Coordinates to Structure

CCP-SAS 2015

Atomistic Modeling for Small Angle Scattering:

A Short Course

May 26-28, 2015

Institut Laue-Langevin, France

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MD

A technique for computing equilibrium and transport properties of a classical many-body system.

Experiment:

sample in instrument, measure over time ... measure longer until data converge.

MD:

model system with N particles, solve **F** = m**a** until properties do not change (Equilibrate) then you “measure” (i.e. average a property) until data converge.

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MD

They can both suffer from the same mistakes

experiment	md
sample not prepared correctly	incorrect starting model structure
measurement too short	simulation too short
system undergoes irreversible change (aggregate etc.)	structure gets stuck in non-ergodic hole
didn’t quite measure what we thought	ahem, a bug in your analysis code

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Pseudo-code

```
read_input_parameters(temp, dt, number_of_timesteps, pressure,
approximation parameters)

initialize(coordinates, velocities)

Loop over timesteps:

    calculate_forces(r)

    integrate_equation_of_motion(r,p) --> propagates r & p

    t = t + dt
```

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F ≡ - del U ---> Verlet Integrator

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$f_x(r) = -\frac{\partial u(r)}{\partial x} = -\left(\frac{x}{r}\right)\left(\frac{\partial u(r)}{\partial r}\right)$$

$$f_x(r) = \frac{48x}{r^2}\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{0.5}{r}\right)^{6}\right]$$

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F ≡ - del U ---> Verlet Integrator

Many more numerical integrators have been evaluated

Verlet
Leapfrog Verlet
Velocity Verlet
4d Verlet
Velocity Verlet 2
. . .

Key --> energy conservation (~10^{-6})

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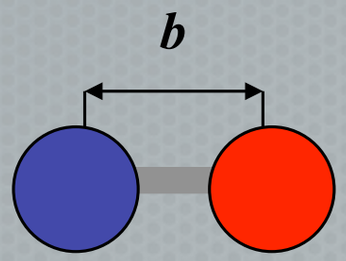
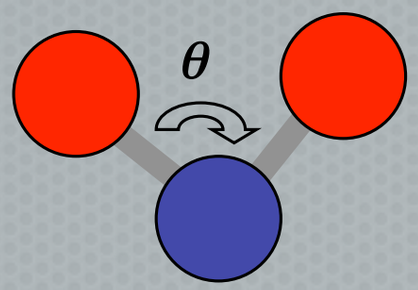
Bonded Systems

Potential

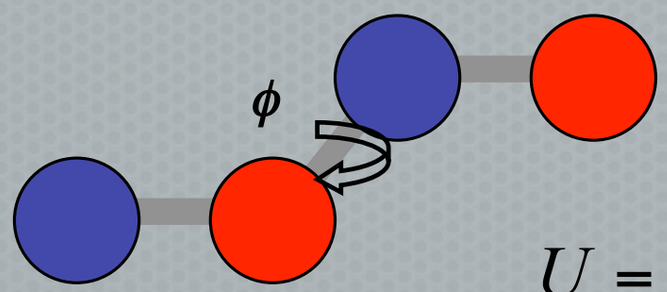
Strong bonded interactions



$$U = K(b - b_0)^2$$

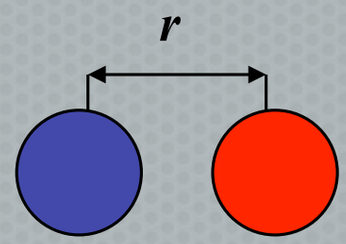


$$U = K(\theta - \theta_0)^2$$

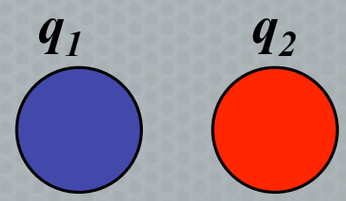


$$U = K(1 - \cos(n\phi))$$

Non bonded interactions



$$U = \left(\frac{A}{r}\right)^{12} - \left(\frac{B}{r}\right)^{6}$$



$$U = \frac{q_1 q_2}{r}$$

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Bonded Systems

$$
\begin{aligned}
V = & \sum_{\text{bonds}} k_b \left(b - b_0\right)^2 + \sum_{\text{angles}} k_\theta \left(\theta - \theta_0\right)^2 + \sum_{\text{dihedrals}} k_\phi \left[1 + \cos\left(n\phi - \delta\right)\right] \\
& + \sum_{\text{impropers}} k_\omega \left(\omega - \omega_0\right)^2 + \sum_{\text{Urey-Bradley}} k_u \left(u - u_0\right)^2 \\
& + \sum_{\text{nonbonded}} \epsilon \left[\left(\frac{R_{\min_{ij}}}{r_{ij}} \right)^{12} - \left(\frac{R_{\min_{ij}}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon r_{ij}}
\end{aligned}
$$

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Approximations

MD calculations take too long...

Many schemes are used to save cpu cycles. The tricks have no physical significance . . .

They should not affect the results of the calculation in any way.

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Approximations

Force (summed over pairs of atoms)

$N(N-1)/2 \dashrightarrow O(N^2)$

tricks to get O(N):

neighbor lists (verlet, cell, etc.)

PME : N ln (N)

Parallelization Methods

Multiple time steps

built-in and mature

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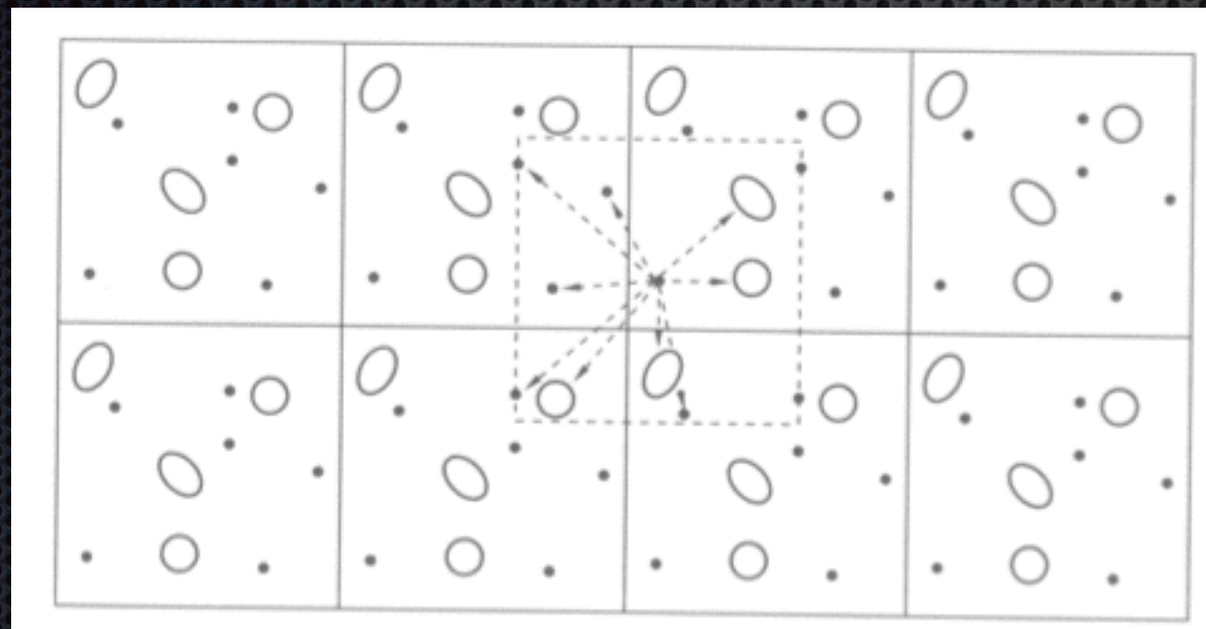
PBC

3D : Fraction @ surface -> $N^{-1/3}$

1000 atoms -> 49% at surface

10^6 atoms -> 6% at surface



But or $O(N^2)$ pair distance calculation just went to infinity

Need cutoffs [rcut < L/2]

MD (truncated & smoothed)

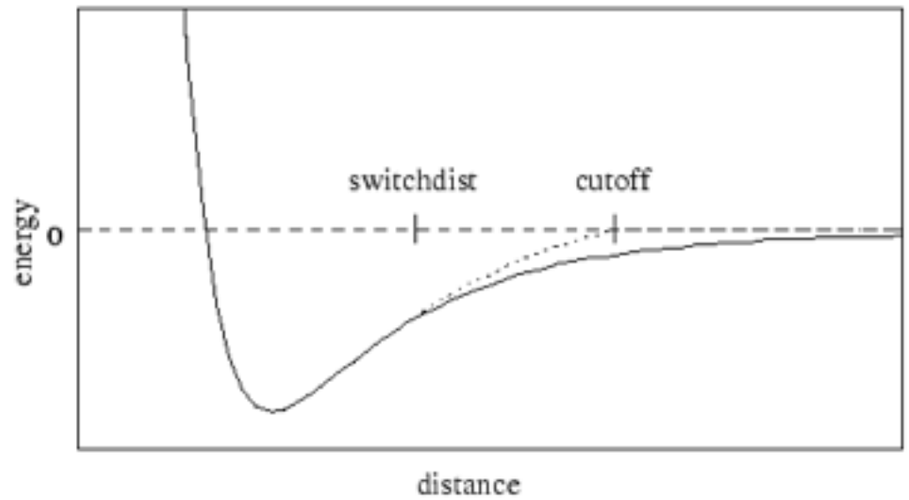


Figure 1: Graph of van der Waals potential with and without the application of the switching function. With the switching function active, the potential is smoothly reduced to 0 at the cutoff distance. Without the switching function, there is a discontinuity where the potential is truncated.

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Summary

Provide the MD “program”

- Coordinates
- Topology (connectivity)
- Force Field Parameters
- Temperature
- Pressure
- Parameters for approximations
  - MTS, NNL, PME, PBC, cutoffs, restraints
- Output information (filenames)

Equilibrate (convergence) … then “measure”

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Barriers: BUILD; EQUILIBRATE; PROPAGATE; ANALYZE

What software package(s) and force-fields do I use?

Starting structure?

How do I clean up the structure?

How do I set up a trajectory (time or space)?

How do I calculate scattering observables correctly?

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Overview

PDB ---> PSF: from coordinates to bonding & structure

Anatomy of PDB file
Binary files
FF topology file
Psfgen (PDB + topology) --> PSF
FF parameter file

PDB + PSF + INPUT FILE : run a NAMD minimization

Minimization (in vacuo)
Adding water & ions
PBC & dynamics parameters
Restarting a simulation (continuation)
Fixed atom simulations & IMD
Output files

Lab I & II preview

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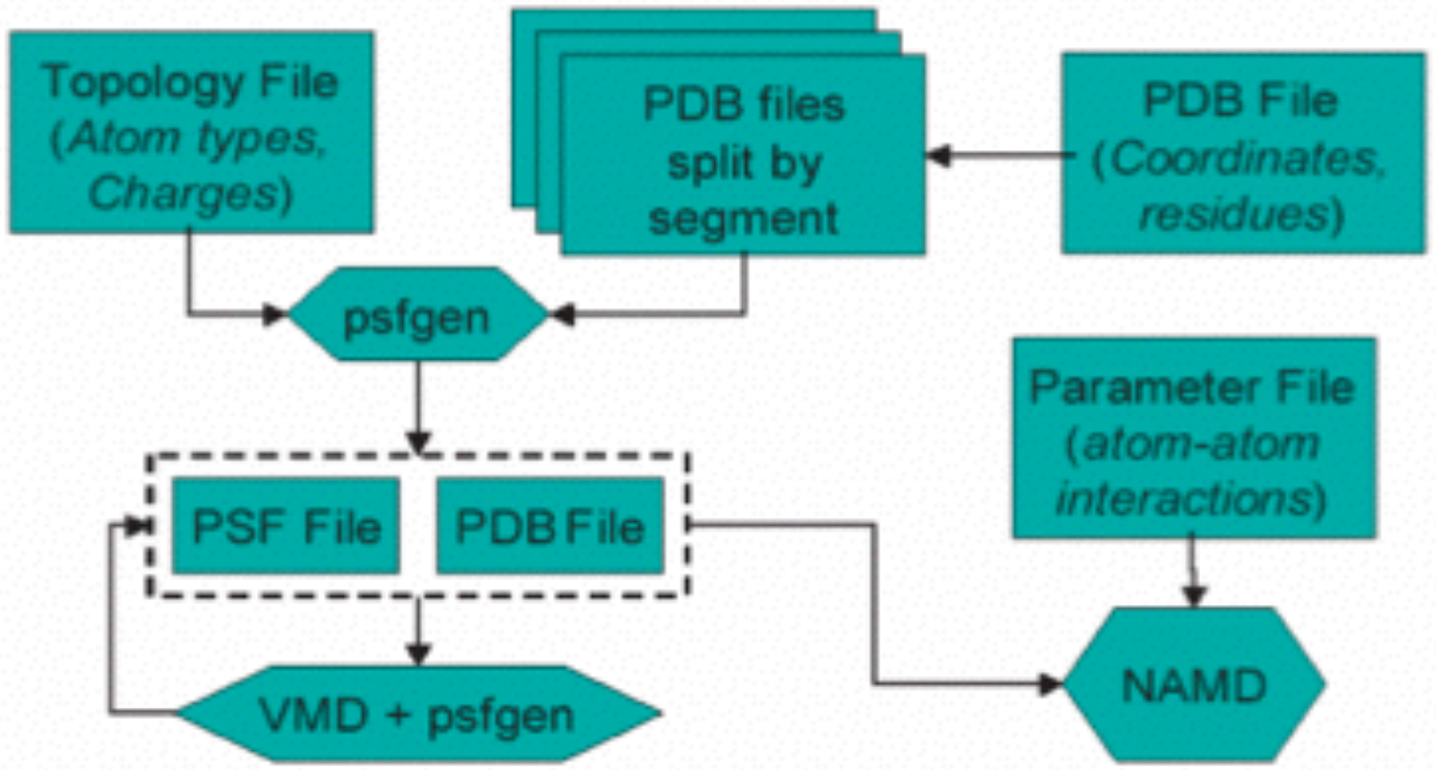
The Process



