Texas A&M HPRC Short Course Series

Setting Up Molecular Dynamics Simulations

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High Performance
Research Computing
DIVISION OF RESEARCH

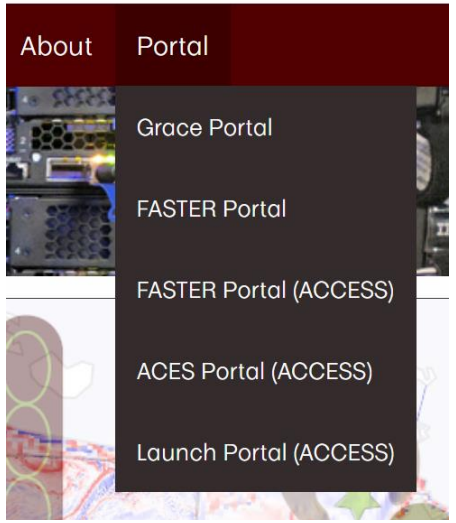
Outline

1. **Grace Basic**
   - File uploading/downloading
   - VNC: VMD
2. **CHARMM-GUI**
   - System preparing
   - Input generating
3. **Setup and perform MD simulations on Grace**
   - Amber
   - GROMACS
   - NAMD
   - OpenMM

Grace Portal

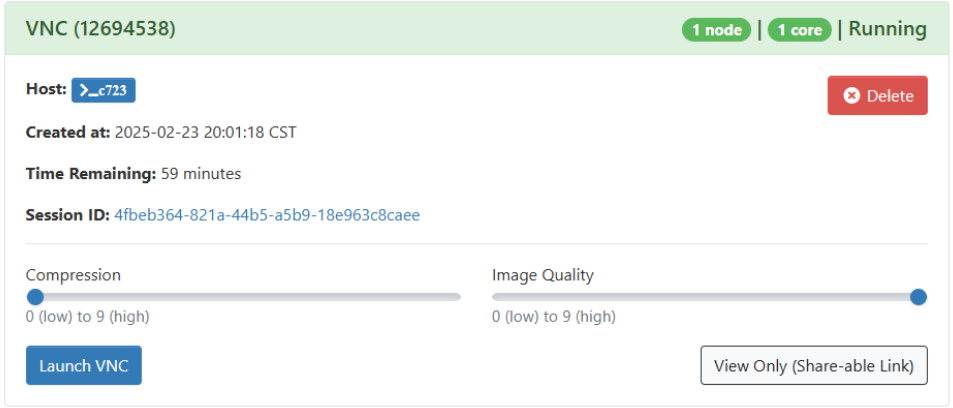
- **Grace: https://hprc.tamu.edu/**

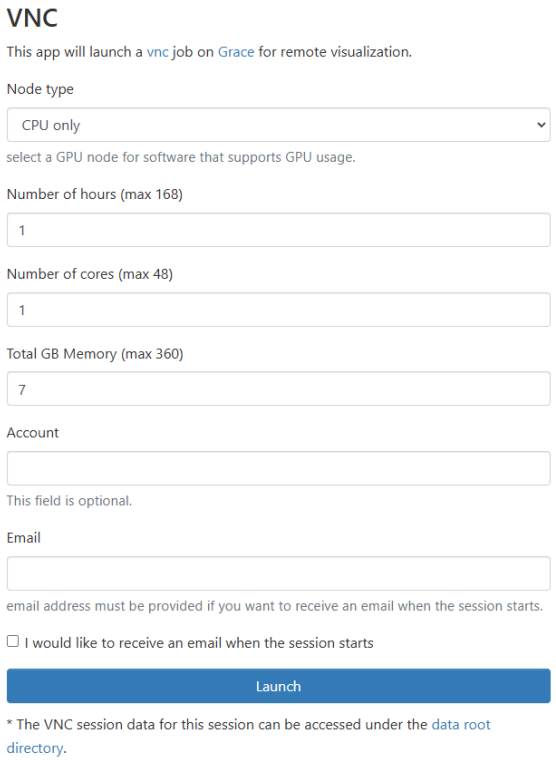
- **OnDemand**
  - Files
  - Clusters:
    $ cd $SCRATCH
    $ cp -r /scratch/training/MD-CHARMMGUI/ ./
  - Interactive Apps -> VNC



