SimTK Molmodel 1.5
Molecular Modeling Workshop

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Schedule

• 8:30-10:00 Molmodel examples (S360)
• 10:00-10:15 Break
• 10:15-11:30 More Molmodel examples (S360)/Using SimTK in neuromuscular simulations(S362)
• 11:30-12:30 Lunch
• 12:30-3:30 Open lab (S360)
• 3:30-5:00 Refreshments (Clark patio)
What is Molmodel?

• Domain-specific modeling layer on Simbody
• Part of SimTK core libraries
• You should have Programmer’s Guide
Principal SimTK Core Libraries

SimTK Molmodel - molecular modeling
SimTK Simbody - order(n) multibody dynamics
SimTK Math - numerical methods and linear algebra
SimTK Common - Vector, Matrix classes and other data structures
SimTK Lapack - linear algebra
Molecular Physical Units

- Length: nanometers (10^{-9} meters)
- Time: picoseconds (10^{-12} seconds)
- Mass: atomic mass units
  \( \frac{1}{(\text{Avogadro’s Constant}) \text{ grams}} \)
Macromolecules, residues, and atoms

- RNA, DNA, and protein are large molecules called *macromolecules*
- Macromolecules consist of chains of *residues*
Simple protein

- Construct protein from sequence
- All atom parameters are built into AMBER99 force field
- Note end caps
Molecular Force Field

• What is a molecular force field?
  – A specification of all forces affecting a dynamic simulation. For conventional molecular simulation this includes non-bonded electrostatic forces and van der Waals forces, and bonded stretch, bend, torsion, and improper torsion parameters.
Top level API for constructing proteins

#include "SimTKmolmodel.h"
Protein("ACDEFGHIKLMNPQRSTVWY");
Protein Exercises

• Compile and run SimpleProtein example program
• Try a different sequence
• Add a second protein (note arguments to adoptCompound())
Simple RNA

- RNA from sequence
- Writing PDB files
RNA Exercises

• Compile and run SimpleRNA example program
• Try a different sequence
• Change the frequency of PDB writing