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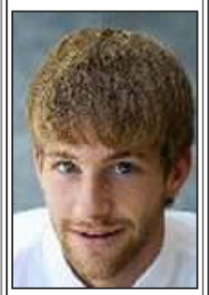

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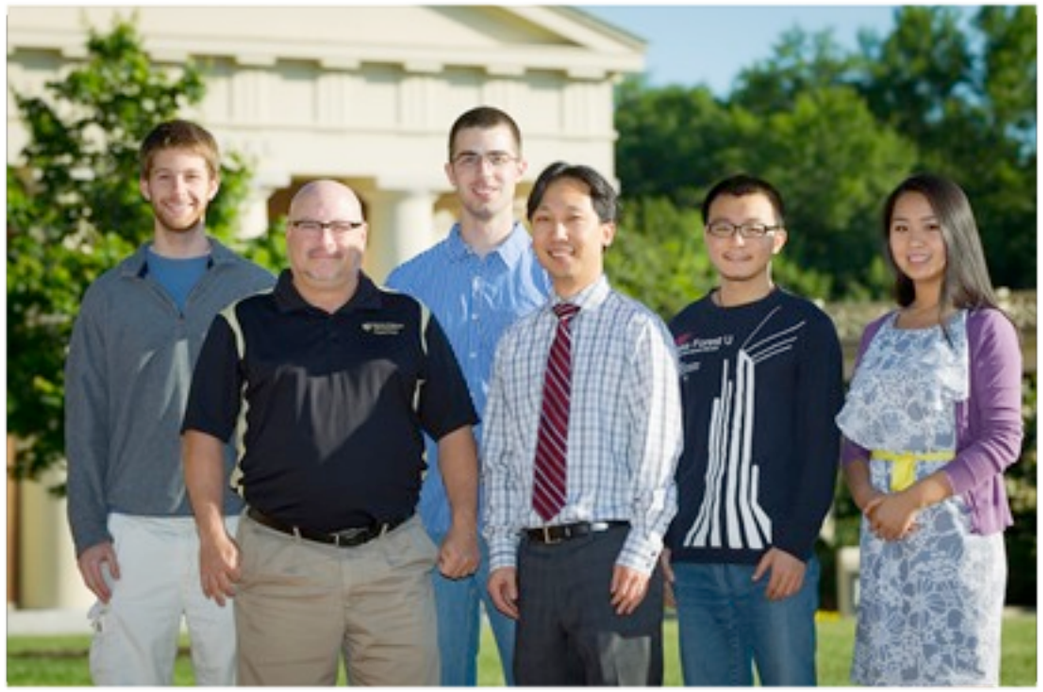

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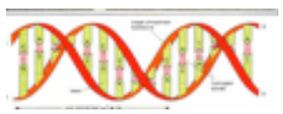
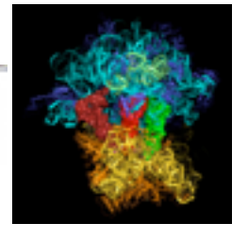
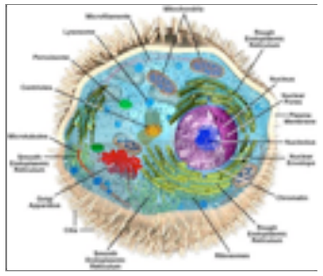
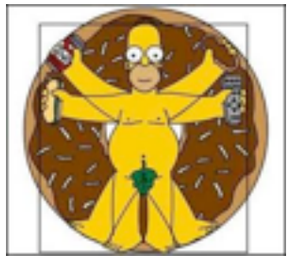
Biology

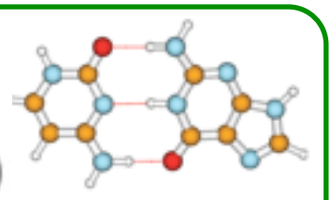





Chemistry

$$E_{Total} = E_{Intra} + E_{Inter}$$

$$E_{Intra} = \sum_{bonds} K_b\left(b - b_0\right)^2 + \sum_{angles} K_\theta\left(\theta - \theta_0\right)^2 + \sum_{torsions} K_\varphi\left(1 + \left(\cos n\varphi - \delta\right)\right)$$

$$E_{Inter} = \sum_{nonbonded} \frac{q_i q_j}{4\pi r_{ij} D} + \varepsilon_{ij}\left[\left(\frac{R_{\min,ij}}{r_{ij}}\right)^{12} - 2\left(\frac{R_{\min,ij}}{r_{ij}}\right)^{6}\right]$$



