Dr. Gregory A. Babbitt

BABBITTLAB@RIT

COMPUTATIONAL MOLECULAR EVOLUTION AND ECOLOGY

some of our students

Erin Coppola BME

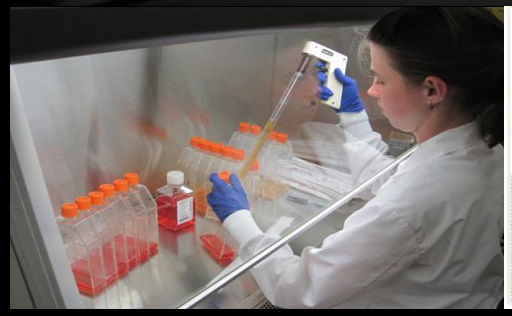
Jamie Mortensen BME

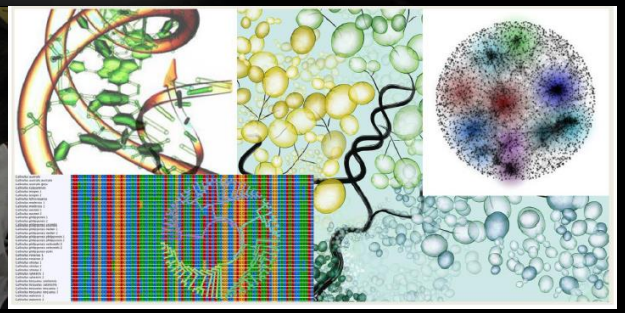
Justin Liao BME

We are a mostly “dry-bench” or computer-based laboratory studying the evolution of the molecular components of cells. Biophysics and biochemistry underlies all molecular processes in the cell, but only some molecular structure and behavior, genetic and epigenetic, can contain information that is subject to heritable change over potentially deep timescales.

