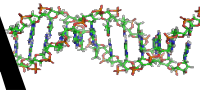
NIST
National Institute of Standards and Technology
U.S. Department of Commerce

WESLEYAN UNIVERSITY

Computer Simulations of DNA Driven Nanoparticle Assemblies



TCBG GPU WORKSHOP

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Fernando Vargas-Lara

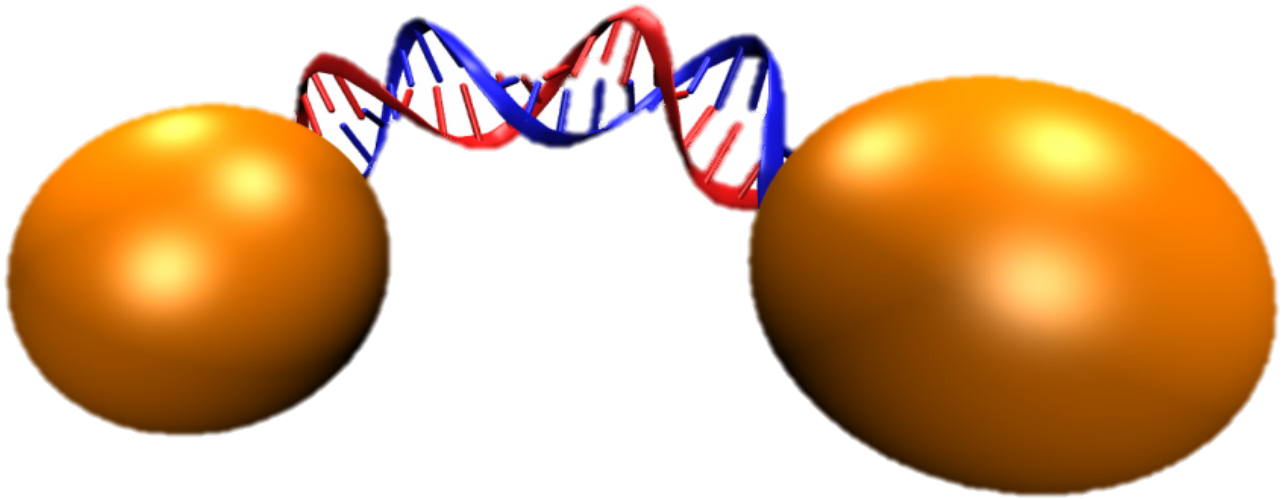
Jack F. Douglas

Materials Science & Engineering Division

Francis W. Starr

Physics Department
Wesleyan University

1. GPU Challenges



CAUTION: All the pictures and movies have been made using VMD

GPU Challenges

Short term goals

1. Migrate ssDNA simple model from C to GPU
2. Translate ZENO from Fortran to GPU
3. Get computing time on TITAN to test 1 &2

