Brownian Dynamics simulations of biological and nanotechnological systems

Chris Maffeo

NCSA monthly software meeting

March 6, 2017

Biological Modeling at Different Scales

spanning orders of magnitude in space and time

system

length scale

individual proteins | molecular assemblies | intra-cellular spaces | prokaryotes | eukaryotes and colonies

1 nm | 10 nm | 100 nm | 1 μm | 10 μm | 1 mm

simulation method

all-atom MD (NAMD)

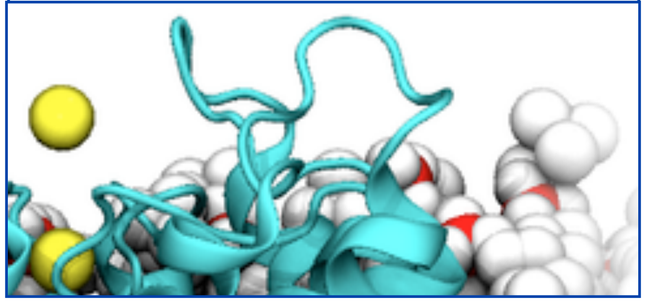
pairwise atomic potentials

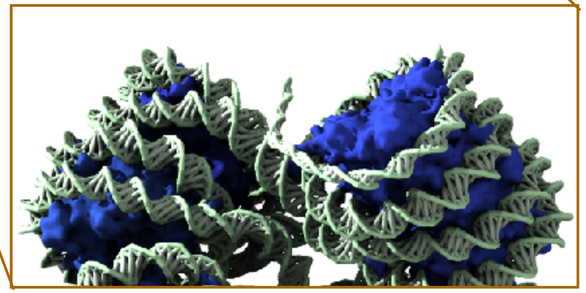
coarse-grained Brownian Dynamics (ARBD)

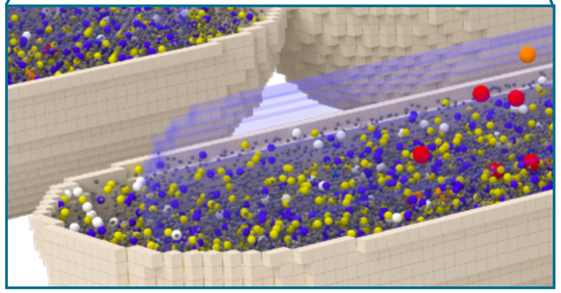
pairwise coarse-grained potentials

reaction–diffusion (Lattice Microbes)

