MMC & SASSIE Overview

Atomistic Modeling of Small-Angle Scattering Data Using SASSIE-web

September 21-23, 2016

Advanced Photon Source

Argonne National Laboratory, Argonne, IL

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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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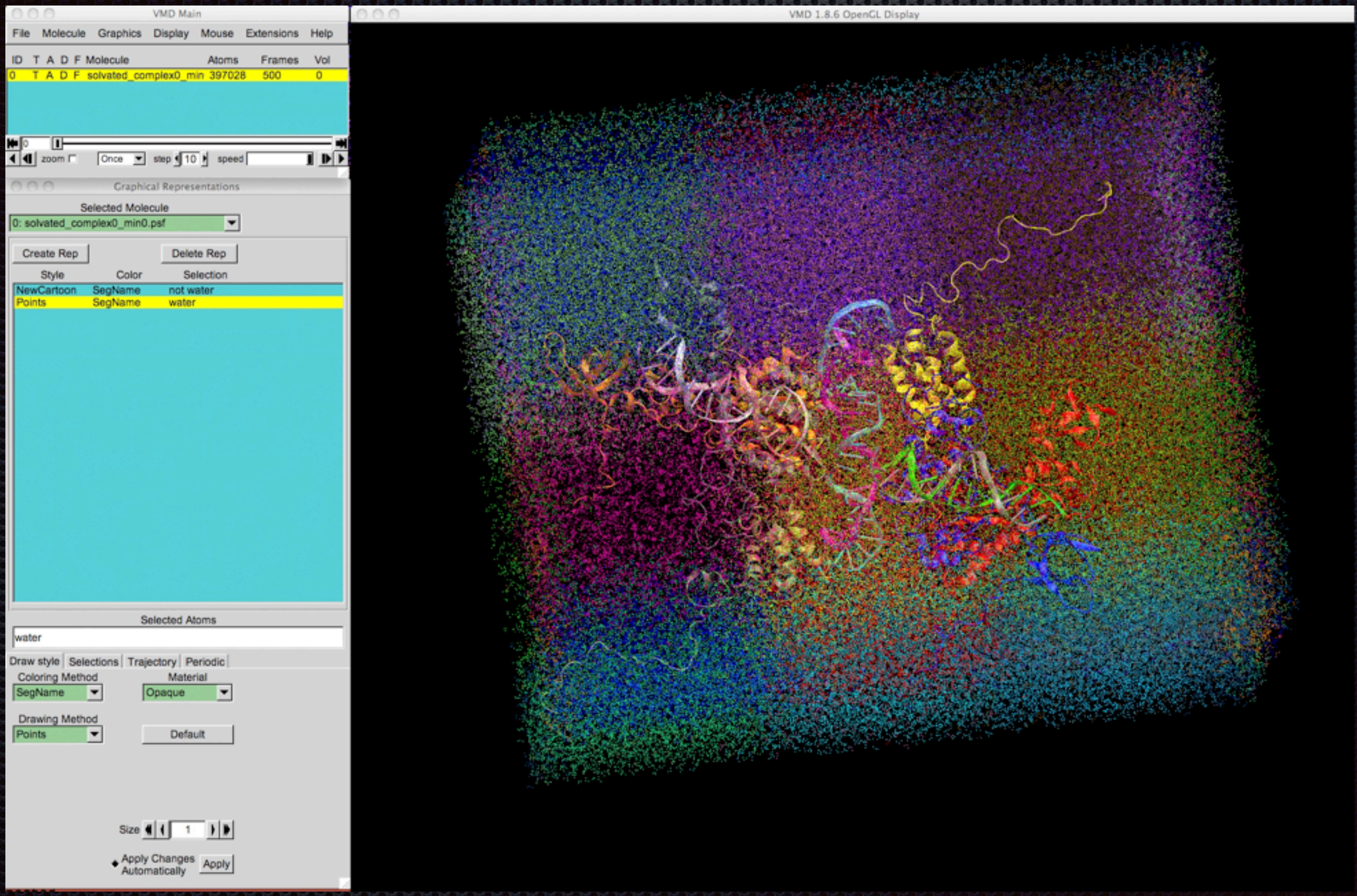
1 ns


VMD Main
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Points SegName water
Selected Atoms
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VMD 1.8.6 OpenGL Display