Physics

$$F_i = m_i a_i = m_i \frac{d^2 r_i}{dt^2} = -\nabla E(R)$$

Mathematics

$$r_i(t + \delta t) = 2r_i(t) - r_i(t + \delta t) + \delta t^2 \frac{F_i(t)}{m_i}$$

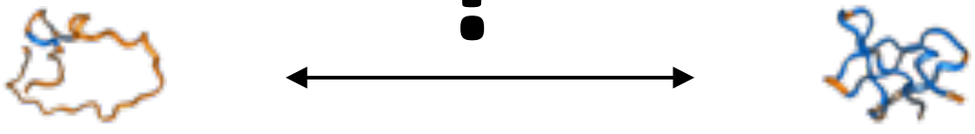
Computer Software

Computer Hardware

What can we directly see?

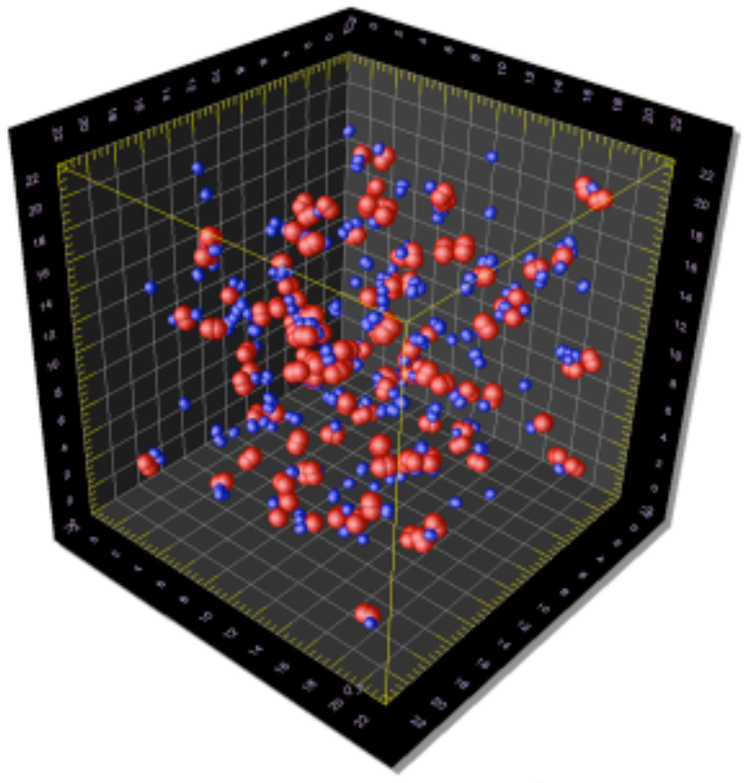
Experiments

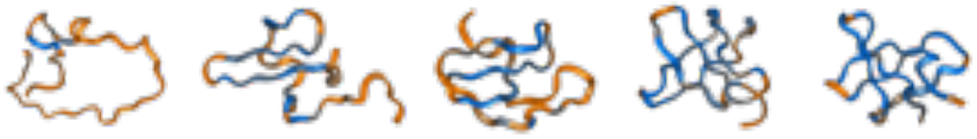
?