Grace Portal

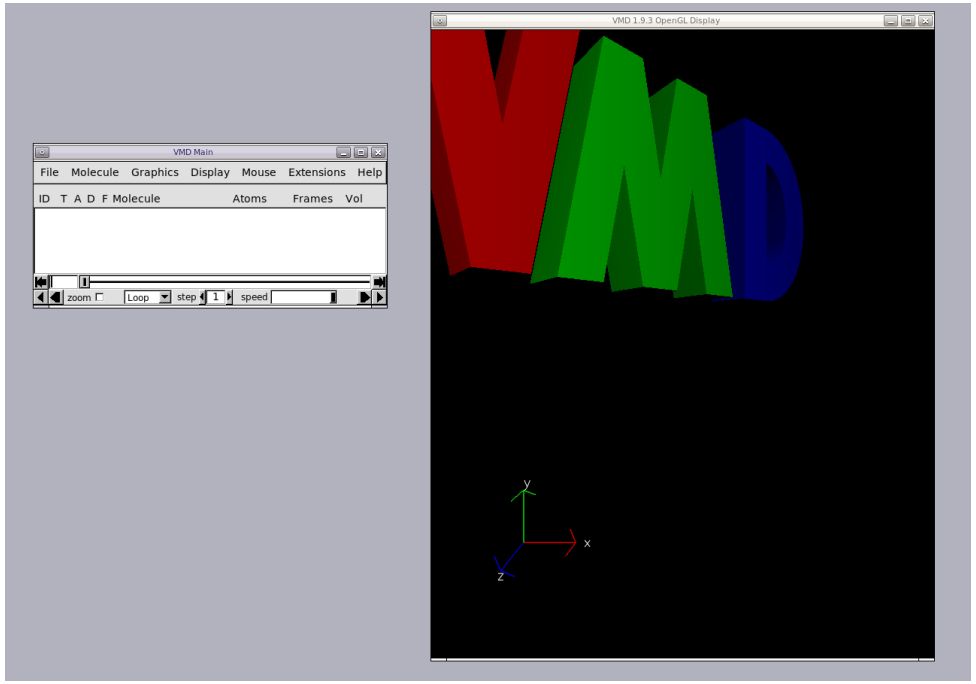
- **OnDemand**
  - Interactive Apps -> VNC
  - VNC: CPU only





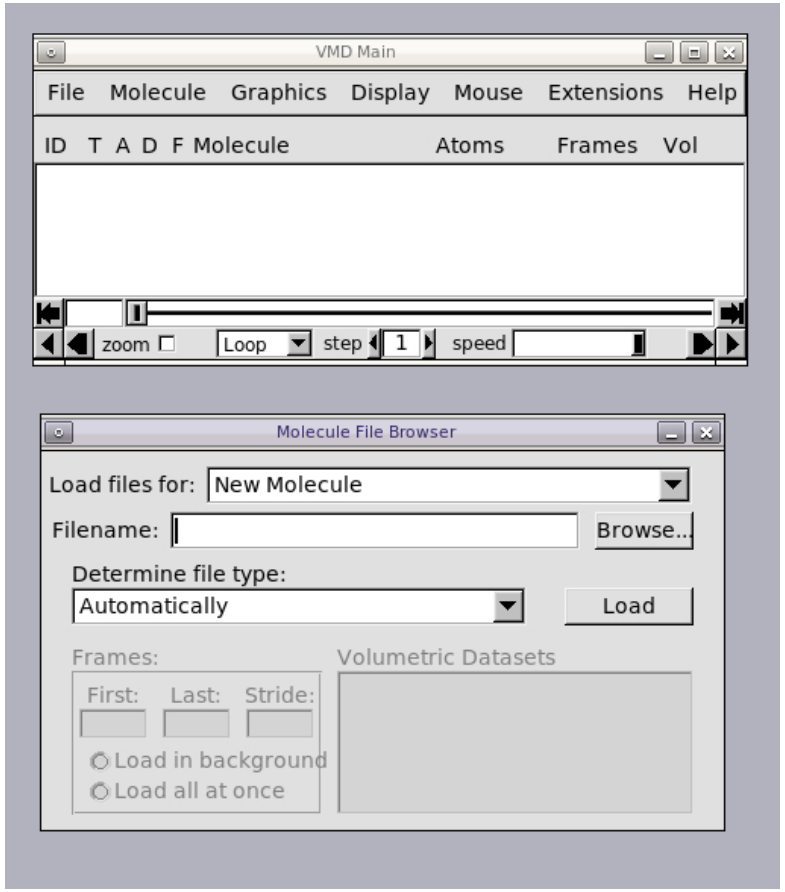
Grace Portal

- **VNC: VMD**
  - $ ml iccifort/2020.1.217
  - $ ml impi/2019.7.217
  - $ ml VMD/1.9.3-Python-2.7.18
  - $ vmd