Mohammed Alawad
Bioinformatics

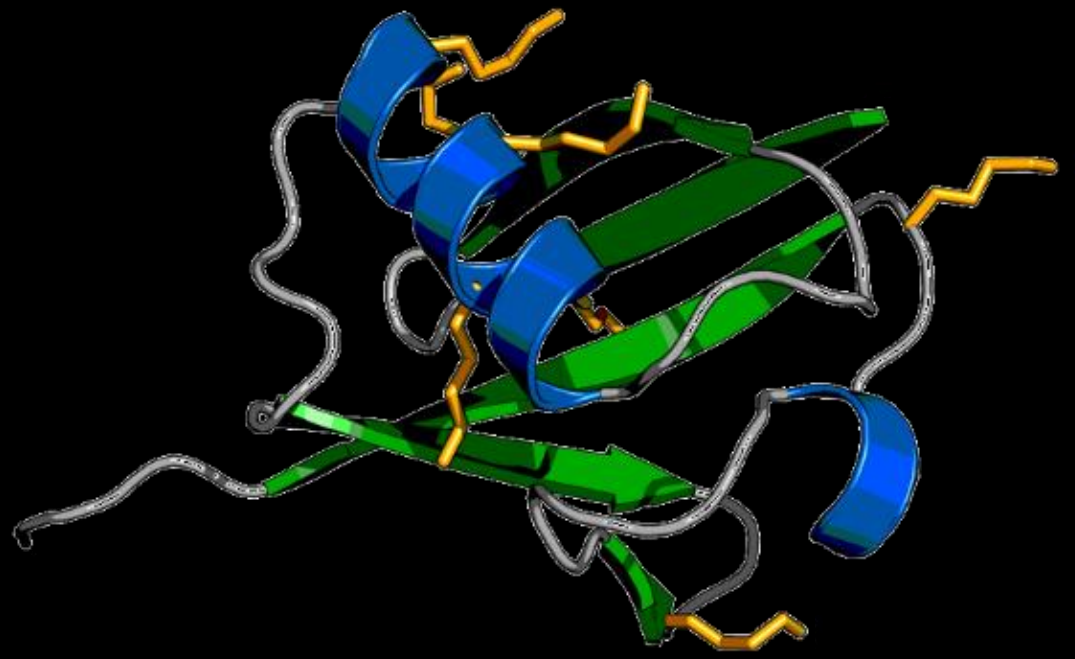
Katharina Schulze
Bioinformatics



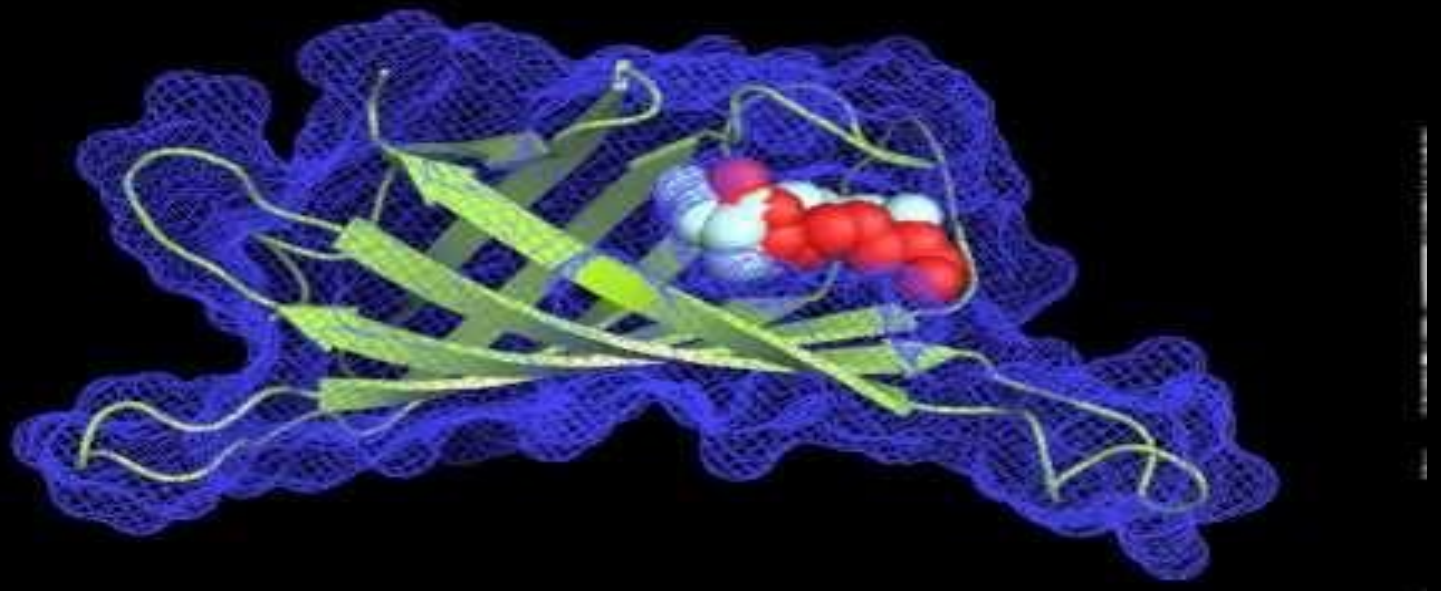


Our long-term research goals are aimed at a more biophysically-grounded understanding of molecular evolution in the cell. We combine biophysical and molecular evolutionary modeling to investigate the boundary between evolvable and non-evolvable biophysics.