Unfolded Folded

Simulations





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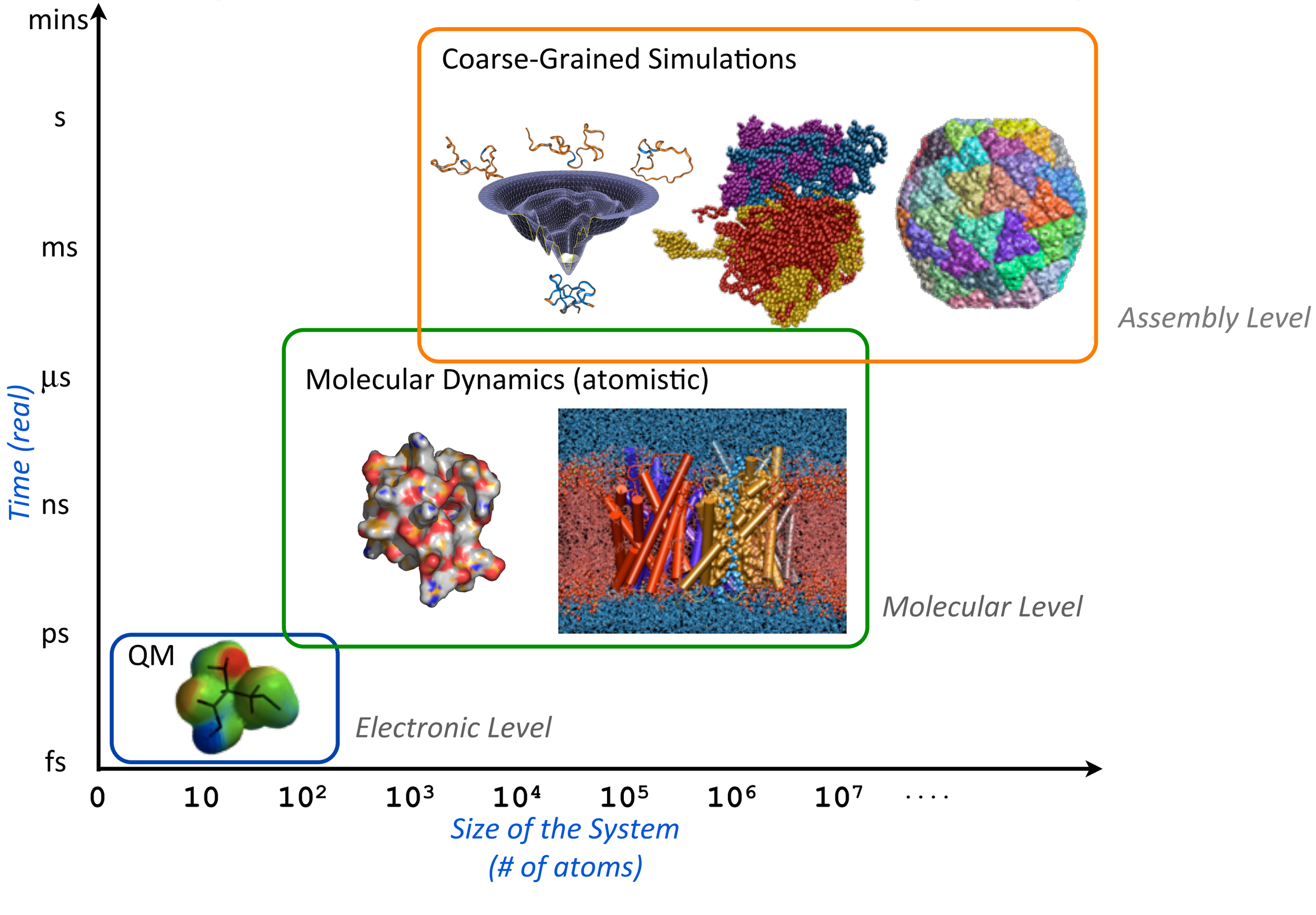
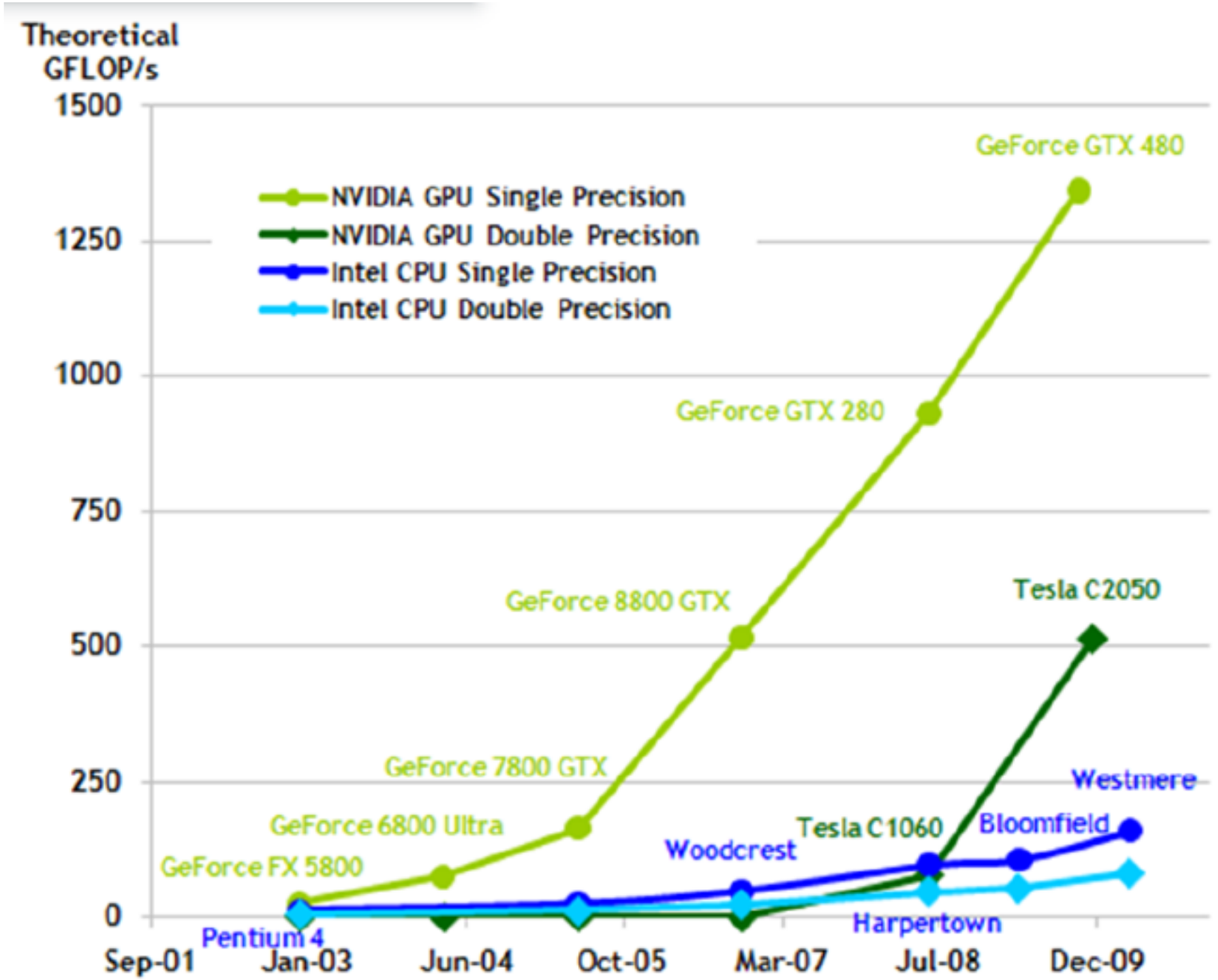
Computer Simulations of Biological Systems

