

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

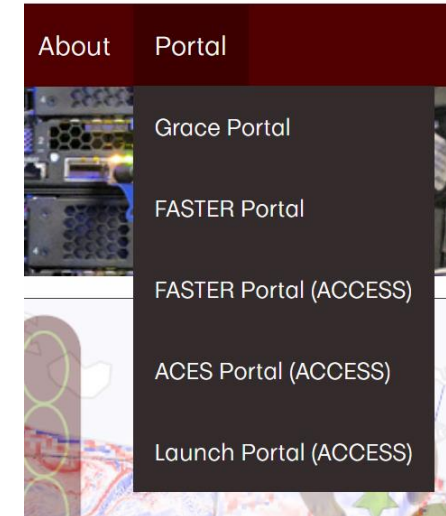
- System preparing
- Input generating

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



TAMU HPRC OnDemand (Grace) Apps ▾ Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Chatbot ▾ Dashboard ▾ Utilities ▾

Grace Portal

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

VNC (12694538)

1 node | 1 core | Running

Host: [>_c723](#)

Delete

Created at: 2025-02-23 20:01:18 CST

Time Remaining: 59 minutes

Session ID: [4fbeb364-821a-44b5-a5b9-18e963c8caee](#)

Compression

0 (low) to 9 (high)

Image Quality

0 (low) to 9 (high)

Launch VNC

View Only (Share-able Link)

VNC

This app will launch a [vnc](#) job on [Grace](#) for remote visualization.

Node type

CPU only

select a GPU node for software that supports GPU usage.

Number of hours (max 168)

1

Number of cores (max 48)

1

Total GB Memory (max 360)

7

Account

This field is optional.

Email

email address must be provided if you want to receive an email when the session starts.

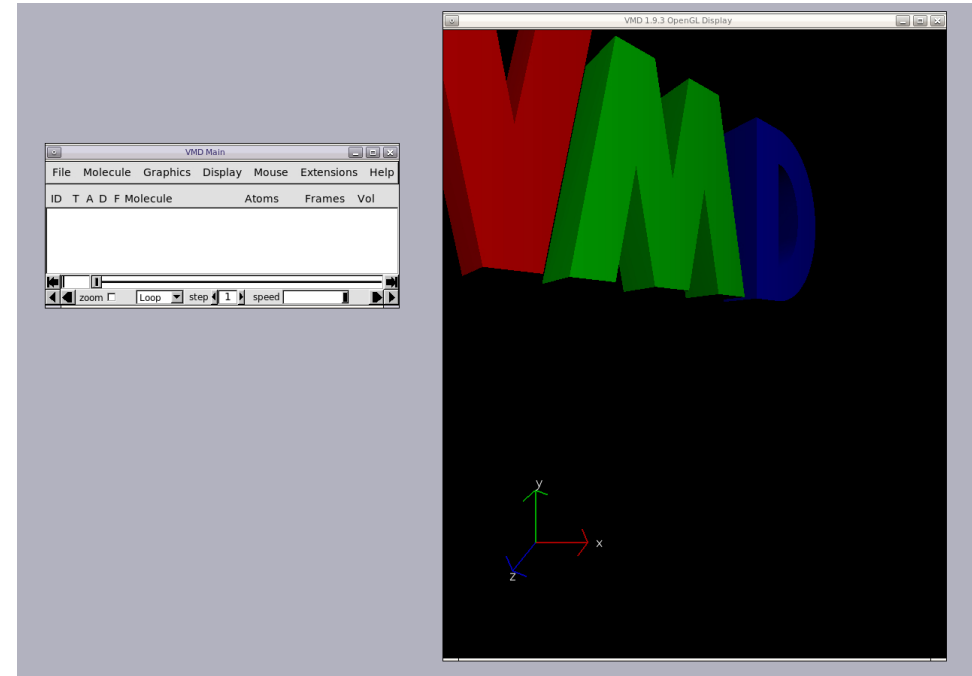
☐ I would like to receive an email when the session starts

Launch

* The VNC session data for this session can be accessed under the [data root directory](#).