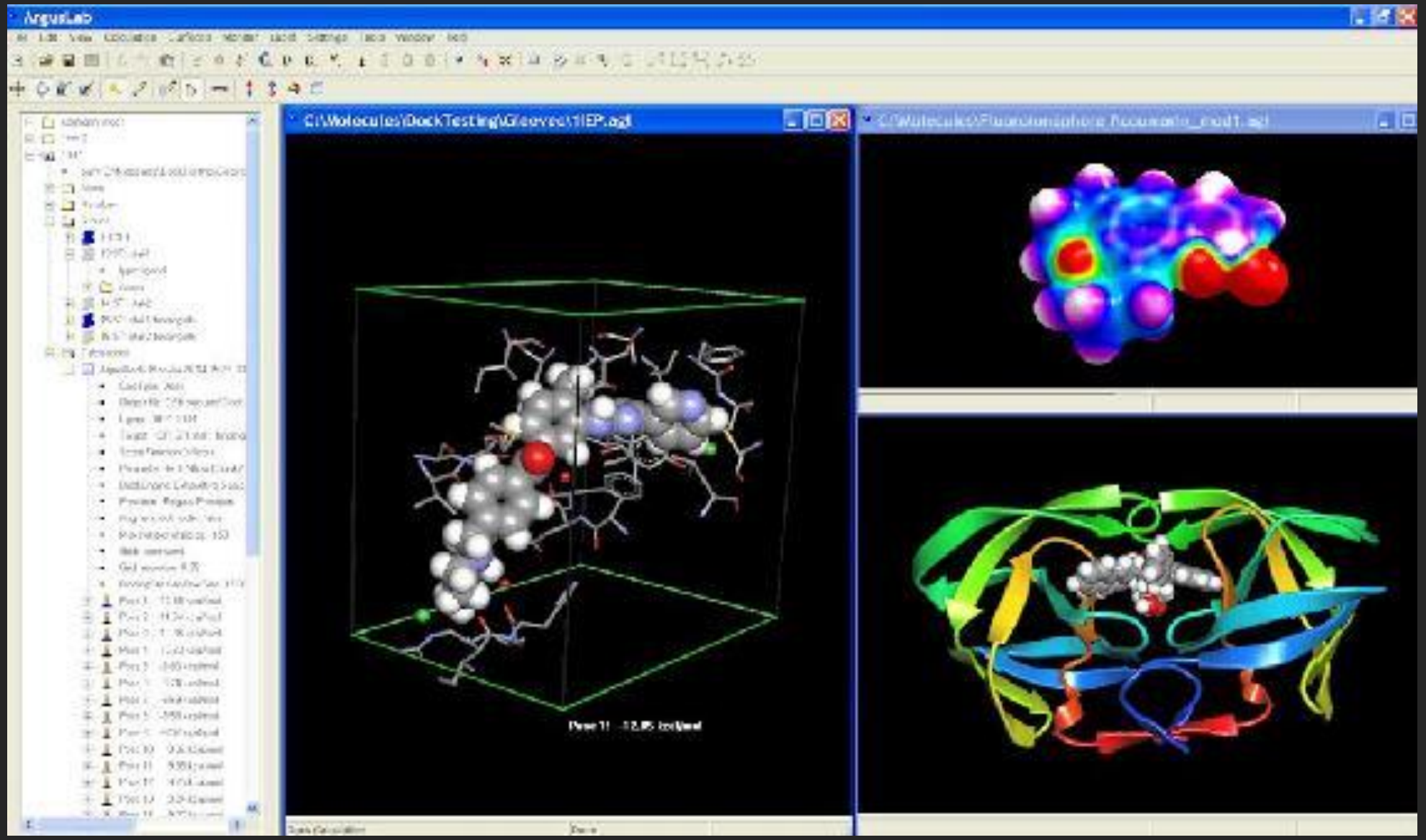
ubiquitin structure



Introduction to Molecular Docking Simulation



