Simulating Bionanotechnology at the Petascale

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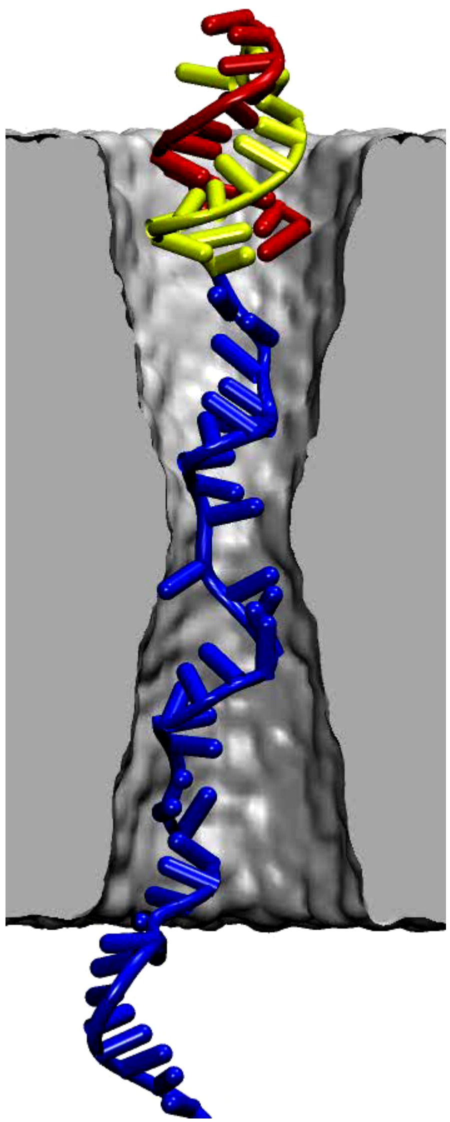
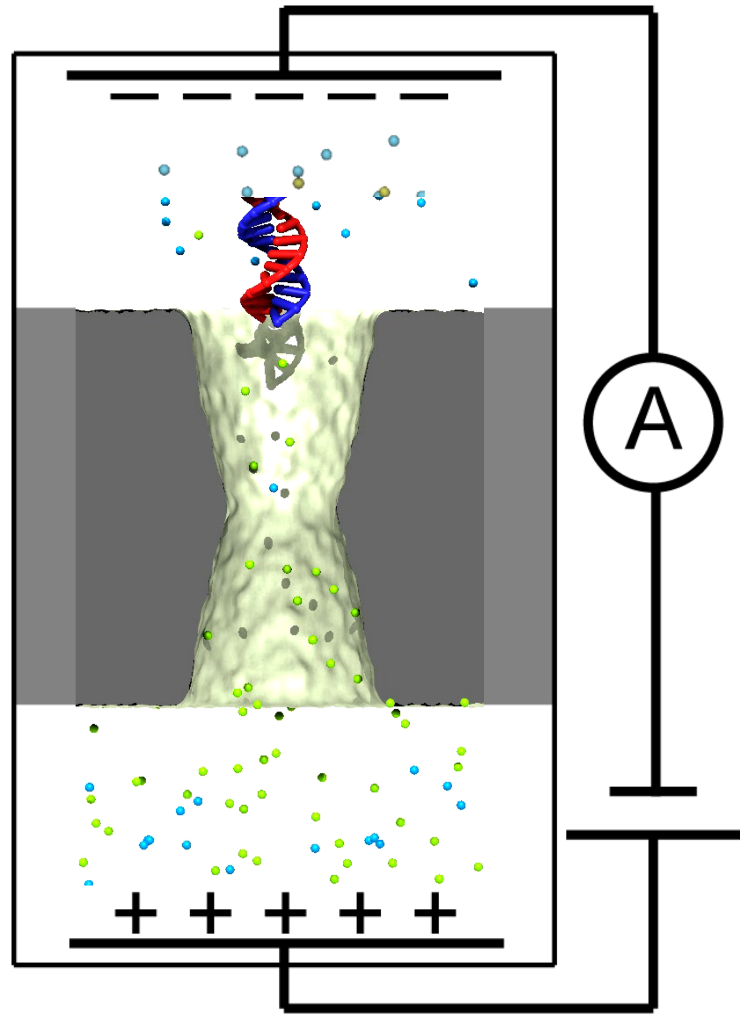
The Computational Microscope