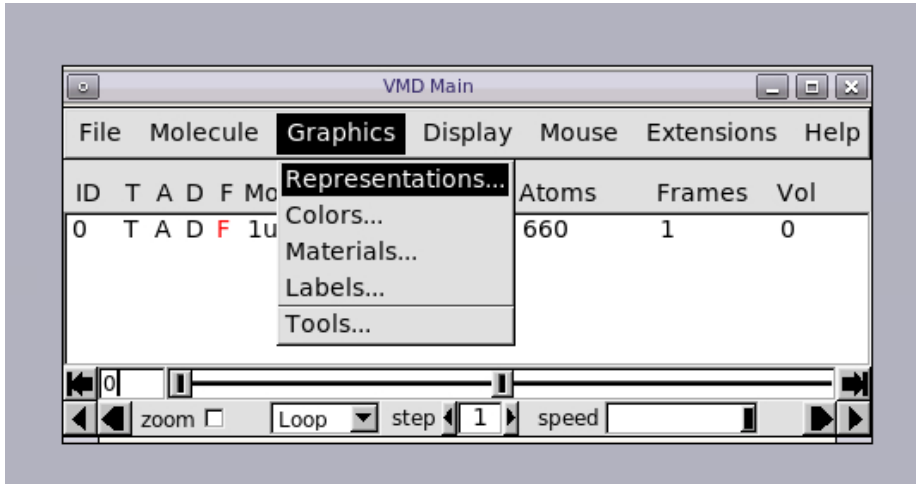
Grace Portal

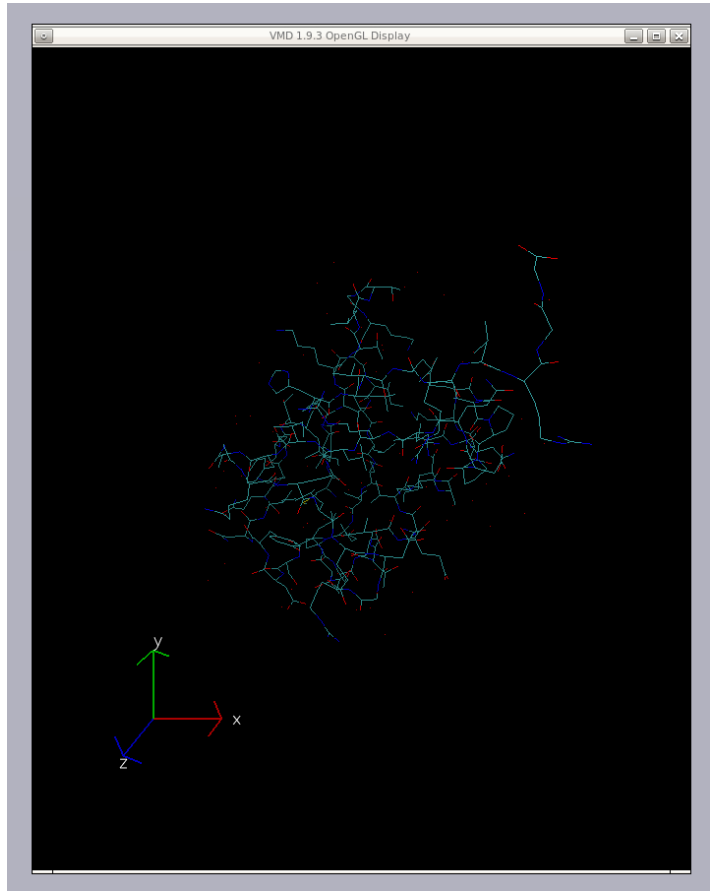
- **VMD**
  - File -> New Molecule…
  - Browse…
  - Path to 1ubq.pdb
  - Load



Grace Portal

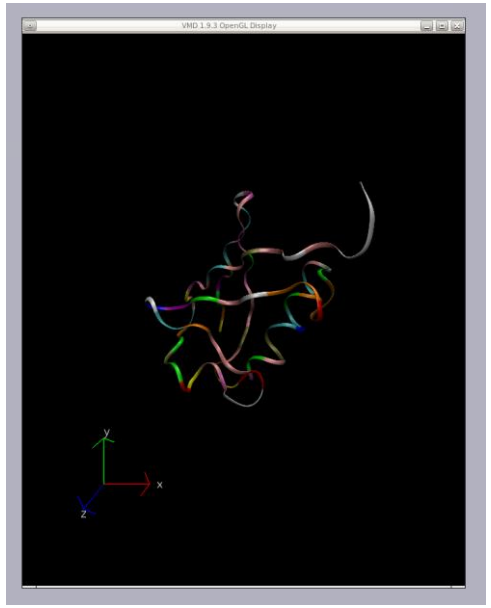
- **VMD**
  - Graphics -> Representations…