Drug docking surveys of small molecule libraries



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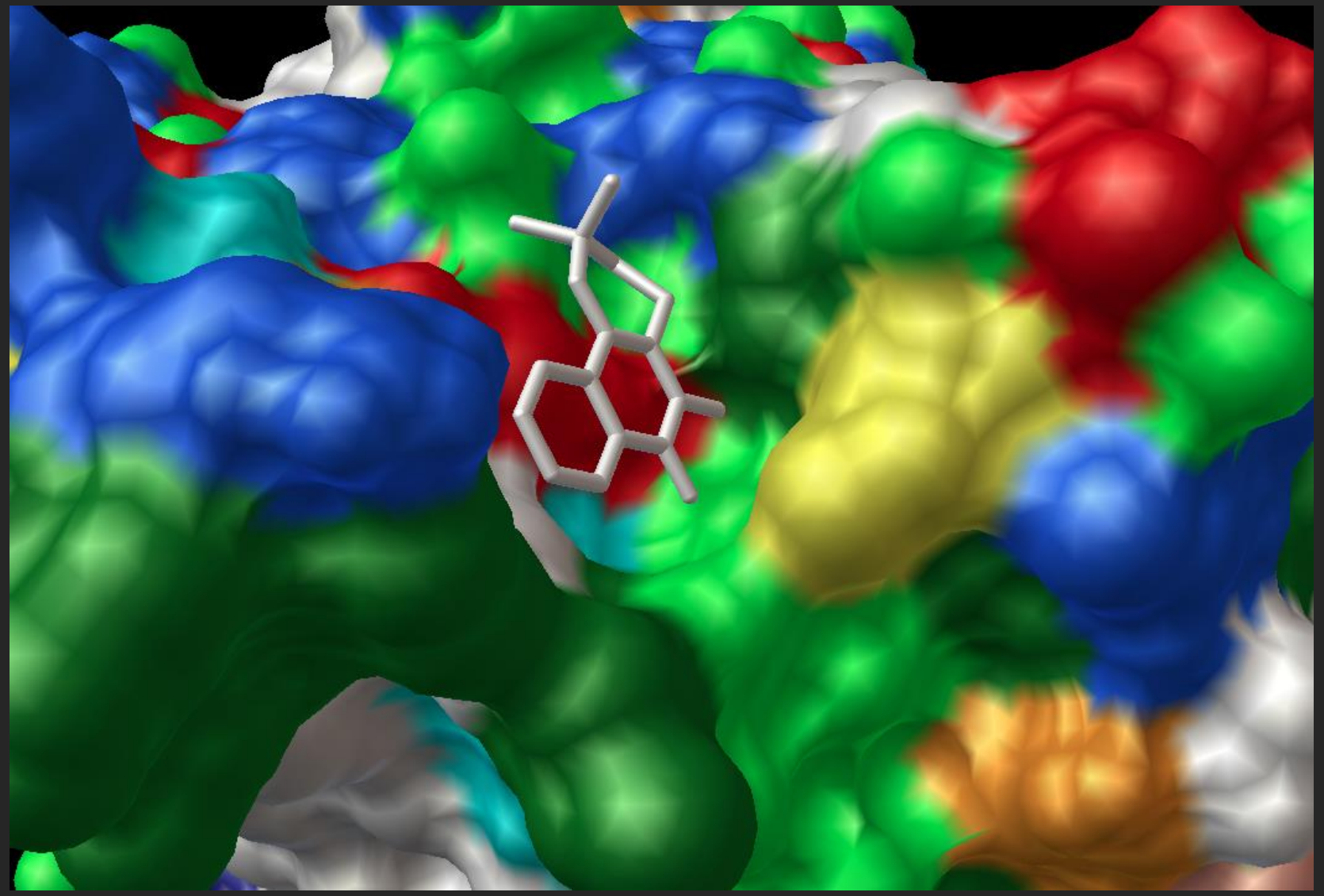
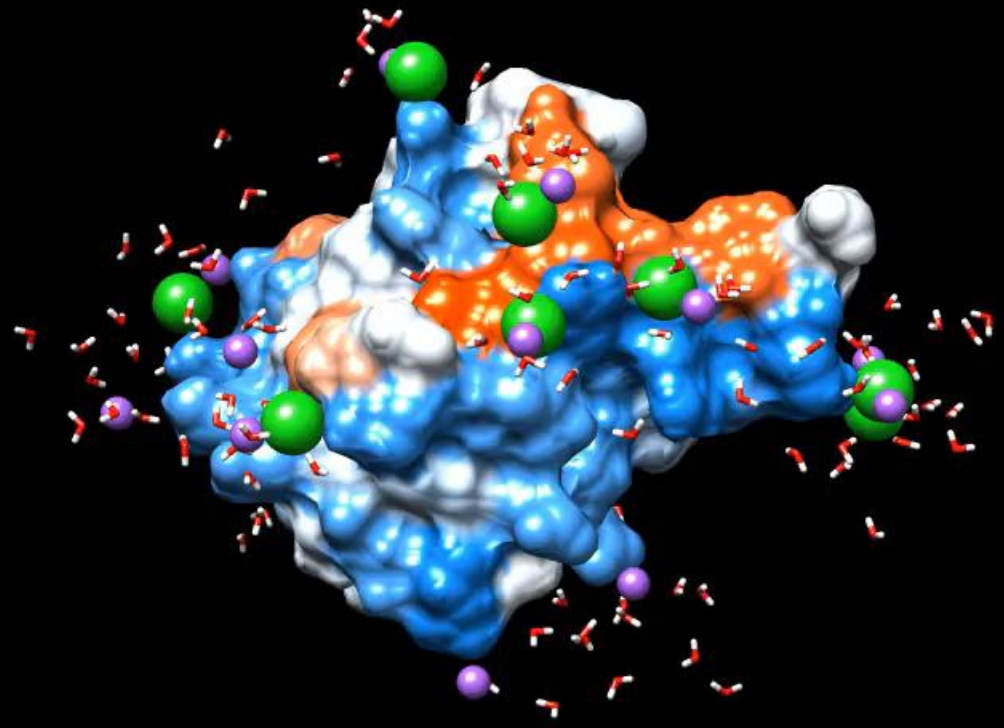
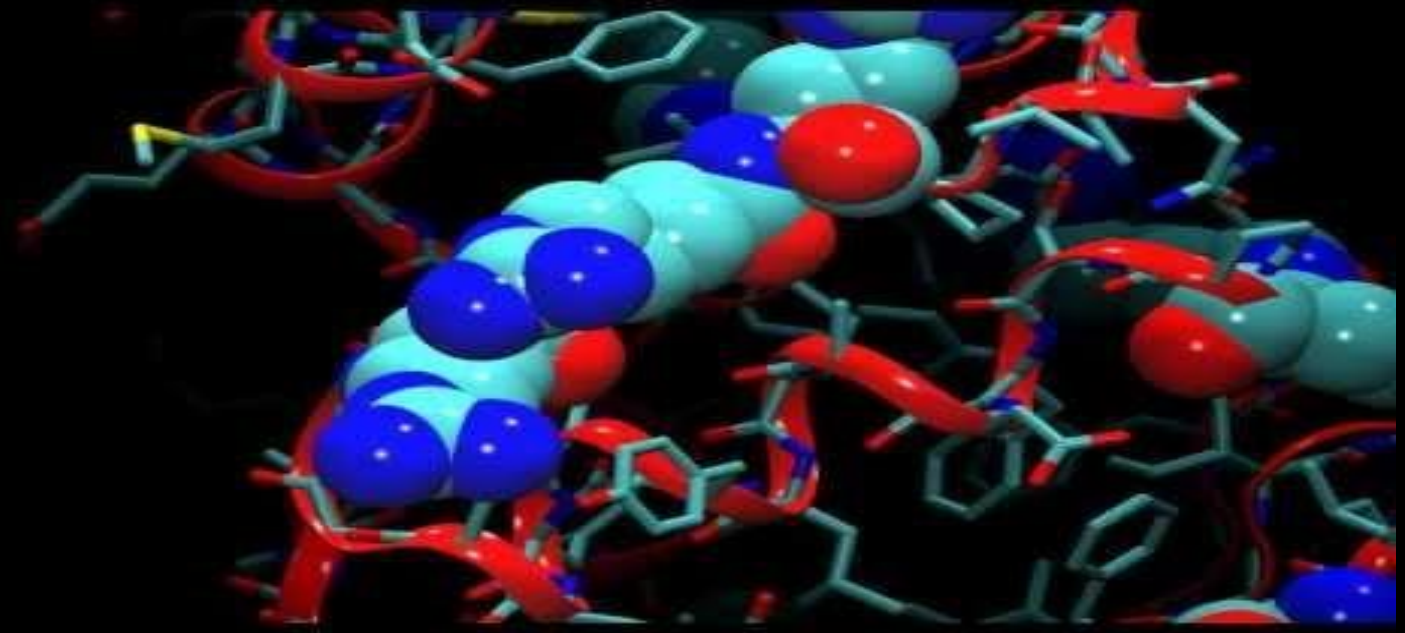