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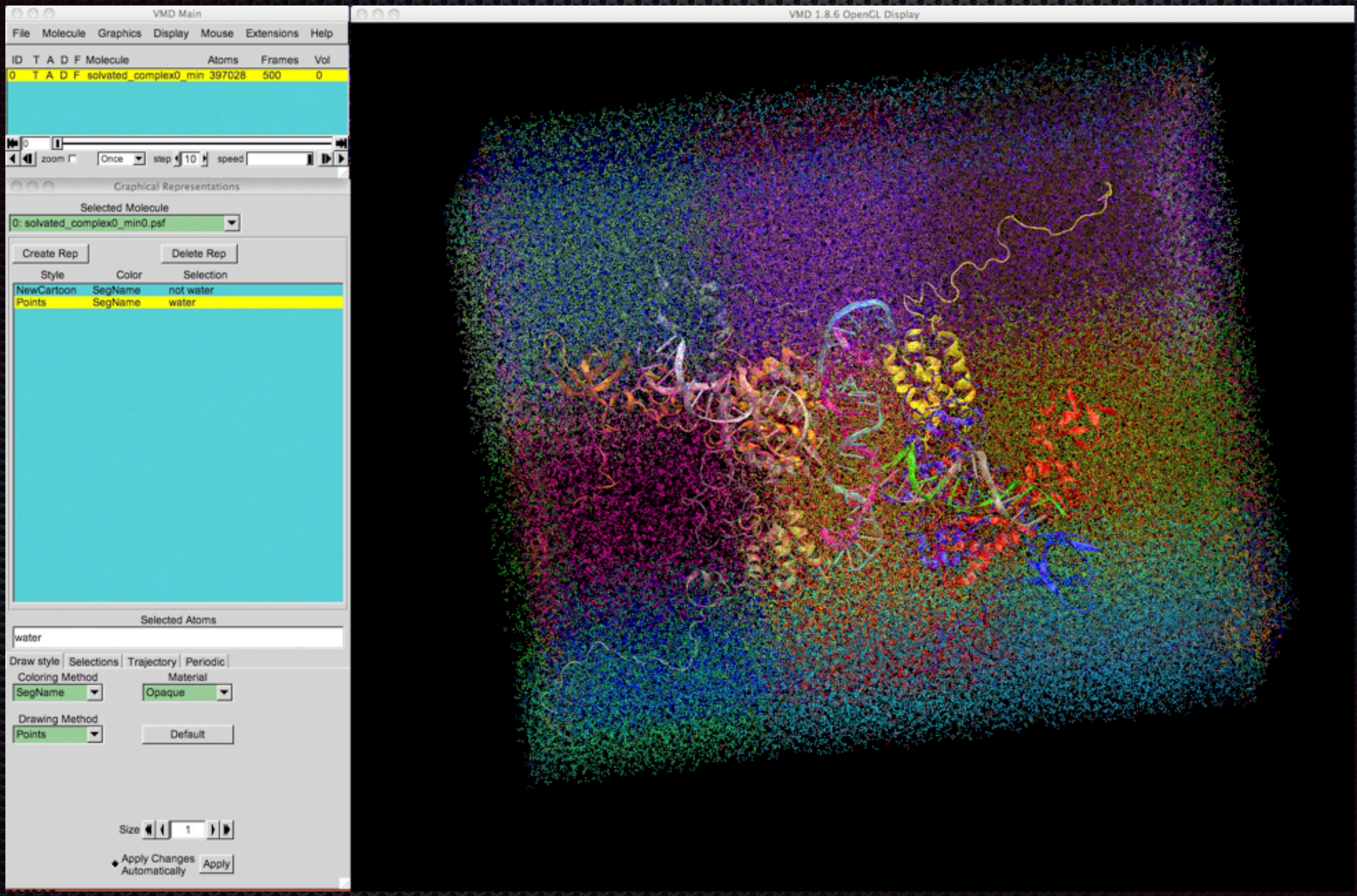
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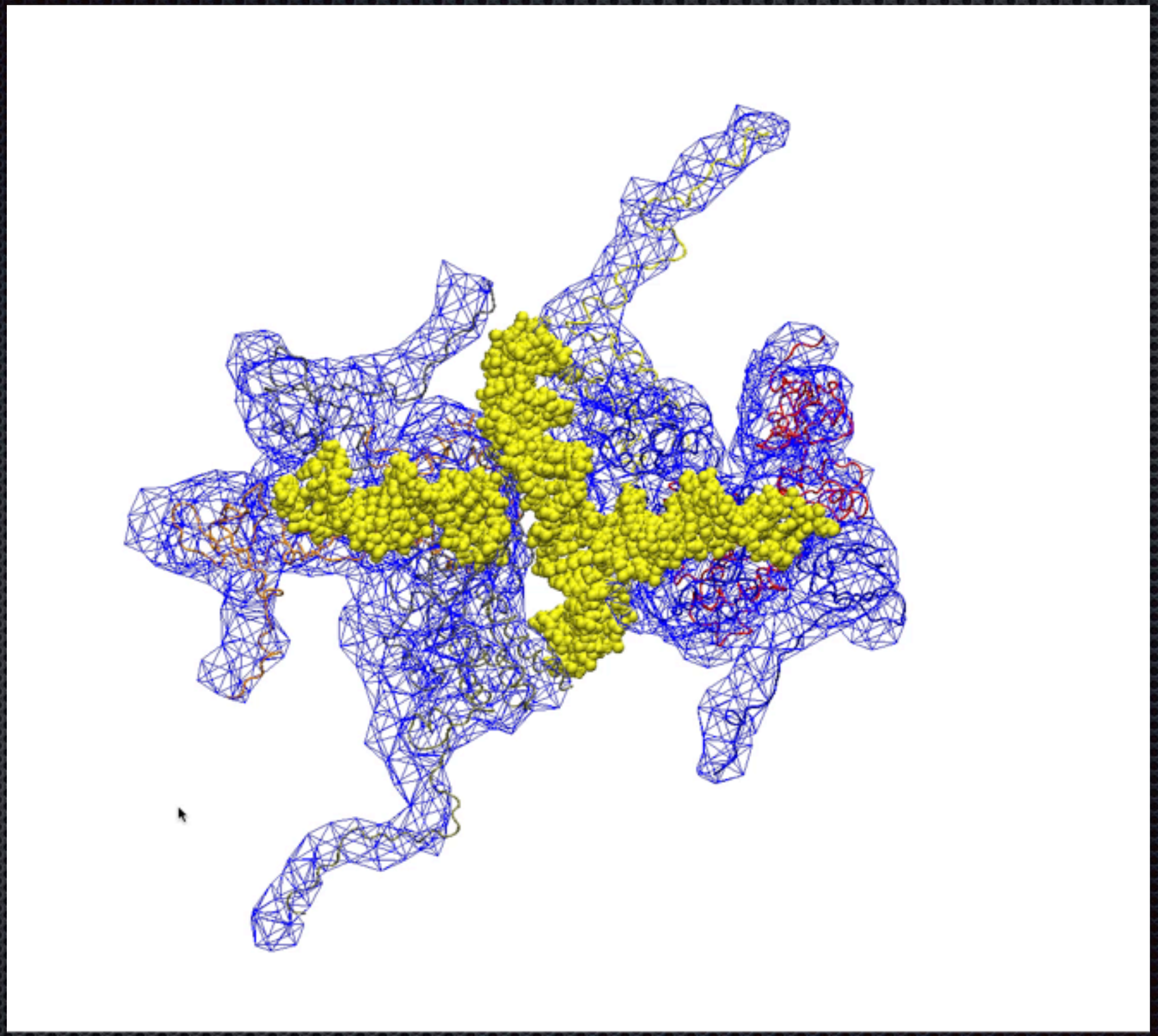
1 ns: 8 CPU 13 days