reaction & diffusion probabilities







timestep & accessible timescale

2 fs timestep

up to 10 μs

20-500 fs timestep

up to 10 ms

μs timestep

up to days

Ingredients for a mesoscopic cell description

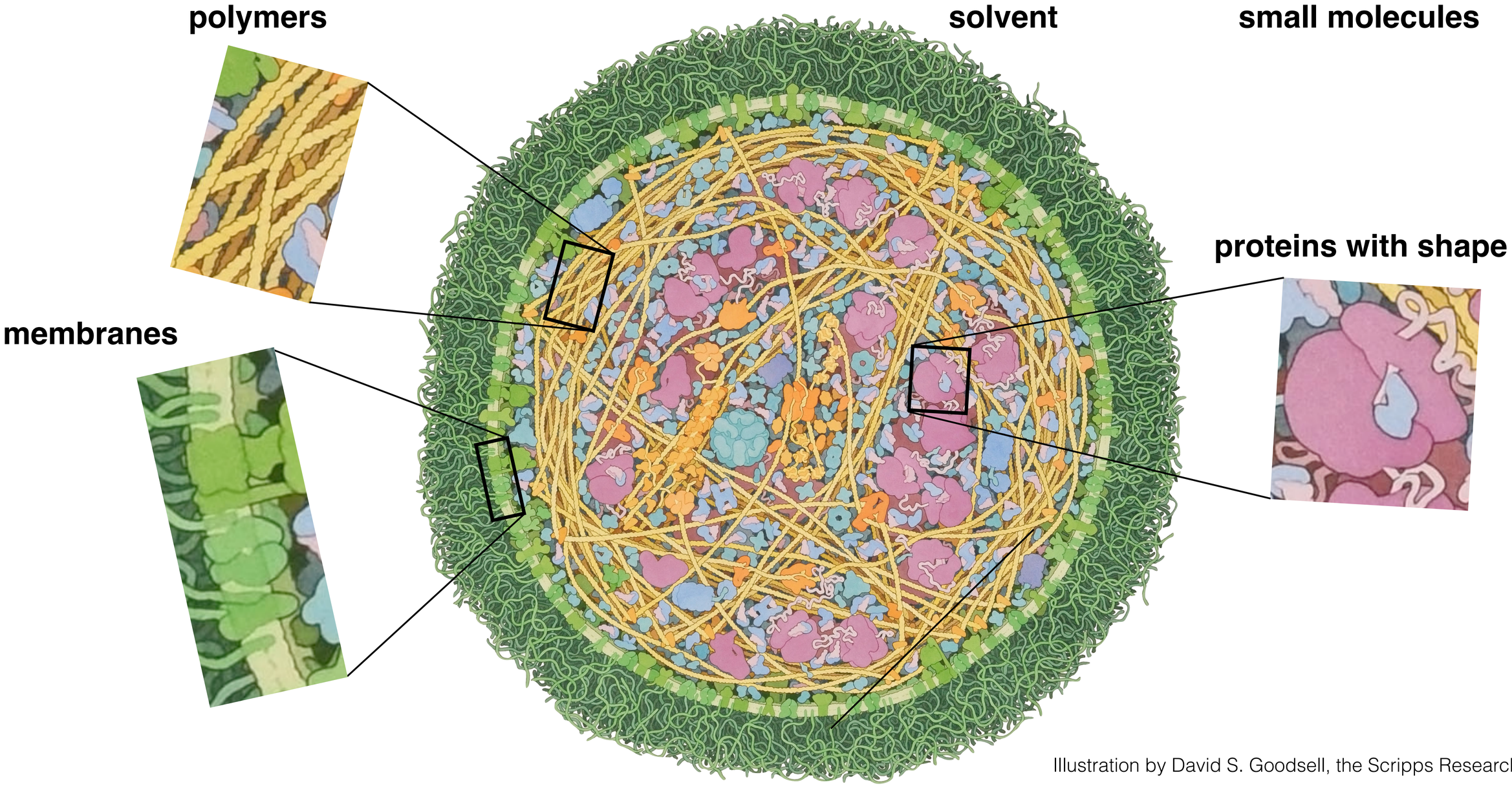


Illustration by David S. Goodsell, the Scripps Research Institute

Representing cell components in a Brownian Dynamics simulation

polymers

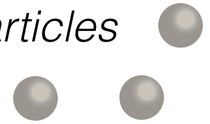
point-like particles connected by bond, angle and dihedral angle potentials

solvent

implicit through tabulated interaction potentials

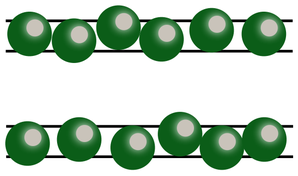
small molecules

point-like particles



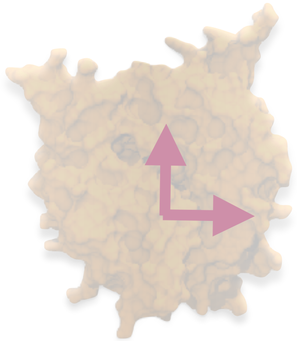
membranes

point-like particles confined by grid-specified potentials

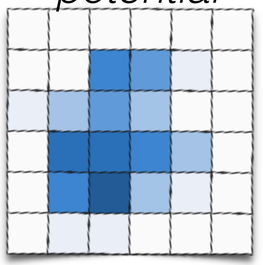


proteins with shape

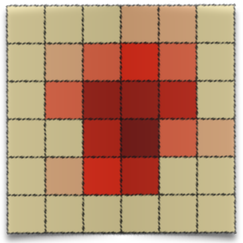
physical particles with grid-specified potentials and densities