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Coord. Files

Protein Data Bank (PDB)

http://www.pdb.org

ftp://ftp.wwpdb.org/pub/pdb/doc/format_descriptions/Format_v32_letter.pdf

Open Babel

http://openbabel.org/wiki/Main_Page

> 110 chemical file formats

- Common cheminformatics formats
  - Canonical SMILES format (can)
  - Chemical Markup Language (cml, mrv)
  - InChI format (inchi)
  - MDL MOL format (mol, mdl, sdf, sd)
  - **Protein Data Bank format (pdb, ent)**
  - SMILES format (smi, smiles)
  - Sybyl Mol2 format (ml2, sy2, mol2)
- Utility formats
  - Compare molecules using InChI (k)
  - Copy raw text (copy)
  - Fastsearch format (fs)
  - Fingerprint format (fpt)
  - General XML format (xml)
  - Generic Output file format (dat, output, out, log)
  - MolPrint2D format (mpd)
  - Multilevel Neighborhoods of Atoms (MNA) (mna)
  - Open Babel molecule report (molreport)
  - Open Babel report format (report)
  - Outputs nothing (nul)
  - Reads raw text (text)
  - Title format (txt)
  - **XYZ cartesian coordinates format (xyz)**
- Other cheminformatics formats
  - Accelrys/MSI Biosym/Insight II CAR format (arc, car)
  - Accelrys/MSI Cerius II MSI format (msi)
  - Accelrys/MSI Quanta CSR format (csr)
  - MCDL format (mcdl)
  - MSI BGF format (bgf)
  - PubChem format (pc)
- Computational chemistry formats
  - ADF cartesian input format (adf)
  - ADF output format (adfout)
  - CAChe MolStruct format (cache, cac)

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Coord. Files

Protein Data Bank (PDB)

http://www.pdb.org

ftp://ftp.wwpdb.org/pub/pdb/doc/format_descriptions/Format_v32_letter.pdf

Open Babel

http://openbabel.org/wiki/Main_Page

> 110 chemical file formats

- Chemical Resource Kit 3D format (crk3d)
- Ghemical format (gpr)
- Molden format (molden, mold, molf)
- PCModel Format (pcm)
- UniChem XYZ format (unixyz)
- ViewMol format (vmol)
- YASARA.org YOB format (yob)

- Kinetics and Thermodynamics formats
  - ChemKin format (ck)
  - Thermo format (tdd, therm)
- Molecular dynamics and docking formats
  - Amber Prep format (prep)
  - Autodock Protein Data Bank (pdbqt)
  - DL-POLY CONFIG (CONFIG)
  - DL-POLY HISTORY (HISTORY)
  - Dock 3.5 Box format (box)
  - GROMOS96 format (gr96)
  - MacroModel format (mmod, mmd)
  - Tinker MM2 format (txyz)
  - XTC format (xtc)
- Volume data formats
  - ADF TAPE41 format (t41)
  - Gaussian cube format (cube, cub)
  - OpenDX cube format for APBS (dx)
- Miscellaneous formats
  - M.F. Sanner's MSMS input format (msms)
- Biological data formats
  - FASTA format (fasta, fa, fsa)
  - PQR format (pqr)
- Obscure formats
  - Alchemy format (alc)
  - CCC format (ccc)
  - Feature format (feat)
  - SMILES FIX format (fix)
  - XED format (xed)

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Anatomy of a PDB file I

HEADER
OBSLTE
TITLE
CAVEAT
COMPND
SOURCE
KEYWDS
EXPDTA
NUMMDL
MDLTYP
AUTHOR
REVDAT
SPRSDE
JRNL
REMARK (1-999)
REMARK 290 Cryst. Sym.
REMARK 300 Biomol.
REMARK 465 Missing AA
REMARK 470 Missing atom(s)
DBREF
SEQADV
SEQRES
MODRES
HET
HETNAM
HETSYN
FORMUL
HELIX
SHEET
SSBOND
LINK
CISPEP
SITE
CRYSTL1
OIGXn
SCALEn
MTRIXn
MODEL (starts a model)
ATOM
ANISOU
TER (ends a chain)
HETATM
ENDMDL (ends a model)
CONECT
MASTER
END

FOCUS:

name of compound
species & tissue
journal citation
sequence
symmetry
missing atoms
modified atoms/bonds
heteroatoms
coords
multiple models

PDB files are not necessarily written with your goals in mind!!!

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Anatomy of a PDB file II

```
         1         2         3         4         5         6         7
1234567890123456789012345678901234567890123456789012345678901234567890
ATOM      1  N   GLN A   1       9.921   8.724   2.612  1.00  0.00      PCLN N
ATOM      2  HT1 GLN A   1       9.866   9.721   2.563  0.00  0.00      PCLN H
ATOM      3  HT2 GLN A   1       9.309   8.315   1.935  0.00  0.00      PCLN H
```

Column(s)	Data Type	Definition	Example
1 - 6	Record Name		"ATOM "
7 - 11	Integer	Atom serial number	" 1"
13 - 16	Atom	Atom name	" N "
17	Character	"altloc"	" "
18 - 20	resName	Residue name	"GLN"
22	chainID	Chain indentifier	"A"
23 - 26	Integer	Residue sequence #	" 1"
27	Character	"iCode"	" "
31 - 38	Real (8.3)	X coord. (ang.)	" 9.921"
39 - 46	Real (8.3)	Y coord. (ang.)	" 8.724"
47 - 54	Real (8.3)	Z coord. (ang.)	" 2.612"
55 - 60	Real (6.2)	Occupancy	" 1.00"
61 - 66	Real (6.2)	Temperature factor	" 0.00"
77 - 78	String	Element symbol (RJ)	" N"
79 - 80	String	Charge	" "
(73 - 76)	String	Segment name	"PCLN"

Anatomy of a PDB file II

```
         1         2         3         4         5         6         7
1234567890123456789012345678901234567890123456789012345678901234567890
ATOM      1  N   GLN A   1       9.921   8.724   2.612  1.00  0.00      PCLN N
ATOM      2  HT1 GLN A   1       9.866   9.721   2.563  0.00  0.00      PCLN H
ATOM      3  HT2 GLN A   1       9.309   8.315   1.935  0.00  0.00      PCLN H
```

Column(s)	Data Type	Definition	Example
1 - 6	Record Name		"ATOM "
7 - 11	Integer	Atom serial number	" 1"
13 - 16	Atom	Atom name	" N "
17	Character	"altloc"	" "
18 - 20	resName	Residue name	"GLN"
22	chainID	Chain indentifier	"A" --> " "
23 - 26	Integer	Residue sequence #	" 1"
27	Character	"iCode"	" "
31 - 38	Real (8.3)	X coord. (ang.)	" 9.921"
39 - 46	Real (8.3)	Y coord. (ang.)	" 8.724"
47 - 54	Real (8.3)	Z coord. (ang.)	" 2.612"
55 - 60	Real (6.2)	Occupancy	" 1.00"
61 - 66	Real (6.2)	Temperature factor	" 0.00"
77 - 78	String	Element symbol (RJ)	" N"
79 - 80	String	Charge	" "
(73 - 76)	String	Segment name	"PCLN"

ftp://ftp.wwpdb.org/pub/pdb/doc/format_descriptions/Format_v32_letter.pdf

PDB Notes

Proteins: N to C terminus
Nucleic acids: 5’ - 3’
No ordering for polysaccharides
Chains terminated by “TER”
MODEL --> ENDMDL
AltLoc --> means there is more than one structure reported (duplicate)

Model can have no more than 99,999 atoms, otherwise split into separate PDB ENTRIES
--> in practice we can have any number of atoms in our files (99999) & (9999)->SEG

Terminal oxygen atoms: OXT (proteins) & O5’ or OP3 (nucleic acids)

MISSING ATOMS/RESIDUES (hydrogens!)
DUPLICATE RESIDUES / ATOMS (AltLoc)
WRONG PROTEIN (e.g. you only want part of a complex)
POST-TRANSLATION MODS (HEME, phosphoserine, etc.)
SEQUENCE (HIS tags, cloning artifacts, etc.)
RS-SR’
N-TERMINAL MODIFICATIONS
X-tal / NMR WATERS / IONS

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Binary Coordinate Files

DCD (CHARMM/NAMD/XPLOR)

TRJ or MDCRD (Amber)

NETCDF (Amber, MMTK)

TRJ (Gromacs)

etc.

"naming" information is not in a binary file, just general system info. and x,y,z coordinates: need PDB or PSF + DCD

Compared to concatenated PDB files (separated by END statements) DCD files are ~ 7 - 10 X smaller

Allows one to optimize file I/O code to speed up saving & reading data

Non-trivial to bootstrap your own code (endian byte ordering, 32/64 bit, . . .)

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Simple Example

PDB of a atom (oh2.pdb)

```
ATOM      1  OH2 TIP3 A   1       0.000   0.000   0.000  1.00  0.00      WAT1 O
```

XYZ of a atom (oh2.xyz)

```
 1

 OH2         2.000000        2.000000        2.000000
```

PDB of a atom moving (oh2_move.pdb)

```
ATOM      1  OH2 TIP3 A   1       0.000   0.000   0.000  1.00  0.00      WAT1 O
END
ATOM      1  OH2 TIP3 A   1       1.000   0.000   0.000  1.00  0.00      WAT1 O
END
ATOM      1  OH2 TIP3 A   1       2.000   0.000   0.000  1.00  0.00      WAT1 O
END
ATOM      1  OH2 TIP3 A   1       3.000   0.000   0.000  1.00  0.00      WAT1 O
END
```

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Simple Example

PDB of a atom (oh2.pdb)

```
ATOM      1                                   .00      WAT1 O
```

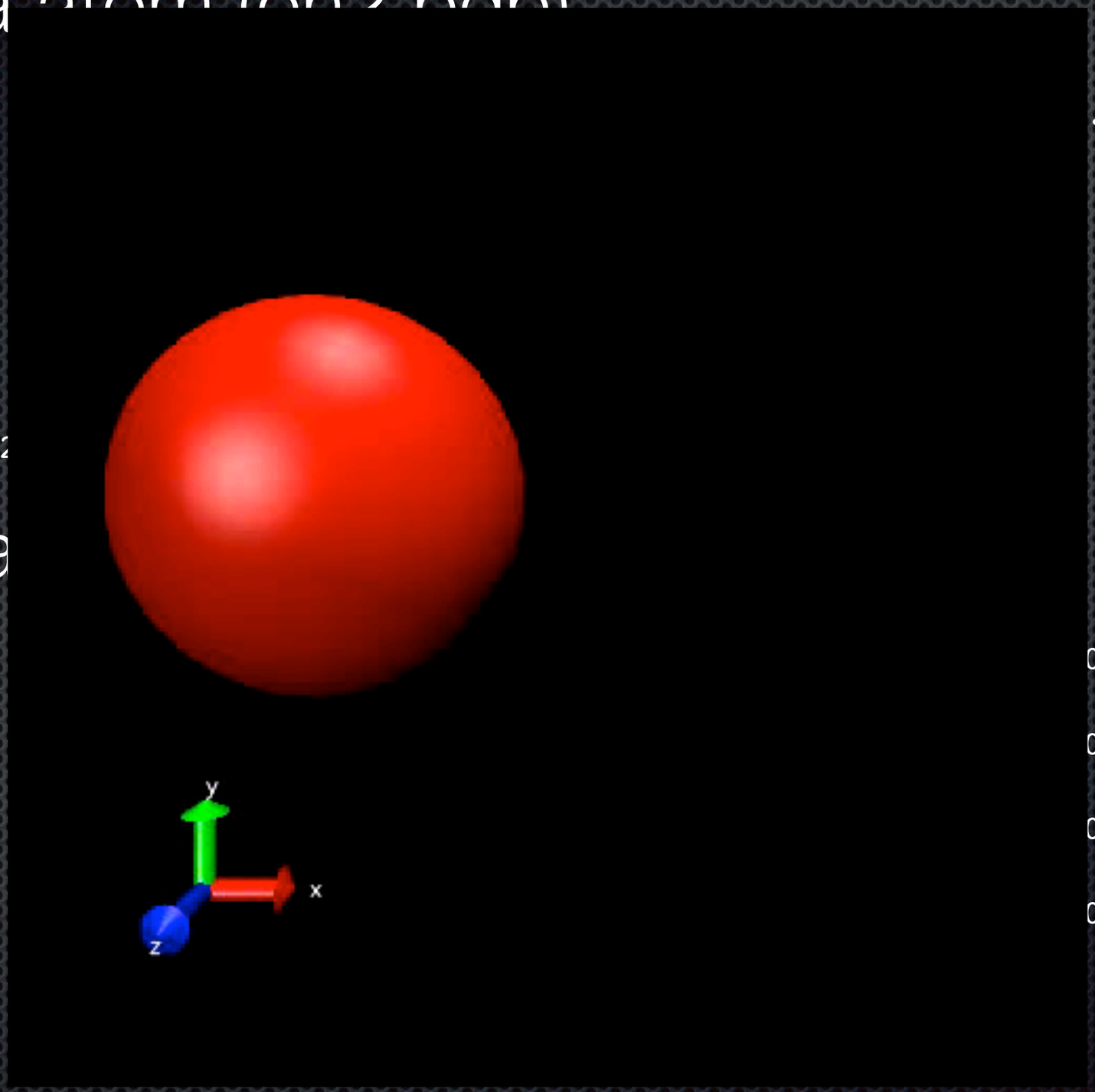
XYZ of a

```
1

OH2        2
```

PDB of a

```
ATOM      1                                   0.00      WAT1 O
END
ATOM      1                                   0.00      WAT1 O
END
ATOM      1                                   0.00      WAT1 O
END
ATOM      1                                   0.00      WAT1 O
END
```



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Onward

Okay, we have coordinates but how do we begin to deal with bonding and forces . . . MD?

PDB
(a file)

Dictionary of building blocks
(a file)
“topology for all systems”

1. PSFGEN
2. CHARMM
(programs)

PSF
(a file)

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Topology File

http://mackerell.umaryland.edu/CHARMM_ff_params.html

Specifically:

top_all27_prot_na.inp

KEYWORDS

MASS : define atom type names and masses

RESI : define building blocks (amino acids, etc.)

PRES : patches to correct / change structure (NTER, CTER, DISU, etc.)