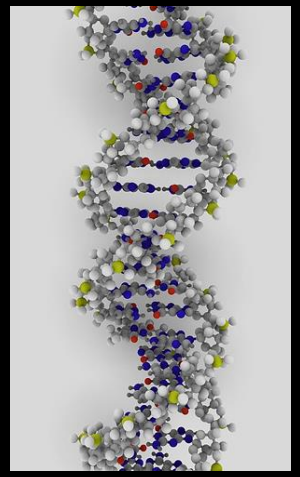
ubiquitin in explicit solvent MD simulation



Introduction to Molecular Dynamics

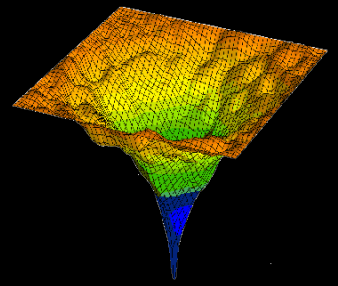


Anatomy of a molecular dynamic simulation

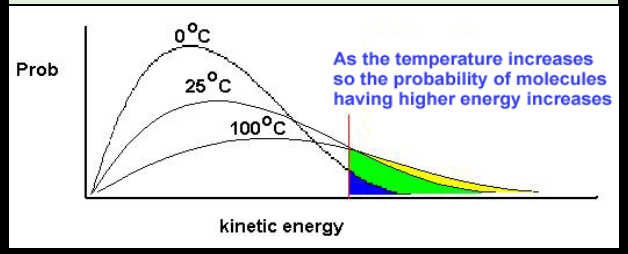


structure = ideal or PDB

minimization of potential energy surface (relaxation)



heating applied to all bonds

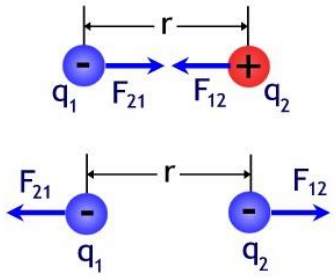


How might one statistically compare results between MD production runs?

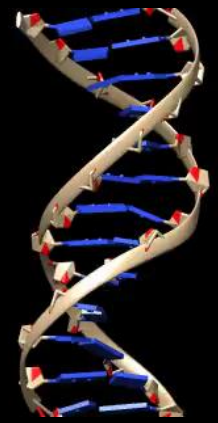
movies and statistics rendered from atomic vector trajectories

