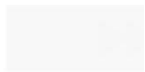
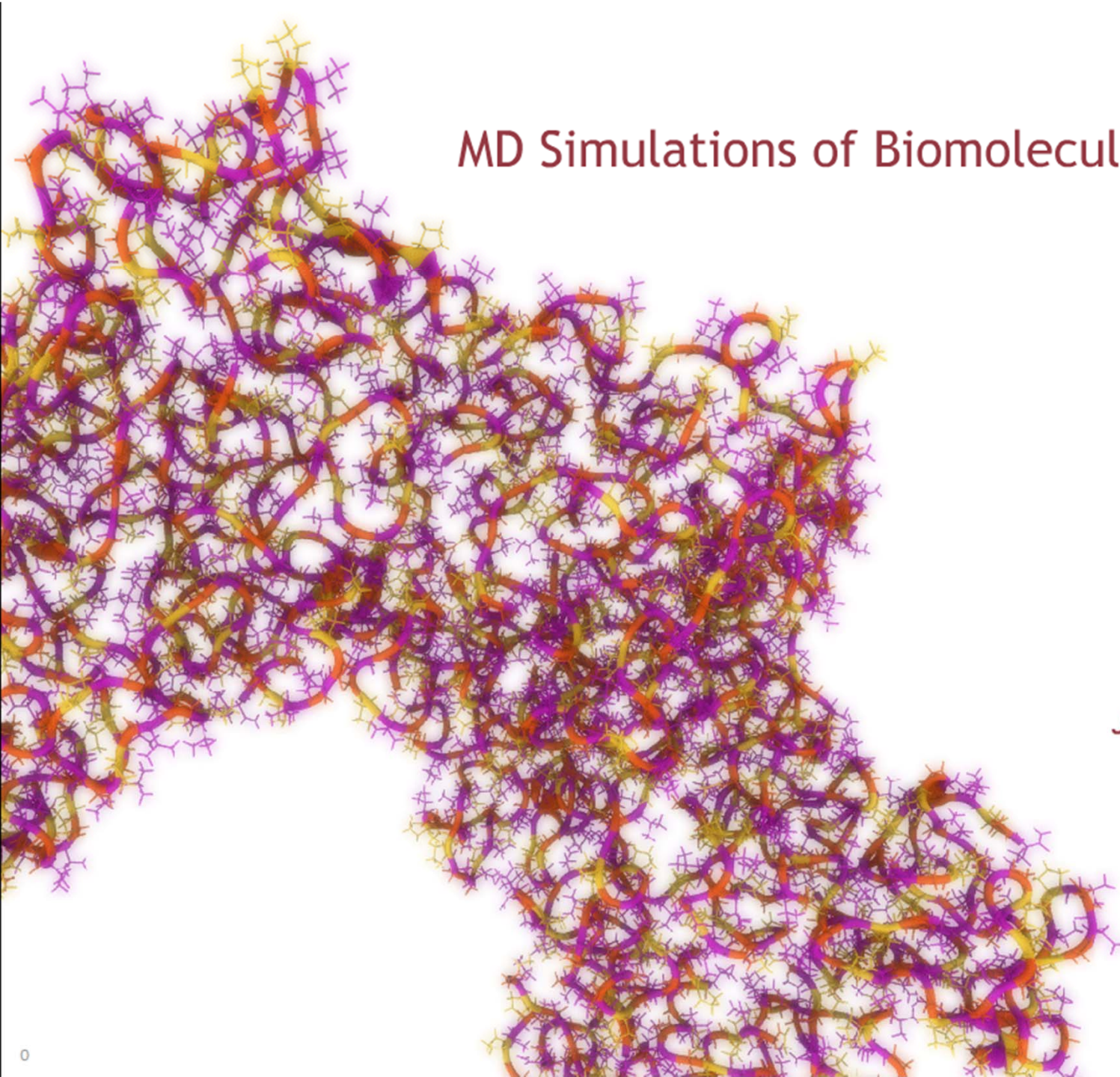