“See” microscopic details

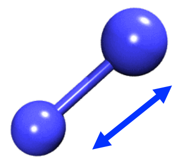


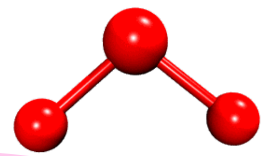
Develop nanopore DNA sequencing



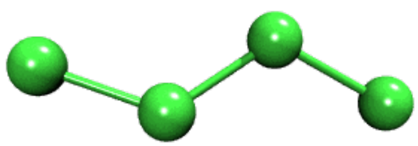
All-atom Molecular Dynamics Simulation

- Newton's second law integrated numerically $$m_i \frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathbf{r}_i(t) = -\nabla_i U\big(\mathbf{r}_1(t), \ldots, \mathbf{r}_N(t)\big)$$
- Simple algebraic form for every type of interaction
- Simulations performed with NAMD (Phillips et al., *J. Comp. Chem*. **26** (2005) 1781–1802.)





heuristic



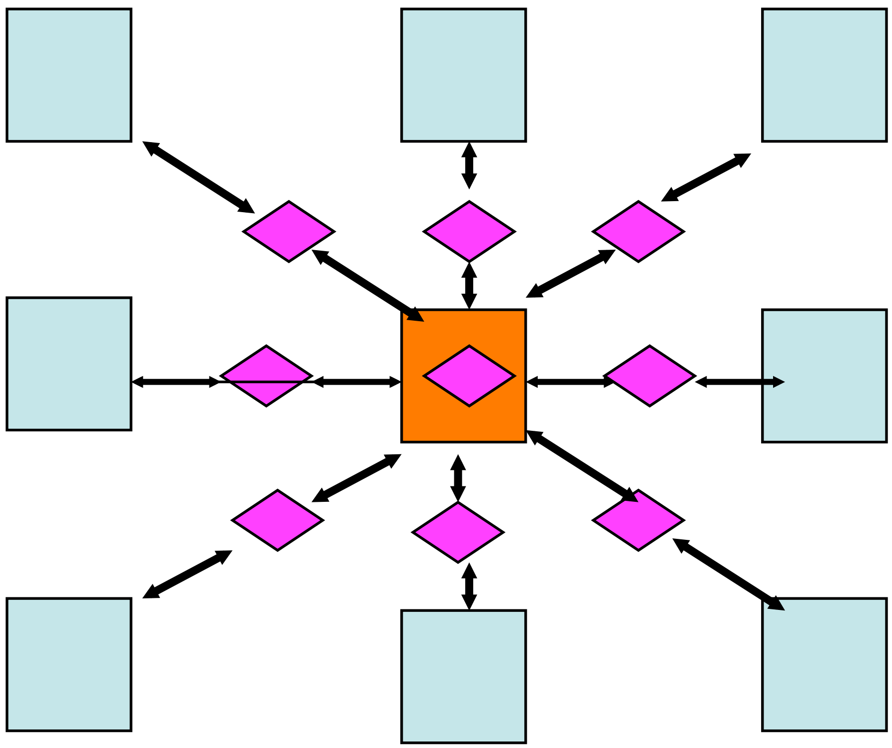
$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} + \underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} + \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}}_{U_{nonbond}}$$