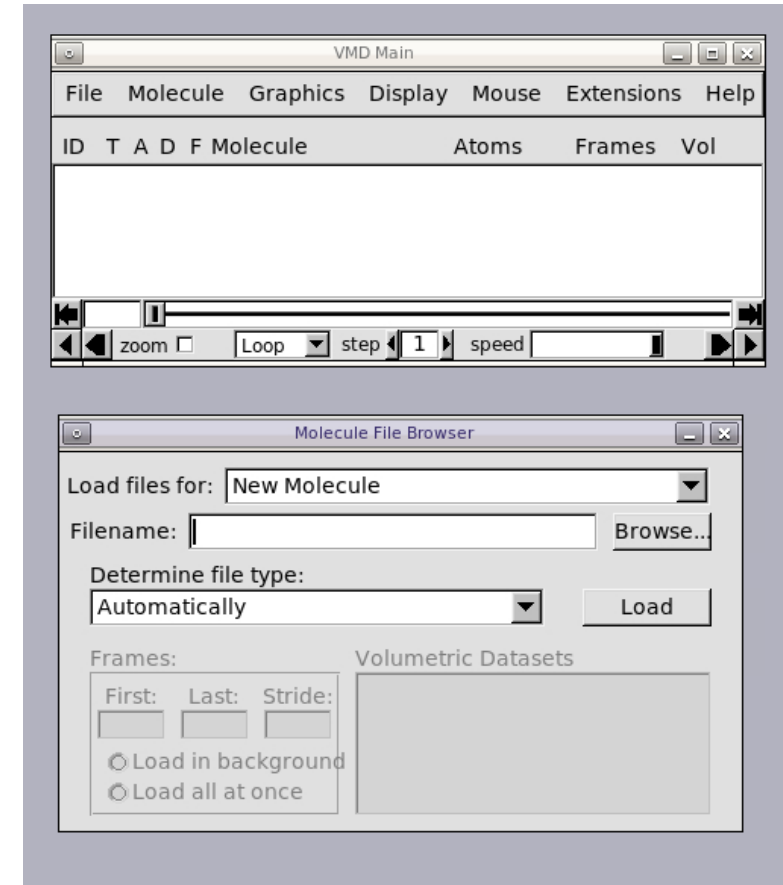
Grace Portal

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



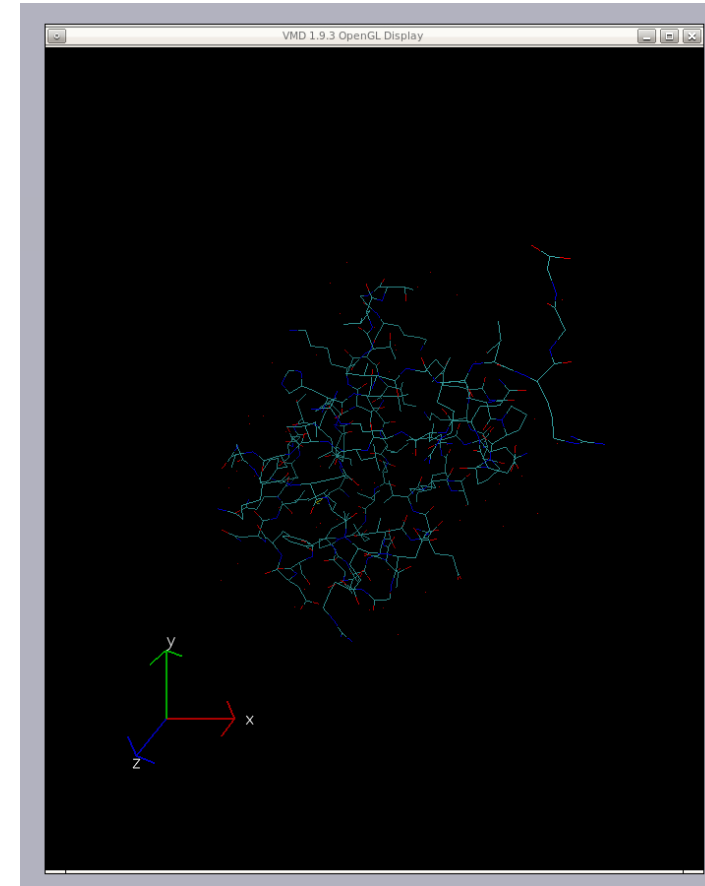
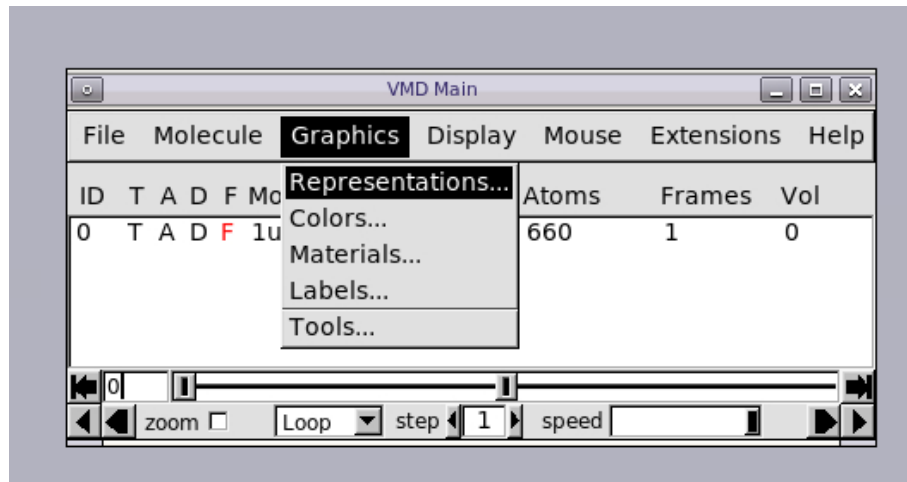