DECL : to deal with joining blocks
proteins: -CA, -C, -O, +N, +HN, +CA
nucl. acids: +P, +O1P, +O2P, +O5', -O3'

DEFA : default patches to apply (NTER, CTER)

AUTO ANGLES DIHE : tells "program" to enumerate angles and dihedrals when blocks are put together

Text file (read top to bottom)

Keyword driven

Comments --> ! or *

Topology file is still only a piece of the puzzle . . .

Need a "parameter" file at some point.

Anatomy of a Topology File I

```
MASS     1 H      1.00800 H ! polar H
MASS     2 HC     1.00800 H ! N-ter H
MASS     3 HA     1.00800 H ! nonpolar H
MASS     4 HT     1.00800 H ! TIPS3P WATER HYDROGEN
MASS     5 HP     1.00800 H ! aromatic H
MASS     6 HB     1.00800 H ! backbone H
MASS     7 HR1    1.00800 H ! his he1, (+) his HG,HD2
MASS     8 HR2    1.00800 H ! (+) his HE1
MASS     9 HR3    1.00800 H ! neutral his HG, HD2
MASS    10 HS     1.00800 H ! thiol hydrogen
MASS    11 HE1    1.00800 H ! for alkene; RHC=CR
MASS    12 HE2    1.00800 H ! for alkene; H2C=CR
MASS    20 C     12.01100 C ! carbonyl C, peptide backbone
MASS    21 CA    12.01100 C ! aromatic C
MASS    22 CT1   12.01100 C ! aliphatic sp3 C for CH
MASS    23 CT2   12.01100 C ! aliphatic sp3 C for CH2
MASS    24 CT3   12.01100 C ! aliphatic sp3 C for CH3
MASS    25 CPH1  12.01100 C ! his CG and CD2 carbons
MASS    26 CPH2  12.01100 C ! his CE1 carbon


. . . etc. . . .
```

“Atom Types” != “PDB Atom Name”

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Anatomy of a Topology File II

```
. . .

RESI CLA       -1.00 ! Chloride Ion
GROUP
ATOM CLA  CLA -1.00
PATCHING FIRST NONE LAST NONE

RESI SOD        1.00 ! Sodium Ion
GROUP
ATOM SOD  SOD  1.00
PATCHING FIRST NONE LAST NONE

RESI CAL        2.00 ! Calcium Ion
GROUP
ATOM CAL  CAL  2.00
PATCHING FIRST NONE LAST NONE


. . .
```

CLA --> expected name in PDB file

CLA --> “atom type” in topology file (MASS)

MINIMAL FORMAT FOR A “RESIDUE”:

```
RESI “NAME”        TOTAL CHARGE
GROUP
ATOM “PDBNAME” “ATOM TYPE NAME” CHARGE
“DEFAULT PATCH STATEMENT”
```

a residue is defined between the initial RESI statement until another “keyword” is found (RESI, MASS, etc.) or EOF . . .

Generally, you don’t edit these files, you USE them . . .

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Anatomy of a Topology File III

RESI:

```
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE

RESI ALA          0.00
GROUP
ATOM N    NH1    -0.47  !      |
ATOM HN   H       0.31  !   HN-N
ATOM CA   CT1     0.07  !      |     HB1
ATOM HA   HB      0.09  !      |    /
GROUP                   !   HA-CA--CB-HB2
ATOM CB   CT3    -0.27  !      |     \
ATOM HB1  HA      0.09  !      |     HB3
ATOM HB2  HA      0.09  !    O=C
ATOM HB3  HA      0.09  !      |
GROUP                   !
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  N  HN  N  CA
BOND C  CA  C  +N  CA HA  CB HB1  CB HB2  CB HB3
DOUBLE O  C
IMPR N -C CA HN  C CA +N O
DONOR HN N
ACCEPTOR O C
IC -C   CA   *N   HN    1.3551 126.4900  180.0000 115.4200  0.9996
IC -C   N    CA   C     1.3551 126.4900  180.0000 114.4400  1.5390
IC N    CA   C    +N    1.4592 114.4400  180.0000 116.8400  1.3558
IC +N   CA   *C   O     1.3558 116.8400  180.0000 122.5200  1.2297
IC CA   C    +N   +CA   1.5390 116.8400  180.0000 126.7700  1.4613
IC N    C    *CA  CB    1.4592 114.4400  123.2300 111.0900  1.5461
IC N    C    *CA  HA    1.4592 114.4400 -120.4500 106.3900  1.0840
IC C    CA   CB   HB1   1.5390 111.0900  177.2500 109.6000  1.1109
IC HB1  CA   *CB  HB2   1.1109 109.6000  119.1300 111.0500  1.1119
IC HB1  CA   *CB  HB3   1.1109 109.6000 -119.5800 111.6100  1.1114

. . .
```

N --> expected name in PDB file

NH1 --> “atom type” in topology file (MASS)

A residue may then be subdivided into GROUps, which contain several atoms whose total charge is neutral or a unit charge. This subdivision is used in the calculation of nonbonded interactions using the group keyword and in the extended electrostatics options.

Anatomy of a Topology File IV

Internal Coordinates:

"optional"

one IC line for each atom in RESI

have information about N-1 & N+1 RESI

```
                          (1-2)    (1-2-3)    (1-2-3-4)  (2-3-4)  (3-4)
                           bond     bond       dihedral    bond     bond
 (1)   (2)   (3)   (4)    length    angle      angle      angle    length

IC -C    CA    *N    HN    1.3551  126.4900   180.0000  115.4200  0.9996
IC -C    N     CA    C     1.3551  126.4900   180.0000  114.4400  1.5390
IC N     CA    C     +N    1.4592  114.4400   180.0000  116.8400  1.3558
IC +N    CA    *C    O     1.3558  116.8400   180.0000  122.5200  1.2297
IC CA    C     +N    +CA   1.5390  116.8400   180.0000  126.7700  1.4613
IC N     C     *CA   CB    1.4592  114.4400   123.2300  111.0900  1.5461
IC N     C     *CA   HA    1.4592  114.4400  -120.4500  106.3900  1.0840
IC C     CA    CB    HB1   1.5390  111.0900   177.2500  109.6000  1.1109
IC HB1   CA    *CB   HB2   1.1109  109.6000   119.1300  111.0500  1.1119
IC HB1   CA    *CB   HB3   1.1109  109.6000  -119.5800  111.6100  1.1114
```

```
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |     HB1
ATOM HA   HB      0.09  !     |    /
GROUP                   !  HA-CA--CB-HB2
ATOM CB   CT3    -0.27  !     |    \
ATOM HB1  HA      0.09  !     |     HB3
ATOM HB2  HA      0.09  !   O=C
ATOM HB3  HA      0.09  !     |
GROUP                   !
ATOM C    C       0.51
ATOM O    O      -0.51
```

position of (1) determined from positions of 2-4

position of (4) determined from positions of 1-3

Thus, given a 3 atom seed all coordinates of RESI can be generated (using the IC definitions)

* --> on 3rd atom delineates an improper IC ("advanced")

Anatomy of a Topology File V

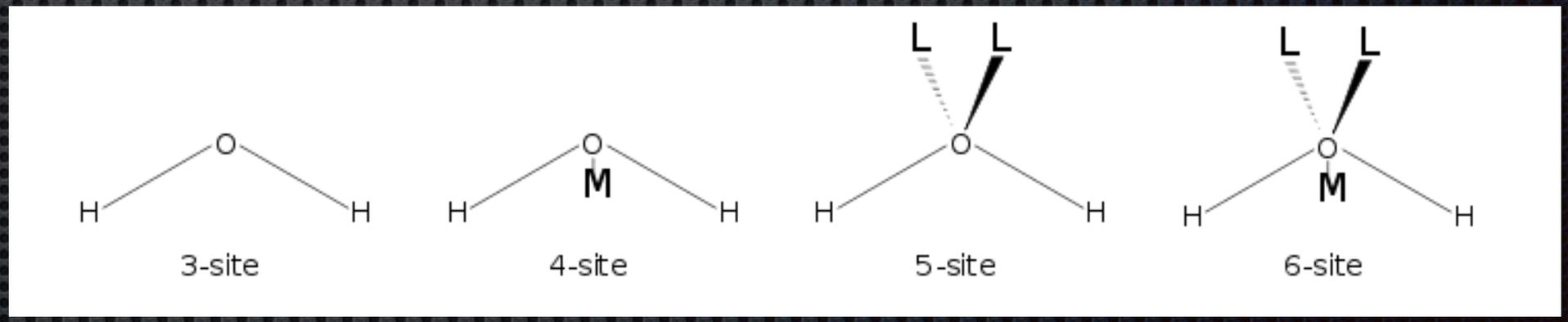
Water

. . .

```
RESI TIP3          0.000 ! tip3p water model, generate using noangle nodihedral
GROUP
ATOM OH2   OT      -0.834
ATOM H1    HT       0.417
ATOM H2    HT       0.417
BOND OH2 H1 OH2 H2 H1 H2     ! the last bond is needed
ANGLE H1 OH2 H2              ! required
ACCEPTOR OH2
PATCHING FIRS NONE LAST NONE
```

. . .

	TIPS[4]	SPC[5]	TIP3P[6]	SPC/E[7]
r(OH), Å	0.9572	1.0	0.9572	1.0
HOH, deg	104.52	109.47	104.52	109.47
A × 10^{-3}, kcal $Å^{12}$/mol	580.0	629.4	582.0	629.4
B, kcal $Å^6$/mol	525.0	625.5	595.0	625.5
q(O)	−0.80	−0.82	−0.834	−0.8476
q(H)	+0.40	+0.41	+0.417	+0.4238



http://en.wikipedia.org/wiki/Water_model

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Anatomy of a Topology File VI

Patches: PRES

```
PRES NTER          1.00 ! standard N-terminus
GROUP                   ! use in generate statement
ATOM N     NH3    -0.30 !
ATOM HT1   HC      0.33 !          HT1
ATOM HT2   HC      0.33 !      (+)/
ATOM HT3   HC      0.33 ! --CA--N--HT2
ATOM CA    CT1     0.21 !   |     \
ATOM HA    HB      0.10 !   HA     HT3
DELETE ATOM HN
BOND HT1 N HT2 N HT3 N
DONOR HT1 N
DONOR HT2 N
DONOR HT3 N
IC HT1  N    CA   C     0.0000  0.0000  180.0000  0.0000  0.0000
IC HT2  CA   *N   HT1   0.0000  0.0000  120.0000  0.0000  0.0000
IC HT3  CA   *N   HT2   0.0000  0.0000  120.0000  0.0000  0.0000
```

ATOM statements here:

(1) **ADD new atoms (HT1, HT2, HT3)**

(2) **MODIFY & CHANGE the type and charge (N, CA, HA)**

Patches are used to:

Alter protonation state (ASPP, GLUP, HS2, ...)

Create RS-SR' bonds (DISU)

Attach HEME groups (PHEM)

Alter terminii (NTER, CTER, GLYP, PROP)

...

Anatomy of a Topology File VII

Patches (cont.): more examples . . .

```
PRES GLYP          1.00 ! Glycine N-terminus
GROUP                   ! use in generate statement
ATOM N    NH3    -0.30 !
ATOM HT1  HC      0.33 !   HA1   HT1
ATOM HT2  HC      0.33 !   | (+)/
ATOM HT3  HC      0.33 ! --CA--N--HT2
ATOM CA   CT2     0.13 !   |    \
ATOM HA1  HB      0.09 !   HA2   HT3
ATOM HA2  HB      0.09 !
DELETE ATOM HN
BOND HT1 N HT2 N HT3 N
DONOR HT1 N
DONOR HT2 N
DONOR HT3 N
IC HT1  N    CA   C     0.0000  0.0000  180.0000  0.0000  0.0000
IC HT2  CA   *N   HT1   0.0000  0.0000  120.0000  0.0000  0.0000
IC HT3  CA   *N   HT2   0.0000  0.0000  120.0000  0.0000  0.0000

PRES PROP          1.00 ! Proline N-Terminal
GROUP                   ! use in generate statement
ATOM N    NP     -0.07 !   HA
ATOM HN1  HC      0.24 !   |
ATOM HN2  HC      0.24 !  -CA   HN1
ATOM CD   CP3     0.16 !  /  \ /
ATOM HD1  HA      0.09 !       N(+)
ATOM HD2  HA      0.09 !      / \
ATOM CA   CP1     0.16 !  -CD    HN2
ATOM HA   HB      0.09 !   | \
BOND HN1 N HN2 N       !  HD1 HD2
DONOR HN1 N
DONOR HN2 N
IC HN1  CA   *N   CD    0.0000  0.0000  120.0000  0.0000  0.0000
IC HN2  CA   *N   HN1   0.0000  0.0000  120.0000  0.0000  0.0000
```

```
PRES ACE           0.00 ! acetylated N-terminus
GROUP                   ! use in generate statement
ATOM CAY  CT3    -0.27 !
ATOM HY1  HA      0.09 ! HY1 HY2 HY3
ATOM HY2  HA      0.09 !    \ | /
ATOM HY3  HA      0.09 !     CAY
GROUP                  !      |
ATOM CY   C       0.51 !     CY=OY
ATOM OY   O      -0.51 !      |
                       !
BOND CY CAY CY N CAY HY1 CAY HY2 CAY HY3
DOUBLE OY CY
IMPR CY CAY N OY
IMPR N CY CA HN
ACCEPTOR OY CY
IC CY   N    CA   C     0.0000  0.0000  -60.0000  0.0000  0.0000
IC CY   CA   *N   HN    0.0000  0.0000  180.0000  0.0000  0.0000
IC CAY  CY   N    CA    0.0000  0.0000  180.0000  0.0000  0.0000
IC N    CAY  *CY  OY    0.0000  0.0000  180.0000  0.0000  0.0000
IC OY   CY   CAY  HY1   0.0000  0.0000  180.0000  0.0000  0.0000
IC OY   CY   CAY  HY2   0.0000  0.0000   60.0000  0.0000  0.0000
IC OY   CY   CAY  HY3   0.0000  0.0000  -60.0000  0.0000  0.0000
```