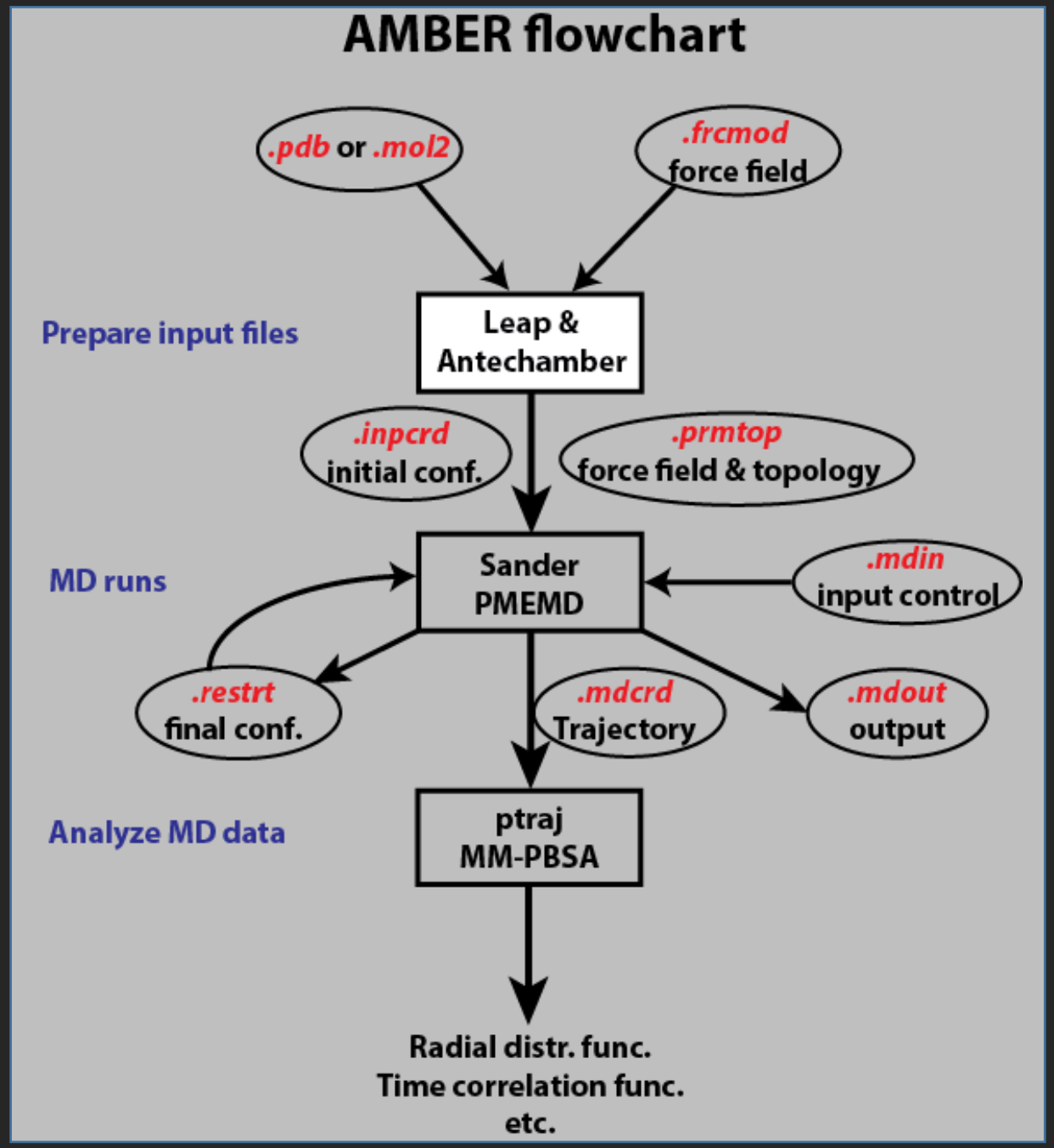
bonded atoms

non-bonded atom



MD equilibration and production run(s) track Newtonian mechanics stepped out in femtoseconds





Simplified schematic of the molecular dynamics algorithm

Give atoms initial $\boldsymbol{r}^{(i=0)}$ and $\boldsymbol{v}^{(i=0)}$, set $\boldsymbol{a} = 0.0$, $t = 0.0$, $i = 0$, choose short Δt

↓

Predictor stage: predict next atom positions:
Move atoms: $\boldsymbol{r}^{p} = \boldsymbol{r}^{(i)} + \boldsymbol{v}^{(i)}\,\Delta t + {}^{1}\!/_{2}\,\boldsymbol{a}\,\Delta\, t^{2}$ + more accurate terms
Update velocities: $\boldsymbol{v}^{p} = \boldsymbol{v}^{(i)} + \boldsymbol{a}\,\Delta t$ + more accurate terms

↓

Get forces $\boldsymbol{F} = -\nabla V(\boldsymbol{r}^{p})$ or $\boldsymbol{F} = \boldsymbol{F}(\Psi(\boldsymbol{r}^{p}))$ and $\boldsymbol{a} = \boldsymbol{F}/m$

↓

Corrector stage: adjust atom positions based on new $\boldsymbol{a}$:
Move atoms: $\boldsymbol{r}^{(i+1)} = \boldsymbol{r}^{p}$ + some function of $(\boldsymbol{a}, \Delta t)$
Update velocities: $\boldsymbol{v}^{(i+1)} = \boldsymbol{v}^{p}$ + some function of $(\boldsymbol{a}, \Delta t)$