from physics

NAMD: Scalable MD

Kale *et al.*, *J. Comp. Phys.* **151** (1999) 283–312

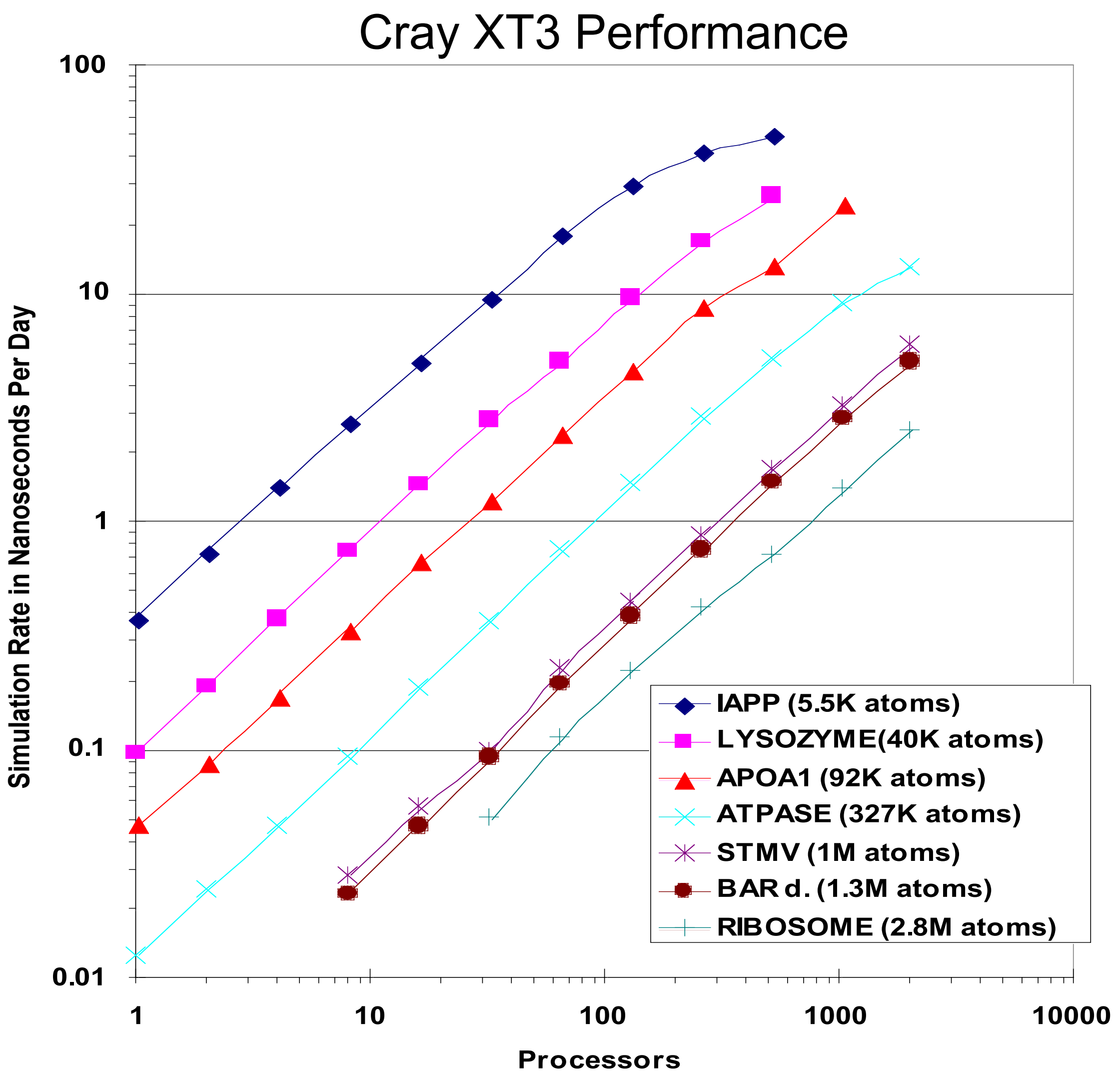
Charmm++: object-oriented parallel system
(charm.cs.uiuc.edu/research/charm/)