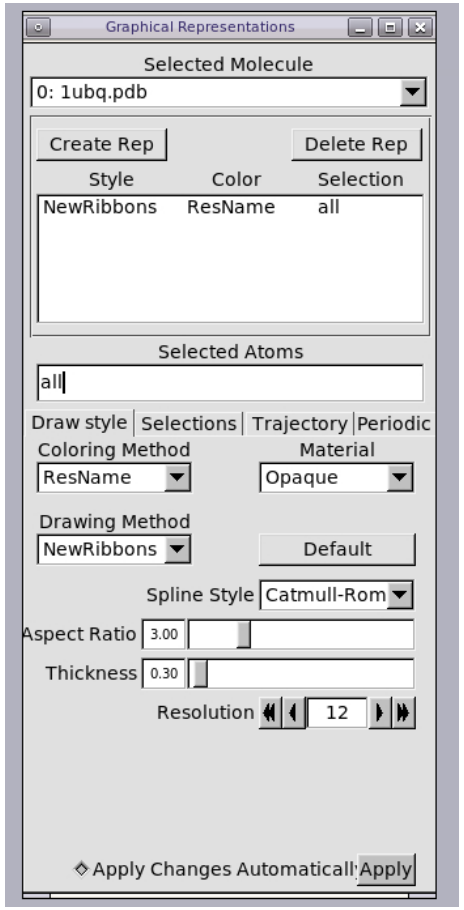




Grace Portal

- **VMD**
  - Coloring Method: ResName
  - Drawing Method: NewRibbons





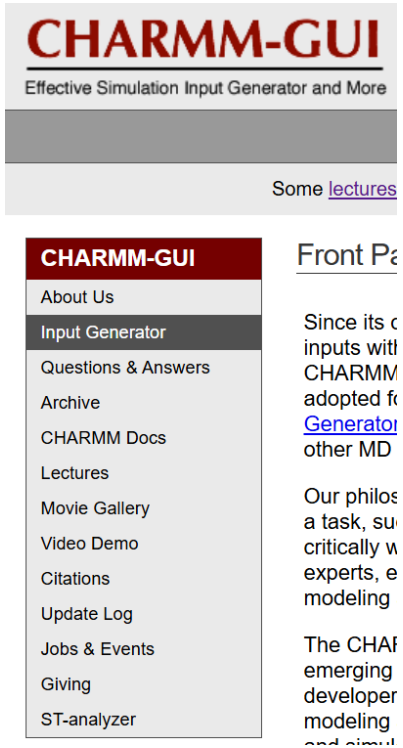
CHARMM-GUI

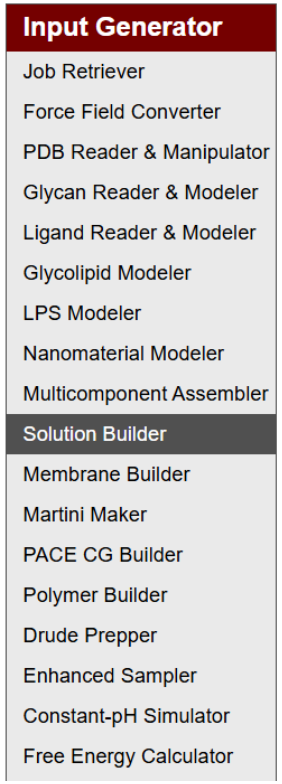
- A typical MD study
  - Prepare your system
  - Pre-production: minimization/heating/equilibration
  - Production MD
  - Post MD Analysis

- CHARMM-GUI: https://www.charmm-gui.org/
  - System preparation
  - Input generator

CHARMM-GUI

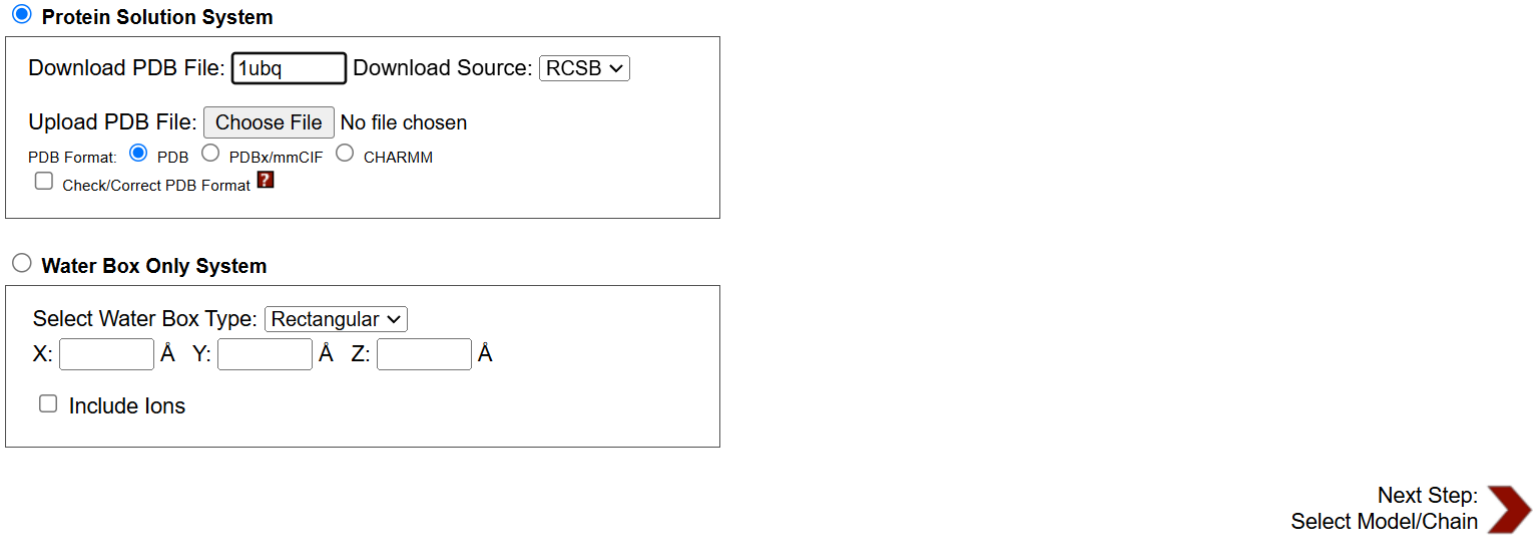
- System preparation
  - -> Input generator
  - -> Solution Builder