potential



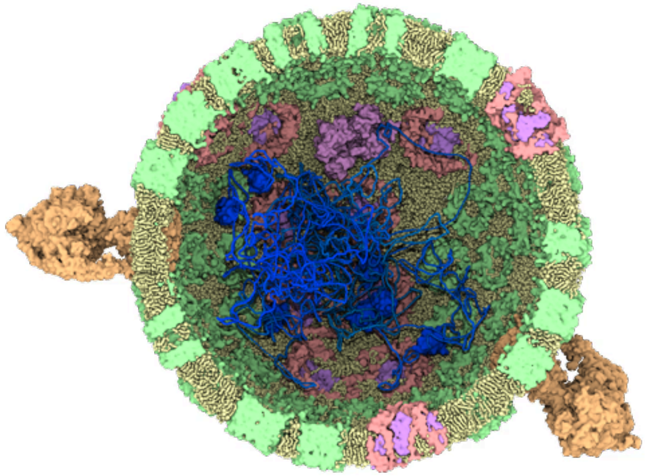
density

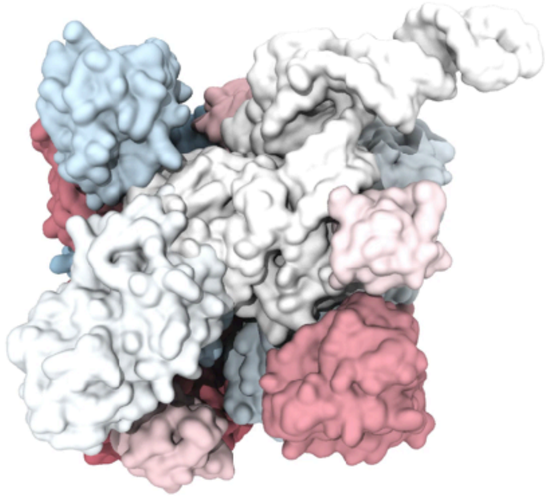


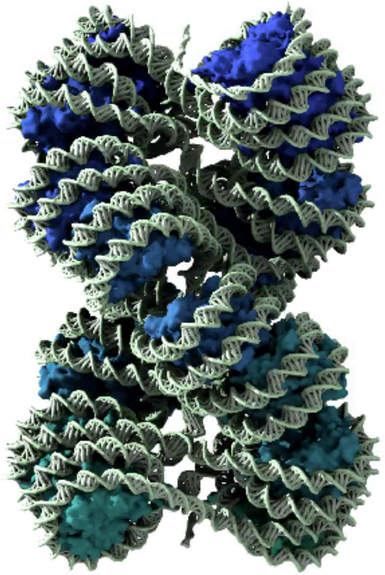
Collaborations using *Atomic Resolution Brownian Dynamics*

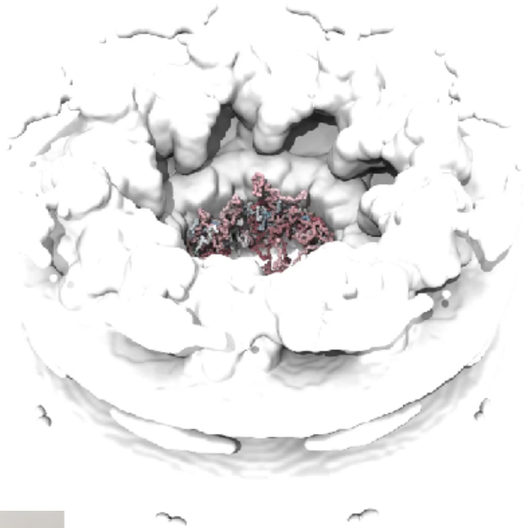
http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=ARBD

Charge transport in the **Chromatophore,** a light harvesting organelle	Crowding in the **cytosol:** model assembly for protein folding	Dynamics and structure of **Chromatin**, a complex of DNA and histones	Structure of the **Nuclear Pore Complex** central mesh, the gateway to the nucleus



