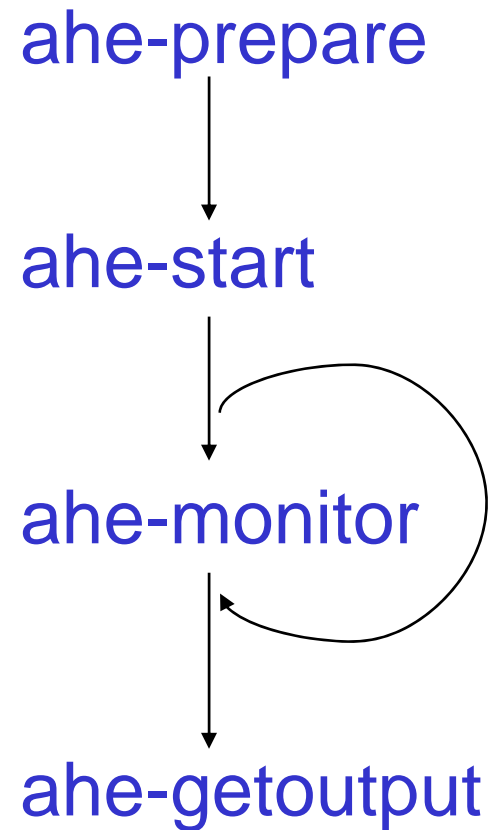


# Scripting Workflows with the Application Hosting Environment

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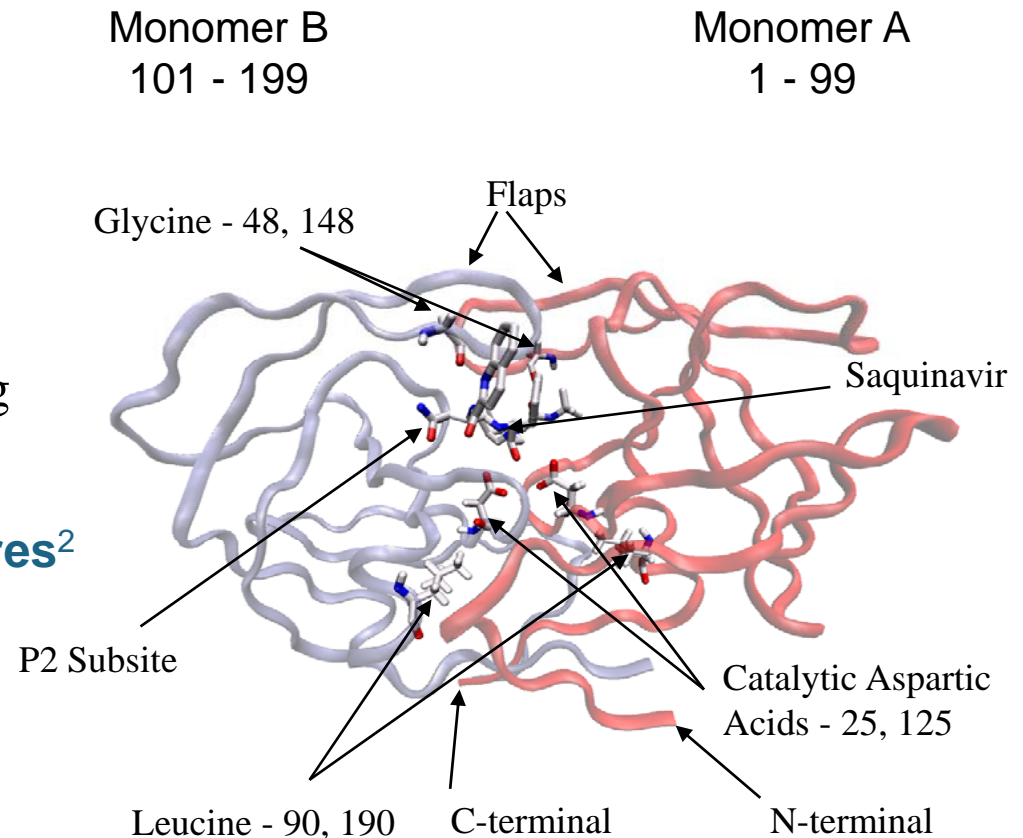
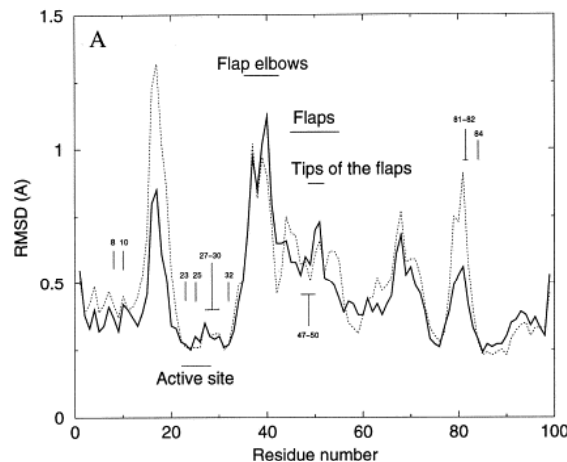
- By calling command line clients from Perl script complex workflows can be achieved
- Easily create chained or ensemble simulations
- For example jobs can be chained together:
  - ahe-prepare → prepare a new simulation for the first step
  - ahe-start → start the step
  - ahe-monitor → poll until step complete
  - ahe-getoutput → download output files
  - repeat for next step

