6.581/20.482

TUESDAY 28 FEB 2006

LECTURE 6: MOLECULAR DYNAMICS & ELECTROSTATICS

OVERVIEW:
1) Remind about E(x)
2) Time Discretization
3) Electrostatics Evaluation
   - Costs Low

Problematic term

$$E(x) = \sum_{\text{bonds}} + \sum_{\substack{\text{bond}\\\text{angles}}} + \sum_{\text{torsions}} + \sum_{\substack{\text{all}\\\text{pairs}}} \frac{B_{ij}}{r^{12}} - \frac{C_{ij}}{r^6} + \sum_{\substack{\text{all}\\\text{pairs}}} \frac{q_i q_j}{r_{ij}}$$

$$m_i \frac{d}{dt} V_{i\{X,Y,Z\}} = -\frac{\partial}{\partial x_{i\{X,Y,Z\}}} E(\vec{x})$$

m_i: ith atomic mass

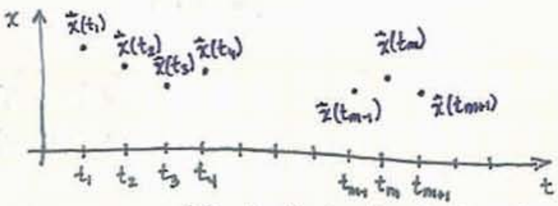
$$M \frac{d}{dt}\vec{V} = -\nabla_{\vec{x}} E(\vec{x})$$

$$\frac{d}{dt}\vec{x} = \vec{V}$$

$\vec{x}$: atomic positions; $\vec{V}$: atomic velocities

System of 2nd order Equations

$$M \frac{d^2}{dt^2}\vec{x} = -\nabla_{\vec{x}} E(\vec{x})$$



$$\frac{d}{dt}\vec{x}(t_m) \simeq \frac{\vec{x}(t_{m+1}) - \vec{x}(t_m)}{t_{m+1} - t_m} \simeq \frac{\vec{x}(t_m) - \vec{x}(t_{m-1})}{t_m - t_{m-1}}$$

$$\Delta t = t_{m+1} - t_m = t_m - t_{m-1}$$

$$\frac{d^2}{dt^2}\vec{x}(t_m) \simeq \frac{\frac{\vec{x}(t_{m+1}) - \vec{x}(t_m)}{\Delta t} - \frac{\vec{x}(t_m) - \vec{x}(t_{m-1})}{\Delta t}}{\Delta t}$$

$$\frac{d}{dt}\vec{v}(t_m) \simeq \underbrace{\frac{\vec{x}(t_{m+1}) - 2\vec{x}(t_m) + \vec{x}(t_{m-1})}{\Delta t^2}}_{\text{verlet}}$$

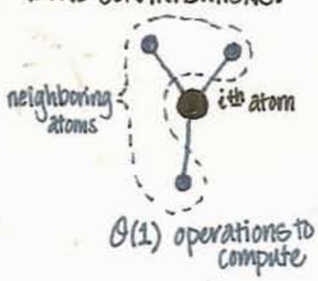
$$M \frac{\vec{x}(t_{m+1}) - 2\vec{x}(t_m) + \vec{x}(t_{m-1})}{\Delta t^2} = -\nabla_{\vec{x}} E(\vec{x})$$

ALGORITHM:

$$\underbrace{x(t_{m+1}) = 2x(t_m) - x(t_{m-1}) - \Delta t^2 M^{-1} E(\vec{x})}_{\text{Explicit Integration Scheme}}$$

on each time step:
Evaluate $E_{(x)}(\vec{x}(t_m))$ + other stuff

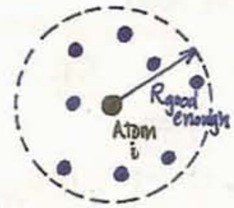
BOND CONTRIBUTIONS:



Inexpensive ~ O(N)

$$E(x) = \overbrace{\sum_{\text{bonds}} + \sum_{\substack{\text{bond}\\\text{angles}}} + \sum_{\text{torsions}}}^{\text{Inexpensive} \sim O(N)} + \sum_{\substack{\text{all}\\\text{pairs}}} \frac{B_{ij}}{r^{12}} - \frac{C_{ij}}{r^6} + \sum_{\substack{\text{all}\\\text{pairs}}} \frac{q_i q_j}{r_{ij}}$$

van der Waals:

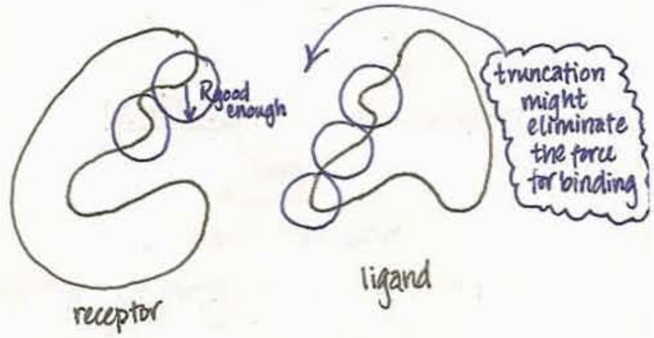


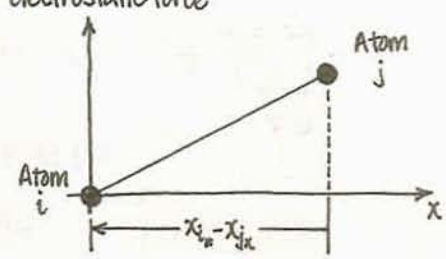
all pairwise interactions O(n) operations per atom ⟹ but truncate ⟹ O(1)

Electrostatics:

electrostatic forces die like $1/R^2$

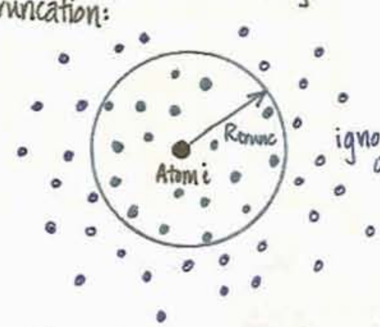
can we truncate?





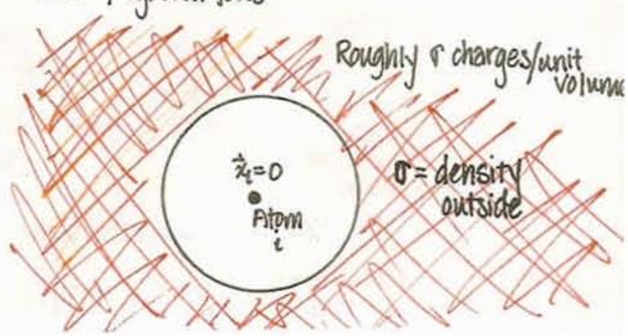
$$F = E_x = -\frac{\partial}{\partial x_{i_x}} \frac{q_i q_j}{|\vec{x}_i - \vec{x}_j|} = \frac{q_i q_j (x_{i_x} - x_{j_x})}{|\vec{x}_i - \vec{x}_j|^3}$$

try truncation:



ignore outside atoms

idea of ignored force:



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Foundations of Algorithms and Computational Techniques in Systems Biology
Professor Bruce Tidor
Professor Jacob K. White

bound on ignored force:

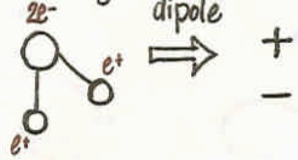
ignoring direction cancellation

$$\text{Force Bound} \simeq \int_{\text{volume outside}} \frac{\sigma(\vec{x})}{|\vec{x}|^2} dV$$

$$\simeq \int_0^{2\pi}\int_0^{\pi}\int_{R_{trunc}}^{\infty} \sigma \frac{1}{R^2} R^2 \sin\phi \, dR\, d\phi\, d\theta$$

$$\simeq \int_0^{2\pi}\int_0^{\pi} \Big[\sigma R\Big]_{R_{trunc}}^{\infty} \sin\phi\, d\phi\, d\theta \rightarrow \infty$$

charge neutrality:



Potential due to dipole: $\dfrac{\vec{p}\cdot(\vec{x}_i-\vec{x}_j)}{|\vec{x}_i-\vec{x}_j|^3}$

dipole moment

force due to dipole $\propto \frac{1}{R^3}$

bound on ignored force (dipole assumption):

$$\text{Force bound} \simeq \int_{\Omega} \frac{\rho(\vec{x})}{R^3} dV$$

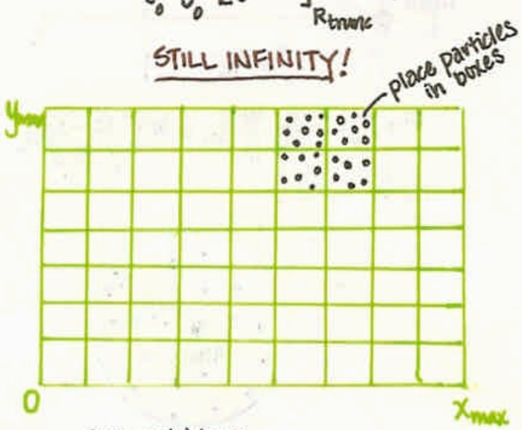
dipole density

$$\simeq \int_0^{2\pi}\int_0^{\pi}\int_{R_{trunc}}^{\infty} \frac{\rho}{R^3} R^2 \sin\phi\, dR\, d\phi\, d\theta$$

$$\simeq \int_0^{2\pi}\int_0^{\pi} \Big[\rho \ln R\Big]_{R_{trunc}}^{\infty} \sin\phi\, d\phi\, d\theta \rightarrow \infty$$

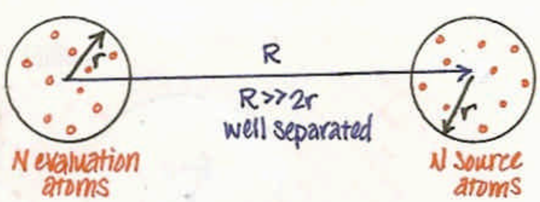
STILL INFINITY!

2-D:



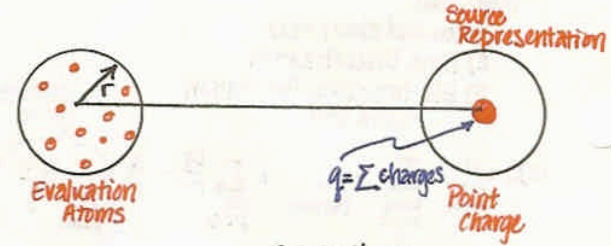
easy neighbors

MULTIPOLE IDEA:



direct force calculation is $O(N^2)$

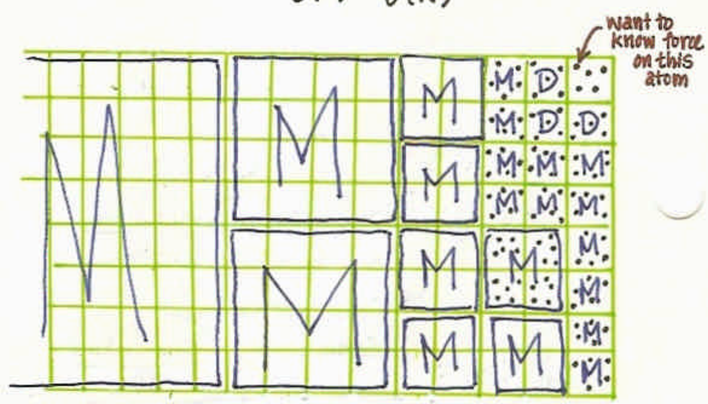
for each of N evaluation atoms: $F_i = \sum_{j \in \text{source atoms}} F_{ij}$



Source Charge Evaluation ~ $O(N)$

Single Charge Evaluation + 3 dipole Evaluations

$O(N) + O(N)$



Multiresolution

$O(N\log N)$