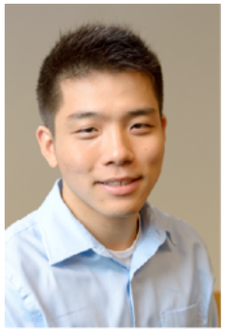






Abhi Singharoy

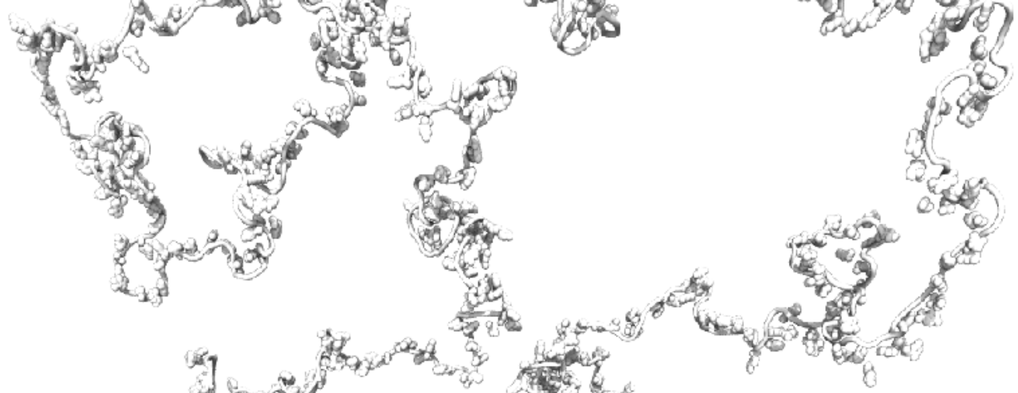
Yi Zhang

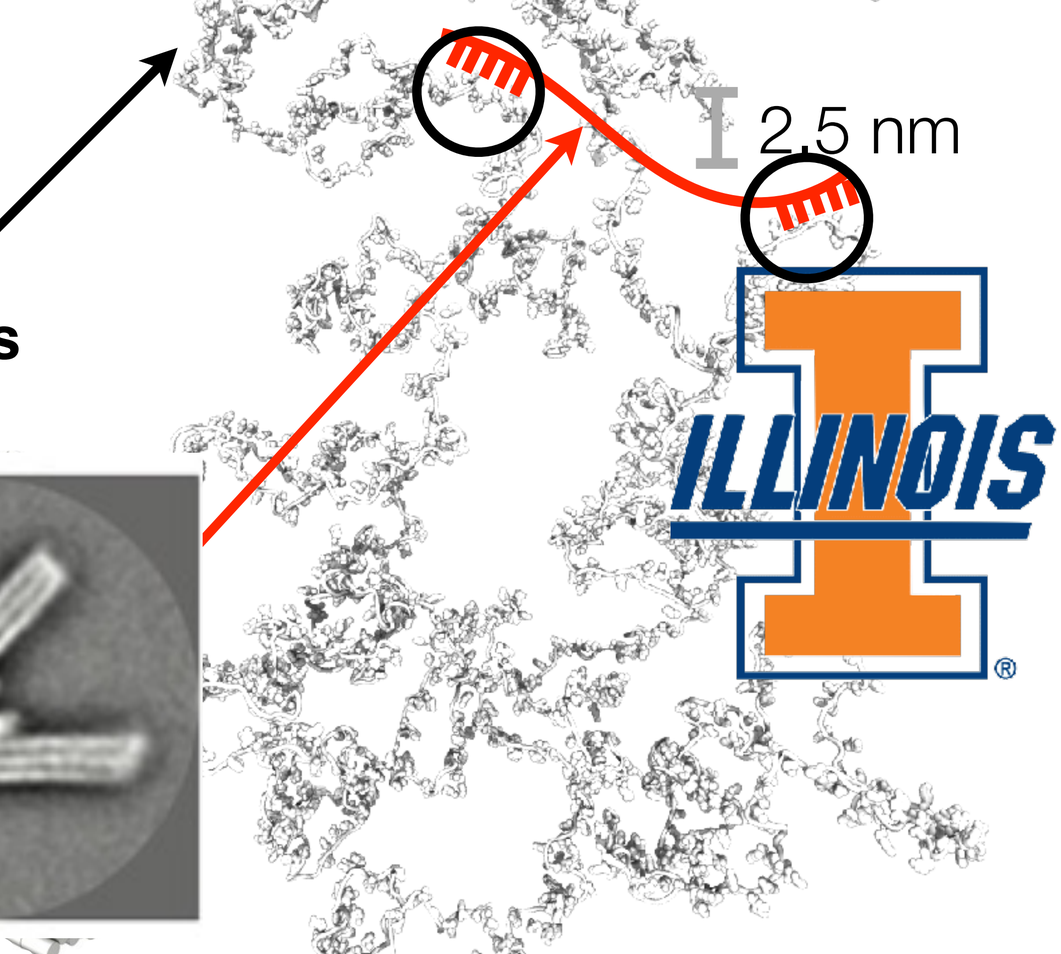


David Winogradoff

DNA origami: nanotechnology to **program** a custom-shape 3D structure of a long viral DNA (>5000 nucleotides) using short synthetic DNA oligomers.

- Nanometer-scale precision