Grace Portal

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



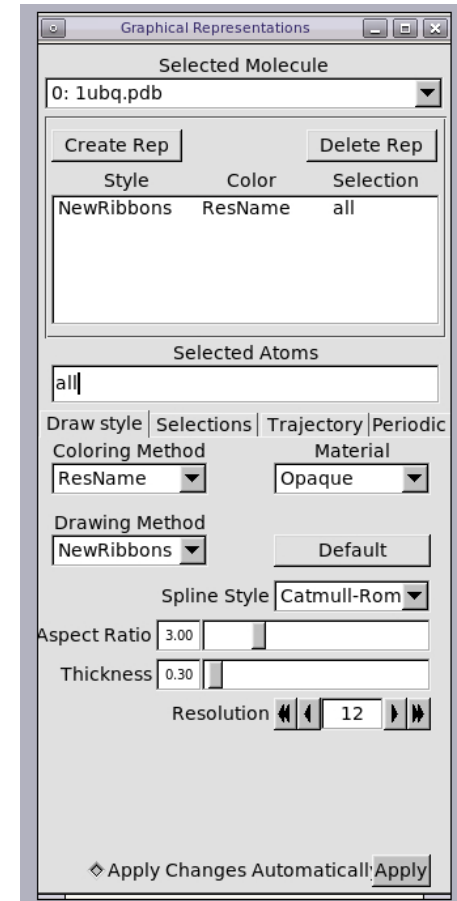
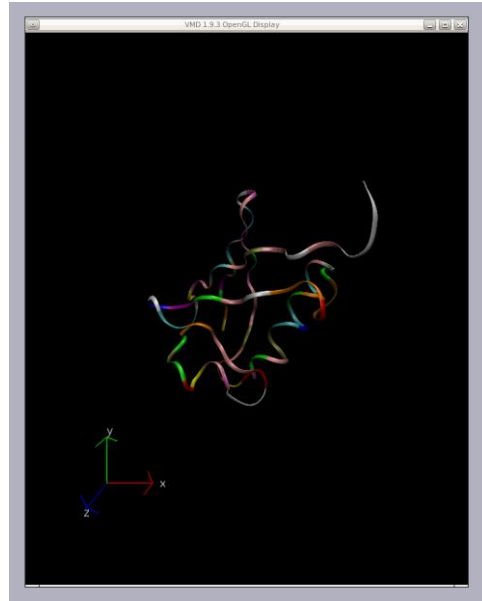
Grace Portal