Anatomy of a Topology File VIII

```
. . .

PRES 5TER          0.00  ! 5'-terminal HYDROXYL patch, from MeOH
                         ! use in generate statement
GROUP
ATOM H5T  HN5      0.43
ATOM O5'  ON5     -0.66
ATOM C5'  CN8B     0.05
ATOM H5'  HN8      0.09
ATOM H5'' HN8      0.09
!
DELETE ATOM P
DELETE ATOM O1P
DELETE ATOM O2P
!
BOND H5T   O5'
DONO H5T   O5'
BILD H5T  O5'   C5'  C4'   0.0000    0.00  180.00    0.00   0.0000


PRES 3TER          0.00  ! 3'terminal HYDROXYL patch, from MeOH
                         ! use in generate statement
GROUP
ATOM C3'  CN7      0.14
ATOM H3'  HN7      0.09
ATOM O3'  ON5     -0.66
ATOM H3T  HN5      0.43
BOND O3'  H3T
DONO H3T  O3'
BILD H3T  O3'   C3'  C4'   0.9600  114.97  148.63  111.92   1.5284


. . .
```

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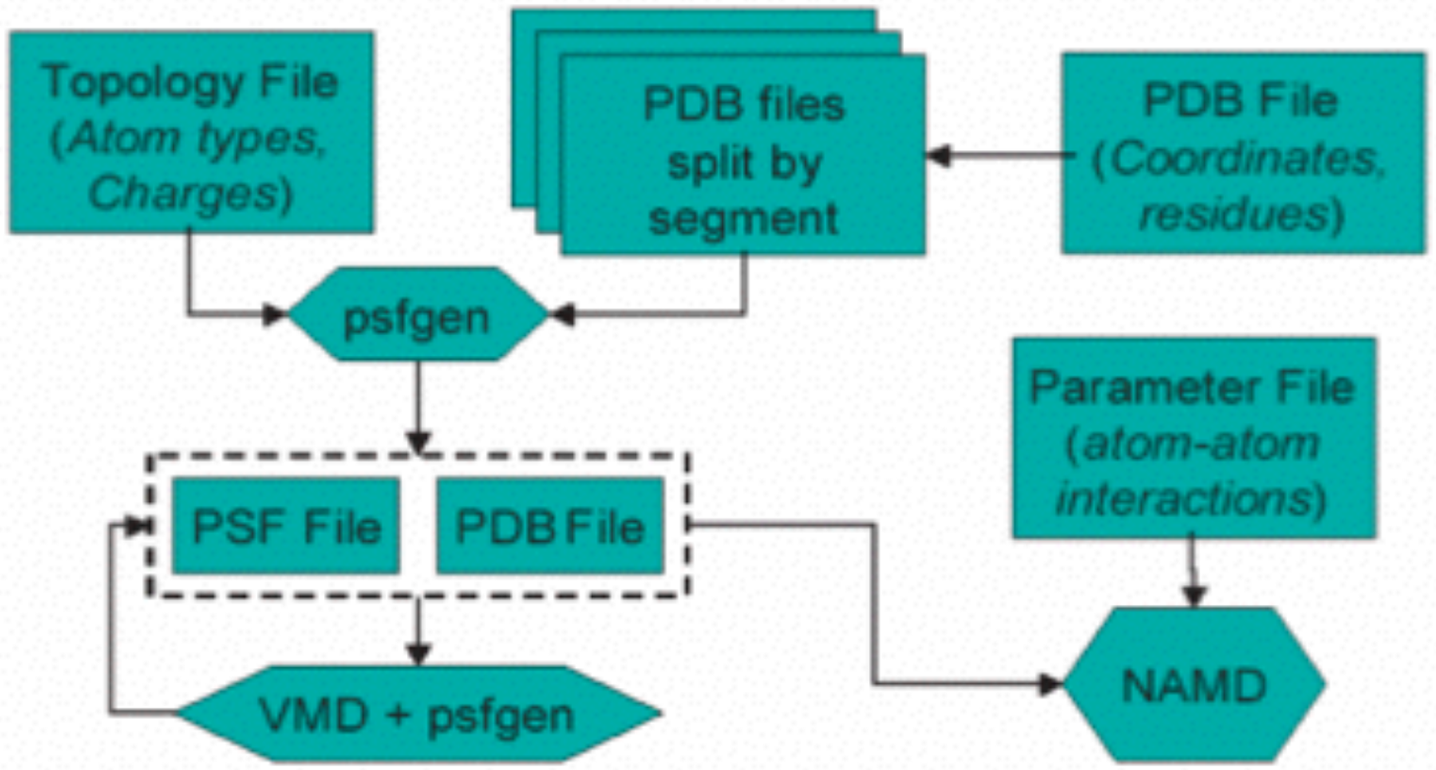
The Process



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PSFGEN

A program to read your structure files (separate PDB files for each segment) and use the topology file ("dictionary") to build the complete system.

The program needs an input file to tell it what to do

USAGE (unix prompt):

>psfgen build_system.psfgen >& build.out &

Sample input file (here named: build_system.psfgen):

```
topology /home/mdschool/toppar/top_all27_prot_na.inp

segment
  auto none

  pdb output_building/oh2.pdb
}
coordpdb output_building/oh2.pdb

guesscoord

writepsf output_building/one_water.psf

writepdb output_building/one_water.pdb
```

path to topology file

define a segment
pre-build command

path to pdb file

path coordinate file (pdb)

use IC to add H etc.

OUTPUT FILES

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PSFGEN II (OUTPUT)

```
ATOM      1  OH2 TIP3 A   1       0.000   0.000   0.000  1.00  0.00      WAT1 O
```

(jc@ocho)psfgen/single_water% cat build.out

. . .

```
Created by CHARMM version 27 1
duplicate residue key CAL will be ignored
duplicate residue key DUM will be ignored
building segment TIP3
disabling angle autogeneration
disabling dihedral autogeneration
reading residues from pdb file output_building/oh2.pdb
extracted 1 residues from pdb file
Info: generating structure...
Info: segment complete.
reading coordinates from pdb file output_building/oh2.pdb for segment TIP3
Info: guessing coordinates for 2 atoms (0 non-hydrogen)
Warning: poorly guessed coordinates for 2 atoms (0 non-hydrogen):
Warning: poorly guessed coordinate for atom H1          TIP3:A          TIP3
Warning: poorly guessed coordinate for atom H2          TIP3:A          TIP3
Info: writing psf file output_building/one_water.psf
total of 3 atoms
total of 3 bonds
total of 1 angles
total of 0 dihedrals
total of 0 impropers
total of 0 cross-terms
Info: psf file complete.
Info: writing pdb file output_building/one_water.pdb
Info: Atoms with guessed coordinates will have occupancy of 0.0.
Info: pdb file complete.
```

HINTS:

“poorly guessed ...”
- search PDB for 0.000
- search PDB for 99999.999

new PDB file:
- important! (H, patches, ... etc.)

NEVER ASSUME that since the script ran that it did what you expected
- inspect output
- inspect output files
- inspect structure (VMD)

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PSFGEN II (OUTPUT)

```
ATOM      1  OH2 TIP3 A   1       0.000   0.000   0.000  1.00  0.00      WAT1 O
```

```
REMARK original generated coordinate pdb file
ATOM      1  OH2 TIP3    0       0.000   0.000   0.000  1.00  0.00       TIP3 O
ATOM      2  H1  TIP3    0       1.000   0.000   0.000  0.00  0.00       TIP3 H
ATOM      3  H2  TIP3    0      -0.326   0.946   0.000  0.00  0.00       TIP3 H
END
```

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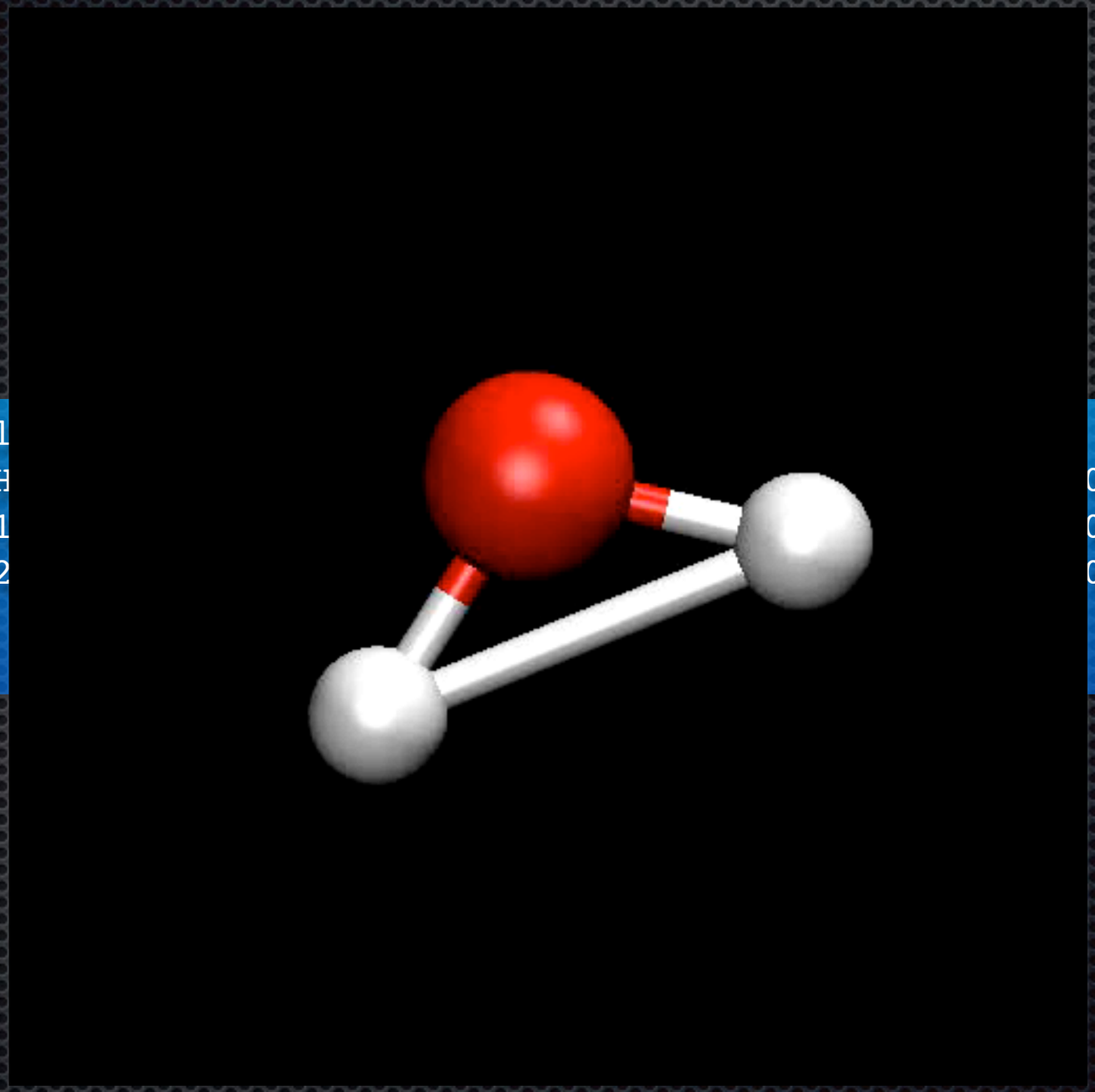
PSFGEN II (OUTPUT)

```
ATOM      1  OH2 TIP3 A   1       0.000   0.000   0.000  1.00  0.00      WAT1 O
```



```
REMARK original
ATOM      1  OH                                    0.00      TIP3 O
ATOM      2  H1                                    0.00      TIP3 H
ATOM      3  H2                                    0.00      TIP3 H
END
```

PSFGEN III

protein

Sample input file (here named: build_system_protein.psfgen):

>psfgen build_system_protein.psfgen >& build_protein.out &

```
topology /home/mdschool/toppar/top_all27_prot_na.inp

alias residue HIS HSE

segment PCLN {
 first NTER
 last CTER
 pdb output_building/icln.pdb
}

coordpdb output_building/icln.pdb PCLN

guesscoord

writepsf output_building/

writepdb output_building/
```

path to topology file

correct naming issues

pre-build commands

path to pdb file (sequence)

path coordinate file (pdb)

use IC to add H etc.

OUTPUT FILES

all terminal patches go in segment area

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PSFGEN IV (OUTPUT)

(jc@ocho)psfgen/protein% cat build_protein.out

. . .

```
Created by CHARMM version 27 1
duplicate residue key CAL will be ignored
duplicate residue key DUM will be ignored
aliasing residue HIS to HSE
building segment PCLN
setting patch for first residue to NTER
setting patch for last residue to CTER
reading residues from pdb file output_building/icln.pdb
extracted 116 residues from pdb file
Info: generating structure...
Info: skipping improper N-C-CA-HN at beginning of segment.
Info: skipping conformation C-N-CA-C at beginning of segment.
Info: skipping conformation C-CA-N-HN at beginning of segment.
Info: skipping bond C-N at end of segment.
Info: skipping improper C-CA-N-O at end of segment.
Info: skipping conformation CA-C-N-CA at end of segment.
Info: skipping conformation N-CA-C-O at end of segment.
Info: skipping conformation N-CA-C-N at end of segment.
Info: segment complete.
reading coordinates from pdb file output_building/icln.pdb for segment PCLN
Warning: failed to set coordinate for atom H     GLN:27   PCLN
Warning: failed to set coordinate for atom HB3   GLN:27   PCLN
Warning: failed to set coordinate for atom HG3   GLN:27   PCLN
Warning: failed to set coordinate for atom H     GLN:28   PCLN
Warning: failed to set coordinate for atom HB3   GLN:28   PCLN
Warning: failed to set coordinate for atom HG3   GLN:28   PCLN
Warning: failed to set coordinate for atom H     GLN:29   PCLN
```

. . .

```
Info: guessing coordinates for 287 atoms (5 non-hydrogen)
Warning: poorly guessed coordinates for 127 atoms (2 non-hydrogen):
         poorly guessed coordinate for atom HT1  GLN:27   PCLN
         poorly guessed coordinate for atom HT2  GLN:27   PCLN
         poorly guessed coordinate for atom HT3  GLN:27   PCLN
```

HINTS:

“Warning: failed to set coor. ...”

pdb <-> topology naming issues (use more alias commands or fix pdb file)

new PDB file:

important! (H, patches, ... etc.)