Long term goals

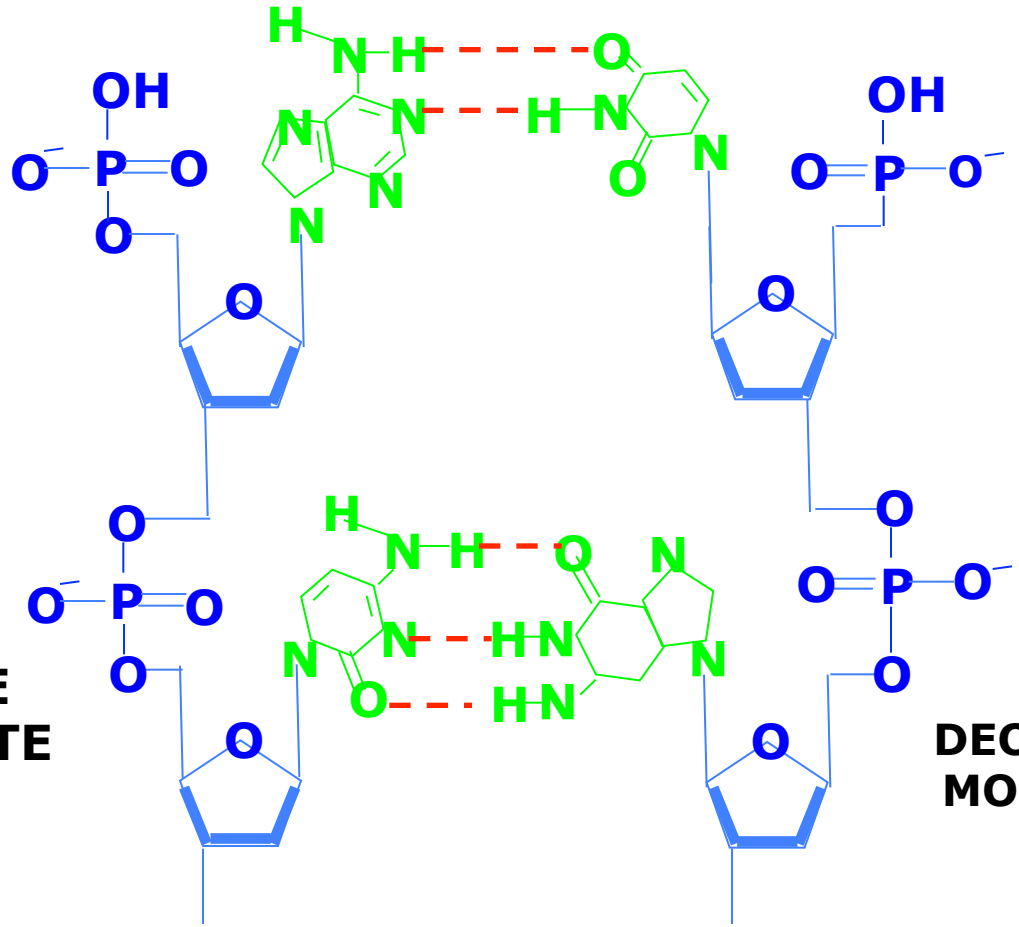
1. Run a megaton of DNA-grafted NPs to study the dynamics of crystallization
2. Determine elec. & mech. properties of large systems using ZENO.
3. Study other MD models using GPU technology

2. Description of the Problem

DNA is a complex molecule!

DEOXYADENOSINE MONOPHOSPHATE (A)

DEOXYTHYMIDINE MONOPHOSPHATE (T)