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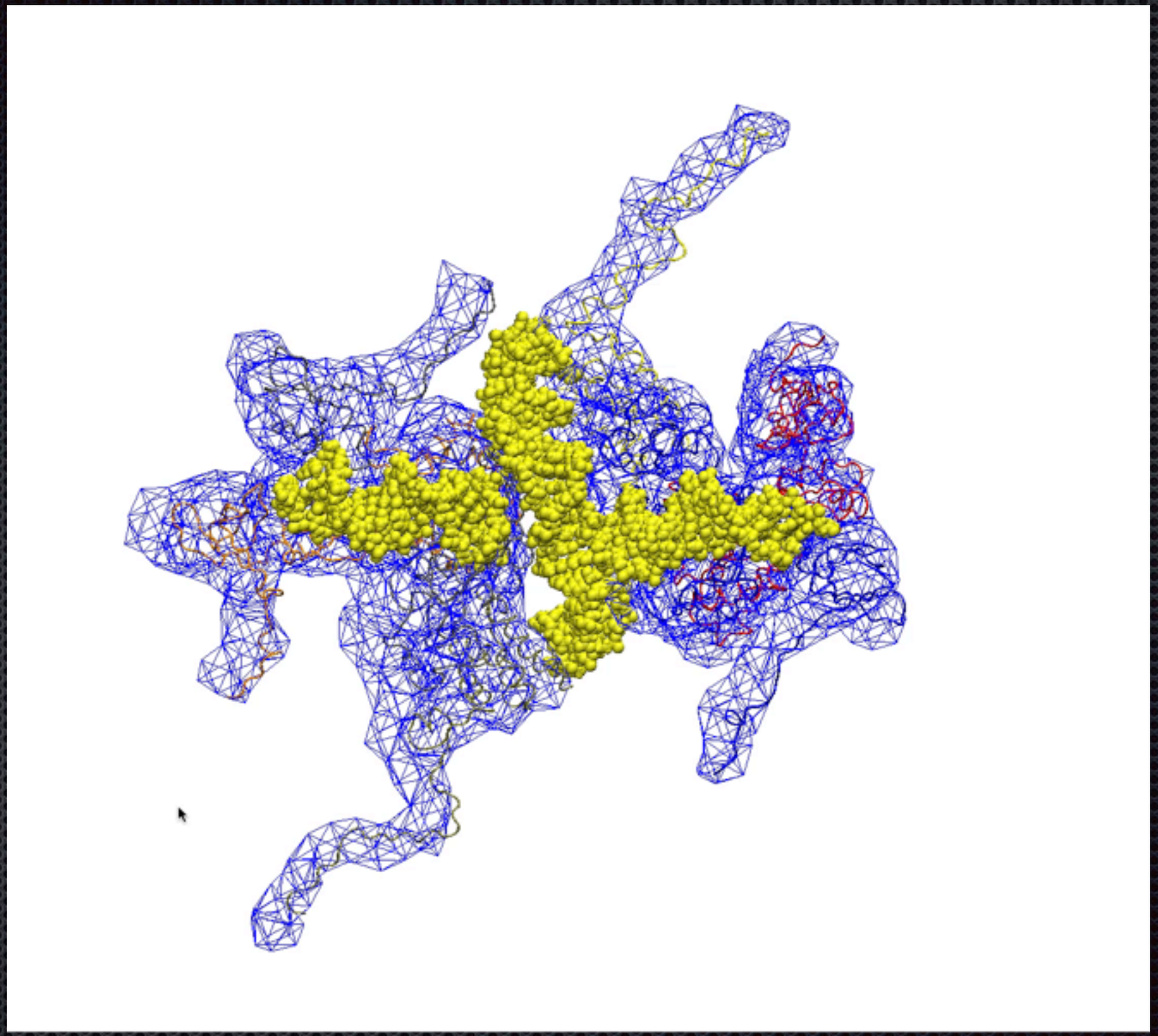

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Options (today)

We don't have ANTON . . . (and even if we did, maybe you don't) . . . and even then 25 us may not be long enough, etc. etc.

For many, yet not all, IDP/ID problems a fully-atomistic simulation is impractical for an average user.

For many, IDP/ID problems, even with massive computational resources, to obtain an answer for a particular starting model is going to take time.

A number of hybrid MD/MC & MC routines exist to sample configuration space yet they are cumbersome to use and not ready for prime time.

Rigid body modeling packages exist (docking, etc.), but they don't handle flexible bits or scattering calcuations.

In 2004 there were fewer options

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MMC

Monte Carlo samples configurations by generating moves (translational, rotational, etc.), within the molecular potential of your system. These structures taken together make up an ensemble of configurations covering "phase space"

There is an equivalence where by calculated observables, let's say for example the density of a system rho = rho (r)

$$\langle \rho_i(r) \rangle_{time} = \langle \rho_i(r) \rangle_{phasespace}$$

This means that the "time-average" of a quantity calculated by MD is equivalent to the "ensemble-average" of the same quantity as calculated by Monte Carlo means. ***For ergodic systems.***

See: Frenkel & Smit for a nice description from QM to CM.

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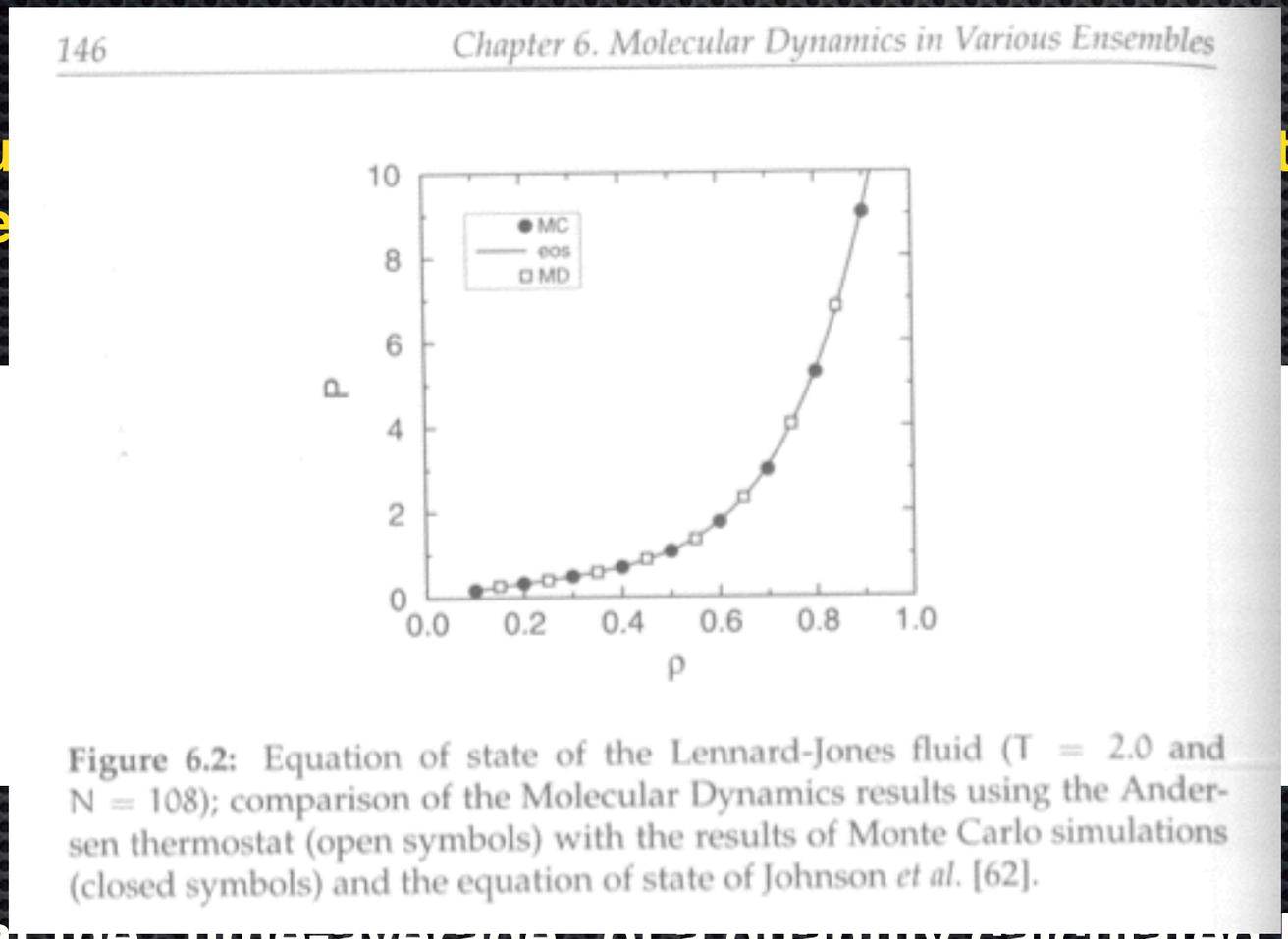