# Constructing a workflow



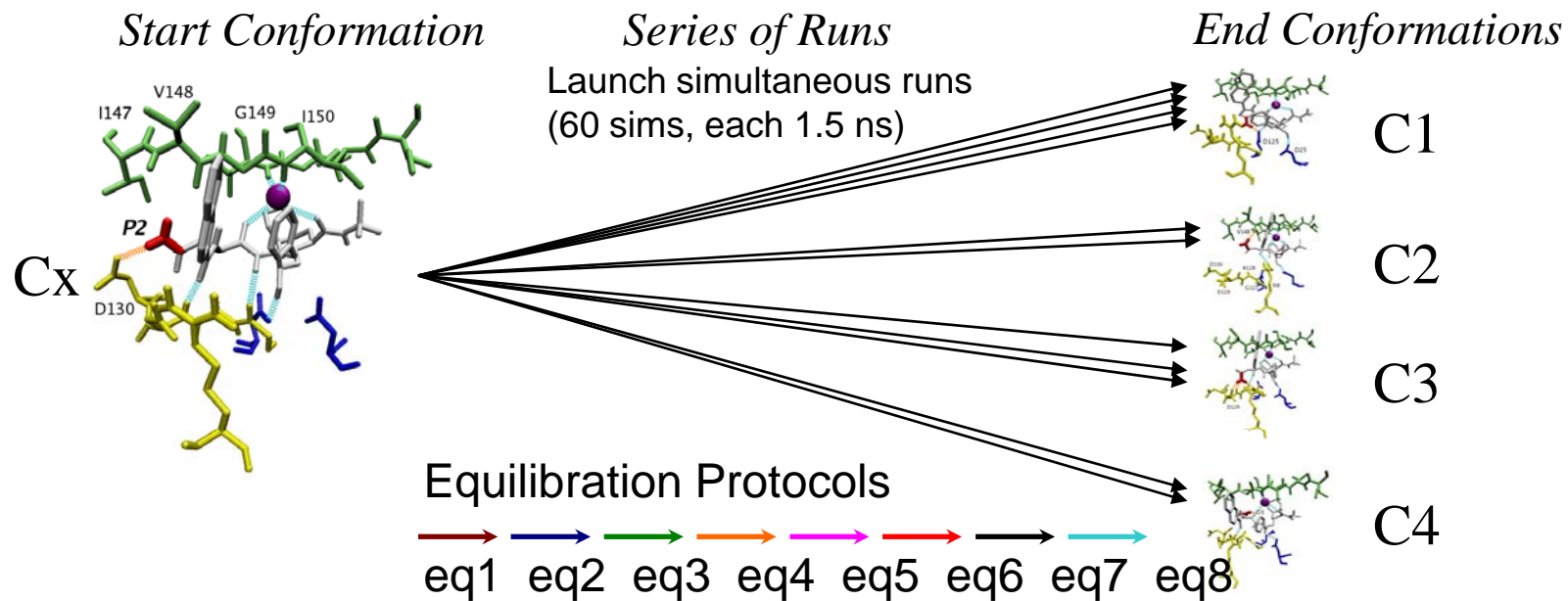
- Enzyme of HIV responsible for protein maturation
- Flexible Flaps open to provide access to active site<sup>1</sup>
- Catalytic Asp Dyad cleaves peptide bond
- Example of Structure Assisted Drug Design – 8 FDA inhibitors

