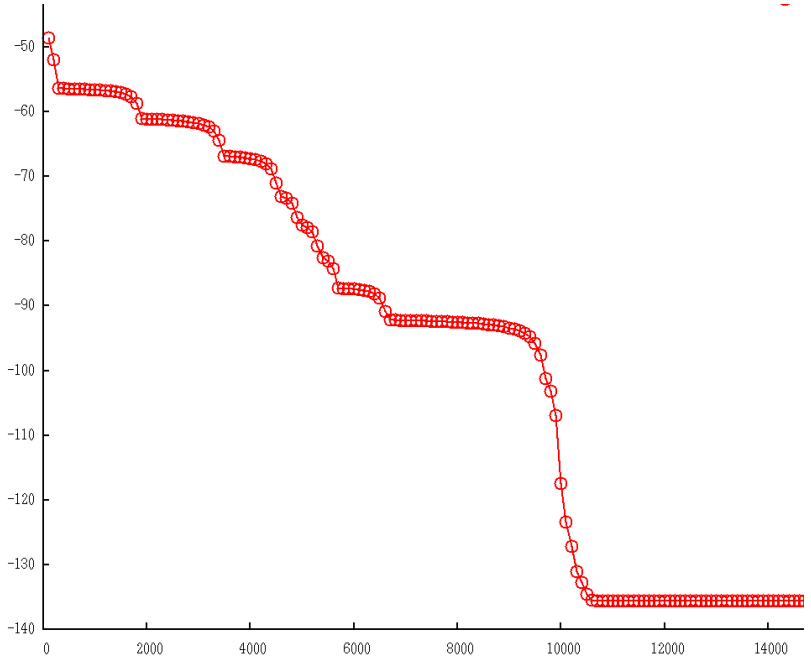
1st MD simulation (LJ clusters)

Approaching to state of minimum energy



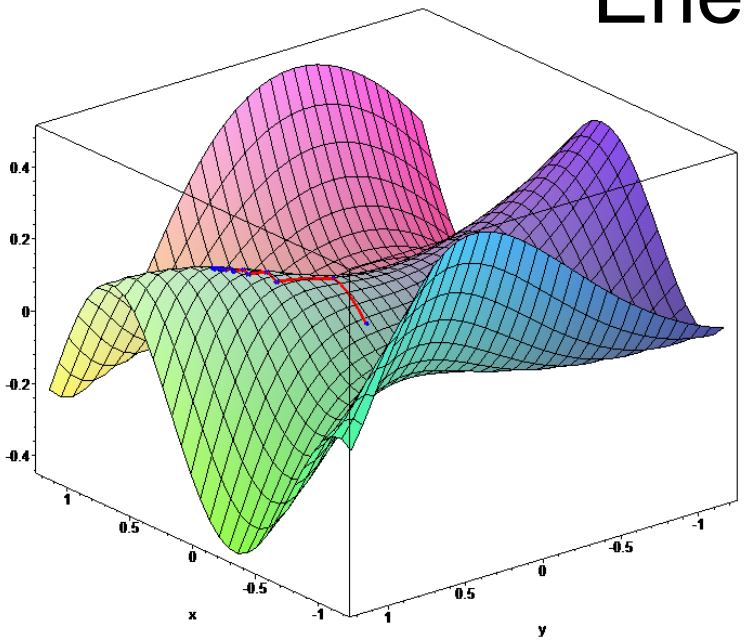
10 atoms (LJ)

Energy

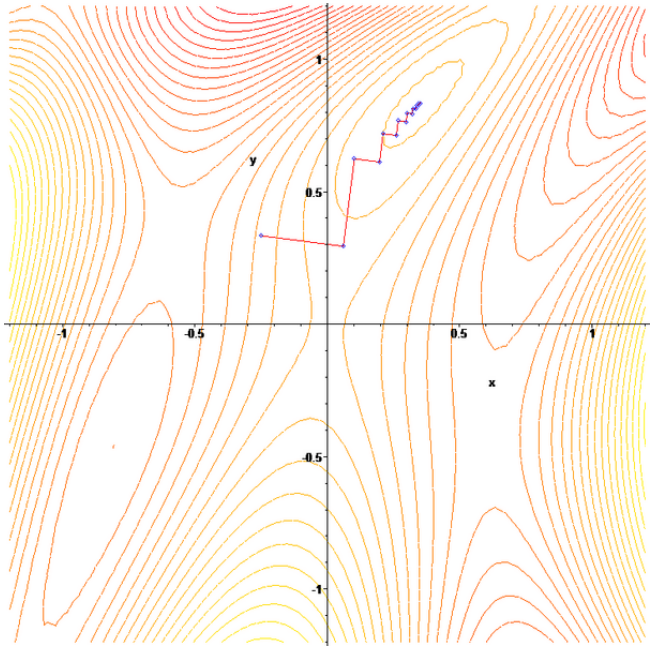


time

Energy minimization approaches



1) local minimum and global minimum
2) relaxed state (at the bottom of the basin in the energy landscape)
3) finding optimal structure: the optimal structure would then be the one with the lowest energy
4) different ``attraction basins" in the energy landscape
5) overcome energy barriers: from one state to another (transition state，过渡态)



Gradient descent

Steepest Descent (SD)

Conjugate Gradient (CG) Methods