Figure 6.2: Equation of state of the Lennard-Jones fluid (T = 2.0 and N = 108); comparison of the Molecular Dynamics results using the Andersen thermostat (open symbols) with the results of Monte Carlo simulations (closed symbols) and the equation of state of Johnson *et al.* [62].

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MC

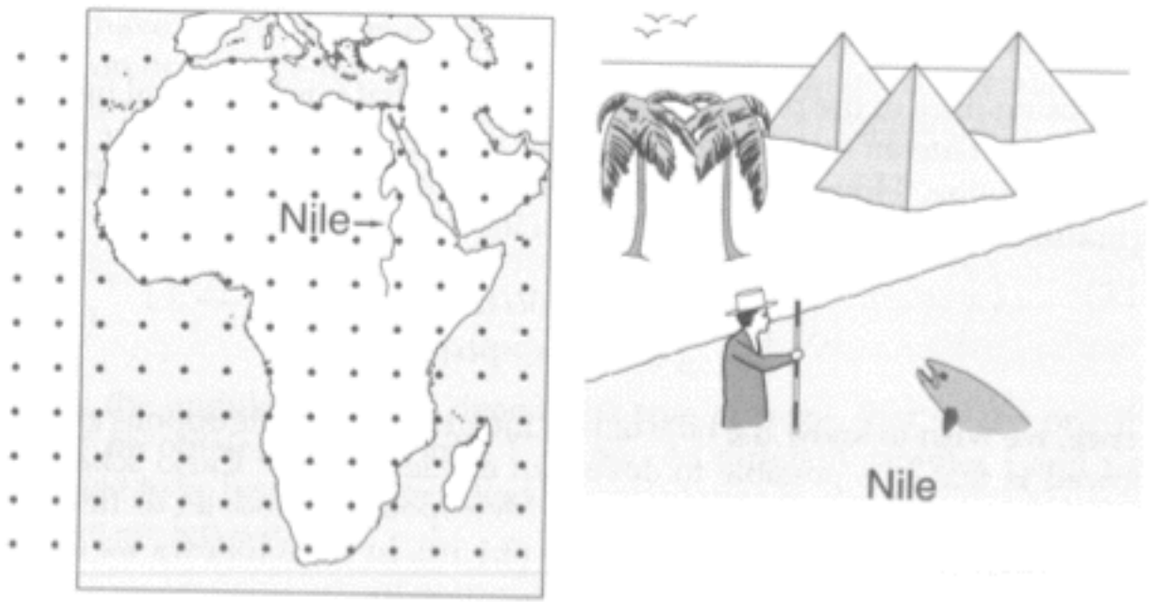

Figure 3.1: Measuring the depth of the Nile: a comparison of conventional quadrature (left), with the Metropolis scheme (right).

Two ways to sample.

(1) Quadrature
You measure the depth of the "Nile" on a equidistant grid. --> get depth

(2) "Metropolis"
a) trial move --> rejected if you are not in the water
(b) trial move is accepted if you are in the water.

For molecular systems the important part of space (r, theta, phi, etc.) is related to the molecular potential.

After every move you measure the depth. The average of all measurements is the depth of the Nile

See: Frenkel & Smit for a nice description of MC (& MD).

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MC

For molecules, we generate points in configuration space with a relative probability proportional to the Boltzmann factor. So for a move from "old == o" to "new == n", the probability that a move is accepted: acc(o->n)

$$\frac{acc(o->n)}{acc(n->o)} = exp\left(-\beta\left[U(n) - U(o)\right]\right)$$

If $U(n) < U(o)$ then the trial move is accepted.

If $U(n) > U(o)$ then the trial move is accepted if $exp\left(-\beta\left[U(n) - U(o)\right]\right) < 1$

```
for i in xrange(number_of_steps):

        x(o) = pick_a_random_atom(random(0,natoms))
        Eold = energy ( x(o) )
        Xnew = x(o) + random(0,1)*delta_x
        Enew = energy( Xnew )
        If Enew < Eold:
            x(o) = Xnew
        elif ( random(0,1) < exp(-beta*(Enew-Eold) ):
            x(o) = Xnew
```

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MC

Size of moves in a Markovian chain:

“A MC sampling scheme is optimal if it yields the lowest statistical error of < A > for a given length of CPU time”

In practice, you merely want to cover configuration space.

For an observable A, the mean square error in A should be inversely proportional to the number of uncorrelated configurations is given amount of CPU time.

The point is that there is no golden rule.

Ad-hoc definitions mean, to me, that I should use common sense.

Each problem type needs to be optimized.

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MMC (with rotation)

So, to have a fully-atomistic MMC (vary all bonds and angles) our averages and hence our energy calculations become numerically much more complicated. For large flexible systems, fully-atomistic MMC is slower than (or as slow as) MD!

$$\langle A \rangle = \frac{\int d\mathbf{p}^N d\mathbf{r}^N exp[-\beta H(\mathbf{p}^N,\mathbf{r}^N)] A(\mathbf{p}^N,\mathbf{q}^N)}{\int d\mathbf{p}^N d\mathbf{r}^N exp[-\beta H(\mathbf{p}^N,\mathbf{r}^N)]}$$

where $H\left(\mathbf{p}^N,\mathbf{r}^N\right) = \sum_j p_j^2/(2m_j) + U(\mathbf{r}^n)$

but for rotational moves (now in generalized coordinates);

$$H\left(\mathbf{p}^N,\mathbf{r}^N\right) = \tfrac{1}{2}\mathbf{p}\cdot G^{-1}\cdot\mathbf{p} + U(\mathbf{r}^n)$$

when when placed into our expression for $\langle A \rangle$
leads to $|G|^{\frac{1}{2}}$ in the numerator.