NEVER ASSUME that since the script ran that it did what you expected

inspect output

inspect output files

inspect structure (VMD)

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```
Info: skipping improper C-CA-N-O at end of segment.
Info: skipping conformation CA-C-N-CA at end of segment.
Info: skipping conformation N-CA-C-O at end of segment.
Info: skipping conformation N-CA-C-N at end of segment.
Info: segment complete.
reading coordinates from pdb file output_building/icln.pdb for segment PCLN
Warning: failed to set coordinate for atom H     GLN:27   PCLN
Warning: failed to set coordinate for atom HB3   GLN:27   PCLN
Warning: failed to set coordinate for atom HG3   GLN:27   PCLN
Warning: failed to set coordinate for atom H     GLN:28   PCLN
Warning: failed to set coordinate for atom HB3   GLN:28   PCLN
Warning: failed to set coordinate for atom HG3   GLN:28   PCLN
Warning: failed to set coordinate for atom H     GLN:29   PCLN

. . .

Info: guessing coordinates for 287 atoms (5 non-hydrogen)
Warning: poorly guessed coordinates for 127 atoms (2 non-hydrogen):
Warning: poorly guessed coordinate for atom HT1  GLN:27   PCLN
Warning: poorly guessed coordinate for atom HT2  GLN:27   PCLN
Warning: poorly guessed coordinate for atom HT3  GLN:27   PCLN
Warning: poorly guessed coordinate for atom HB1  GLN:27   PCLN
Warning: poorly guessed coordinate for atom HG1  GLN:27   PCLN
Warning: poorly guessed coordinate for atom HB1  GLN:28   PCLN
Warning: poorly guessed coordinate for atom HG1  GLN:28   PCLN
Warning: poorly guessed coordinate for atom HB1  GLN:29   PCLN

. . .

Info: writing psf file output_building/new_icln.psf
total of 1745 atoms
total of 1762 bonds
total of 3177 angles
total of 4651 dihedrals
total of 297 impropers
total of 0 cross-terms
Info: psf file complete.
Info: writing pdb file output_building/new_icln.pdb
Info: Atoms with guessed coordinates will have occupancy of 0.0.
Info: pdb file complete.
PCLN:27
PCLN:112
```

HINTS:

"Warning: failed to set coor. ..."

pdb <-> topology naming issues (use more alias commands or fix pdb file)

new PDB file:

important! (H, patches, ... etc.)

NEVER ASSUME that since the script ran that it did what you expected

inspect output

inspect output files

inspect structure (VMD)

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Original pdb file (icln.pdb)

```
ATOM      1  N   GLN A  27
ATOM      2  CA  GLN A  27
ATOM      3  C   GLN A  27
ATOM      4  O   GLN A  27
ATOM      5  CB  GLN A  27
ATOM      6  CG  GLN A  27
ATOM      7  CD  GLN A  27
ATOM      8  OE1 GLN A  27
ATOM      9  NE2 GLN A  27
ATOM     10  H   GLN A  27
ATOM     11  HA  GLN A  27
ATOM     12  HB2 GLN A  27
ATOM     13  HB3 GLN A  27
ATOM     14  HG2 GLN A  27
ATOM     15  HG3 GLN A  27
ATOM     16 HE21 GLN A  27
ATOM     17 HE22 GLN A  27
 . . .
```

Topology for RESI GLN

```
RESI GLN          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |   HB1 HG1 OE1   HE21 (cis to OE1)
ATOM HA   HB      0.09  !     |   |   |   ||    /
GROUP                   !  HA-CA--CB--CG--CD--NE2
ATOM CB   CT2    -0.18  !     |   |   |         \
ATOM HB1  HA      0.09  !     |   HB2 HG2       HE22 (trans to OE1)
ATOM HB2  HA      0.09  !   O=C
GROUP                   !     |
ATOM CG   CT2    -0.18
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
GROUP
ATOM CD   CC      0.55
ATOM OE1  O      -0.55
GROUP
ATOM NE2  NH2    -0.62
ATOM HE21 H       0.32
ATOM HE22 H       0.30
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
```

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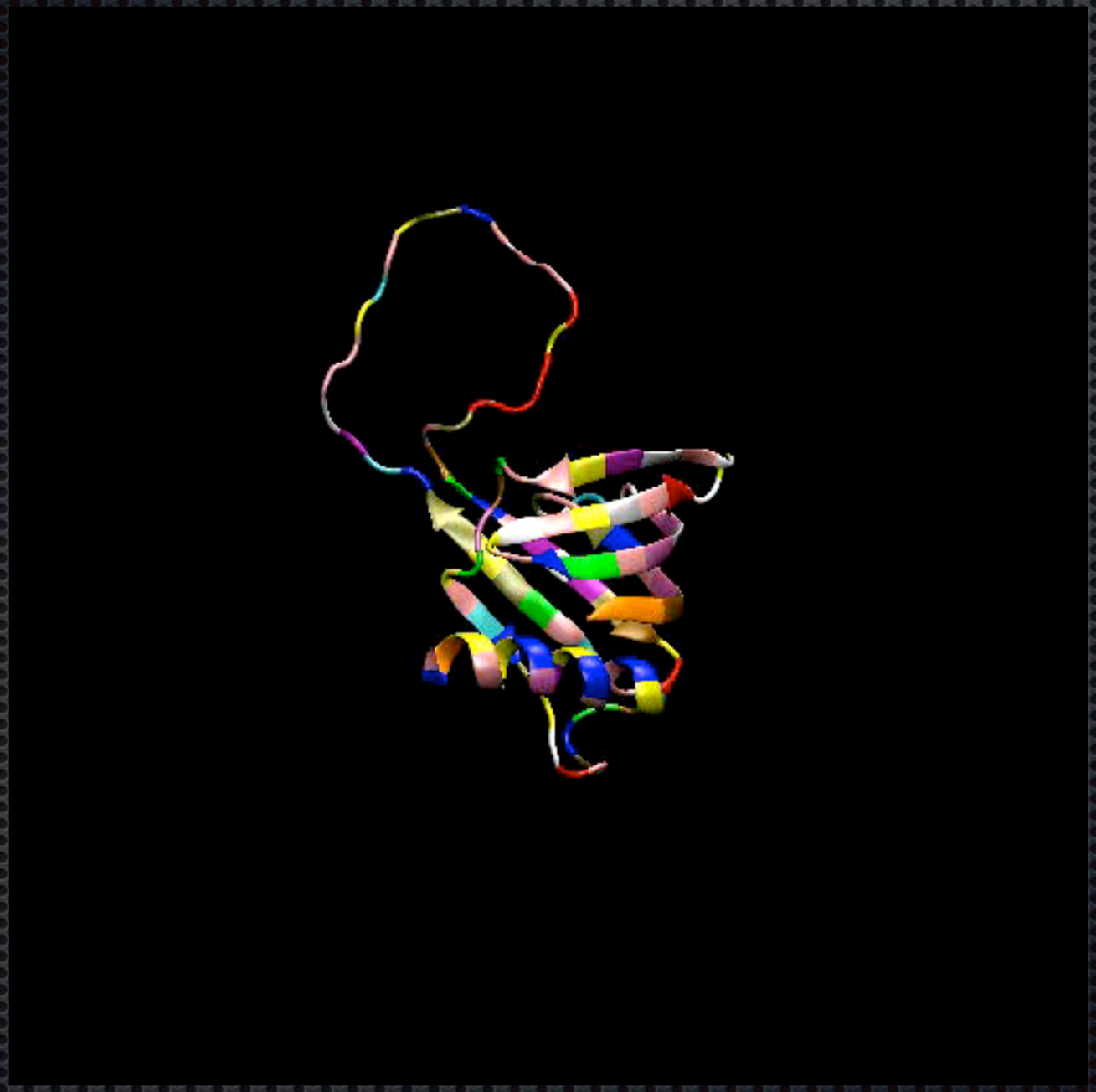

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PSFGEN V

protein II (with patches)

Sample input file (here named: build_system_protein_II.psfgen):

>psfgen build_system_protein_II.psfgen >& build_protein_II.out &

```
topology /home/mdschool1/toppar/top_all27_prot_na.inp

alias residue HIS HSE
alias atom ILE CD1 CD

segment HYDR {
 first NTER
 last CTER
 pdb output_building/hydrolase.pdb
}

coordpdb output_building/hydrolase.pdb HYDR

patch DISU HYDR:22  HYDR:157
patch DISU HYDR:42  HYDR:58
patch DISU HYDR:128 HYDR:232
patch DISU HYDR:136 HYDR:201
patch DISU HYDR:168 HYDR:182
patch DISU HYDR:191 HYDR:220

guesscoord

writepsf output_building/new_hydrolase.psf

writepdb output_building/new_hydrolase.pdb
```

path to topology file

correct naming issues

pre-build commands

path to pdb file (sequence)

path coordinate file (pdb)

post-build commands

use IC to add H etc.

OUTPUT FILES

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PSFGEN VI (OUTPUT)

```
(jc@ocho)psfgen/protein% cat build_protein_II.out

. . .

Created by CHARMM version 27 1
duplicate residue key CAL will be ignored
duplicate residue key DUM will be ignored
aliasing residue HIS to HSE
aliasing residue ILE atom CD1 to CD
building segment HYDR
setting patch for first residue to NTER
setting patch for last residue to CTER
reading residues from pdb file output_building/hydrolase.pdb
extracted 220 residues from pdb file
Info: generating structure...
Info: skipping improper N-C-CA-HN at beginning of segment.
Info: skipping conformation C-N-CA-C at beginning of segment.
Info: skipping conformation C-CA-N-HN at beginning of segment.
Info: skipping bond C-N at end of segment.
Info: skipping improper C-CA-N-O at end of segment.
Info: skipping conformation CA-C-N-CA at end of segment.
Info: skipping conformation N-CA-C-O at end of segment.
Info: skipping conformation N-CA-C-N at end of segment.
Info: segment complete.
reading coordinates from pdb file output_building/hydrolase.pdb for segment HYDR
Warning: failed to set coordinate for atom O     ASN:245        HYDR
Warning: failed to set coordinate for atom OXT   ASN:245        HYDR
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
Info: guessing coordinates for 1563 atoms (2 non-hydrogen)
Warning: poorly guessed coordinates for 19 atoms (2 non-hydrogen):
Warning: poorly guessed coordinate for atom HT1  ILE:16   HYDR
Warning: poorly guessed coordinate for atom HT2  ILE:16   HYDR
Warning: poorly guessed coordinate for atom HT3  ILE:16   HYDR
```

HINTS:

"Warning: failed to set coor. ..."
pdb <-> topology naming issues (use more alias commands or fix pdb file)

new PDB file:
important! (H, patches, ... etc.)

NEVER ASSUME that since the script ran that it did what you expected
inspect output
inspect output files
inspect structure (VMD)

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```
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
applying patch DISU to 2 residues
Info: guessing coordinates for 1563 atoms (2 non-hydrogen)
Warning: poorly guessed coordinates for 19 atoms (2 non-hydrogen):
Warning: poorly guessed coordinate for atom HT1  ILE:16   HYDR
Warning: poorly guessed coordinate for atom HT2  ILE:16   HYDR
Warning: poorly guessed coordinate for atom HT3  ILE:16   HYDR
Warning: poorly guessed coordinate for atom HG   LEU:33   HYDR
Warning: poorly guessed coordinate for atom HG   LEU:46   HYDR
Warning: poorly guessed coordinate for atom HG   LEU:67   HYDR
Warning: poorly guessed coordinate for atom HG   LEU:99   HYDR
Warning: poorly guessed coordinate for atom HG   LEU:105        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:108        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:114        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:123        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:137        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:155        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:158        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:163        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:185        HYDR
Warning: poorly guessed coordinate for atom HG   LEU:209        HYDR
Warning: poorly guessed coordinate for atom OT1  ASN:245        HYDR
Warning: poorly guessed coordinate for atom OT2  ASN:245        HYDR
Info: writing psf file output_building/new_hydrolase.psf
total of 3160 atoms
total of 3196 bonds
total of 5767 angles
total of 8444 dihedrals
total of 569 impropers
total of 0 cross-terms
Info: psf file complete.
Info: writing pdb file output_building/new_hydrolase.pdb
Info: Atoms with guessed coordinates will have occupancy of 0.0.

HYDR:245
HYDR:22 HYDR:157
HYDR:42 HYDR:58
HYDR:128 HYDR:232
HYDR:136 HYDR:201
HYDR:168 HYDR:182
91 HYDR:220
```

HINTS:

“Warning: failed to set coor. ...”

pdb <-> topology naming issues (use more alias commands or fix pdb file)

new PDB file:

important! (H, patches, ... etc.)

