

Molecular simulations of biomolecules

Remote Lecture #3

software options
getting started with Amber

CCB 550, Spring 2020

The computational chemistry software landscape

- Quantum chemistry options

- Gaussian
- ORCA
- QChem
- pyscf
- grimme_lab/xtb
- TeraChem
- CP2K
- quantum espresso

- MD packages

- Amber
- CHARMM
- gromacs
- Tinker
- openMM

- Other software

- Chimera
- pymol
- Avogadro

<https://www.nomad-coe.eu/externals/codes>

Finding Amber (and other software) on Amarel

`module avail` (nothing related to Amber)

Use "module spider" to find all possible modules.

`module spider`

amber: amber/14 amber/16

AMBER: Assisted Model Building with Energy Refinement

module spider amber/16

amber: amber/16

Description:

AMBER: Assisted Model Building with Energy Refinement

You will need to load all module(s) on any one of the lines below before the "amber/16" module is available to load.

intel/16.0.3 mvapich2/2.1 cuda/7.5

intel/17.0.0 mvapich2/2.2 cuda/7.5

intel/17.0.1 mvapich2/2.2 cuda/7.5

Help:

This module loads the environment to run Amber 16 ...

`module load intel/17.0.1 mvapich2/2.2 cuda/7.5 amber/16`

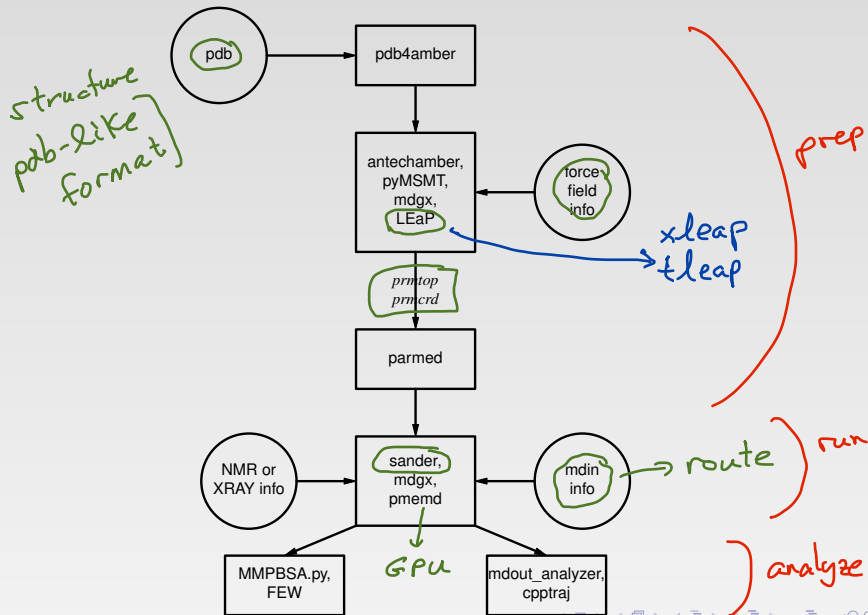
`module list`

Currently Loaded Modules: 1) gcc/5.4 2) intel/17.0.1 3) mvapich2/2.2
4) cuda/7.5 5) amber/16

`which tleap`

/opt/sw/packages/intel-17.0.1/mvapich2-2.2/cuda-7.5/amber/16/bin/tleap

Information flow in molecular and biomolecular simulations



Setting up a simple protein simulation in Amber/tleap

In order to prepare a molecule within LEaP for AMBER, three basic tasks need to be completed.

- 1 Any needed UNIT or PARMSET objects must be loaded;
- 2 The molecule must be constructed within LEaP;
- 3 The user must output topology and coordinate files from LEaP to use in AMBER.

The most typical command sequence is the following:

```
source leaprc.protein.ff14SB (load a force field)
x = loadPdb trypsin.pdb (load in a structure)
.... add in cross-links, solvate, etc.
saveAmberParm x prmtop prmcrd (save files)
```

More about running tleap—getting help

```
Welcome to LEaP!
```

```
(no leaprc in search path)
```

```
> help
```

```
Help is available on the following subjects:
```

_cmd_options_	_types_	add	addAtomTypes
addH	addIons	addIons2	addIonsRand
addPath	addPdbAtomMap	addPdbResMap	alias
alignAxes	bond	bondByDistance	center
charge	check	clearPdbAtomMap	clearPdbResMap
clearVariables	combine	copy	createAtom
createParmset	createResidue	createUnit	crossLink
debugOff	debugOn	debugStatus	deleteBond
deleteOffLibEntry	deleteRestraint	desc	deSelect
displayPdbAtomMap	displayPdbResMap	edit	flip
groupSelectedAtoms	help	impose	list
listOff	loadAmberParams	loadAmberPrep	loadMol2
loadMol3	loadOff	loadPdb	loadPdbUsingSeq
logFile	matchVariables	measureGeom	quit
relax	remove	restrainAngle	restrainBond
restrainTorsion	saveAmberParm	saveAmberParmNetcdf	saveAmberParmPert
saveAmberParmPol	saveAmberParmPolPert	saveAmberPrep	saveMol2
saveMol3	saveOff	saveOffParm	savePdb
scaleCharges	select	sequence	set
set_default	setBox	showdefault	solvateBox
solvateCap	solvateDontClip	solvateOct	solvateShell
source	transform	translate	verbosity
zMatrix			

Information flow inside teap

Term	Input Files		Parameters		Output Files	
	.pdb	.mol2	.lib, .mol2	.dat, .frmod	.prmtop	.crd
Molecules	✓	✓	✓		✓	
Atom Names	✓	✓	✓		✓	
Atom Types		✓	✓	✓	✓	
Charges		✓	✓		✓	
Connections	✓	✓	✓		✓	
Coordinates	✓	✓	✓			✓
Masses				✓	✓	
Bond Params				✓	✓	
NonB Params				✓	✓	

More information flow in tleap

Structure File	Library Files	Parameter Files
Molecules Atom Names Connections Coordinates	Units (Residues) Atom Names Atom Types Charges Connections Coordinates Masses Bonded Params Nonbond Params	Atom Types Masses Bonded Params Nonbond Params

Topology	Coordinates
Units (Residues) Atom Names Atom Types Charges Connections Masses Bonded Params Nonbond Params	Coordinates

→
→
→

Input for a sample MD run

```
#!/bin/bash
cat<<EOF >mdin
md for orthorhombic
&cntrl
  imin=0, maxcyc=200, ntmin=2, nscm=20000,
  ntp=20000, ntwx=100000, ntwr=100000,
  cut=9., ioutfm=1, nt xo=2,
  ntx=5, irest=1, tempi=0., temp0=298.,
  ntt=3, gamma_ln=10.,
  ntb=1, ntp=0, ntc=2, ntf=2, tol=0.0000001, taup=1.0d15,
  nstlim=2000000, dt=.004, ig=-1, ntave=0,
  ntr=0, restraint_wt=0.01,
  restraintmask="@1-1135500&!@H=,EPW"
```

route coord

EOF

```
sander -O -i mdin -ref md-1.x \
  -c md$in.x -o md$out.o -r md$out.x -x md$out.nc
```

prmcord

log file

final coordinates

trajectory inter. coords.