- High yield
- No expensive fabrication facilities.

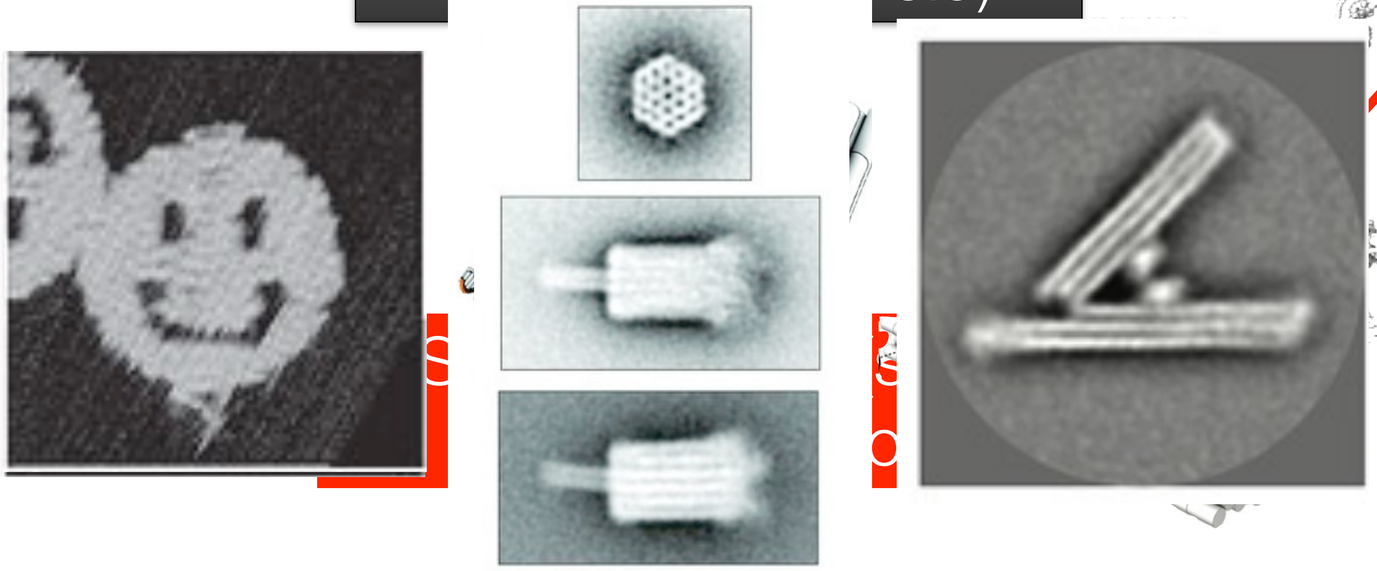




Animation: Jejoong Yoo

Custom shapes, channels, and sensors

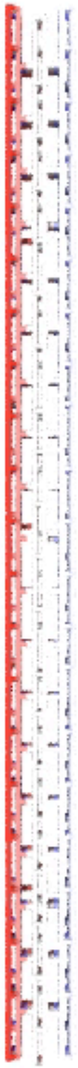
Viral DNA (scaffold)



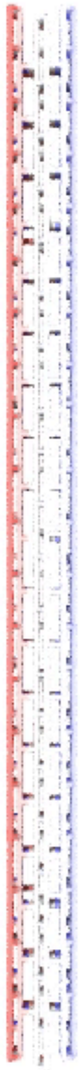
For illustration, an unfolding trajectory at a high temperature is played backward.

