SimTK Molmodel 1.5 Molecular Modeling Workshop

September 26, 2008

Christopher Bruns

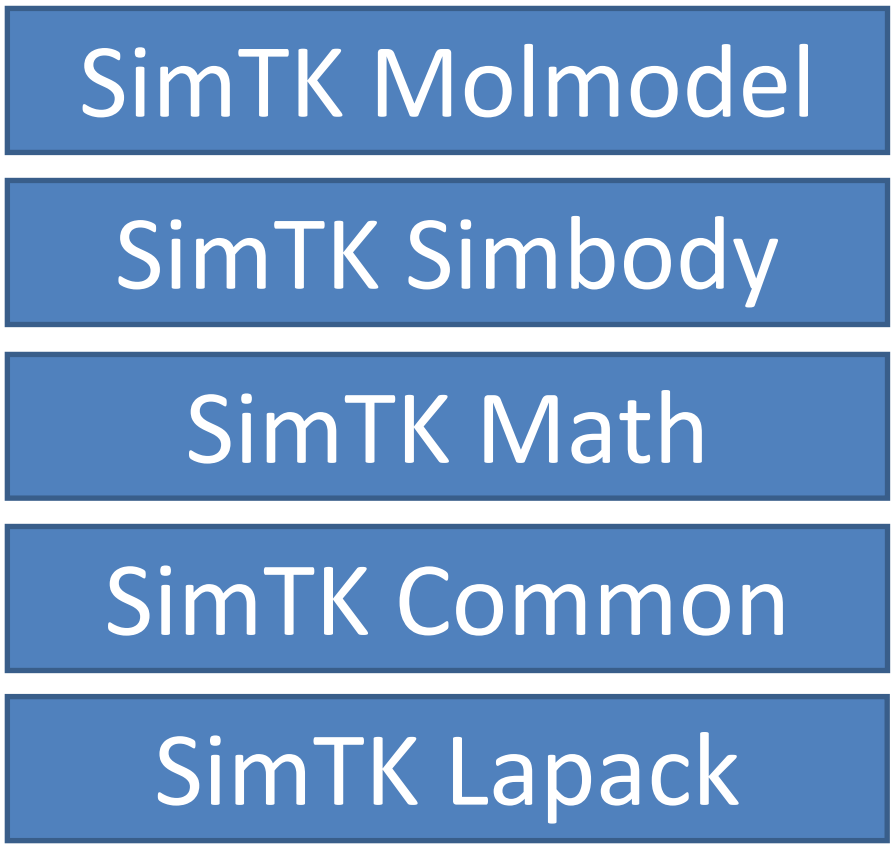
Schedule

- 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



molecular modeling

order(n) multibody dynamics

numerical methods and linear algebra

Vector, Matrix classes and other data structures

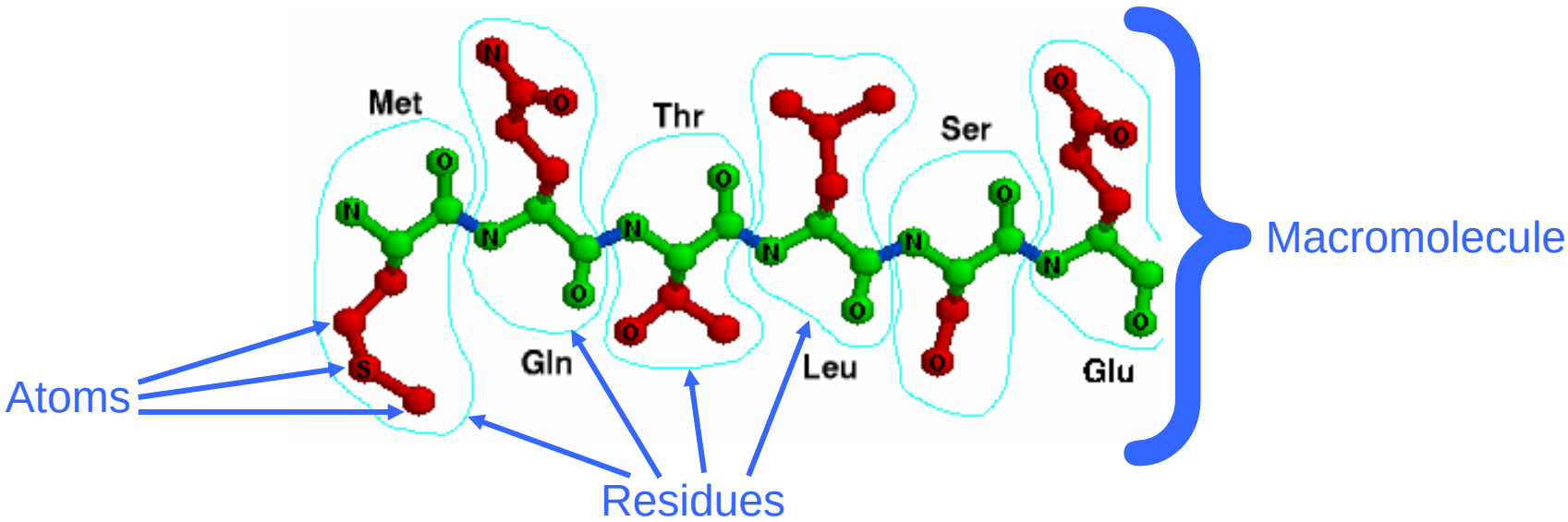
linear algebra

Molecular Physical Units