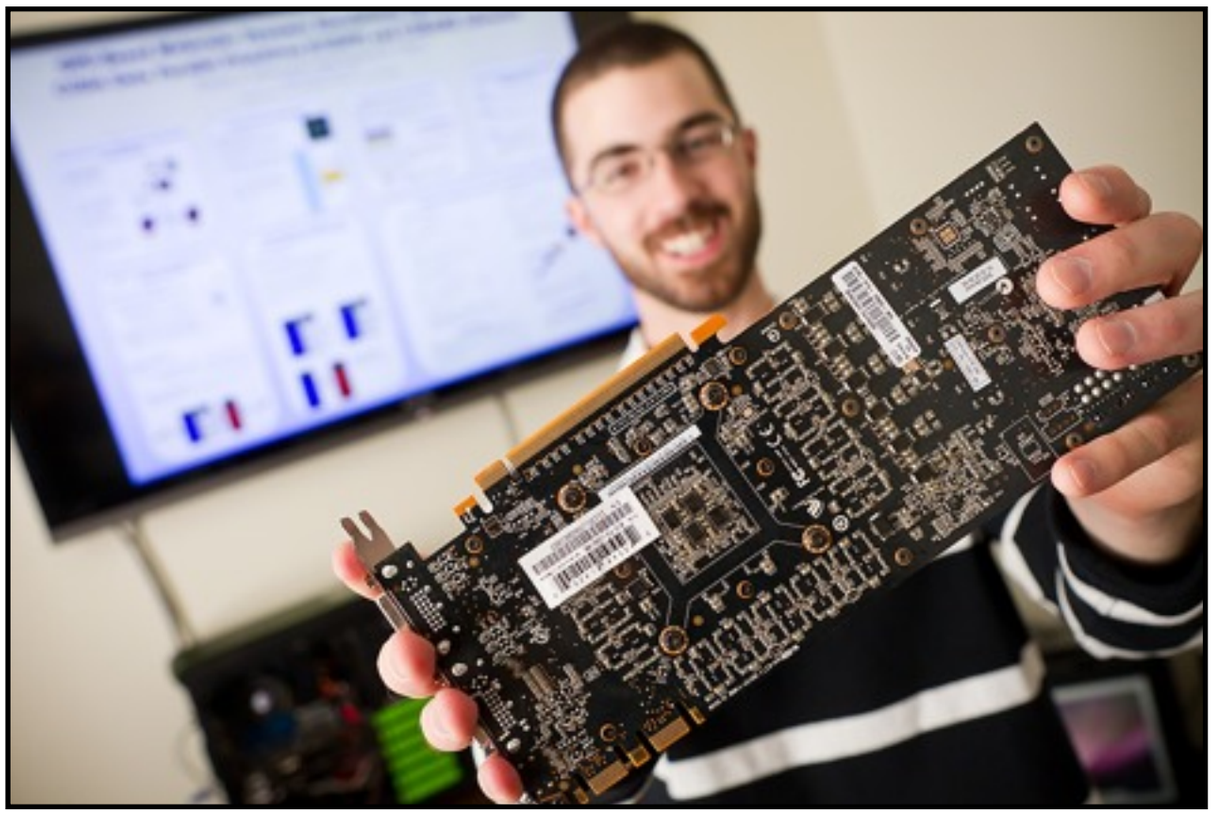


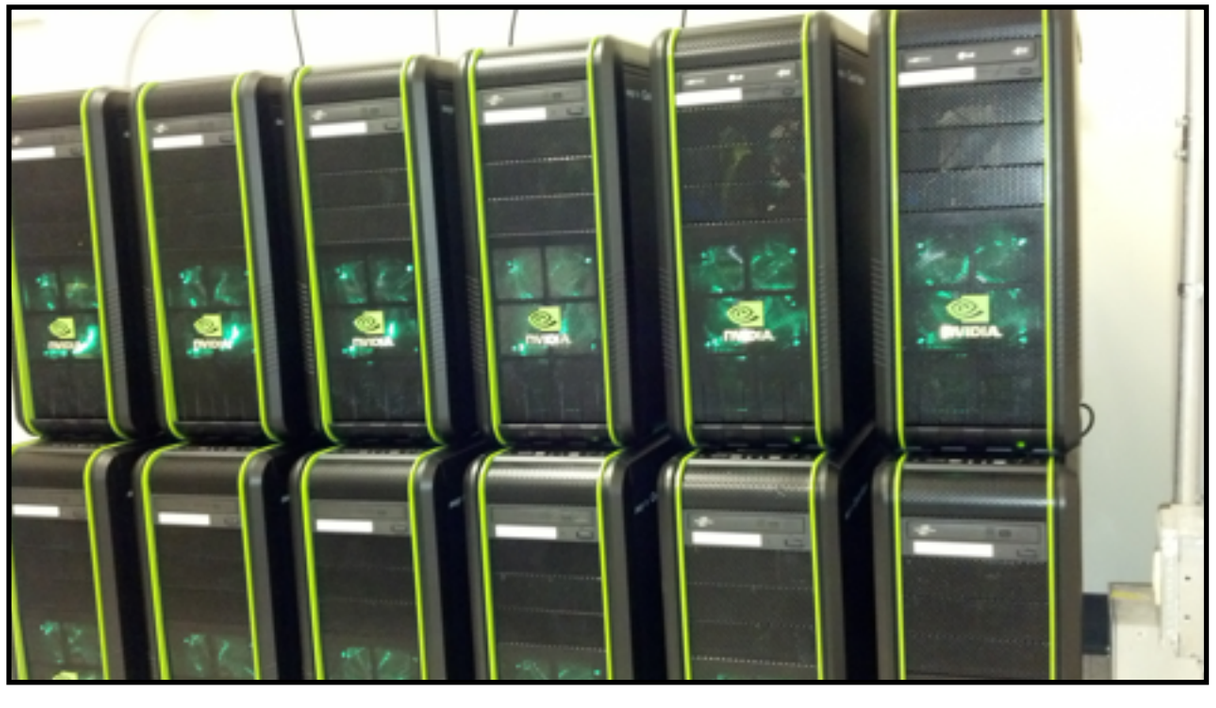
CPU vs. GPU Performance Track Record



Many-core GPU performance is faster and increasing more quickly than Single-core CPUs

GPU Hardware Setup





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Videogame GPUs reappropriated for biological simulations

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Video games take role in treating cancer at Wake Forest

5:54 pm, February 16, 2012, by Ryan Sullivan and Brent Campbell

WAKE FOREST UNIVERSITY

News Center

PUBLISHED: FEBRUARY 16, 2012

Can a video game cure cancer?

By ALICIA ROBERTS

Anqi Zou ('12) never thought she would thank video gamers for showing her the way to exciting discoveries in molecular biology.

But here she is, acknowledging that the technology she uses to show the inner workings of cells was originally perfected to create realistic images on gaming screens worldwide.

Computer science and physics professor Samuel Cho (center) works with his students, graduate student Tyson Lipscomb (left) and senior Anqi Zou ('12).

TYSON LIPSCOMB
WFU GRADUATE STUDENT
FROM VIDEO GAMES TO CURING CANCER

M, N.C. — In a research lab at Wake Forest University, the cure for cancer
deo games.

n assistant professor of physics and computer science, uses graphics

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ARTICLE

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Folding of Human Telomerase RNA Pseudoknot Using Ion-Jump and Temperature-Quench Simulations

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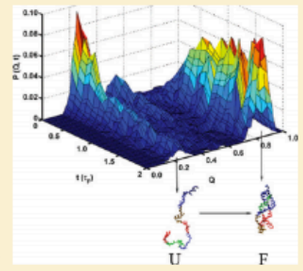
ABSTRACT: Globally RNA folding occurs in multiple stages involving chain compaction and subsequent rearrangement by a number of parallel routes to the folded state. However, the sequence-dependent details of the folding pathways and the link between collapse and folding are poorly understood. To obtain a comprehensive picture of the thermodynamics and folding kinetics we used molecular simulations of coarse-grained