- **VMD**
 - Graphics -> Representations...



Grace Portal

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

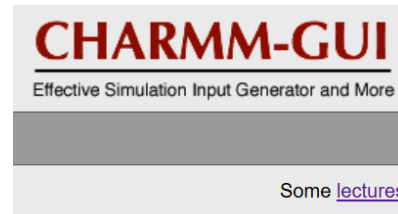


CHARMM-GUI

- 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
About Us
Input Generator
Questions & Answers
Archive
CHARMM Docs
Lectures
Movie Gallery
Video Demo
Citations
Update Log
Jobs & Events
Giving
ST-analyzer

Front Page

Since its creation, CHARMM-GUI has been adopted for many other MD simulations.

Our philosophy is to make a task, such as building a system, critically with experts, e.g., for modeling.

The CHARMM-GUI team is an emerging developer community for modeling and simulation.

Input Generator
Job Retriever
Force Field Converter
PDB Reader & Manipulator
Glycan Reader & Modeler
Ligand Reader & Modeler
Glycolipid Modeler
LPS Modeler
Nanomaterial Modeler
Multicomponent Assembler
Solution Builder
Membrane Builder
Martini Maker
PACE CG Builder
Polymer Builder
Drude Prepper
Enhanced Sampler
Constant-pH Simulator
Free Energy Calculator

CHARMM-GUI

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

☒ **Protein Solution System**

Download PDB File: Download Source: ▼

Upload PDB File: No file chosen

PDB Format: ☒ PDB ☐ PDBx/mmCIF ☐ CHARMM

☐ Check/Correct PDB Format ?

☐ **Water Box Only System**

Select Water Box Type: ▼

X: Å Y: Å Z: Å

☐ Include Ions

Next Step: 
Select Model/Chain

CHARMM-GUI

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

Solution Builder

PDB Info	CHARMM PDB	Solvator	PBC Setup	Input Generator
Title	STRUCTURE OF UBIQUITIN REFINED AT 1.8 ANGSTROMS RESOLUTION			
PDB ID	1UBQ			
Type	Protein			
Experimental Method	X-RAY			

Model/Chain Selection Option:

Click on the chains you want to select.