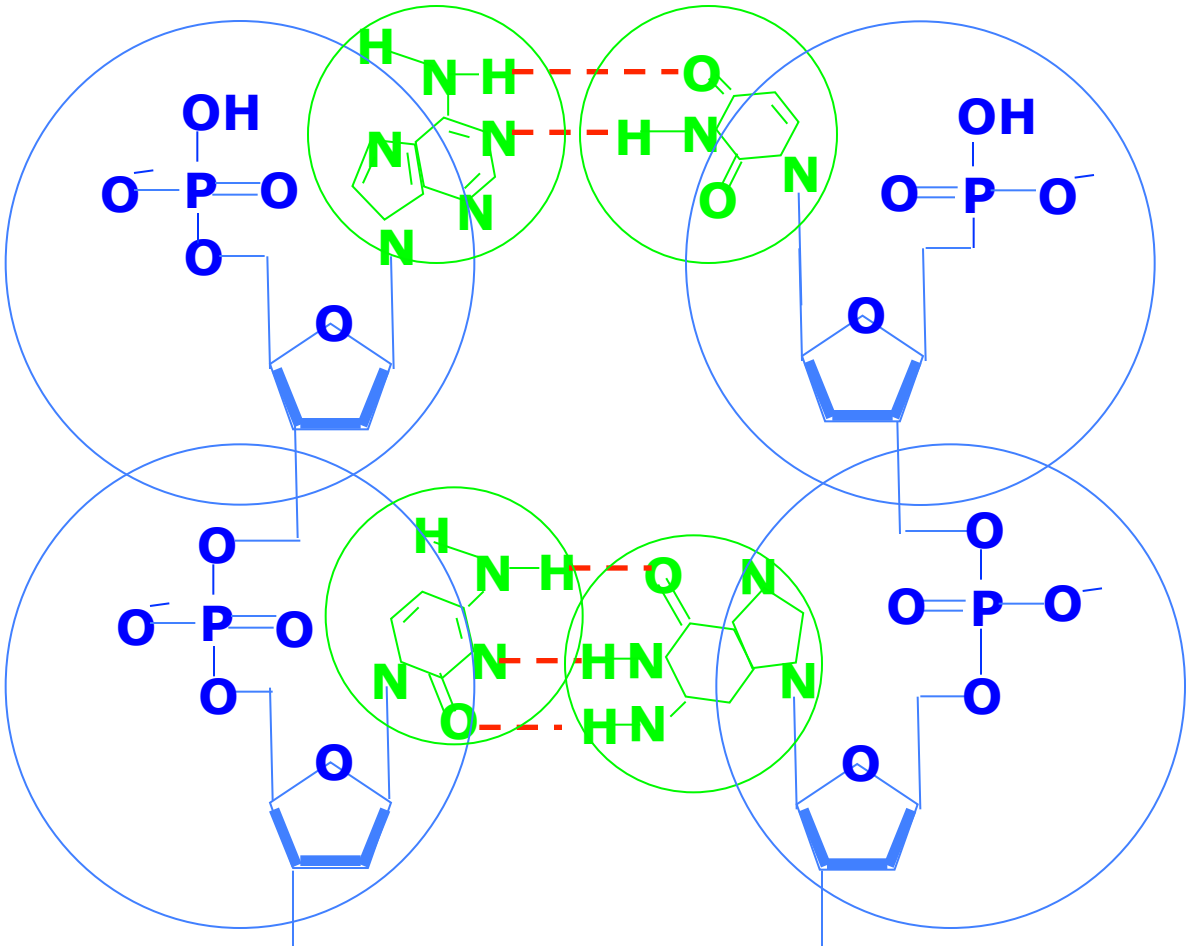


DEOXYCYTIDINE MONOPHOSPHATE (C)

DEOXYGUANOSINE MONOPHOSPHATE (G)