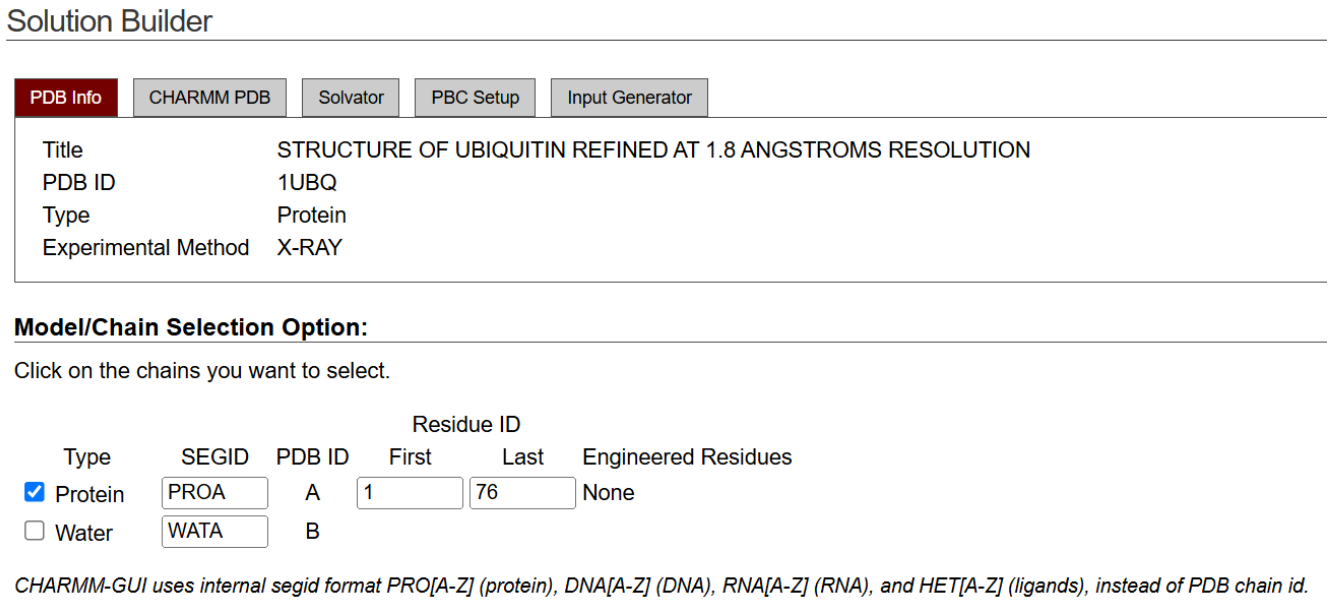
CHARMM-GUI

- Protein Solution System
  - 1ubq
  - Next Step: Select Model/Chain



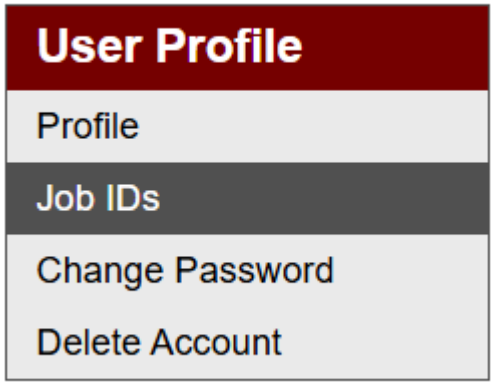
CHARMM-GUI

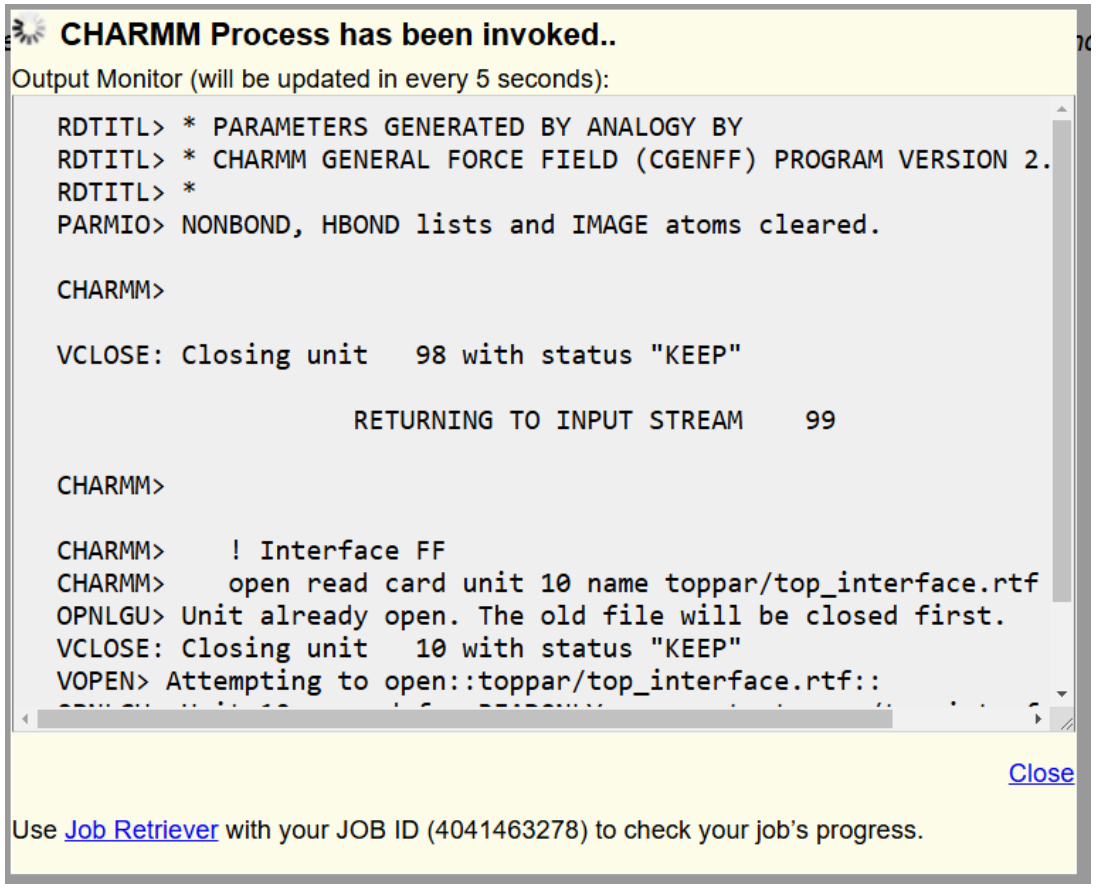
- Protein Solution System
  - Include water or not
  - Next Step: Manipulate PDB