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MMC with frozen dof

An alternative strategy is to only sample the configurational landscape accessible by rotating the dihedral bonds of macromolecules.

Use the CHARMM force-field to sample only the dihedral potential using the Metropolis criterion, then if you have interesting result, you minimize the entire ensemble of structures.

Sampling on a grid (40 degree spacing for HIV-1 Gag) --> 10^67 configurations are required.

Sampling from Ramachandran plot is fundamentally limiting.

Advantages:

Generate configurations quickly to test hypotheses.

Structures are minimized and ready for further analyses IF YOU WISH.

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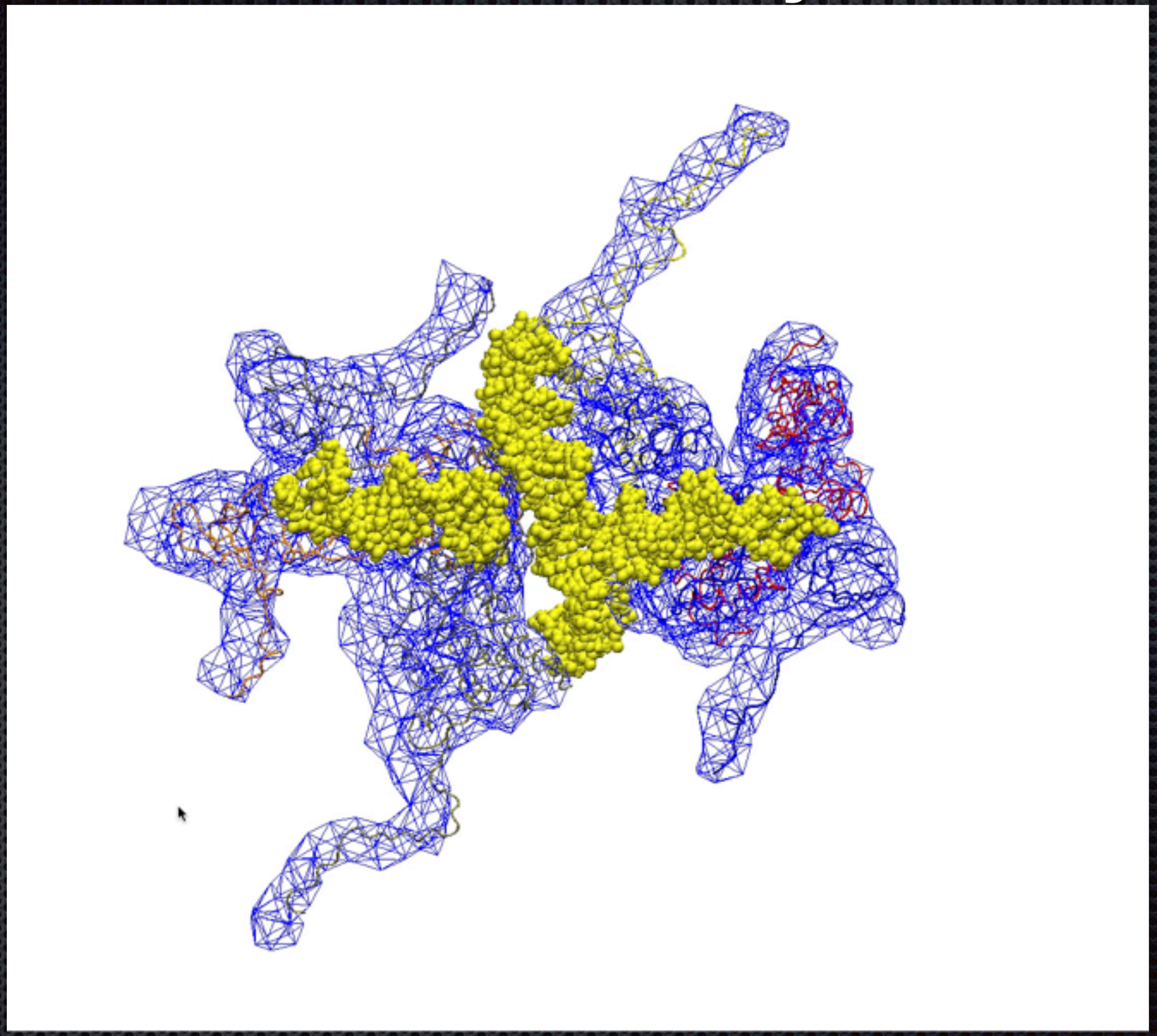
1 ns: 8 CPU 13 days



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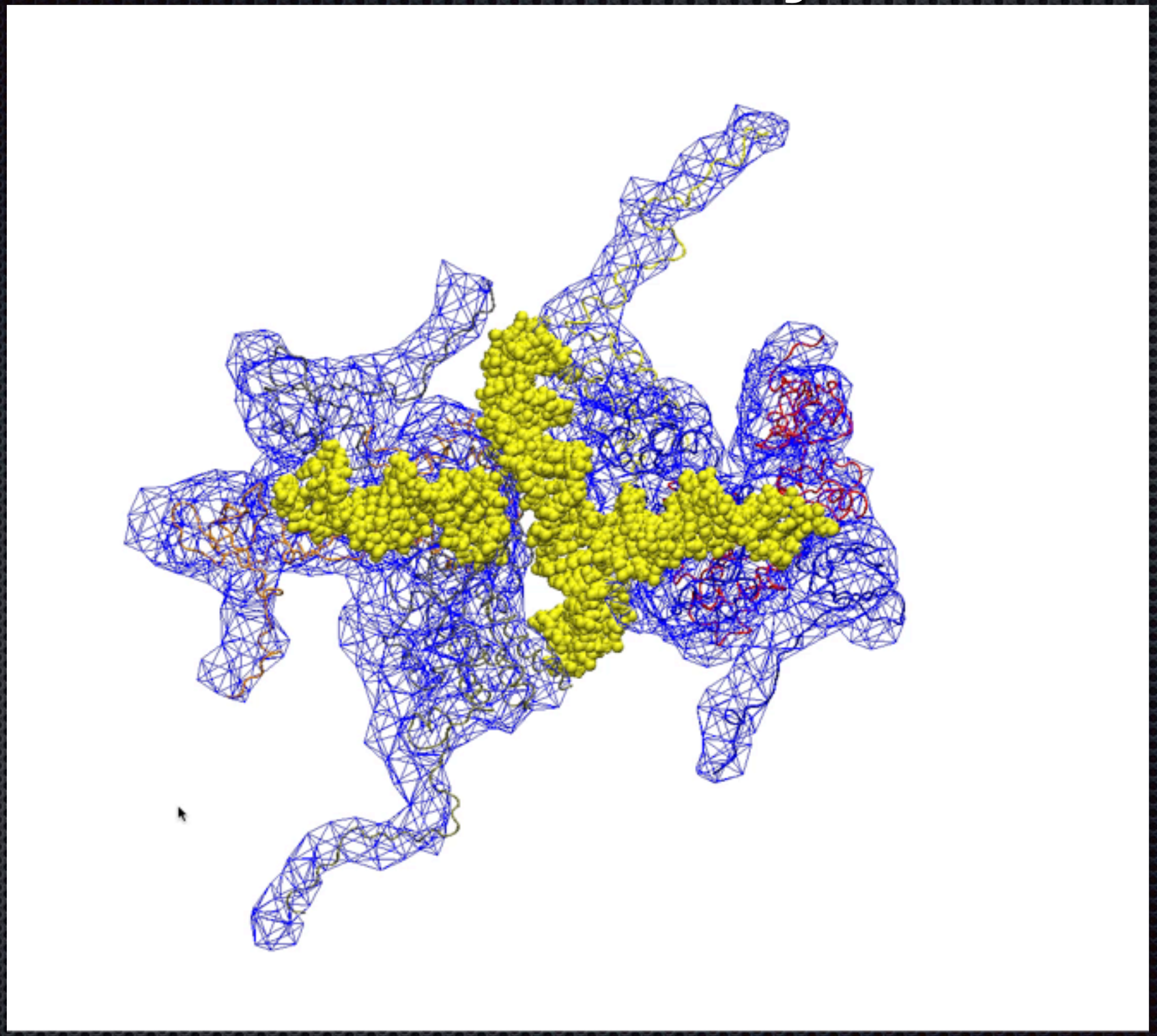
1 ns: 8 CPU 13 days