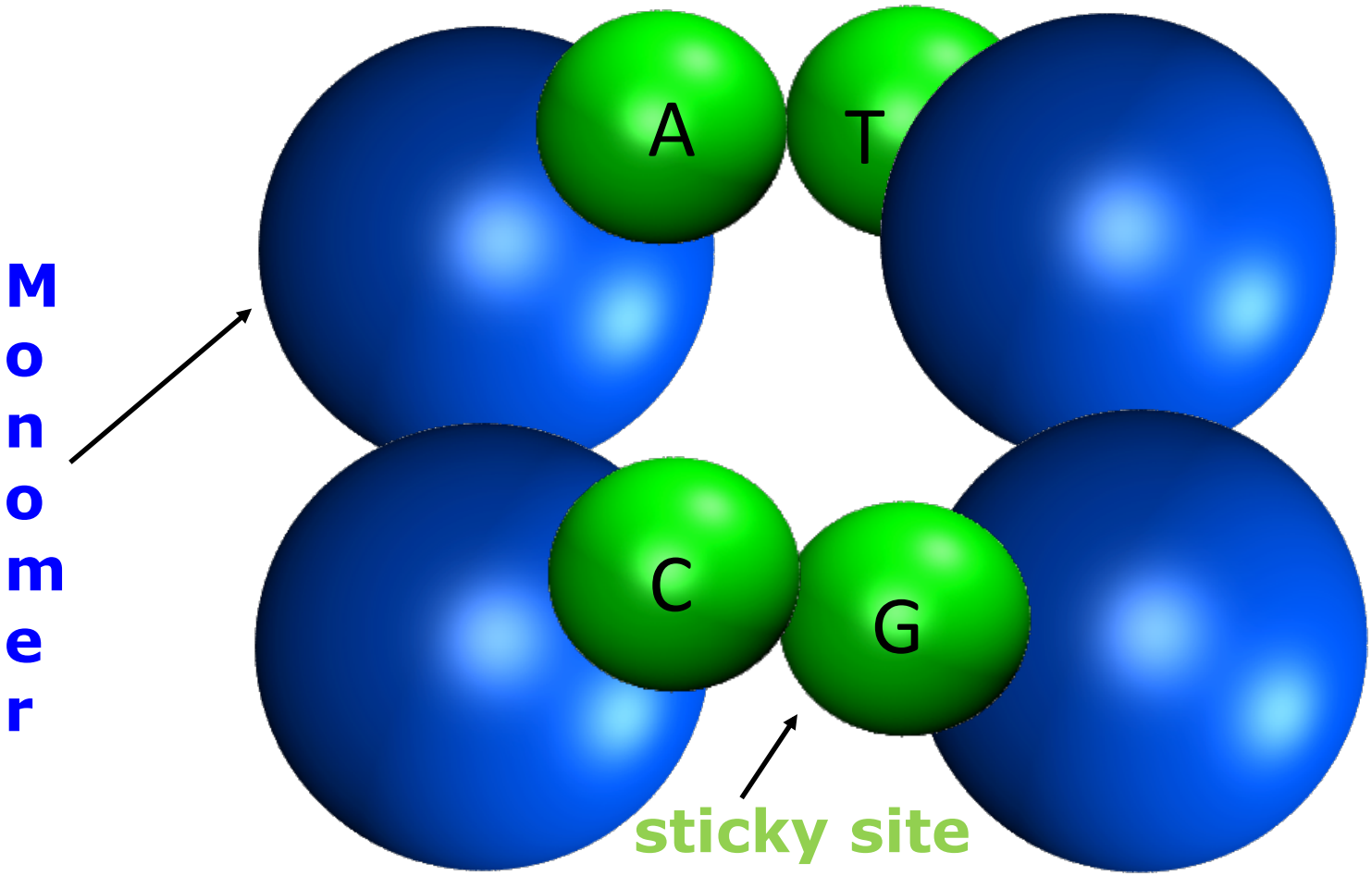
Simple DNA Strand Model

Starr & Sciortino, J. Phys. Condens. Matt. 18, L347 (2006)



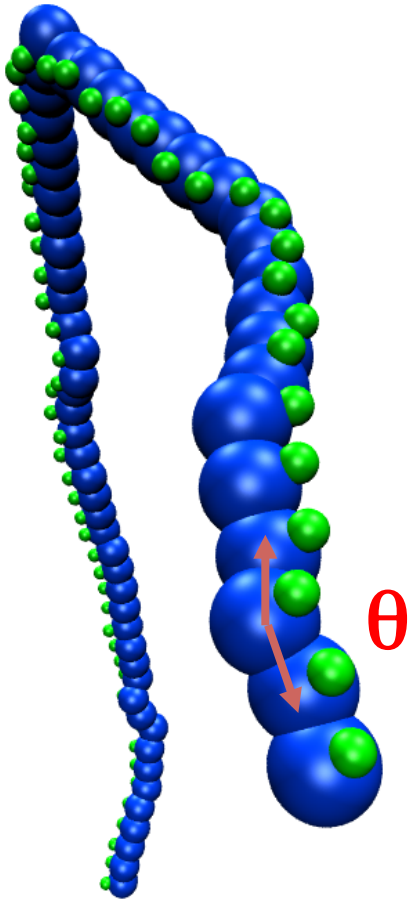
Simple DNA Strand Model

Parameterized to reproduce the **rigidity** and the **natural self-assembly** double-stranded DNA



Simple DNA Strand Model

Interaction Potentials

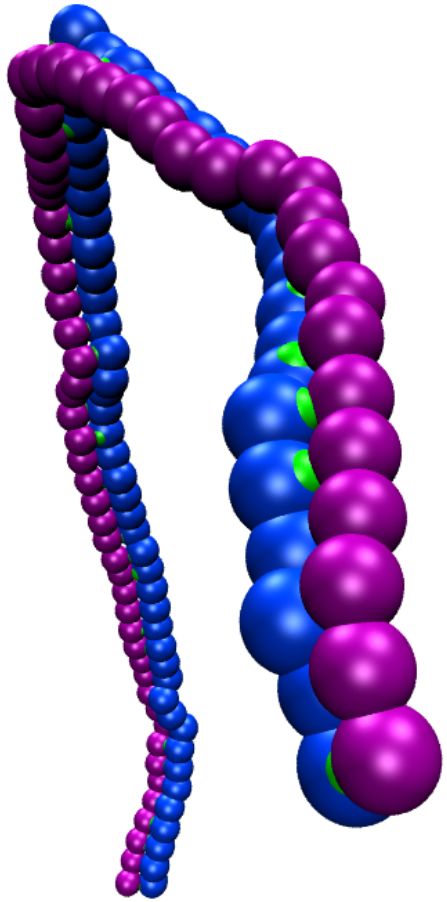


- All Pair sites via truncating and shifting LJ
- Neighboring monomers via FENE
- To model the characteristic rigidity:

$$V_L = k_{linear}[1 + \cos(\theta)]$$

- Small spheres carry A,C,G,T identities

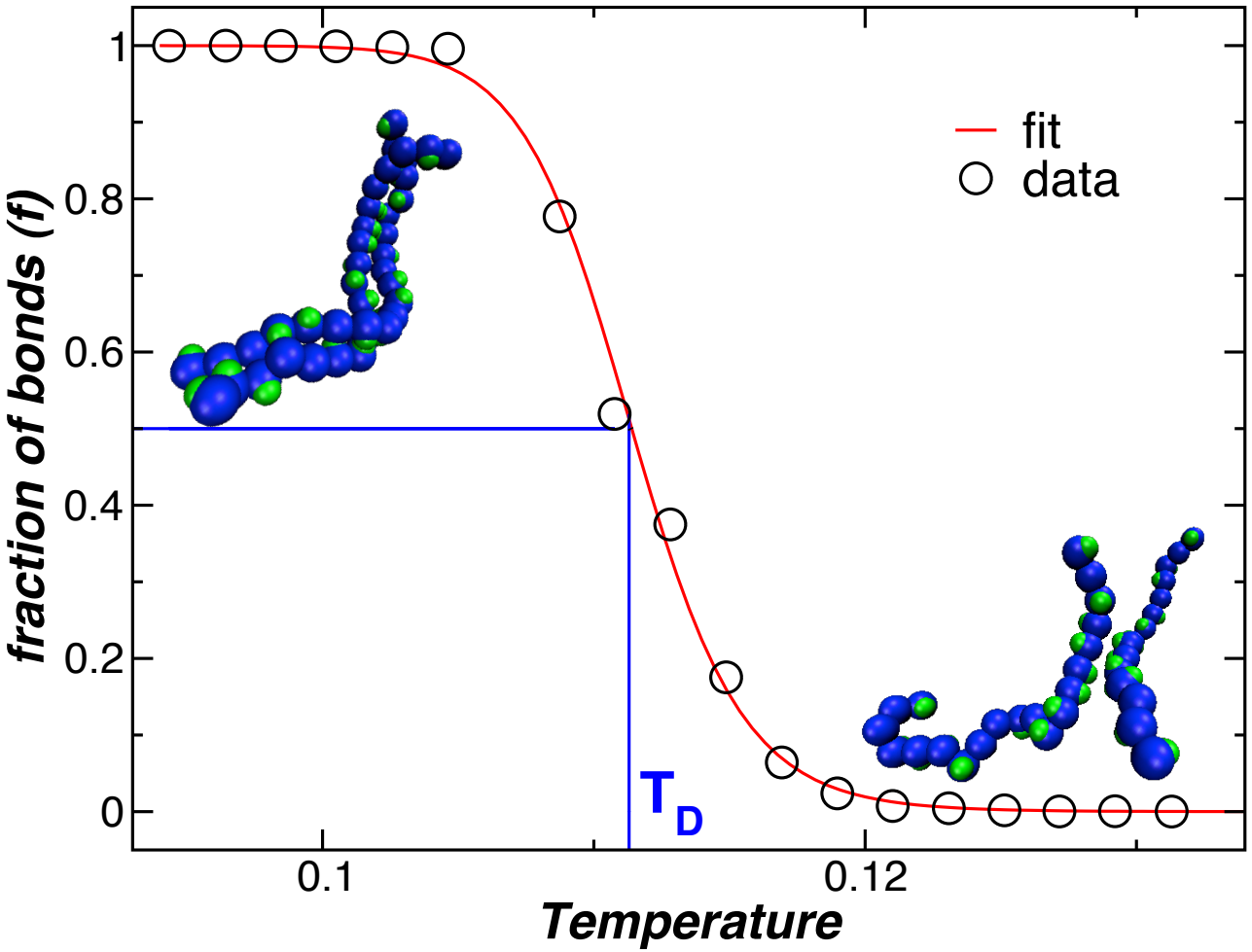
Simple DNA Strand Model



At low temperature, two complementary strands self-assembly forming dsDNA

Simple DNA Strand Model

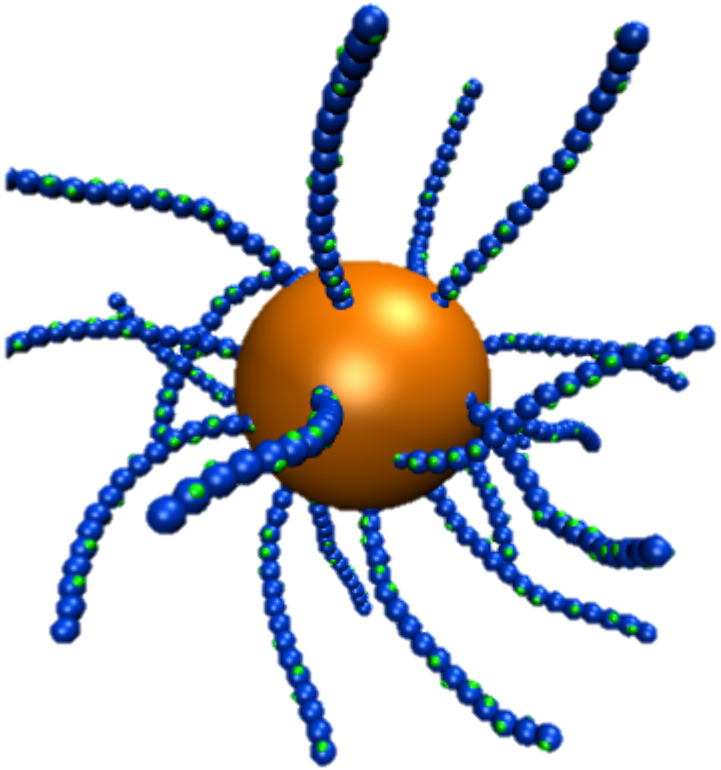
Fraction of bonds (f) as a function of the temperature