MD Simulations of Biomolecular Systems

Sarah Rauscher
January 12, 2011



1. Biomolecular Simulations:

- research interests of the Pomès lab
- MD simulations of proteins

2. Simulations on the SciNet GPC:

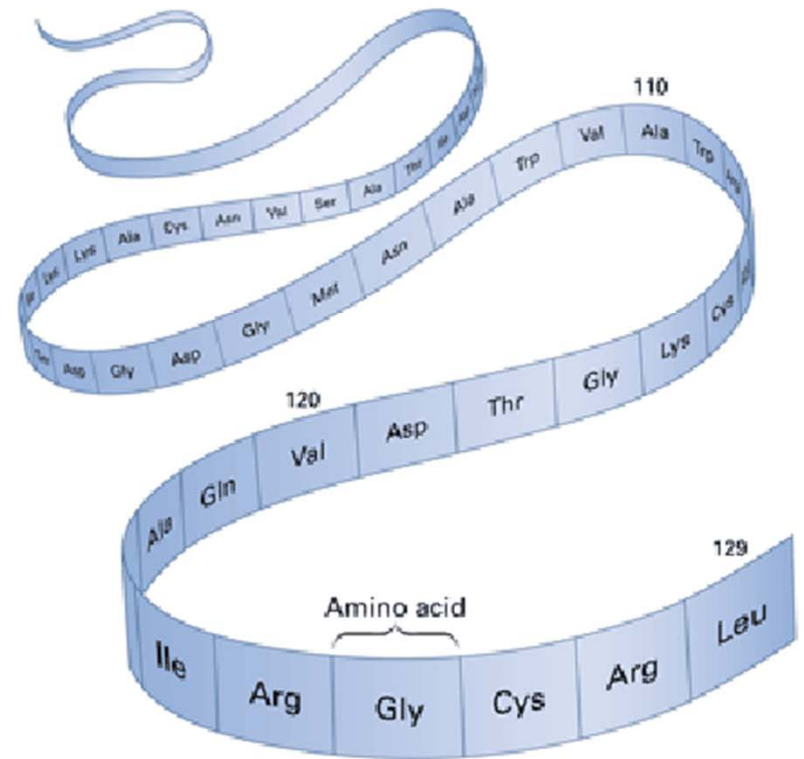
- challenges in "scaling up"
- strategies

3. Questions

Proteins are
the "machinery of life"