NEVER ASSUME that since the script ran that it did what you expected

inspect output

inspect output files

inspect structure (VMD)

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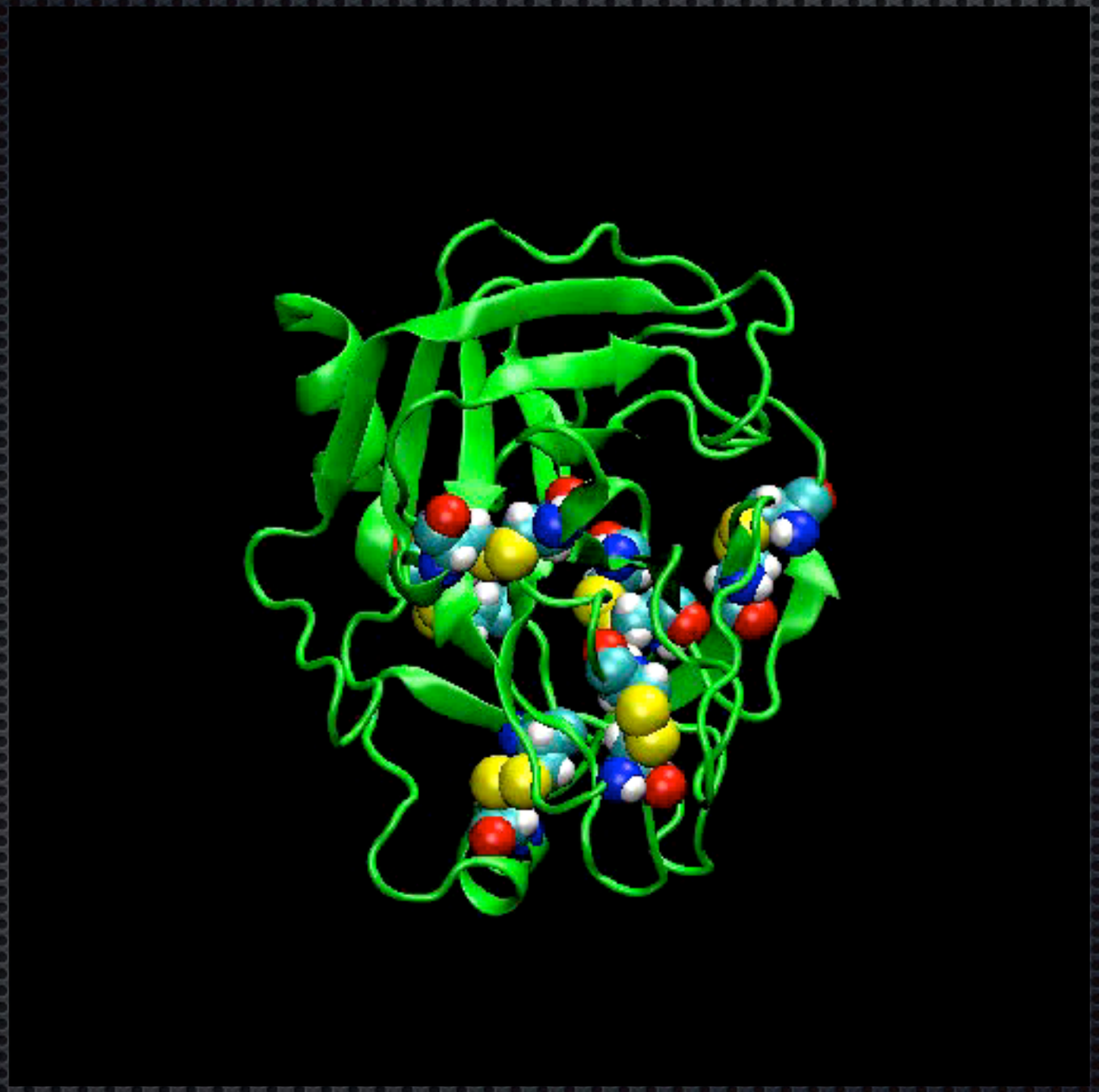

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PSFGEN VII

protein III (multiple segments with patches)

Sample input file (here named: build_system_protein_III.psfgen):

>psfgen build_system_protein_III.psfgen >& build_protein_III.out &

```
topology /home/mdschool/toppar/top_all27_prot_na.inp

alias residue HIS HSE
alias atom ILE CD1 CD

segment FIXA {
 first NTER
 last CTER
 pdb output_building/chain_a.pdb
}
coordpdb output_building/chain_a.pdb FIXA

segment FIXB {
 first NTER
 last CTER
 pdb output_building/chain_b.pdb
}
coordpdb output_building/chain_b.pdb FIXB

patch DISU FIXA:42  FIXA:58
patch DISU FIXA:122 FIXB:132
patch DISU FIXA:168 FIXA:182
patch DISU FIXA:191 FIXA:220
patch DISU FIXB:88  FIXB:99
patch DISU FIXB:95  FIXB:109
patch DISU FIXB:111 FIXB:124

guesscoord

writepsf output_building/new_factorIXA.psf

writepdb output_building/new_factorIXA.pdb
```

path to topology file

correct naming issues

pre-build commands

path to pdb file (sequence)

path coordinate file I (pdb)

pre-build commands

path to pdb file II (sequence)

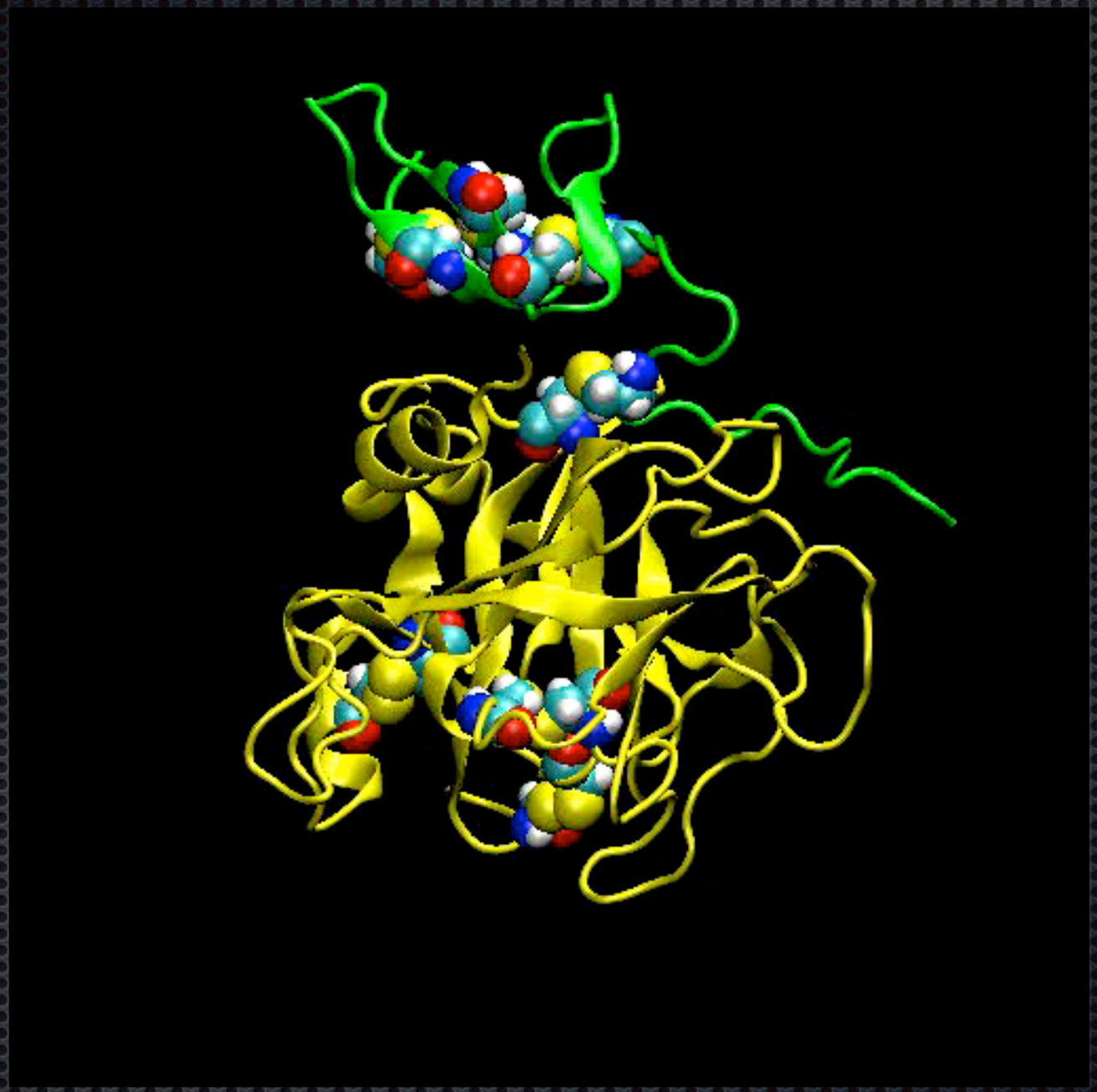
path coordinate file II (pdb)

post-build commands

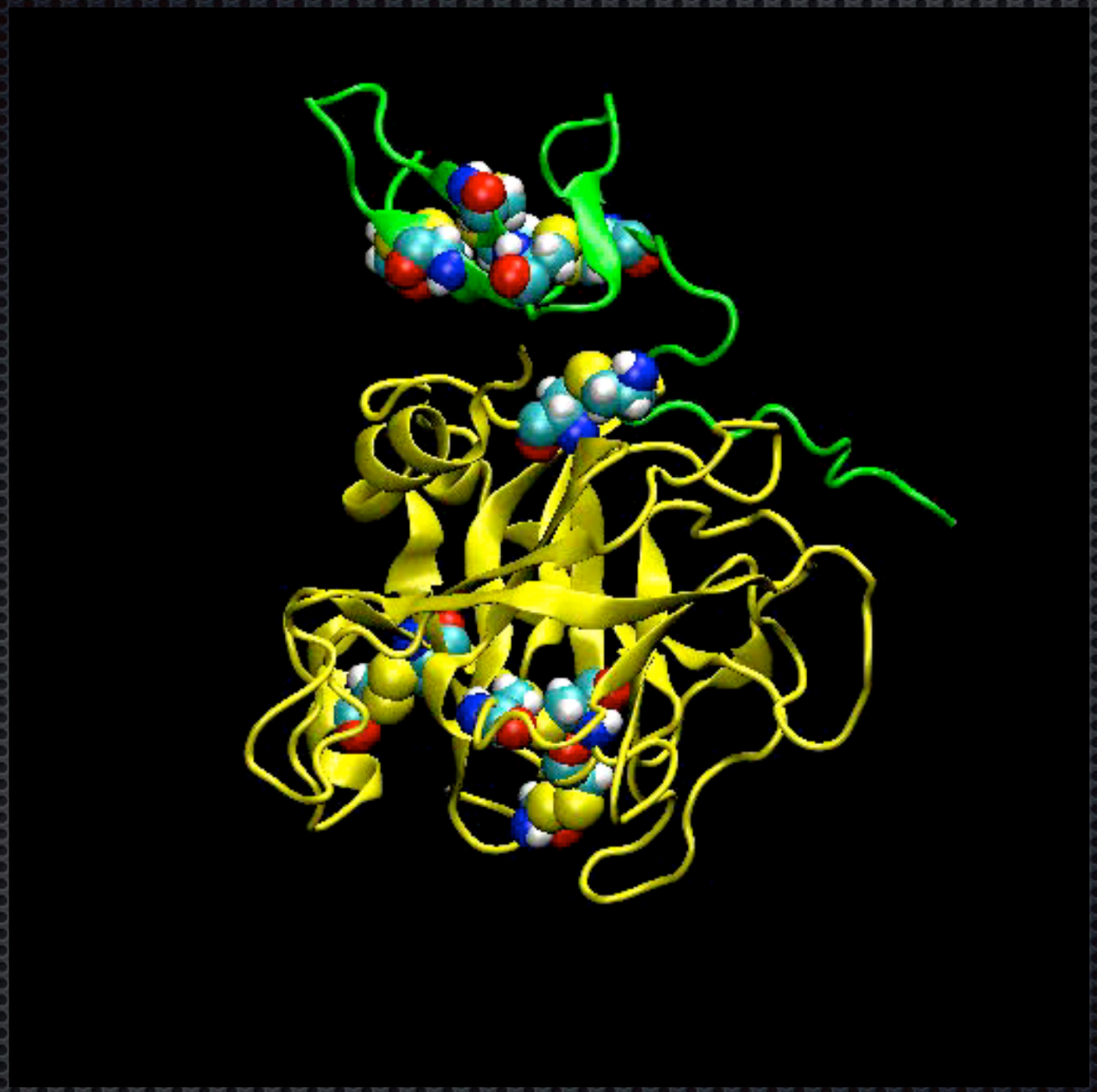
use IC to add H etc.

OUTPUT FILES

PSFGEN VIII (OUTPUT)



PSFGEN VIII (OUTPUT)



PSFGEN IX

protein/dna complex

Sample input file (here named: build_system_protein_dna_complex.psfgen):

>psfgen build_system_protein_dna_complex.psfgen >& build_protein_dna_complex.out &

```
topology /home/mdschool1/toppar/top_all27_prot_na.inp

alias residue HIS HSE
alias atom ILE CD1 CD
alias atom SER HG HG1
alias atom CYS HG HG1
alias atom THY C5A C5M

segment INT1 {
 first NTER
 last CTER
 pdb output_building/fixed_int1.pdb
}
coordpdb output_building/fixed_int1.pdb INT1

segment INT2 {
 first NTER
 last CTER
 pdb output_building/fixed_int2.pdb
}
coordpdb output_building/fixed_int2.pdb INT2

segment INT3 {
 first NTER
 last CTER
 pdb output_building/fixed_int3.pdb
}
coordpdb output_building/fixed_int3.pdb INT3

segment INT4 {
 first NTER
 last CTER
```

System:

4 Integrase proteins

2 LEDGF proteins

3 pieces of DNA (6 chains)*

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```
 first 5TER
 last 3TER
 pdb output_building/dna1.pdb
}
coordpdb output_building/dna1.pdb DNA1

segment DNA2 {
 first 5TER
 last 3TER
 pdb output_building/dna2.pdb
}
coordpdb output_building/dna2.pdb DNA2

segment DNA3 {
 first 5TER
 last 3TER
 pdb output_building/dna3.pdb
}
coordpdb output_building/dna3.pdb DNA3

segment DNA4 {
 first 5TER
 last 3TER
 pdb output_building/dna4.pdb
}
coordpdb output_building/dna4.pdb DNA4

segment DNA5 {
 first 5TER
 last 3TER
 pdb output_building/dna5.pdb
}
coordpdb output_building/dna5.pdb DNA5

segment DNA6 {
 first 5TER
 last 3TER
 pdb output_building/dna6.pdb
}
coordpdb output_building/dna6.pdb DNA6

guesscoord

writepsf output_building/new_complex.psf
writepdb output_building/new_complex.pdb
```

System:

4 Integrase proteins

2 LEDGF proteins

3 pieces of DNA (6 chains)*

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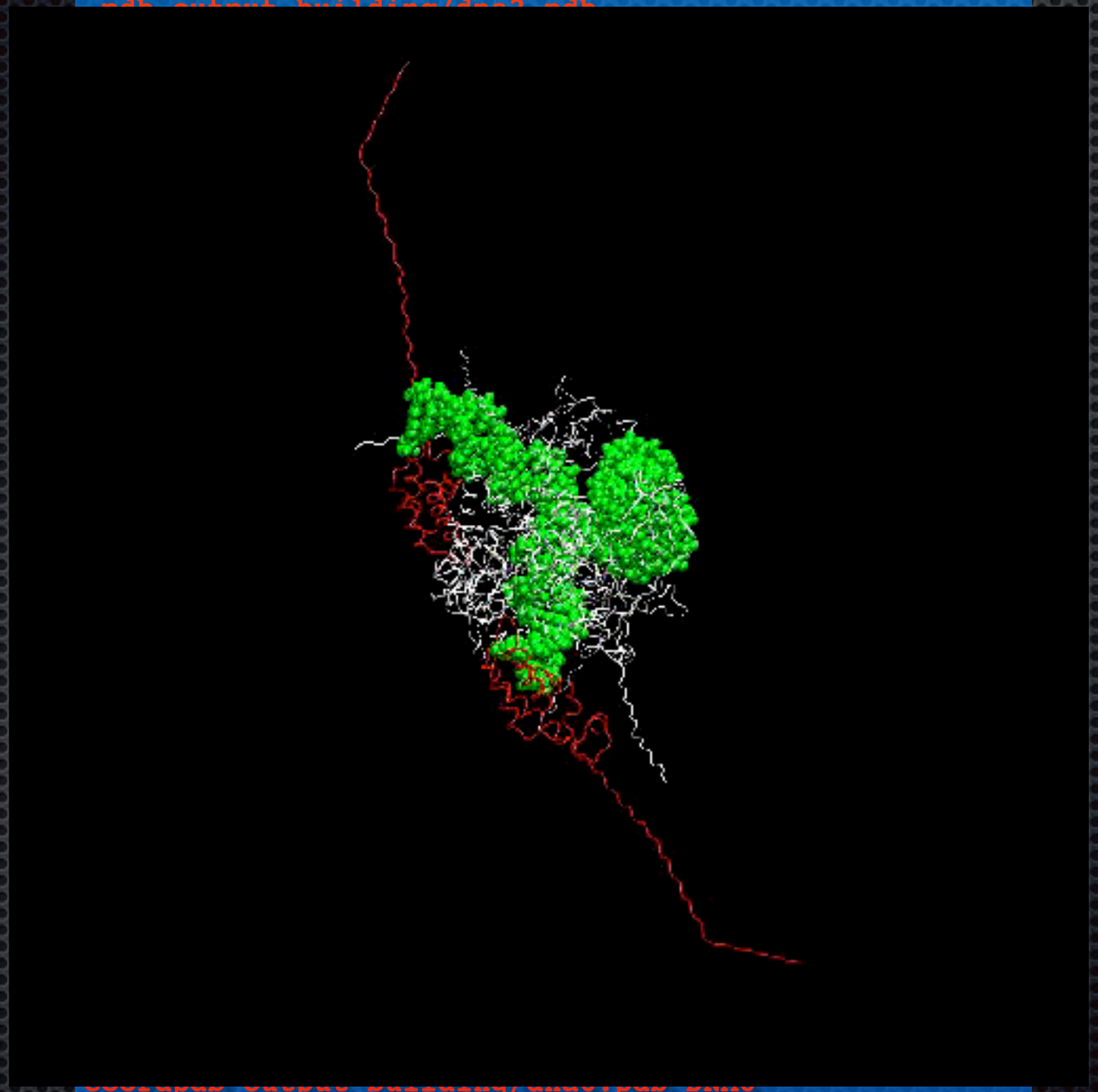
```
 first 5TER
 last 3TER
 pdb output_building/dna1.pdb
}
coordpdb output_building/dna1.pdb DNA1

segment DNA2 {
 first 5TER
 last 3TER
```



System:

4 Integrase proteins

2 LEDGF proteins

3 pieces of DNA (6 chains)*

```
guesscoord

writepsf output_building/new_complex.psf
writepdb output_building/new_complex.pdb
```

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Actually, for DNA you need to apply two patches (one specific patch for each residue type for every residue individually):

DEO1 : PYRIMIDINES

DEO2: PURINES

LAB_2: (today) . . . part III

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PSF File of Water

```
PSF

       3 !NTITLE
 REMARKS original generated structure x-plor psf file
 REMARKS topology /Users/curtisj/research/toppar/top_all27_prot_na.inp
 REMARKS segment TIP3 { first NONE; last NONE; auto none  }

       3 !NATOM
       1 TIP3 A    TIP3 OH2  OT    -0.834000       15.9994           0
       2 TIP3 A    TIP3 H1   HT     0.417000        1.0080           0
       3 TIP3 A    TIP3 H2   HT     0.417000        1.0080           0

       3 !NBOND: bonds
       1       2       1       3       2       3

       1 !NTHETA: angles
       2       1       3

       0 !NPHI: dihedrals


       0 !NIMPHI: impropers


  . . . etc. . . .
```

“Atom Types” != “PDB Atom Name”

PSF File of Protein I

```
PSF

       6 !NTITLE
 REMARKS original generated structure x-plor psf file
 REMARKS 2 patches were applied to the molecule.
 REMARKS topology /Users/curtisj/research/toppar/top_all27_prot_na.inp
 REMARKS segment PCLN { first NTER; last CTER; auto angles dihedrals }
 REMARKS patch NTER PCLN:27
 REMARKS patch CTER PCLN:142

    1745 !NATOM
       1 PCLN 27   GLN  N    NH3   -0.300000       14.0070           0
       2 PCLN 27   GLN  HT1  HC     0.330000        1.0080           0
       3 PCLN 27   GLN  HT2  HC     0.330000        1.0080           0
       4 PCLN 27   GLN  HT3  HC     0.330000        1.0080           0
       5 PCLN 27   GLN  CA   CT1    0.210000       12.0110           0
       6 PCLN 27   GLN  HA   HB     0.100000        1.0080           0
       7 PCLN 27   GLN  CB   CT2   -0.180000       12.0110           0
       8 PCLN 27   GLN  HB1  HA     0.090000        1.0080           0
       9 PCLN 27   GLN  HB2  HA     0.090000        1.0080           0
      10 PCLN 27   GLN  CG   CT2   -0.180000       12.0110           0
      11 PCLN 27   GLN  HG1  HA     0.090000        1.0080           0
      12 PCLN 27   GLN  HG2  HA     0.090000        1.0080           0

. . .

    1744 PCLN 142  LEU  HD22 HA     0.090000        1.0080           0
    1745 PCLN 142  LEU  HD23 HA     0.090000        1.0080           0
```

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PSF File of Protein II

```
. . .

      1762 !NBOND: bonds
         1         5         2         1         3         1         4         1
         5         6         7         5         7         8         7         9
        10         7        10        11        10        12        13        10
        13        14        15        13        15        16        15        17
        18         5        18        20        19        18        20        21
        20        22        22        23        24        22        24        25
        24        26        27        24        27        28        27        29

. . .

      1738      1740      1738      1741      1742      1736      1742      1743
      1742      1744      1742      1745

. . .
```

PSF File of Protein III

```
. . .

    3177 !NTHETA: angles
       1       5       6       1       5      18       2       1       5
       2       1       4       2       1       3       3       1       5
       3       1       4       4       1       5       5      18      19
       5      18      20       5       7       9       5       7       8
       5       7      10       7      10      12       7      10      11
       7      10      13       7       5       6       7       5      18

. . .

       1739    1738    1740    1740    1738    1741    1742    1736    1737
       1743    1742    1745    1743    1742    1744    1744    1742    1745

. . .
```

PSF File of Protein IV

```
. . .

      4651 !NPHI: dihedrals
         1         5         7        10         1         5         7         8
         1         5         7         9         1         5        18        20
         1         5        18        19         2         1         5         7
         2         1         5        18         2         1         5         6
         3         1         5         7         3         1         5        18
         3         1         5         6         4         1         5         7

. . .

         1739      1738      1736      1742      1740      1738      1736      1742
         1741      1738      1736      1742

. . .
```

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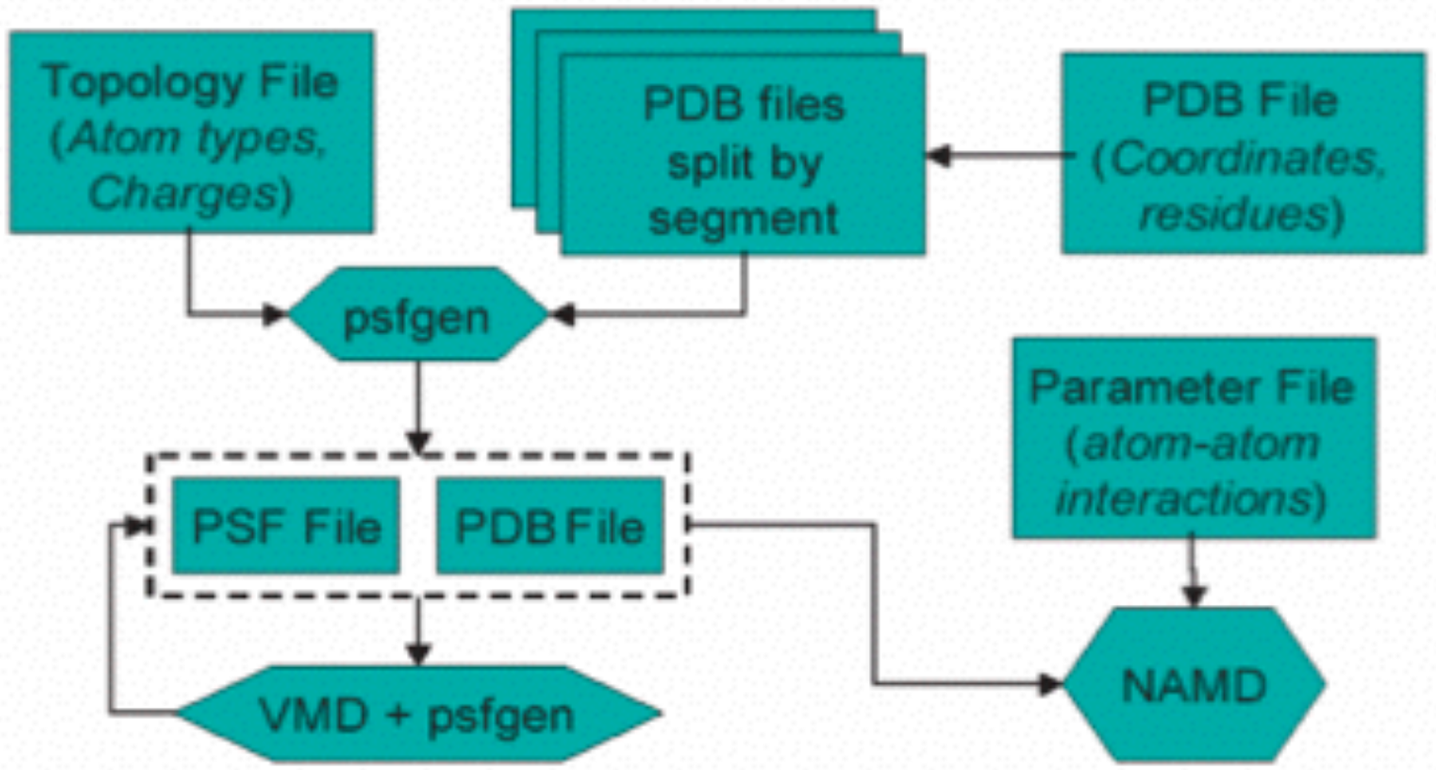
PSF File of Protein V

```
. . .

       297 !NIMPHI: impropers
        13       15       10       14       13       10       15       14
        15       13       16       17       15       13       17       16
        18        5       20       19       20       18       22       21
        30       32       27       31       30       27       32       31
        32       30       33       34       32       30       34       33
        35       22       37       36       37       35       39       38

. . .

         1724     1718     1729     1725     1726     1731     1728     1727
         1729     1724     1731     1730

. . .
```

The Process



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Parameter File I

```
BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
!
!Carbon Dioxide
CST  OST   937.96      1.1600 ! JES
!Heme to Sulfate (PSUL) link
SS   FE    250.0       2.3200 !force constant chosen so
           !equilbrium bond length optimized to reproduce
           !CSD survey values of
           !2.341pm0.01 (mean, standard error)
           !adm jr., 7/01
C    C     600.000      1.3350 ! ALLOW ARO HEM
           ! Heme vinyl substituent (KK, from propene (JCS))
CA   CA    305.000      1.3750 ! ALLOW   ARO
           ! benzene, JES 8/25/89
CE1  CE1   440.000      1.3400   !
           ! for butene; from propene, yin/adm jr., 12/95
CE1  CE2   500.000      1.3420   !
           ! for propene, yin/adm jr., 12/95
CE1  CT2   365.000      1.5020   !
           ! for butene; from propene, yin/adm jr., 12/95
. . .
```

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Parameter File II

```
ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
!
!Carbon Dioxide, JES
OST  CST  OST    3000.00  180.0000 ! CO2, JES

CA   CA   CA    40.000    120.00   35.00   2.41620 ! ALLOW   ARO
                ! JES 8/25/89
CE1  CE1  CT2    48.00    123.50   !
                ! for 2-butene, yin/adm jr., 12/95
CE1  CE1  CT3    48.00    123.50   !
                ! for 2-butene, yin/adm jr., 12/95

. . .
```

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Parameter File III

```
DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
C    CT1  NH1  C        0.2000  1   180.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
C    CT2  NH1  C          0.2000  1   180.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
C    N    CP1  C          0.8000  3     0.00 ! ALLOW PRO PEP
                ! 6-31g* AcProNH2, ProNH2, 6-31g*//3-21g AcProNHCH3 RLD
4/23/93
CA   CA   CA   CA         3.1000  2   180.00 ! ALLOW   ARO
                ! JES 8/25/89
CA   CPT  CPT  CA         3.1000  2   180.00 ! ALLOW   ARO
                ! JWK 05/14/91 fit to indole


. . .
```

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Parameter File IV