- Spatially decompose data and communication
- Independent but related decomp. of force computation
- Charm++ parallel objects for iterative, measurement-based load balancing

Slide material courtesy of Jim Phillips (www.ks.uiuc.edu/namd)

NAMD Performance



- NAMD already scales to 10M atoms or thousands of processors
- Challenge: >100M atom systems and 300k processors
- IBM Blue Waters

Illinois Petascale Computing Facility

Slide material courtesy of Jim Phillips (www.ks.uiuc.edu/namd)

Challenges

1. Long-range electrostatic interactions

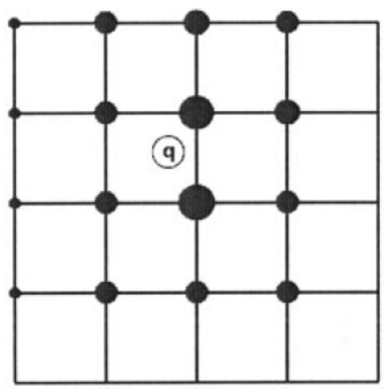
2. Output Data!

Long-rage Electrostatic Interactions

- Long-range electrostatic interactions (naively O(N^2))

$$U_{\text{Coulomb}} = \sum_i \sum_{j>i} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

- Particle-Mesh Ewald (PME) method:
  - Split computation into real and Fourier space
  - Short-range computed explicitly
  - Long-range:



Charge distributed on discrete grid

Reciprocal sum computed using FFT

O(N log N)

FFT communication overhead for large systems:
>10M atoms => 1024×1024×1024 grid

Switch to multilevel summation?

www.ideals.illinois.edu/handle/2142/11173

Output Data

- Write system configuration every 10 ps (5000 MD steps)
- 50–100 ns/day and 100M atoms =>
  1.2 TB per day
- Optimize parallel I/O

Too much data!
Storage space?
Download takes more time than simulation!

Solutions:

1. Write full system less often, skip some water
   Need new file formats and analysis programs
2. Write less often: Perform some analysis on the fly
3. Identify interesting events like High Energy

Brownian Dynamics

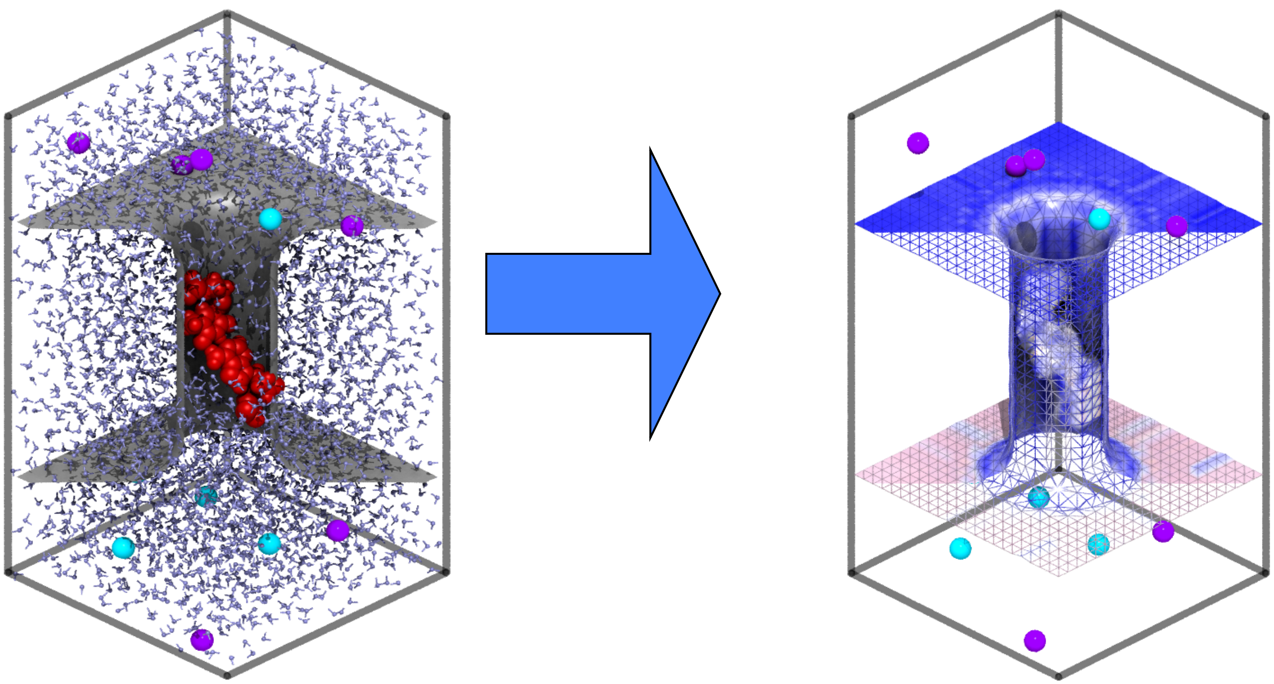
Update Rule: (Ermak and McCammon (1978) J. Chem. Phys. 69:4).