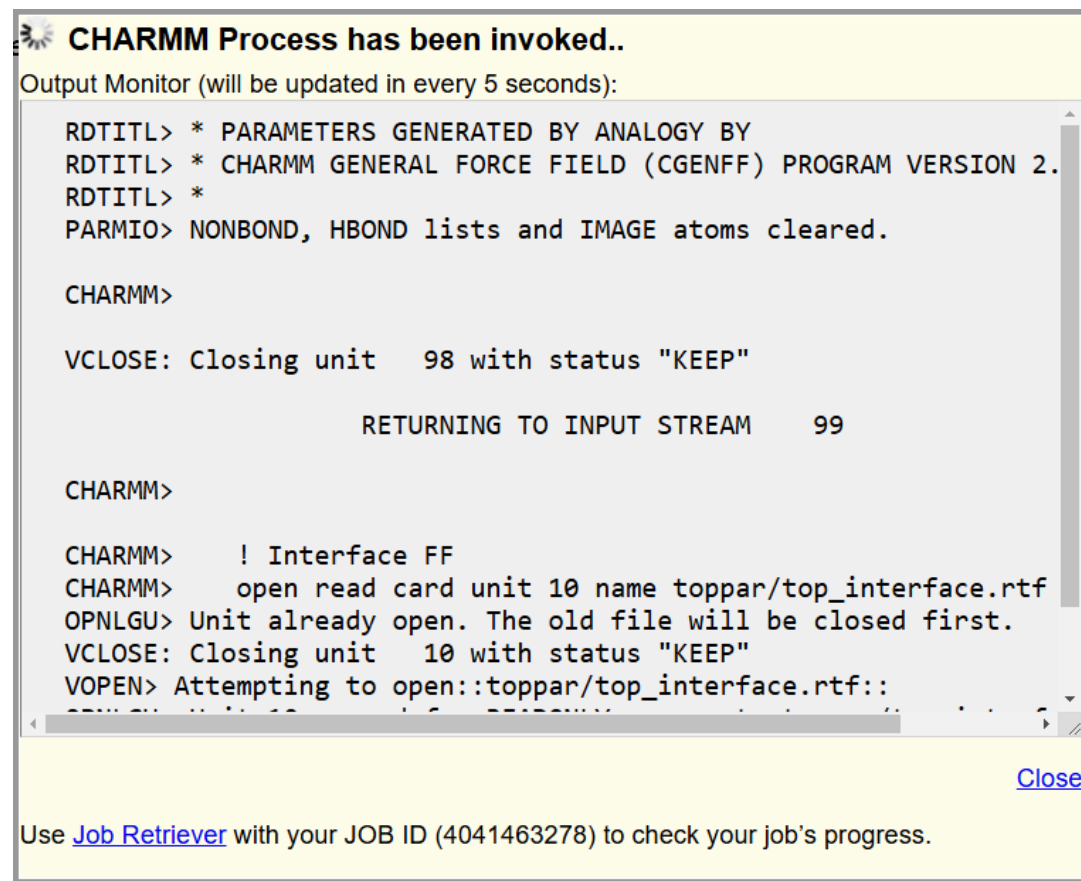
Type	SEGID	PDB ID	Residue ID		Engineered Residues
			First	Last	
☒ Protein	PROA	A	1	76	None
☐ Water	WATA	B			

CHARMM-GUI uses internal segid format PRO[A-Z] (protein), DNA[A-Z] (DNA), RNA[A-Z] (RNA), and HET[A-Z] (ligands), instead of PDB chain id.

CHARMM-GUI

- CHARMM
- Retrieve your job by JOB ID

User Profile
Profile
Job IDs
Change Password
Delete Account



CHARMM Process has been invoked..

Output Monitor (will be updated in every 5 seconds):

```
RDITL> * PARAMETERS GENERATED BY ANALOGY BY
RDITL> * CHARMM GENERAL FORCE FIELD (CGENFF) PROGRAM VERSION 2.
RDITL> *
PARMIO> NONBOND, HBOND lists and IMAGE atoms cleared.

CHARMM>

VCLOSE: Closing unit   98 with status "KEEP"

                RETURNING TO INPUT STREAM      99

CHARMM>

CHARMM>   ! Interface FF
CHARMM>   open read card unit 10 name toppar/top_interface.rtf
OPNLGU> Unit already open. The old file will be closed first.
VCLOSE: Closing unit   10 with status "KEEP"
VOPEN> Attempting to open::toppar/top_interface.rtf::
```

[Close](#)

Use [Job Retriever](#) with your JOB ID (4041463278) to check your job's progress.

CHARMM-GUI

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

Solution Builder

PDB Info		CHARMM PDB	Solvator	PBC Setup	Input Generator
Title	STRUCTURE OF UBIQUITIN REFINED AT 1.8 ANGSTROMS RESOLUTION				
PDB ID	1UBQ				
Type	Protein				
Experimental Method	X-RAY				

PDB Manipulation Options:

- ☒ System pH:
- ☒ Terminal group patching:

First Last

PROA ☐ Cyclic peptide?