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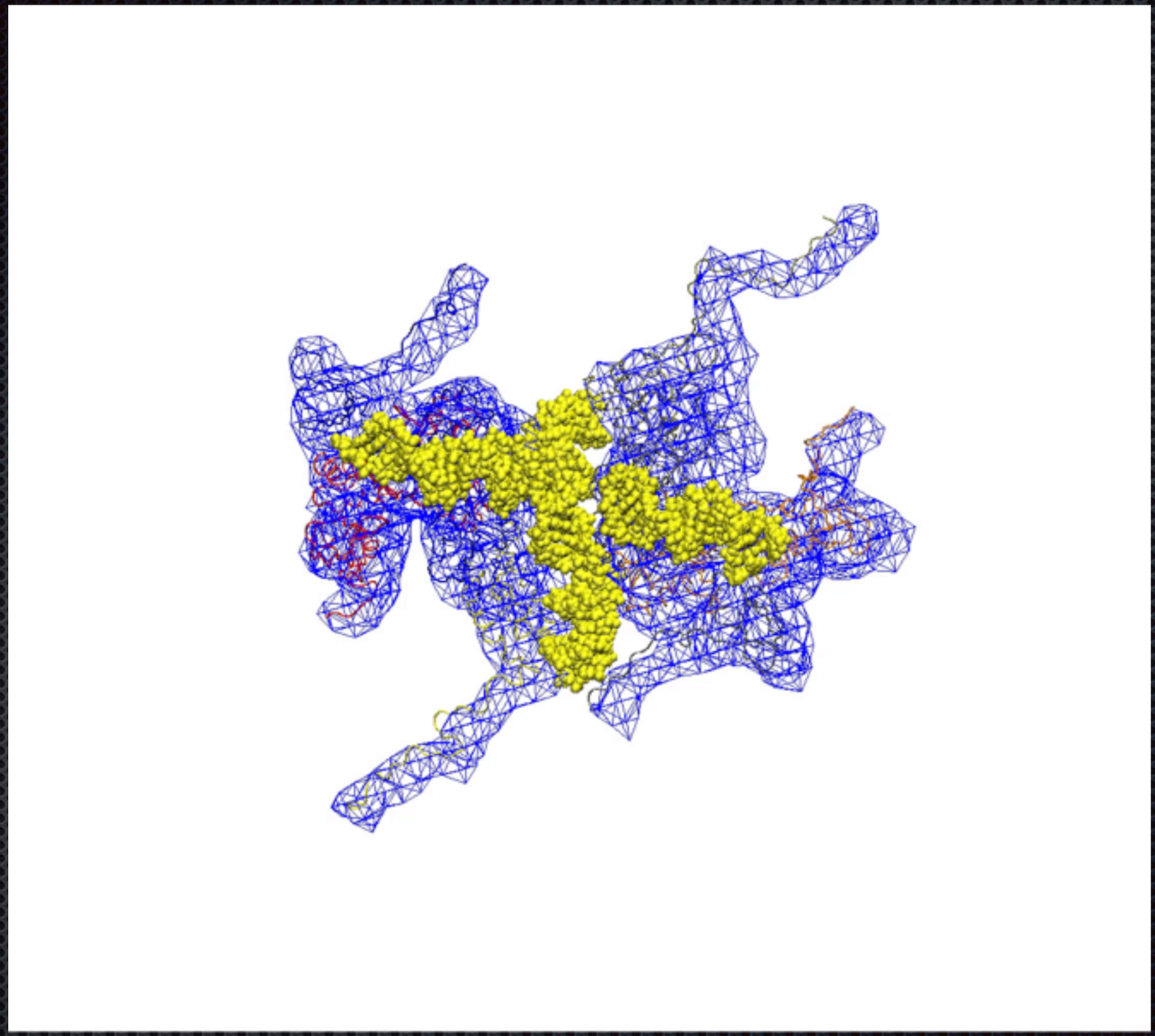
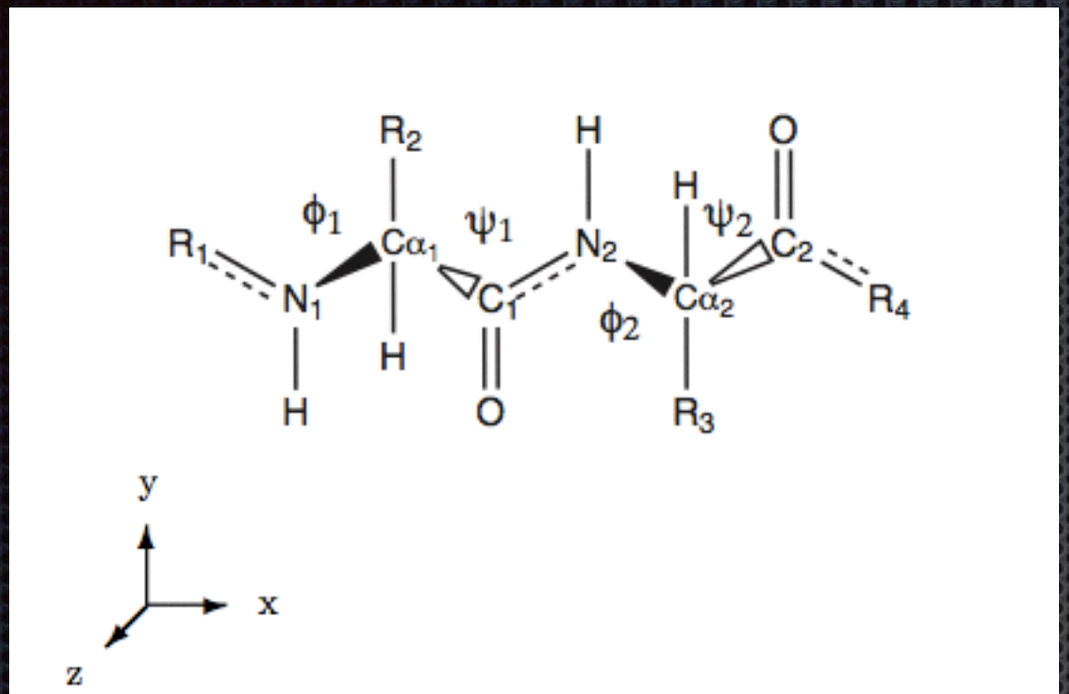
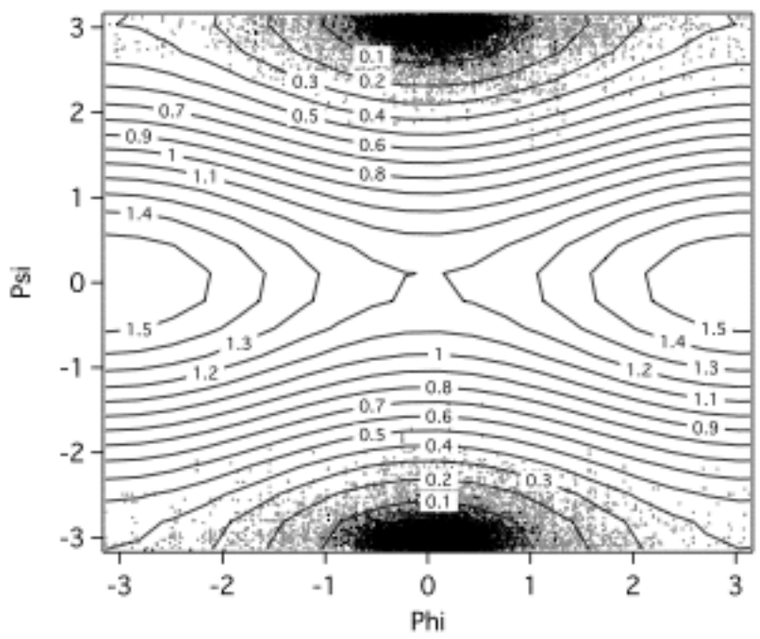
15 min. then 45 min. : 1 CPU