ARBD can be used routinely to check design of DNA origami

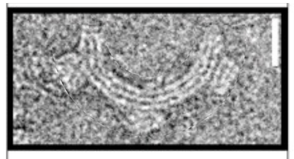
0 degrees



30 degrees

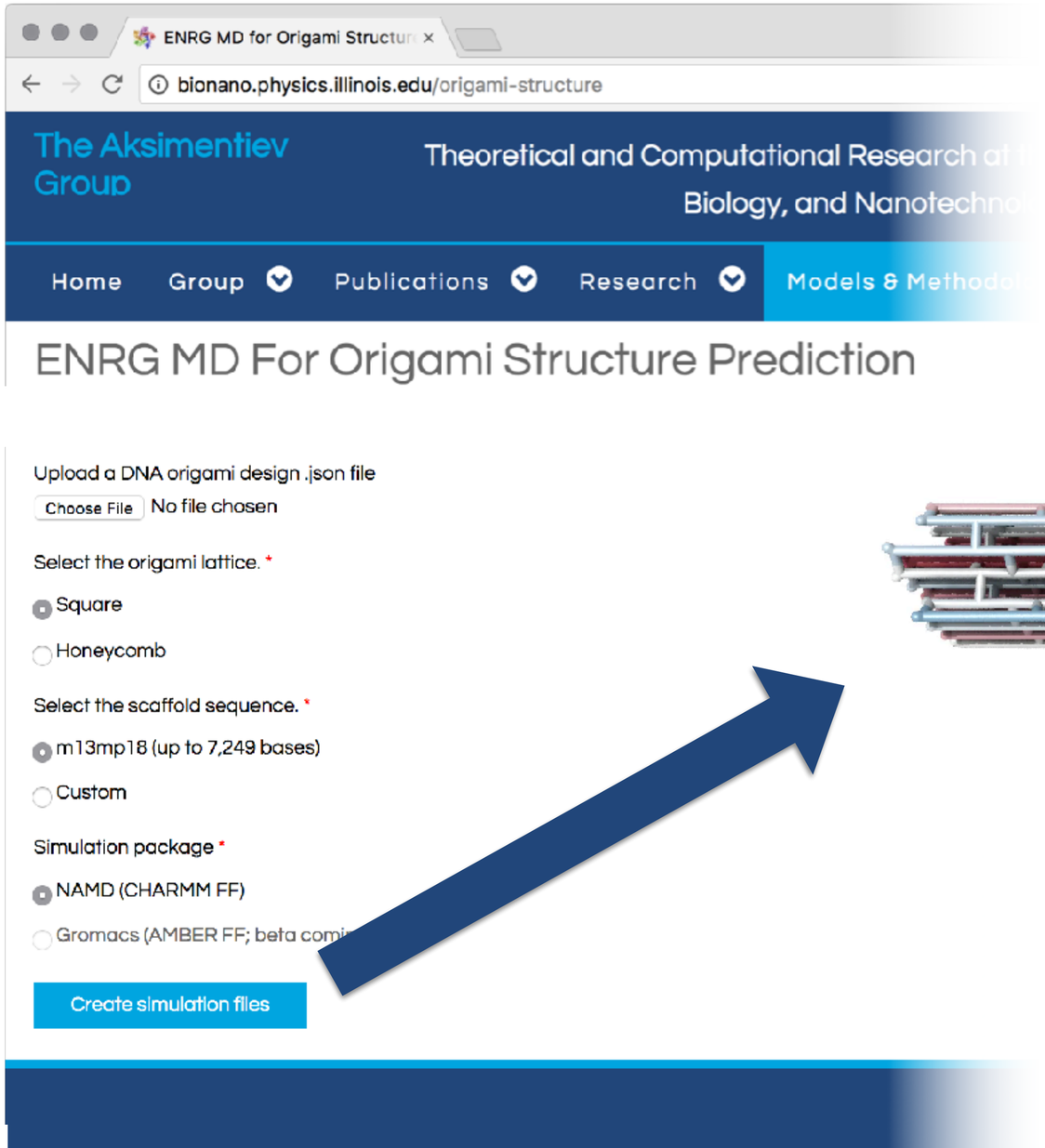


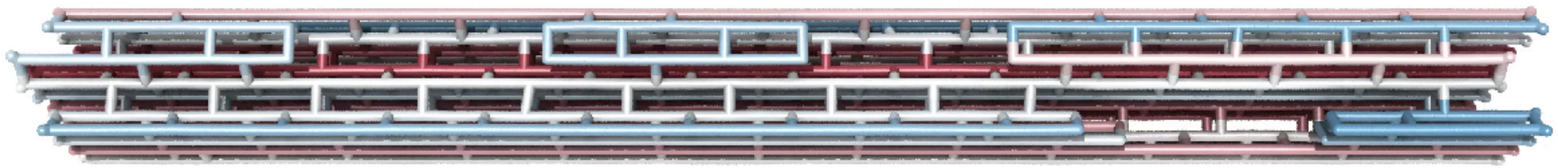
60 degrees



half “gear”

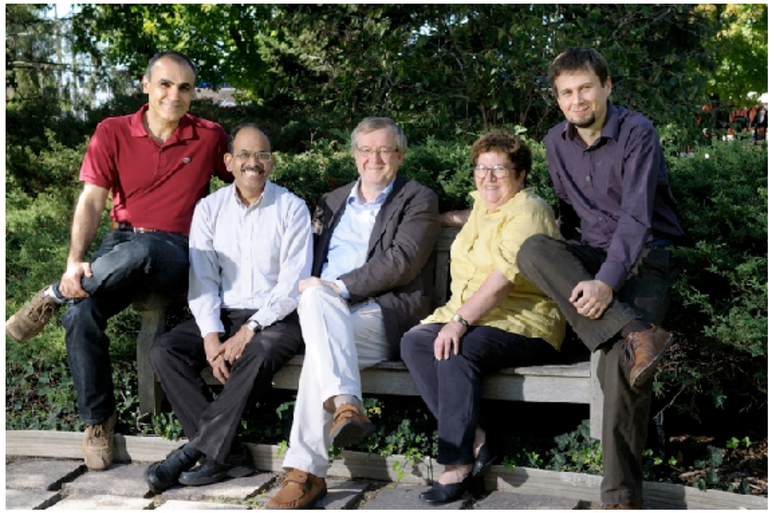
ARBD can be used routinely to check design of DNA origami





Acknowledgements

NIH Center for Macromolecular Modeling and Bioinformatics



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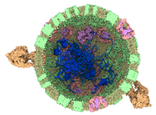
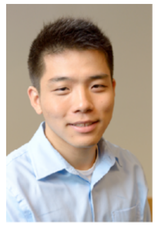
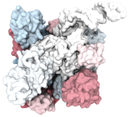
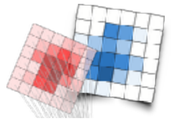




Yi Zhang



Aksimentiev group



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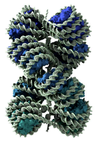
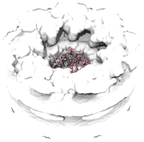
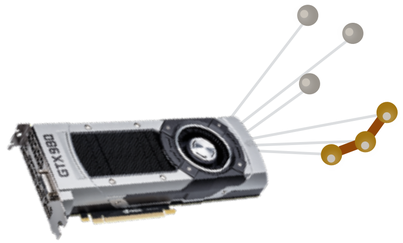




Vladomyr Kindratenko



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BLUE WATERS

Center for the Physics of Living Cells

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