model of a pseudoknot found in the conserved core domain of the human telomerase (hTR) by varying both temperature (T) and ion concentration (C). The phase diagram in the $[T,C]$ plane shows that the boundary separating the folded and unfolded state for the finite 47-nucleotide system is relatively sharp, implying that from a thermodynamic perspective hTR behaves as an apparent two-state system. However, the folding kinetics following single C-jump or T-quench is complicated, involving multiple channels to the native state. Although globally folding kinetics triggered by T-quench and C-jump are similar, the kinetics of chain compaction are vastly different, which reflects the role of initial conditions in directing folding and collapse. Remarkably, even after substantial reduction in the overall size of hTR, the ensemble of compact conformations are far from being nativelike, suggesting that the search for the folded state occurs among the ensemble of low-energy fluidlike globules. The rate of unfolding, which occurs in a single step, is faster upon C-decrease compared to a jump in temperature. To identify "hidden" states that are visited during the folding process we performed simulations by periodically interrupting the approach to the folded state by lowering C. These simulations show that hTR reaches the folded state through a small number of connected clusters that are repeatedly visited during the pulse sequence in which the folding or unfolding is interrupted. The results from interrupted folding simulations, which are in accord with non-equilibrium single-molecule folding of a large ribozyme, show that multiple probes are needed to reveal the invisible states that are sampled by RNA as it folds. Although we have illustrated the complexity of RNA folding using hTR as a case study, general arguments and qualitative comparisons to time-resolved scattering experiments on *Azoarcus* group I ribozyme and single-molecule non-equilibrium periodic ion-jump experiments establish the generality of our findings.



