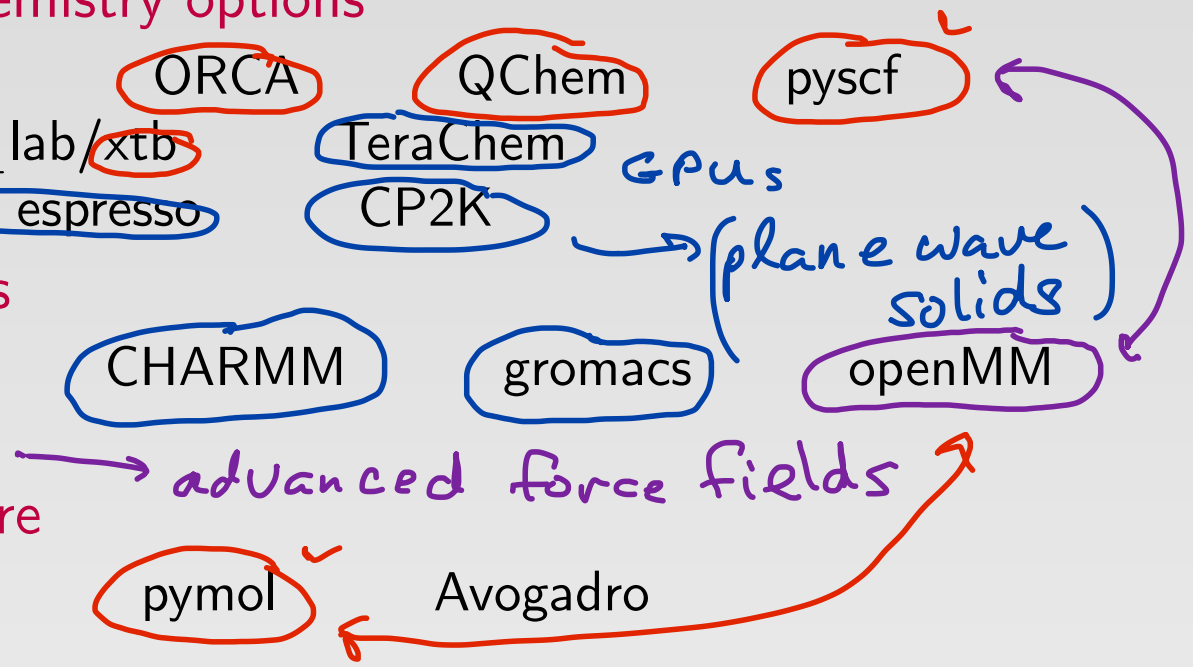
Molecular simulations of biomolecules
Remote Lecture #3

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
  - quantum espresso
  - CP2K
- MD packages
  - Amber
  - CHARMM
  - gromacs
  - openMM
  - Tinker
- Other software
  - Chimera
  - pymol
  - Avogadro

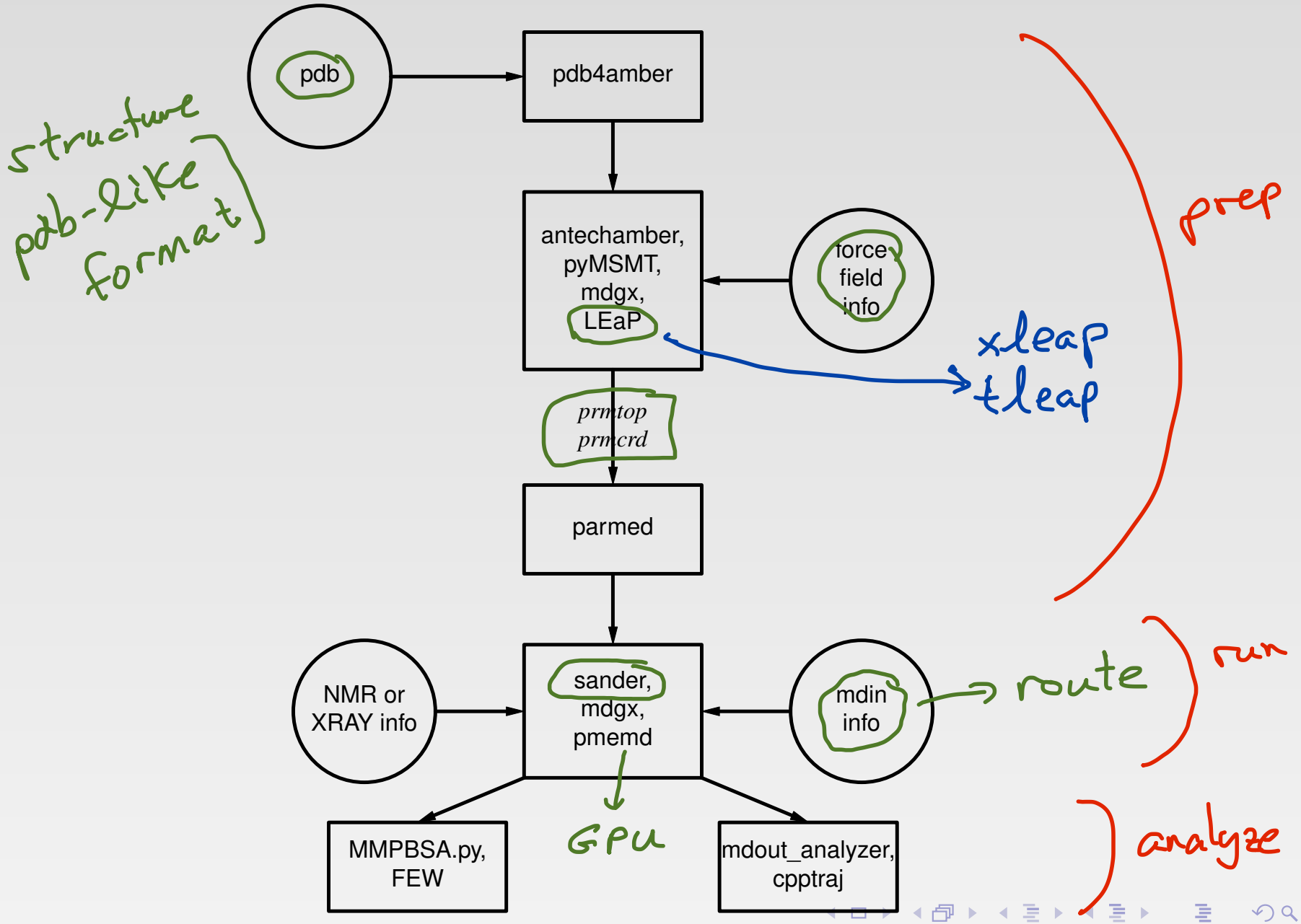


https://www.nomad-coe.eu/externals/codes

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    saveAmberParmPolPertsaveAmberPrep       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 tleap

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

generally come from leaprc

fixed during simul.

More information flow in tleap

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

inputs

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

outputs

Input for a sample MD run

```
#!/bin/bash
cat<<EOF >mdin
md for orthorhombic
 &cntrl
   imin=0, maxcyc=200, ntmin=2, nscm=20000,
   ntpr=20000, ntwx=100000, ntwr=100000,
   cut=9., ioutfm=1, ntxo=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"
 /
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
```

shell script

"here" file

title

creates mdin

route card

-p prmtop

trajectory inter. coords.

run

prmcrd

log file

final coordinates