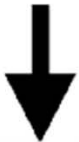
Proteins are
polymers of amino acids



Amino acid sequence



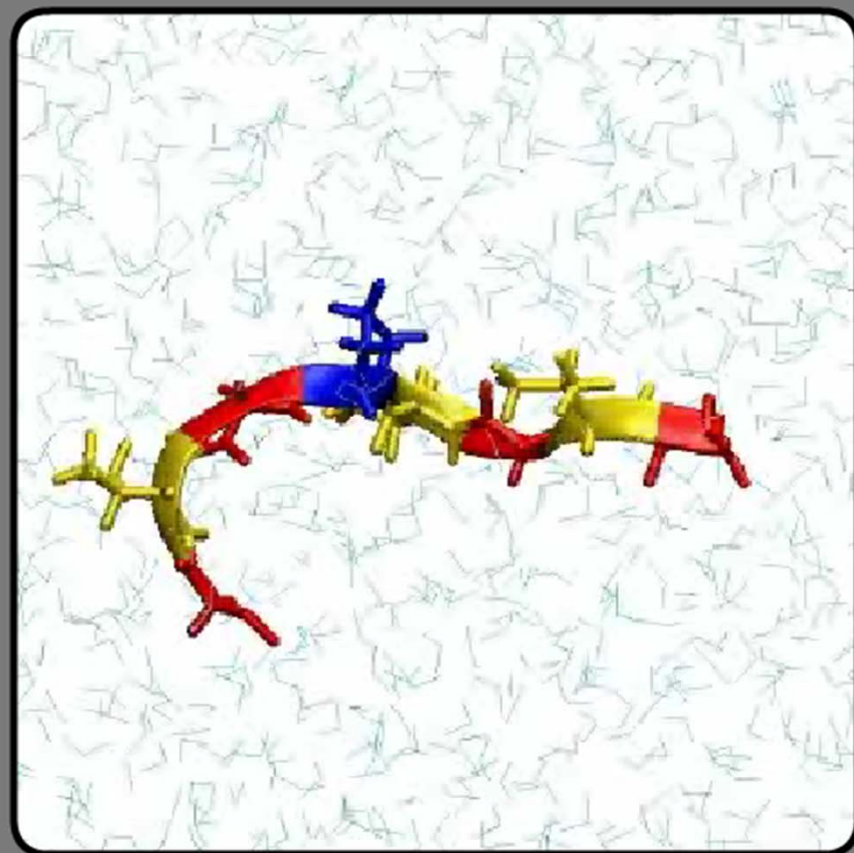
3D structure



Biological function

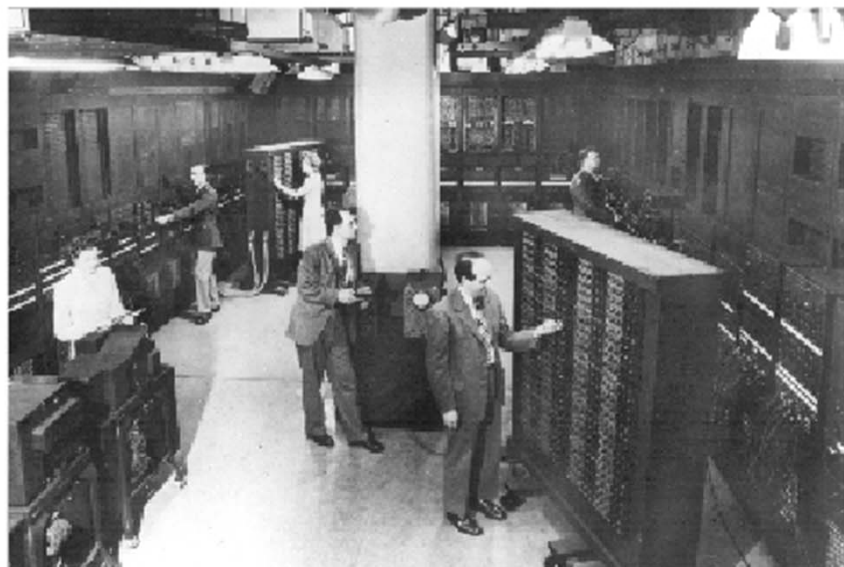


Molecular Dynamics - Time Trajectories



SciNet allowed us to 'Scale Up' our simulations ...