Present Addresses

[#]Departments of Physics and Computer Science, Wake Forest University, Winston-Salem, North Carolina 27109, United States.

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Spotlights

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Spotlights on Recent *JACS* Publications

RAPID, REAL-TIME CELL SECRETION ASSAY SYSTEM

Cytokines—proteins involved in communication between cells and important as markers for medical diagnoses—are essential to immunological research. Many cytokine analysis techniques take a long time, must be repeated for each marker, or cannot be used in a large-scale study. Now, Matthew S. Luchansky and Ryan C. Bailey have developed a fast and simple new system that allows concentrations of multiple analyte molecules to be detected in real time (DOI: 10.1021/ja2087618).

The team used their biosensing chip to simultaneously quantitate several human cytokines from cell culture samples.

NEW RNA SIMULATION KNOWS WHEN TO FOLD 'EM

Ribonucleic acid (RNA) is vital to a wide range of processes in nearly all living cells, including reaction catalysis, regulation of gene expression, and communication of cellular signals. How RNA folds into precise, active structures has a role in its function. To better understand this process, D. Thirumalai and co-workers have presented new computer simulations for the folding and unfolding kinetics of human telomerase (hTR), a RNA responsible for adding junk DNA to the end of our chromosomes to prevent the loss of important coding information (DOI: 10.1021/ja2092823).

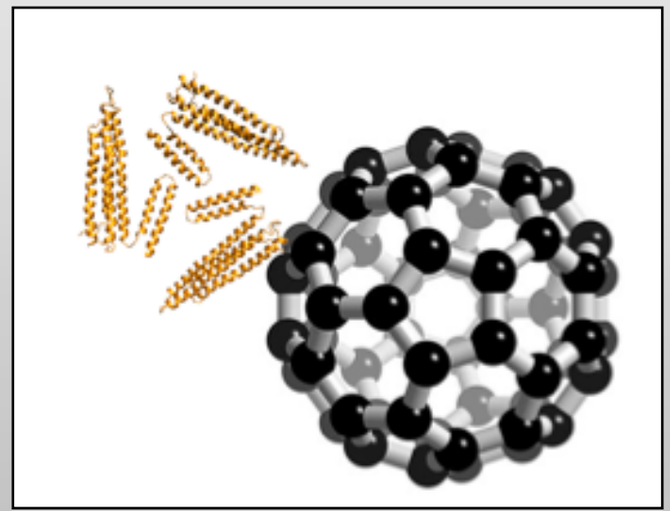
Current Biophysics Projects

Protein-RNA Interactions

- Collaborator: Rebecca Alexander (Wake Forest Univ., Dept. of Chemistry)
- Level: Undergraduate

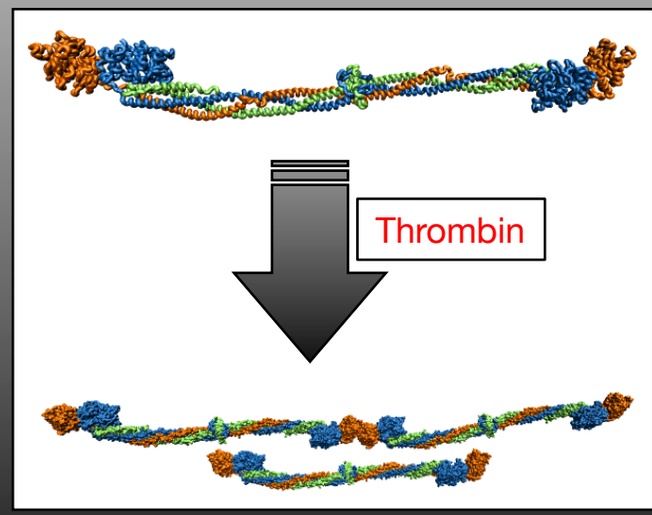
Protein-Nanoparticle Interactions

- Collaborator: Pu-Chun Ke (Clemson Univ., Dept. of Physics)
- Level: Undergraduate, Graduate