$$f = 1 - \frac{1}{1 + e^{\frac{\Delta H - T\Delta S}{T}}}$$

The transition temperature T_D, is the temperature at which half of the bonds that hold the dsDNA permanent intact.

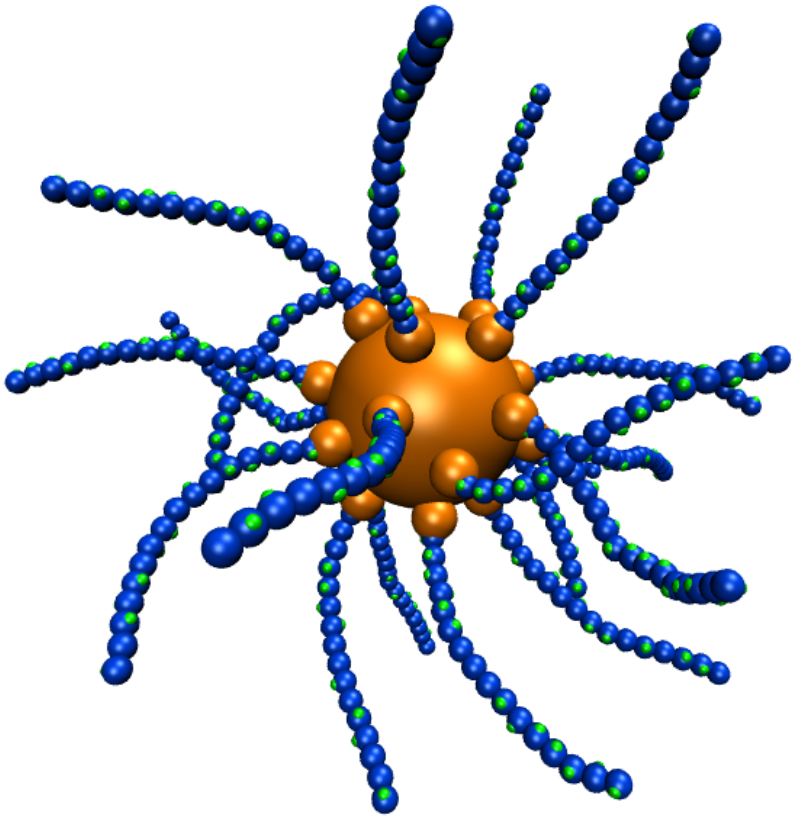
Nanoparticle Core Model



Nanoparticle with:

✓ Spherical Symmetry

Nanoparticle Core Model



Nanoparticle with:

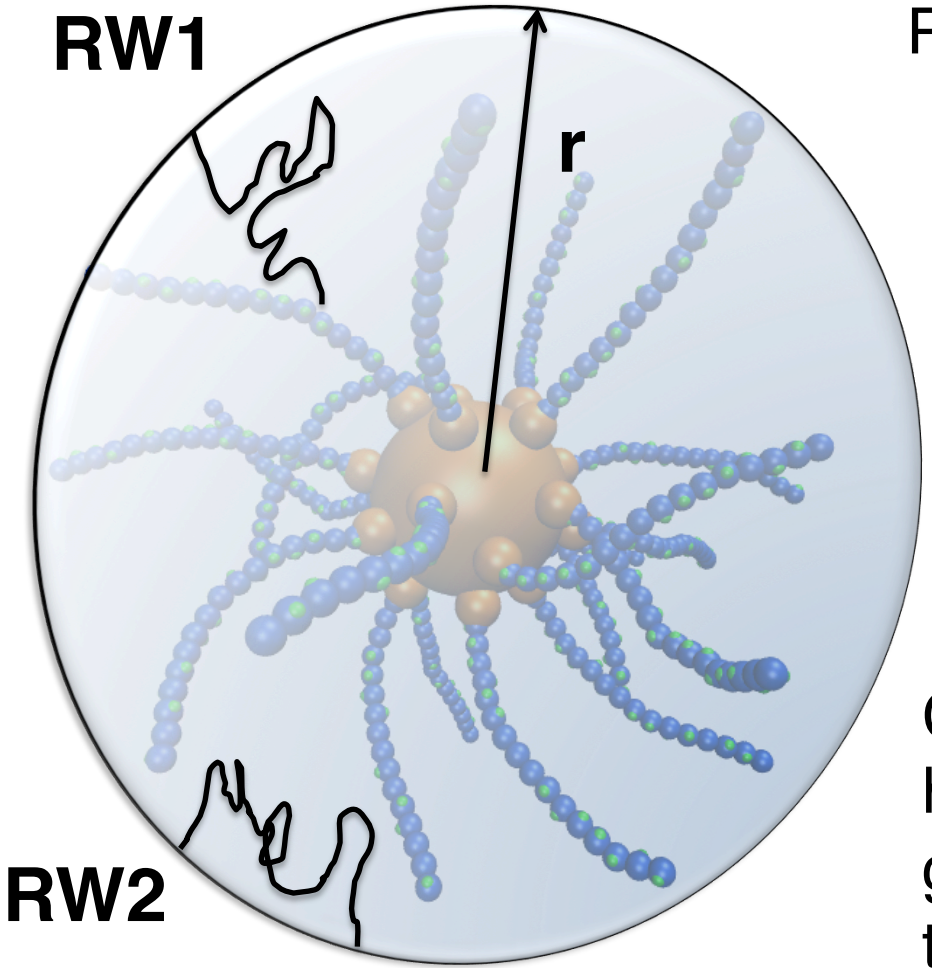
✓ Spherical Symmetry

✓ Regular Solid
- Icosahedron
- Dodecahedron
- Icosidodecahedron

ZENO

A Monte Carlo numerical path integrator

(Integrates Laplace's equation with Dirichlet's b.c)



Probabilistic definition of R_H

$$R_H = \lim_{|r|\to\infty} (|r| P_r)$$

Douglas & Zhou & Hubbard, Phys. Rev. E , 49,5319,(1994)

Computes: friction coefficient, hydrodynamic radius, radius of gyration, capacity, polarizabilty tensor, intrinsic conductivity, intrinsic viscosity...of **arbitrarily shaped objects**

3. Key Algorithms

Key Algorithms

ssDNA Model

- ✓ Molecular Dynamic Simulations (NVT)
- ✓ Velocity-Verlet method to integrate Newton's Equation
- ✓ Periodic Boundary Conditions
- ✓ Neighbour List
- ✓ Nose-Hoover thermostat
- ✓ **MPI parallel computing**