Lucy



Lucy \approx 88 CPUs

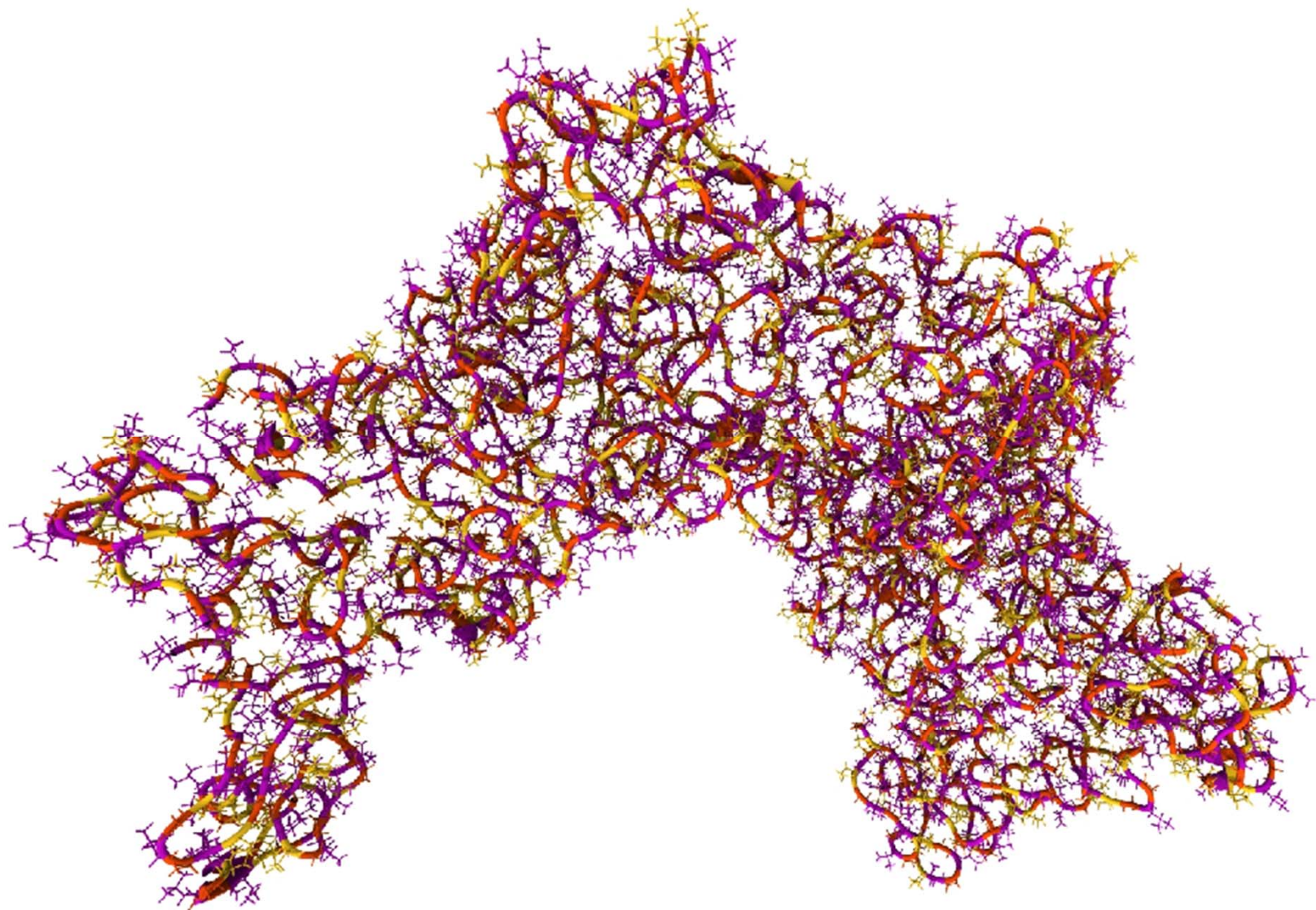
SciNet



SciNet \approx 1800 x Lucy

1. Larger systems, longer timescales (IB nodes)
 - more biologically relevant
 - e.g. large aggregate of elastin

Simulating a Large Aggregate of Elastin

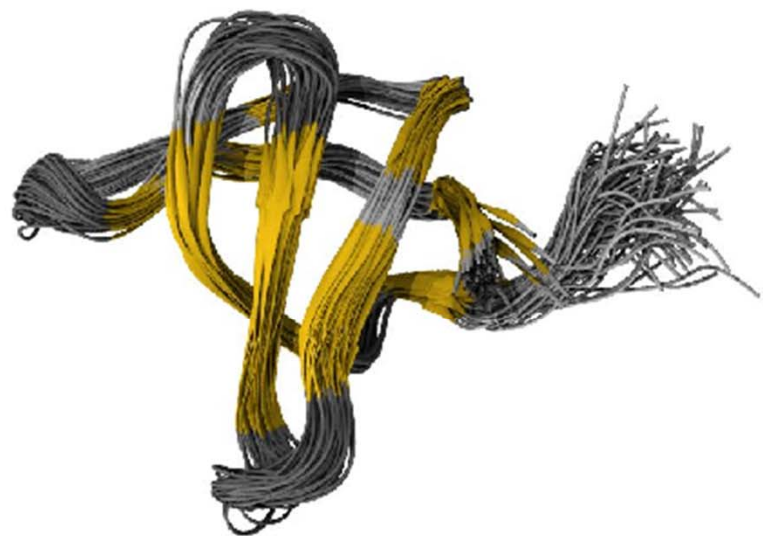


1. Larger systems, longer timescales (IB nodes)
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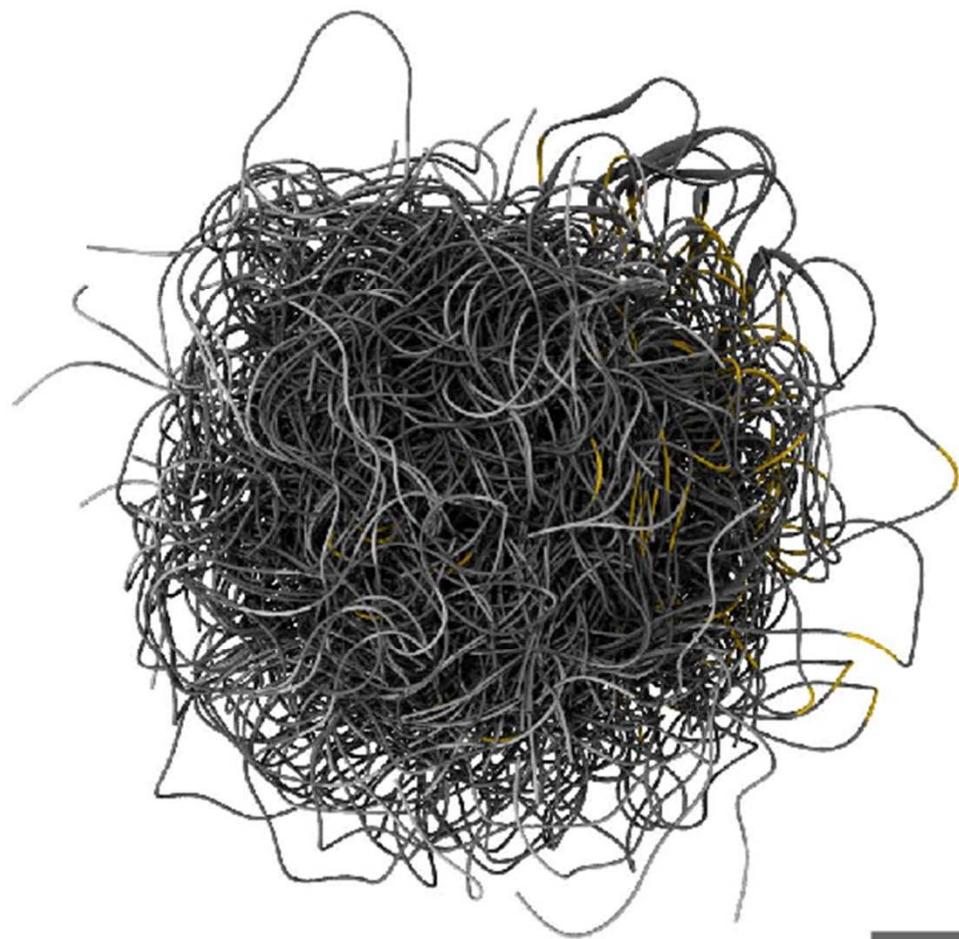
2. Many replicas of a system (Gig-E nodes)
 - improvements in statistics
 - e.g. the unfolded state of a protein

Simulations of Folded and Unfolded States

Folded State



Unfolded State



1. More data (100's of TB vs. 100's of GB)
 - Increased need for in-house dedicated storage and other allocations
 - Huge (!) amount of data to transfer, manage, and analyze

2. More filesystem I/O
 - Redesigned code to minimize I/O (using /dev/shm)



Questions