Ion Diffusivity

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \frac{D_i \Delta t}{k_{\mathrm{B}} T} \nabla_i \underbrace{W(\mathbf{r}_1(t), \mathbf{r}_2(t), \ldots)}_{\text{Potential of Mean Force}} + \underbrace{\sqrt{2 D_i \Delta t}\ \mathbf{R}(t)}_{\text{Stochastic Motion}}$$

All-atom MD Model

Coarser BD Model



Reduced Degrees of Freedom

Extracting BD Inputs from MD

$$W(\mathbf{r}_1, \mathbf{r}_2, \ldots) = \sum_{ij} W_{ij}^{\text{ion-ion}}(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_i W_i^{\text{map}}(\mathbf{r}_i)$$

T
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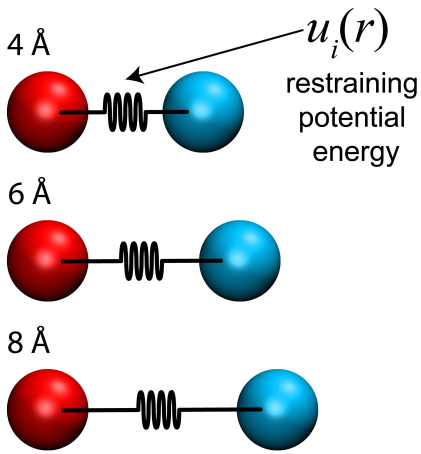
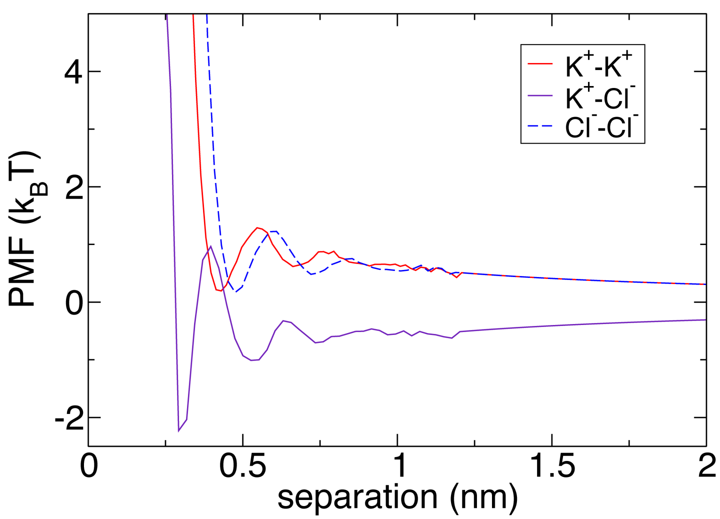
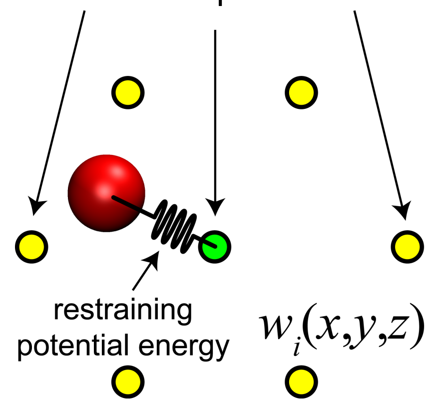
Ion–Ion PMF