- Length: nanometers (10^{-9} meters)
- Time: picoseconds (10^{-12} seconds)
- Mass: atomic mass units (1/(Avogadro'sConstant) grams)

Macromolecules, residues, and atoms

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



Simple protein

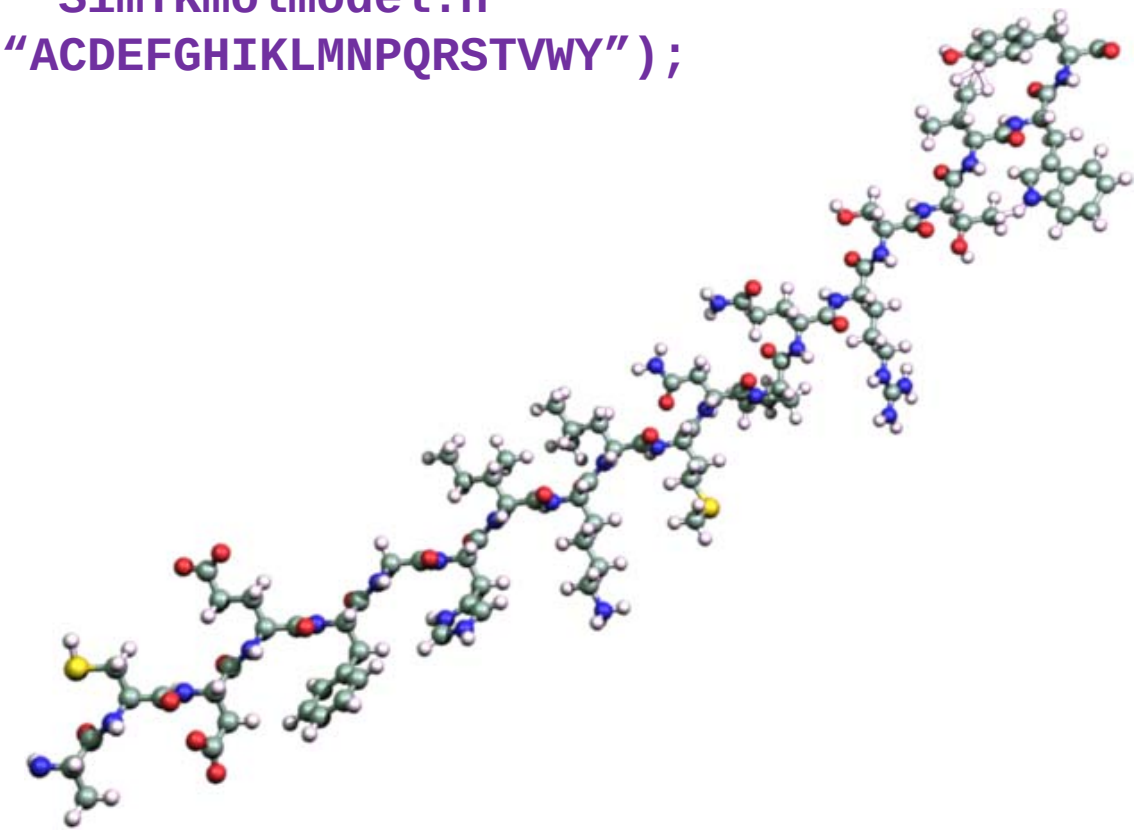
- Construct protein from sequence
- All atom parameters are built into AMBER99 force field
- Note end caps

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