↓

Apply boundary conditions, temperature and pressure control as needed

↓

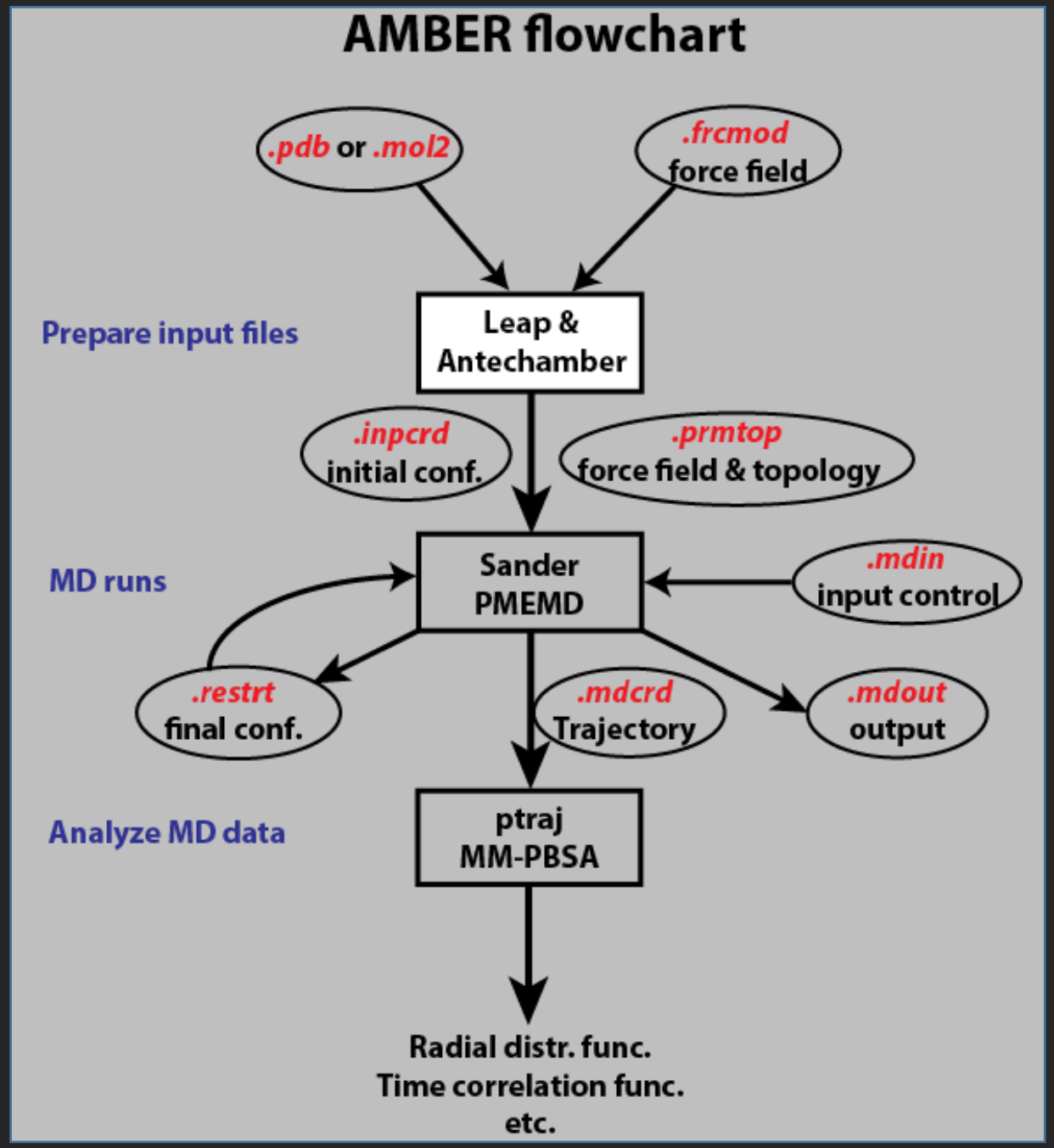
Calculate and output physical quantities of interest

↓

Move time and iteration step forward: $t = t + \Delta t$, $i = i + 1$

↓

Repeat as long as you need



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