backbone torsion sampling





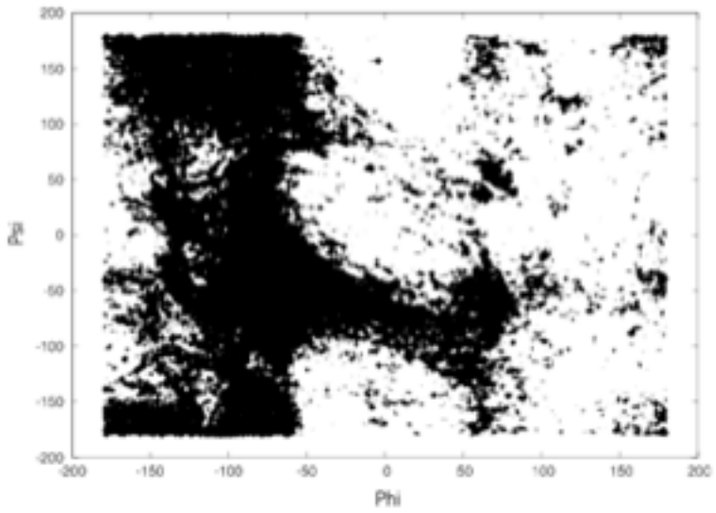


Fig. 5. The values of accepted angular values of ϕ and ψ for the 65 amino-acids located in the five flexible regions of the 10^5 energy minimized full-length HIV-1 Gag protein structures. Angles are shown in degrees.

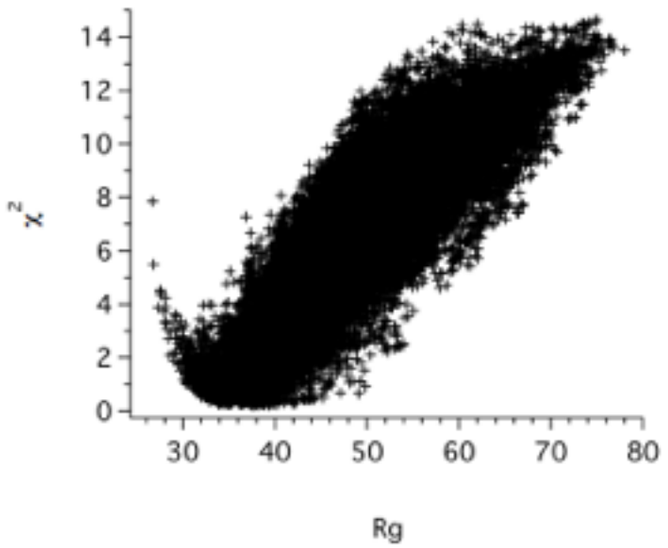


Fig. 6. A plot of χ^2 versus Rg obtained from 10^5 non-overlapping full-length HIV-1 Gag protein structures.