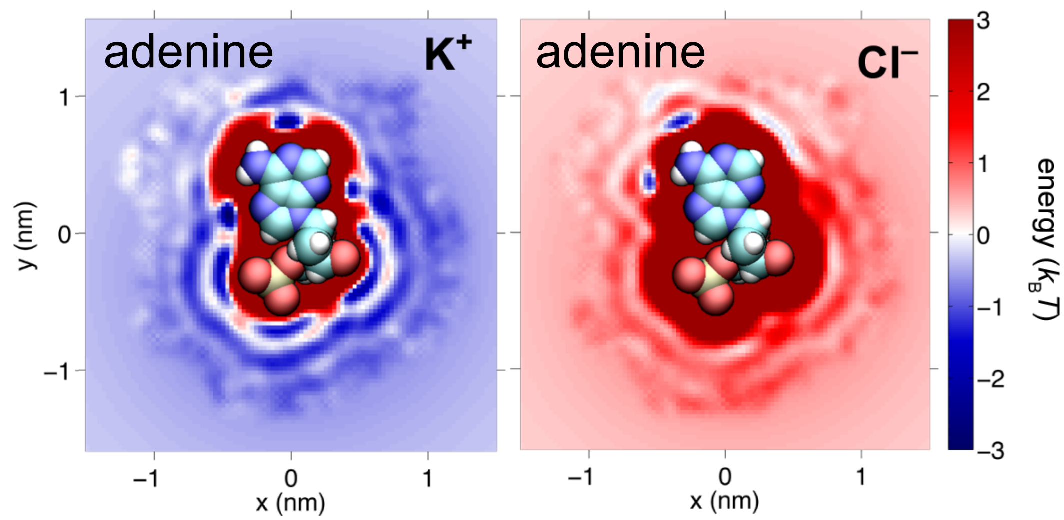


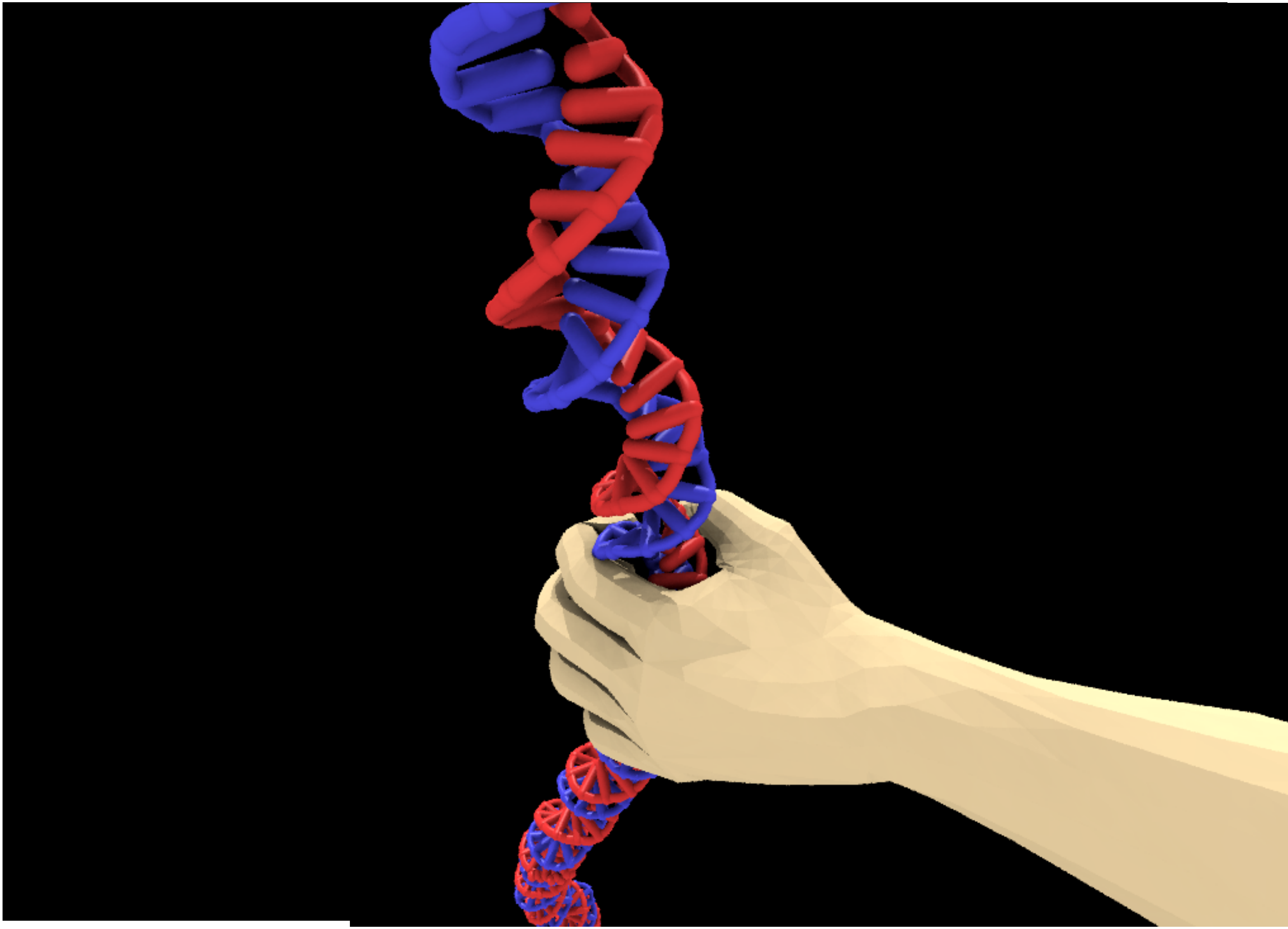


3D Nucleotide–Ion PMF

The ion is restrained to each lattice point in turn.







Molecular Dynamics and Parallel Computation

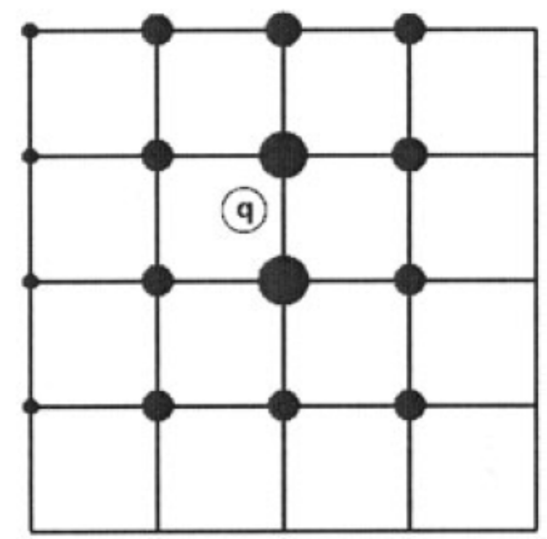
- Form of van der Waals forces permits truncation of potential

$$U_{\mathrm{vdW}} = \sum_{i} \sum_{j>i} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

- Truncation of Coulomb forces unrealistic

$$U_{\mathrm{Coulomb}} = \sum_{i} \sum_{j>i} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

Use PME:



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