Fibrinogen Elasticity

- Collaborators: Martin Guthold (Wake Forest Univ., Dept. of Physics), Valeri Barsegov (University of Massachusetts)
- Level: Graduate

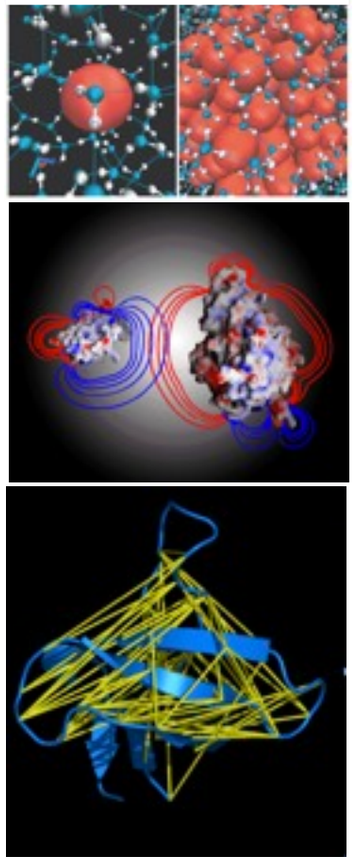


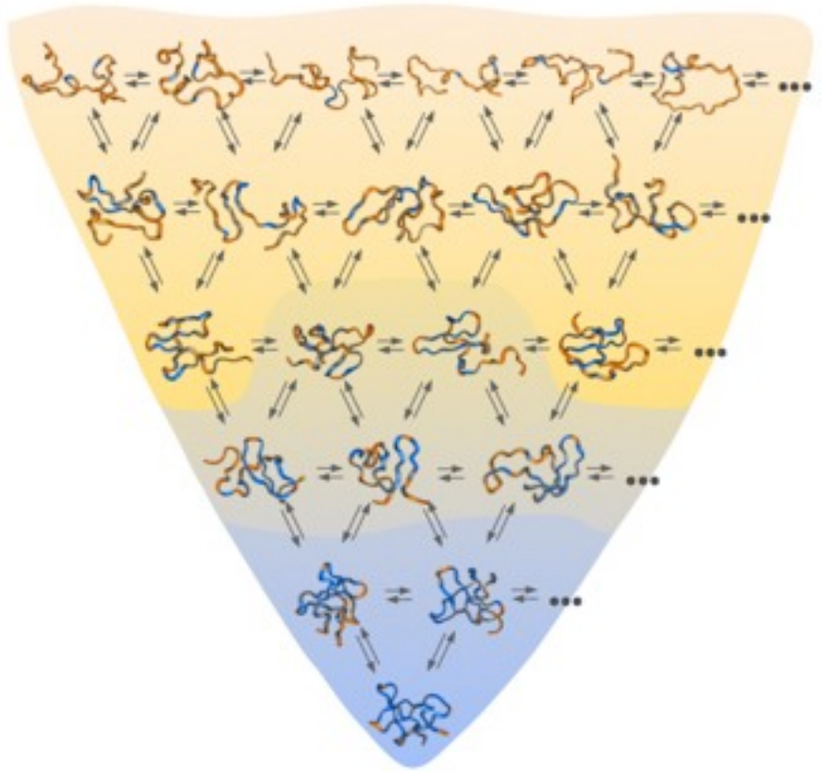
Qualifications:

- Interest in Biophysics, Computer Science, and/or Biochemistry.
- Some computer programming experience preferred.
- Unafraid to talk to people outside your discipline about your research.
- Must commit to one year of research (undergraduate only).

PHY 320/620: Physics of Biological Macromolecules

- TuTh 9:30-10:45am
- Manchester 244
- Pre-/Co-requisites:
  - PHY 113/114
- Questions?
  Contact me:
  choss@wfu.edu





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November 7, 2012

Charles Brooks, III
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Departments of Chemistry and Biophysics
January 30, 2013