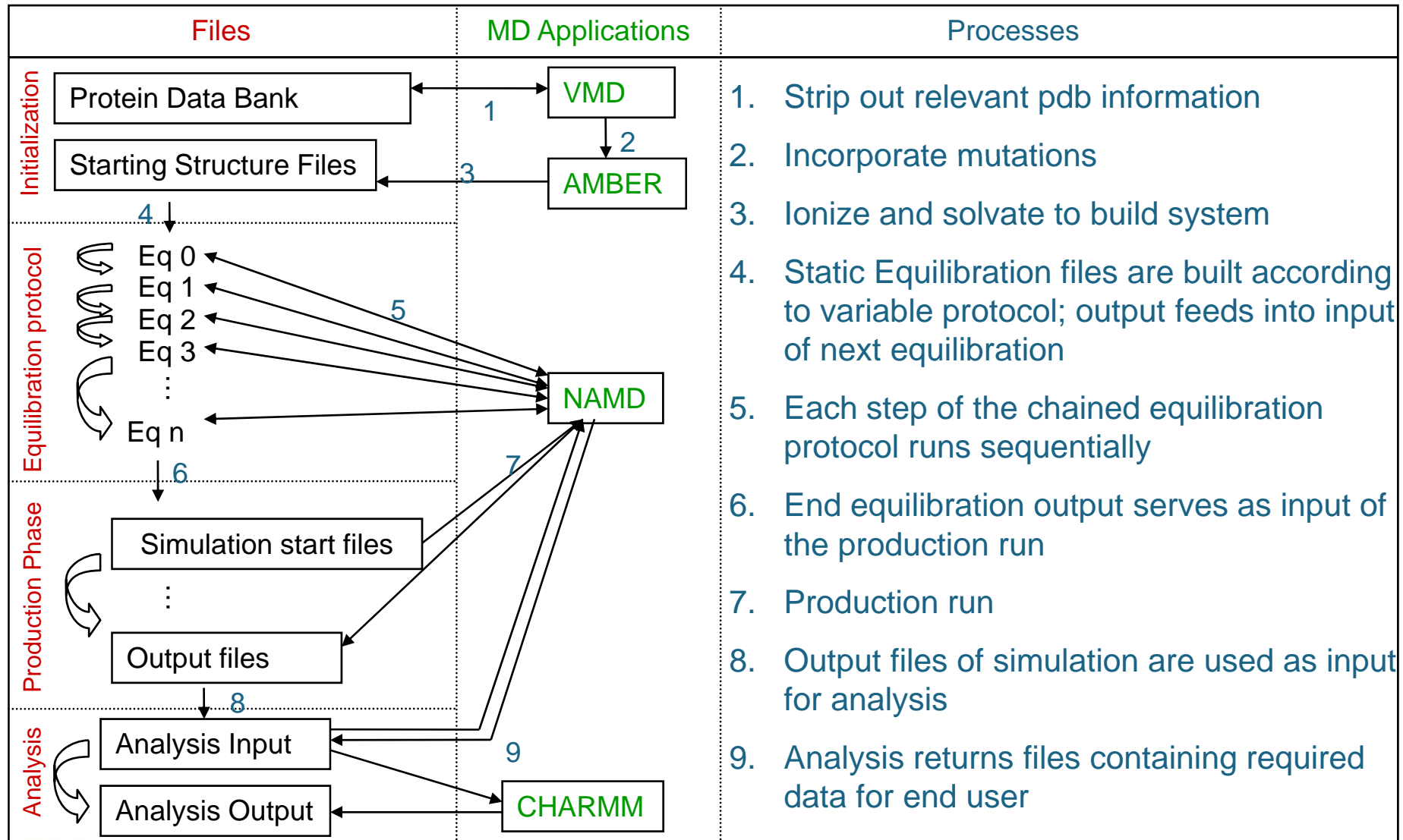
## RMSD of existing crystal structures<sup>2</sup>



## Ensemble MD is suited for HPC GRID

- Simulate each system many times from same starting position
- Each run has randomized atomic energies fitting a certain temperature
- Allows conformational sampling





# Practical 2

## Using Perl:

- Write script to automate preparing and starting a job, and staging files
- Write script to distribute jobs around a number of resources
- Write script to chain jobs, one after the other

<http://www.realitygrid.org/AHE/training/brunel/ex2/>