CHARMM-GUI

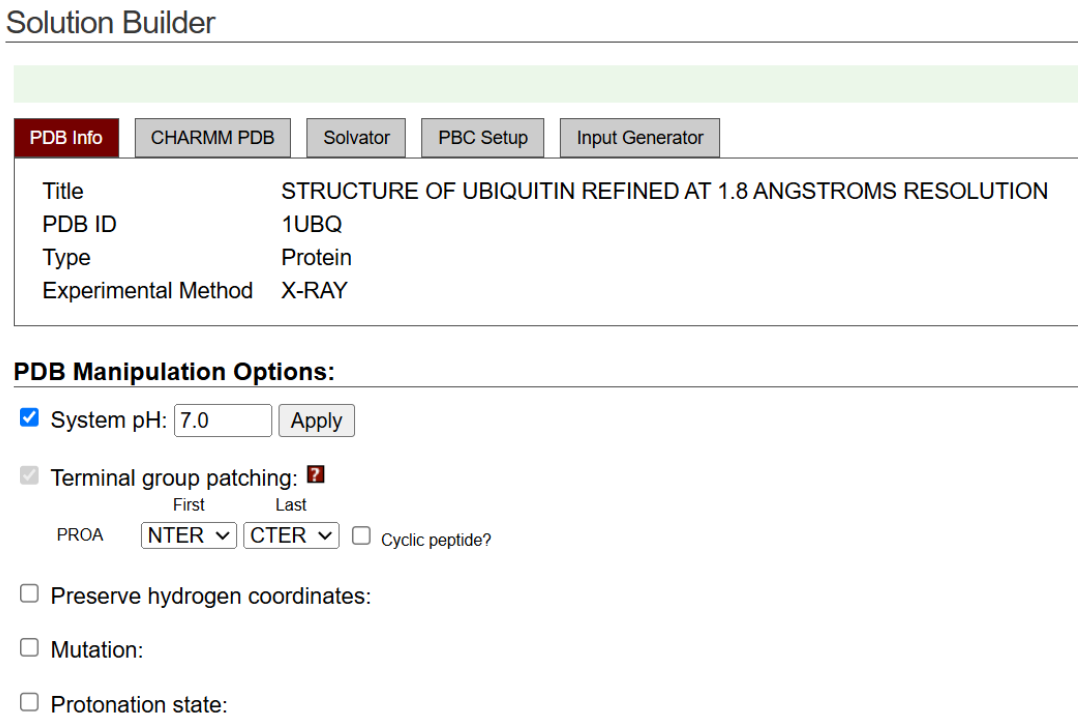
- CHARMM
- Retrieve your job by JOB ID





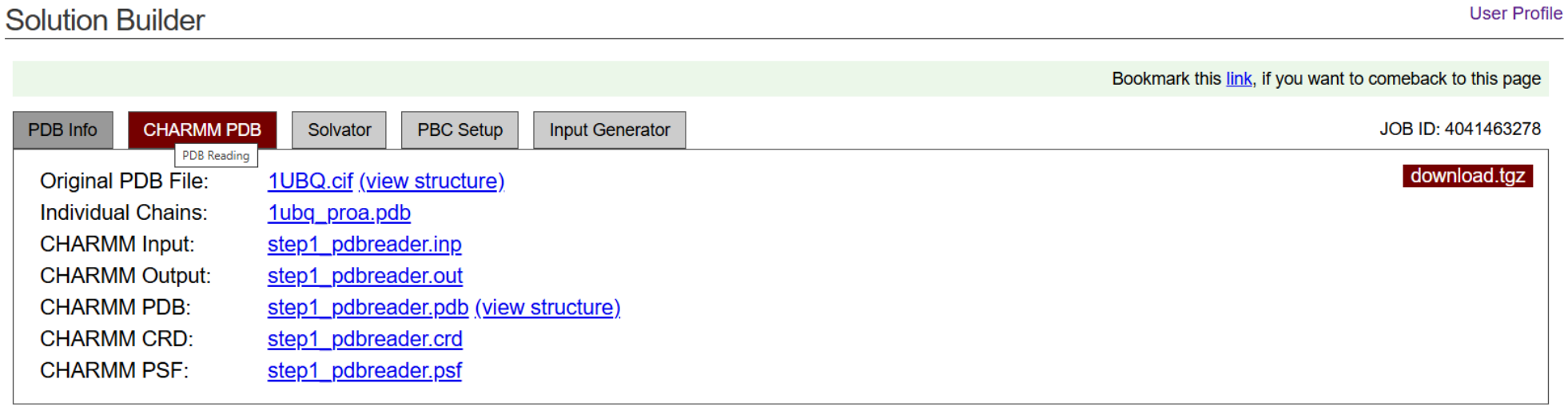
CHARMM-GUI

- Protein Solution System
  - PDB Manipulation
  - Next Step: Generate PDB



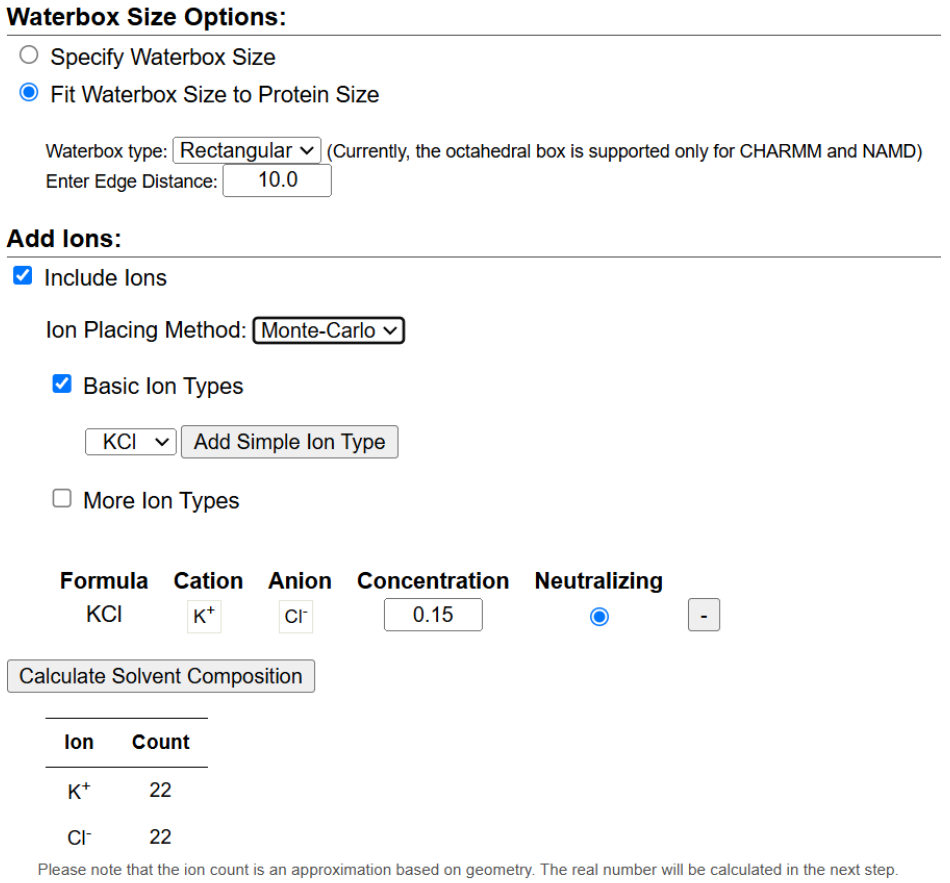
CHARMM-GUI

- Download and view input/output files
- Practice: VMD - confirm water removed



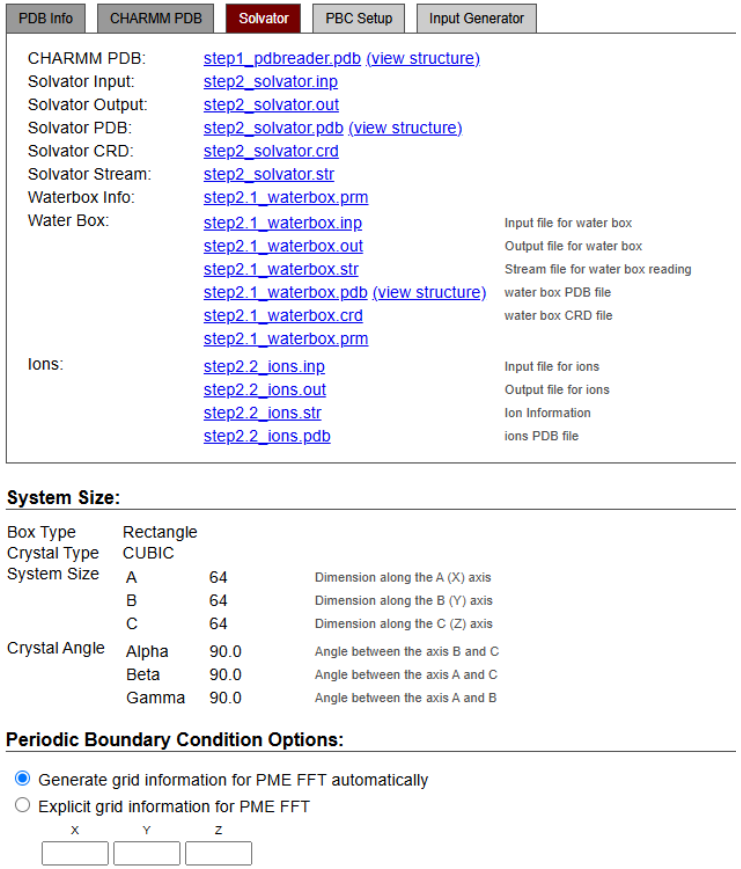
CHARMM-GUI

- Solution Builder
  - Waterbox size
  - Waterbox type
  - Ion types
  - Ion concentration



CHARMM-GUI

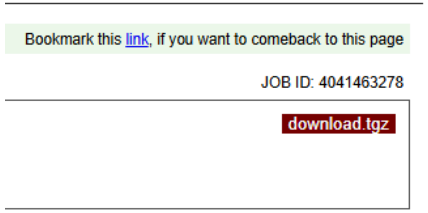
- Solution Builder
  - Check waterbox size
  - VMD: view and check