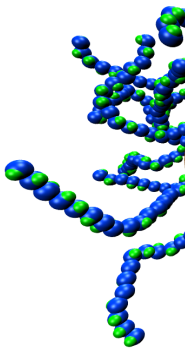
ZENO

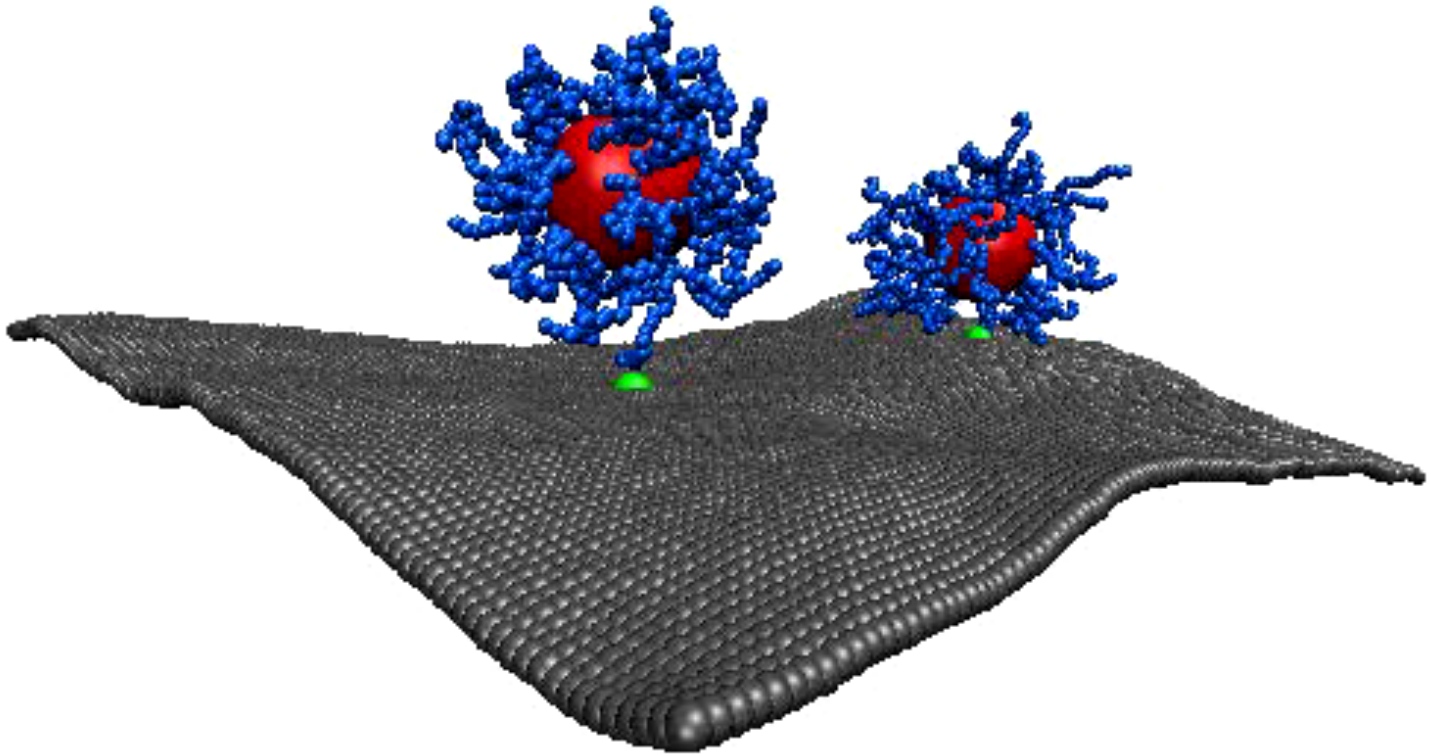
- ✓ Monte Carlo

4. Research Contribution

Some

stals





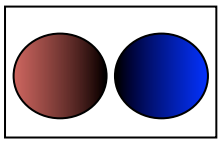
Janus N

s

to-head,
-tail bindin

Sequence

AN NA^{C}



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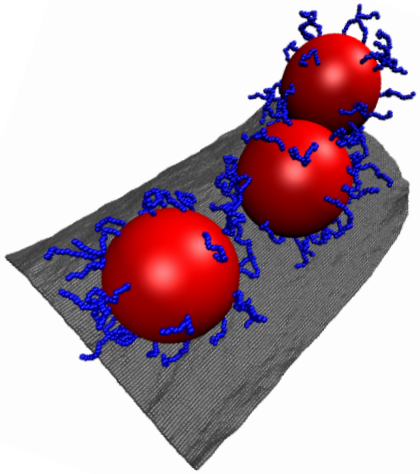
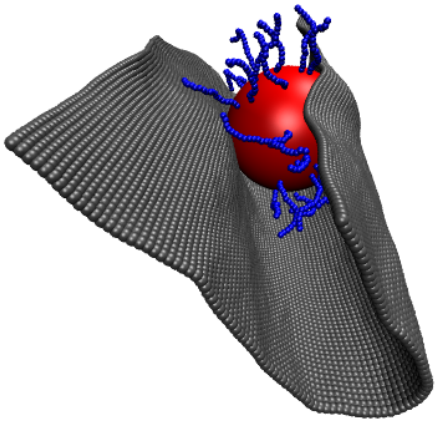
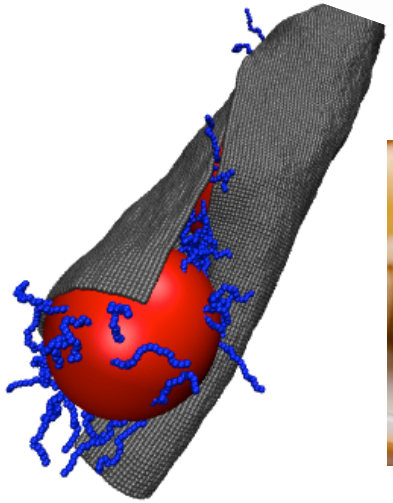
More applications of the model

Soft Tacos



Hard Tacos





Burritos