```
IMPROPER
!
!V(improper) = Kpsi(psi - psi0)**2
!
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is ignored
!
!atom types           Kpsi                   psi0
!
CPB  CPA  NPH  CPA    20.8000         0      0.0000 ! ALLOW HEM
                ! Heme (6-liganded): porphyrin macrocycle (KK 05/13/91)
CPB  X    X    CE1    90.0000          0      0.0000 ! ALLOW HEM
                ! Heme (6-liganded): substituents (KK 05/13/91)
CT2  X    X    CPB    90.0000          0      0.0000 ! ALLOW HEM
                ! Heme (6-liganded): substituents (KK 05/13/91)
CT3  X    X    CPB    90.0000          0      0.0000 ! ALLOW HEM
                ! Heme (6-liganded): substituents (KK 05/13/91)
!HA   C    C     HA     20.0000          0      0.0000 ! ALLOW   PEP POL ARO
                ! Heme vinyl substituent (KK, from propene (JCS))


. . .
```

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Parameter File V

```
NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-4
!
!carbons
C       0.000000  -0.110000     2.000000 ! ALLOW   PEP POL ARO
                ! NMA pure solvent, adm jr., 3/3/93
CA      0.000000  -0.070000     1.992400 ! ALLOW   ARO
                ! benzene (JES)
CC      0.000000  -0.070000     2.000000 ! ALLOW   PEP POL ARO
                ! adm jr. 3/3/92, acetic acid heat of solvation
CD      0.000000  -0.070000     2.000000 ! ALLOW  POL
                ! adm jr. 3/19/92, acetate a.i. and dH of solvation



. . .
```

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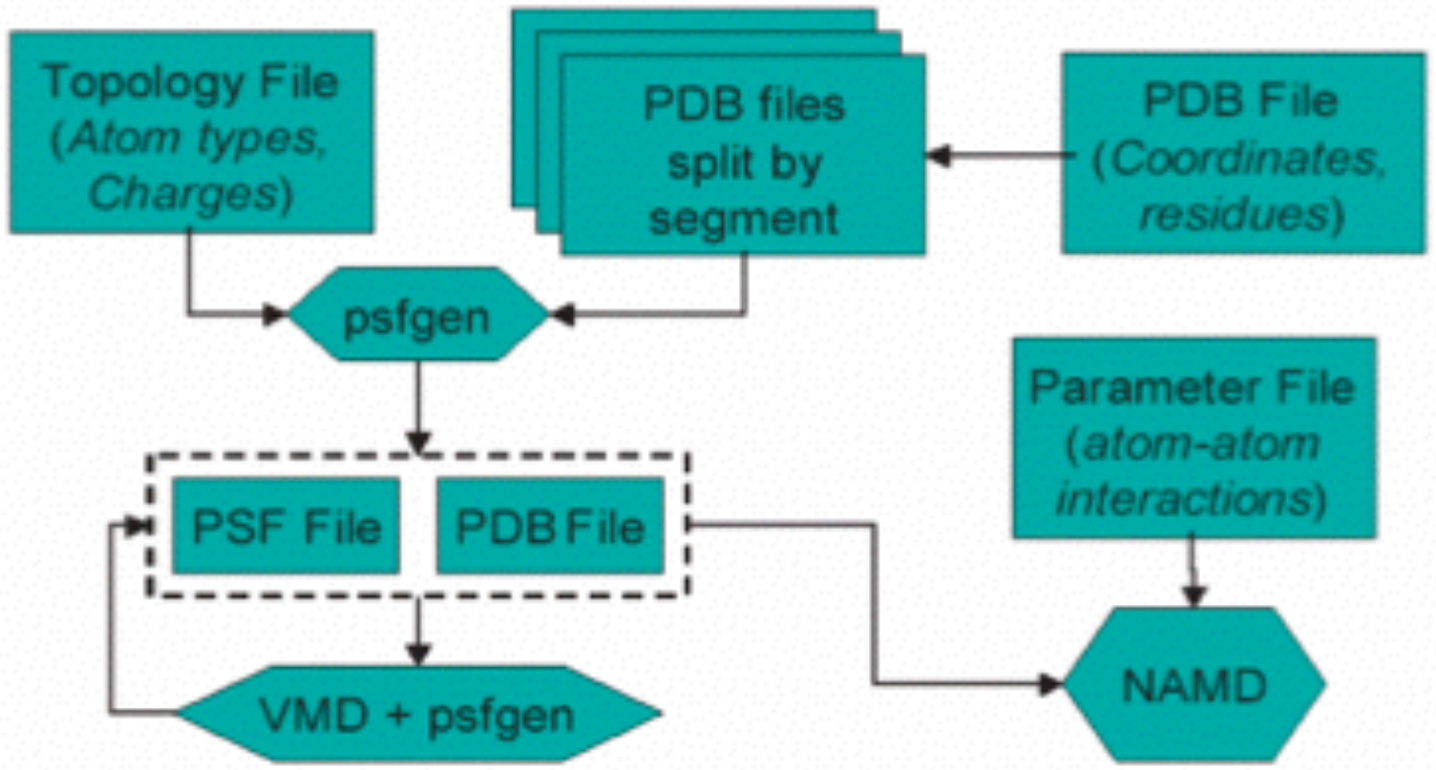
The Process



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NAMD

UIUC:

http://www.ks.uiuc.edu/Research/namd/

Open source (binaries and code) . . . no re-distribution

Many hardware platforms (desktop, GPU, Clusters, etc.)

Superior parallel performance (Charm++, infiniband, myranet, etc.)

SImple input file syntax and expandable via TCL scripting

Charmm / Amber / Coarse Grain / etc. FF

Excellent tutorials and support

Linked w/ VMD (visualization & control)

Runs many types of MD simulations

- NVE, NVT, NPT
- Constant area
- Steered MD
- Interactive MD (IMD)
- MD Flexible Fitting
- Free-Energy
- etc.

- **AIX-POWER-lapi** (IBM POWER clusters)
- **AIX-POWER-multicore** (IBM POWER single node)
- **Linux-x86** (32-bit Intel/AMD with ethernet)
- **Linux-x86-TCP** (TCP may be better on gigabit)
- **Linux-x86_64-multicore** (64-bit Intel/AMD single node)
- **Linux-x86_64** (64-bit Intel/AMD with ethernet)
- **Linux-x86_64-TCP** (TCP may be better on gigabit)
- **Linux-x86_64-ibverbs** (InfiniBand via OpenFabrics OFED, no MPI needed)
- **Linux-x86_64-ibverbs-smp** (InfiniBand plus shared memory, no MPI needed)
- **Linux-x86_64-CUDA** (NVIDIA CUDA acceleration)
- **Linux-x86_64-ibverbs-CUDA** (NVIDIA CUDA with InfiniBand)
- **MacOSX-x86** (Mac OS X for Intel processors)
- **MacOSX-PPC** (Mac OS X for PowerPC)
- **Solaris-x86_64**
- **Win32** (Windows XP, etc.)
- **Win64-MPI** (Windows HPC Server)

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NAMD II

namd binary + input file => new coords.

PDB
PSF
PAR

MD parameters

1. Minimization
2. MD (time)
3. Directed MD

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NAMD INPUT FILE

```
# sample NAMD configuration file for Minimization

# molecular system
coordinates             output/new_icln.pdb
structure               output/new_icln.psf
temperature             300

# force field
paratypecharmm          on
parameters              /home/mdschool/toppar/par_all27_prot_na.inp

# approximations
exclude                 scaled1-4
1-4scaling              1.0
switching               on
switchdist              10
cutoff                  12

# output

outputname              output/min0
binaryoutput            no

# run control

minimize                1000
```

PDB

PSF

PAR

MD parameters

RUNNING NAMD

USAGE (unix prompt):

Start a run:

```
>namd2 min0 >&  min0.out &
```

Check status:

```
>tail -90f min0.out
```

Multi-processor run:

```
>charmrun ++local ++p 2  /usr/local/bin/namd/namd2 min0 >&  min0.out &
```

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CHARMM INPUT FILE

```
* title
*

open unit 1 read form name ~/toppar/top_all27_prot_na.inp
read rtf card unit 1
close unit 1

open unit 1 read form name ~/toppar/par_all27_prot_na.inp
read param card unit 1
close unit 1

open unit 1 read card name traI_308_to_380.pdb
read sequence pdb unit 1
close unit 1

generate TRAA first glyp last cter setup

open unit 1 read card name linker1_phyre_1.pdb
read unit 1 coor pdb
close unit 1

!ic seed
ic fill preserve
ic param
ic build

open unit 1 write form name new_linker1_phyre_1_plus_tail.pdb
write coor pdb unit 1
* fixed TRAA
* by jc 05/24/11
```

```
close unit 1

!ic seed
ic fill preserve
ic param
ic build

open unit 1 write form name new_linker1_phyre_1_plus_tail.pdb
write coor pdb unit 1
* fixed TRAA
* by jc 05/24/11

close unit 1

OPEN UNIT 1 WRITe CARD NAME new_linker1_phyre_1_plus_tail.psf
WRITe PSF CARD UNIT 1
*PSF File
*
```

```
close unit 1

! Perform the minimisation.
Minimise Abnr Nstep 5000 Nprint 50 Tolgrd 0.1 Inbfrq 0 Imgfrq 0

! Test the first derivatives.
Test First Step 0.000001 Tol 0.000001

! Save the optimised coordinates.
Open write card unit 17 name new_min_fixed_full0.pdb
Write coor pdb unit 17
* minimized full PARP
* by jc 9/27/10
*
close unit 17
```

AMBER INPUT FILE

```
#!/bin/csh -f

cat > mdin <<EOF
  MD run, Temp=300K, start                                    #06-07-00#
 11 A water box, const eps=1.0,
 nscm=0, npscal=1, frameon=1 - pointing LP's as in Jim's code
 const pressure MD, seperate temp coupling
 &cntrl
  irest=1, ibelly=0, imin=0,
  ipol=1,
  ntx=5, ntxo=1, ig=71277, tempi=0.00,
  ntb=2,
  ntt=0, temp0=300.0, tautp=0.2,
  ntp=1,    pres0=1.0, comp=44.6, taup=0.2,
  nscm=0,
  nstlim=10,  t=1170.0, dt=0.001,
  ntc=2,    tol=0.0000005,
  ntf=2,    nsnb=5,
  cut=9.0, dielc=1.0,
  ntpr=1, ntwx=5,  ntwv=5, ntwe=5,
  ioutfm=0,
  ntr=0,    ntave=100,  ntrx=1
 /
 &ewald
    ew_type = 0, verbose=0,
    vdwmeth=1, maxiter=10, indmeth = 3, diptau = 1.0,
    frameon=1, irstdip=1, scaldip=0,
 /
EOF

set output = mdout.ubiquitin
```

```
 ipol=1,
 ntx=5, ntxo=1, ig=71277, tempi=0.00,
 ntb=2,
 ntt=0, temp0=300.0, tautp=0.2,
 ntp=1,    pres0=1.0, comp=44.6, taup=0.2,
 nscm=0,
 nstlim=10,  t=1170.0, dt=0.001,
 ntc=2,    tol=0.0000005,
 ntf=2,    nsnb=5,
 cut=9.0, dielc=1.0,
 ntpr=1, ntwx=5,  ntwv=5, ntwe=5,
 ioutfm=0,
 ntr=0,    ntave=100,  ntrx=1
/
&ewald
   ew_type = 0, verbose=0,
   vdwmeth=1, maxiter=10, indmeth = 3, diptau = 1.0,
   frameon=1, irstdip=1, scaldip=0,
 /
EOF

set output = mdout.ubiquitin

$DO_PARALLEL $TESTsander -O -i mdin -p prmtop -c inpcrd -o $output || goto
error

../dacdif $output.save $output
# ../dacdif -t 2 rstdip.save rstdip
# ../dacdif -t 2 restrt.save restrt
../dacdif -t 2 mden.save mden
../dacdif mdcrd.save mdcrd
../dacdif -t 2 mdvel.save mdvel
/bin/rm -f mdin mdinfo
exit(0)
```

CPMD INPUT FILE

```
&CPMD
 MOLECULAR DYNAMICS
 RESTART WAVEFUNCTION COORDINATES LATEST
 MAXSTEP
  100
 STORE
  10
 EMASS
  800.0
 TEMPERATURE
  10.0
 MOVIE
 STRUCTURE BONDS ANGLES
&END

&SYSTEM
 SYMMETRY
  0
 POISSON SOLVER TUCKERMAN
 CELL ABSOLUTE DEGREE
  32.0 32.0 32.0 90.0 90.0 90.0
 CUTOFF
  70.
 CHARGE
  -2.0
&END

&DFT
  FUNCTIONAL BLYP
&END
```

```
&CPMD
 MOLECULAR DYNAMICS
 RESTART WAVEFUNCTION COORDINATES LATEST
 MAXSTEP
  100
 STORE
  10
 EMASS
  800.0
 TEMPERATURE
  10.0
 MOVIE
 STRUCTURE BONDS ANGLES
&END

&SYSTEM
 SYMMETRY
  0
 POISSON SOLVER TUCKERMAN
 CELL ABSOLUTE DEGREE
  32.0 32.0 32.0 90.0 90.0 90.0
 CUTOFF
  70.
 CHARGE
  -2.0
&END

&DFT
  FUNCTIONAL BLYP
&END
```

```
 SYMMETRY
  0
 POISSON SOLVER TUCKERMAN
 CELL ABSOLUTE DEGREE
  32.0 32.0 32.0 90.0 90.0 90.0
 CUTOFF
  70.
 CHARGE
  -2.0
&END

&DFT
  FUNCTIONAL BLYP
&END

&ATOMS
*S-q6              GOEDECKER
 0 0 0
  1
2.108937    -1.441863    -1.341704
*O_MT_BLYP       KLEINMAN-BYLANDER
 LMAX=P LOC=P
17
0.000000     0.000000     0.000000
4.512669     0.120945    -1.283126
1.441863    -2.114603    -3.998664
2.570030    -3.953307     0.132280
-2.619161    -2.553024     3.970312
5.867605    -7.723315    -5.092820
3.061359     -.893838     3.688743
 -.166295    -8.443304    -3.548911
7.819691    -5.767457      .211645
```

SUMMARY

WHEW!!! So many details!!!

What have we accomplished?

You have now seen the way that coordinates are handled and how FF are integrated to describe a molecular (atomic) system. **This is a general method!**

Break

LAB 0 --> Software installation & intro to SASSIE-web

Lunch

LAB I --> Overview of VMD and PDB Scan

Break

LAB II --> YOU generate systems (PDB->PSF-> NAMD)

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