  - Next Step: Setup PBC



CHARMM-GUI

- Input Generation
  - NAMD
  - GROMACS
  - AMBER
  - OpenMM

- Next Step: Generate Inputs!
- download tgz:



Input Generation Options:

The input generation scheme has been changed recer

- [x] NAMD
- [x] GROMACS
- [x] AMBER
- [x] OpenMM
- [ ] CHARMM/OpenMM
- [ ] GENESIS
- [ ] Desmond
- [ ] LAMMPS
- [ ] Tinker

Equilibration Input Generation Options:

- (•) NVT Ensemble

Dynamics Input Generation Options:

- (•) NPT Ensemble
- ( ) NVT Ensemble

Temperature: 303.15 K

Grace: MD Simulations

- Upload and unzip “charmm-gui-tgz”: $ tar -xvzf charmm-gui.tgz

- Example: Amber
  - Upload or move “amber-charmmgui-grace.sub” to “amber” directory
  - “amber-charmmgui-grace.sub”: minimization/equilibration/production
  - Submit “amber-charmmgui-grace.sub”

- Try GROMACS, NAMD, and OpenMM

- Compare time/result

Future MD Course: Suggestion

- Software details: Amber, NAMD, OpenMM, CHARMM, Gromacs

- Free energy methods: Umbrella Sampling, Steered MD, Adaptive Biased Force Method, Replica Exchange MD, Metadynamics, String Method

- Post MD analysis:
  - Trajectory analysis: MSD, RDF, …
  - Structural analysis: RMSD, RMSF, …
  - PCA, Cluster analysis, …

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