☐ Preserve hydrogen coordinates:

☐ Mutation:

☐ Protonation state:

CHARMM-GUI

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

Solution Builder

[User Profile](#)

Bookmark this [link](#), if you want to comeback to this page

PDB Info

CHARMM PDB

Solvator

PBC Setup

Input Generator

JOB ID: 4041463278

PDB Reading

Original PDB File: [1UBQ.cif \(view structure\)](#)

Individual Chains: [1ubq_proa.pdb](#)

CHARMM Input: [step1_pdbreader.inp](#)

CHARMM Output: [step1_pdbreader.out](#)

CHARMM PDB: [step1_pdbreader.pdb \(view structure\)](#)

CHARMM CRD: [step1_pdbreader.crd](#)

CHARMM PSF: [step1_pdbreader.psf](#)

[download.tgz](#)

CHARMM-GUI

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

Waterbox Size Options:

- ☐ Specify Waterbox Size
☒ Fit Waterbox Size to Protein Size

Waterbox type: Rectangular ▾ (Currently, the octahedral box is supported only for CHARMM and NAMD)
Enter Edge Distance: 10.0

Add Ions:

- ☒ Include Ions

Ion Placing Method: Monte-Carlo ▾

- ☒ Basic Ion Types

KCl ▾ Add Simple Ion Type

- ☐ More Ion Types

Formula **Cation** **Anion** **Concentration** **Neutralizing**

KCl K⁺ Cl⁻ 0.15 ☒ -

Calculate Solvent Composition

Ion	Count
K ⁺	22
Cl ⁻	22

Please note that the ion count is an approximation based on geometry. The real number will be calculated in the next step.

CHARMM-GUI

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

PDB Info	CHARMM PDB	Solvator	PBC Setup	Input Generator
CHARMM PDB: step1_pdbreader.pdb (view structure)				
Solvator Input: step2_solvator.inp				
Solvator Output: step2_solvator.out				
Solvator PDB: step2_solvator.pdb (view structure)				
Solvator CRD: step2_solvator.crd				
Solvator Stream: step2_solvator.str				
Waterbox Info: step2.1_waterbox.prm				
Water Box: step2.1_waterbox.inp Input file for water box				
step2.1_waterbox.out Output file for water box				
step2.1_waterbox.str Stream file for water box reading				
step2.1_waterbox.pdb (view structure) water box PDB file				
step2.1_waterbox.crd water box CRD file				
step2.1_waterbox.prm				
Ions: step2.2_ions.inp Input file for ions				
step2.2_ions.out Output file for ions				
step2.2_ions.str Ion Information				
step2.2_ions.pdb ions PDB file				

System Size:

Box Type	Rectangle		
Crystal Type	CUBIC		
System Size	A	64	Dimension along the A (X) axis
	B	64	Dimension along the B (Y) axis
	C	64	Dimension along the C (Z) axis
Crystal Angle	Alpha	90.0	Angle between the axis B and C
	Beta	90.0	Angle between the axis A and C
	Gamma	90.0	Angle between the axis A and B

Periodic Boundary Condition Options:

☒ Generate grid information for PME FFT automatically

☐ Explicit grid information for PME FFT

X	Y	Z

CHARMM-GUI

- Input Generation
 - NAMD
 - GROMACS
 - AMBER
 - OpenMM
- Next Step: Generate Inputs!
- download tgz:

Bookmark this [link](#), if you want to comeback to this page

JOB ID: 4041463278

[download.tgz](#)

Input Generation Options:

The input generation scheme has been changed recei

- ☒ NAMD
- ☒ GROMACS
- ☒ AMBER
- ☒ OpenMM
- ☐ CHARMM/OpenMM
- ☐ GENESIS
- ☐ Desmond
- ☐ LAMMPS
- ☐ Tinker

Equilibration Input Generation Options:

- ☒ NVT Ensemble

Dynamics Input Generation Options:

- ☒ NPT Ensemble
- ☐ NVT Ensemble

Temperature: 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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