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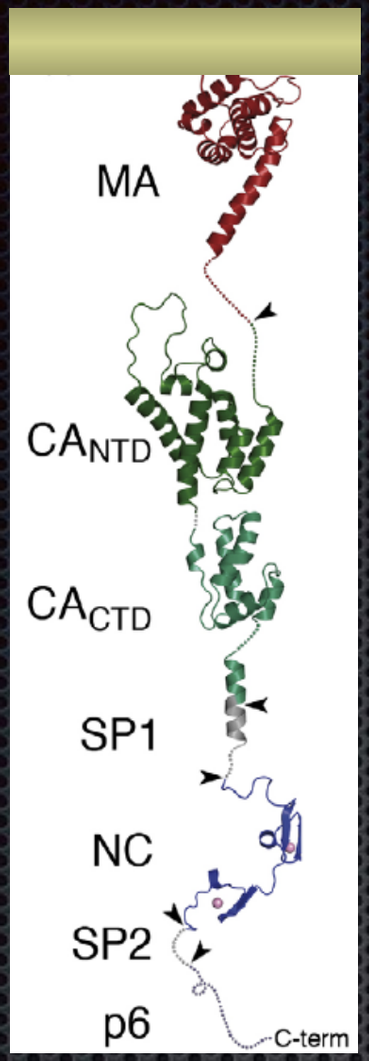
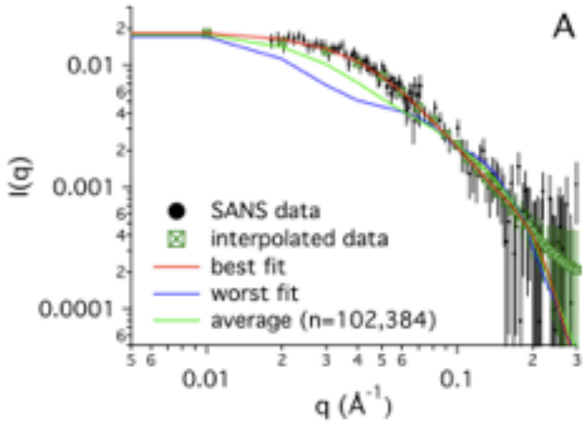
representative envelope/st.



123-144 (21)
278-283 (5)
354-378 (24)
378-389 (11)
408-412 (4)



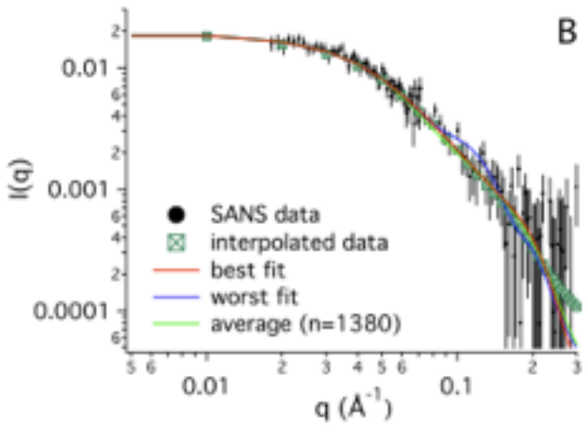


Fig. 7. The plot of experimental and theoretical SANS profiles obtained from 10^5 non-overlapping full-length HIV-1 Gag protein structures.

shown in Figure 6. Here, χ^2 is calculated using

$$\chi^2 = \frac{1}{(N-1)} \frac{\sum_Q (I_{exp}(Q) - I_{calculated}(Q))^2}{\sigma_{exp}(Q)^2} \quad (7)$$

where $I_{exp}(Q)$ is the experimentally determined SANS profile, $I_{calculated}(Q)$ is the value obtained using SASSIE, $\sigma_{exp}(Q)$ is the experimentally determined Q-dependent variance, and the sum was taken over $N = 19$ grid points of momentum transfer, Q. A plot of the best, worst, average, and experimental SANS profiles is shown in Figure 7.

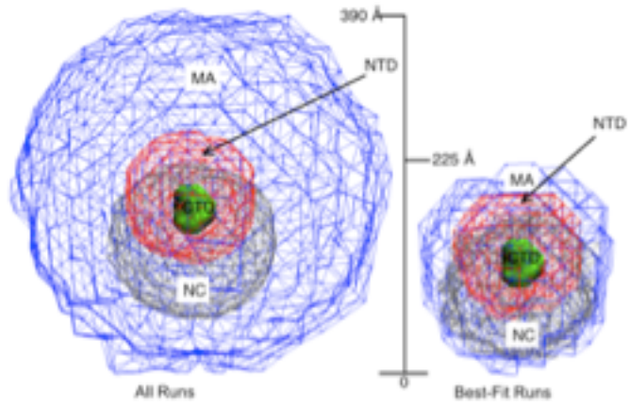


Fig. 8. Iso-density plots of all non-overlapping HIV-1 Gag structures (left: "All Runs") and structures with $\chi^2 \approx 1.0$ (right: "Best-Fit Runs"). The different regions of Gag are colored for clarity (MA:blue, NTD:red, CTD:green, and NC:grey). Structures used to generate the plots were aligned on the alpha-carbon atoms of the CTD region.

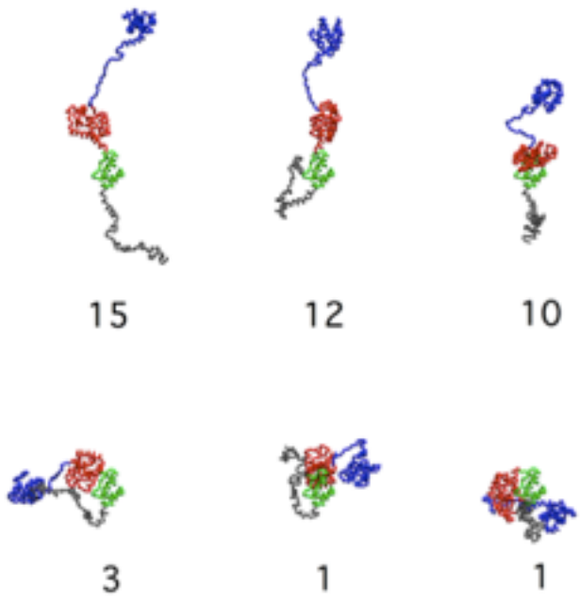


Fig. 9. Tube representations of example HIV-1 Gag structures with χ^2 values shown below each structure. The different regions of Gag are colored for clarity (MA:blue, NTD:red, CTD:green, and NC:grey). Structures are aligned on the alpha-carbon atoms of the CTD region.

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sassie-web

https://sassie-web.chem.utk.edu/sassie2

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sassie-web -- Build

Software to clean-up structure files

and

generate force field topology files

Build -- evaluate and clean up structure files

PDB Scan Generates a report that characterizes the user supplied PDB file (alpha).

PDB Rx Attempts to correct mistakes in user supplied PDB file (alpha).

CG Builder Tools to assist the generation of coarse-grain structures (alpha).

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sassie-web -- Simulate

Monomer Monte Carlo: single chain protein or ss-NA (think IDP / ID-NA)

Complex Monte Carlo: multiple single chain protein or ss-NA (think IDP / ID-NA complexes)

Energy Minimization: anything FF supports (NAMD)

Torsion Angle MD: protein/NA/Carbs. FF supports (CHARMM)

Docking: anything FF supports
Two-Body Grid: anything FF supports

Rigid body

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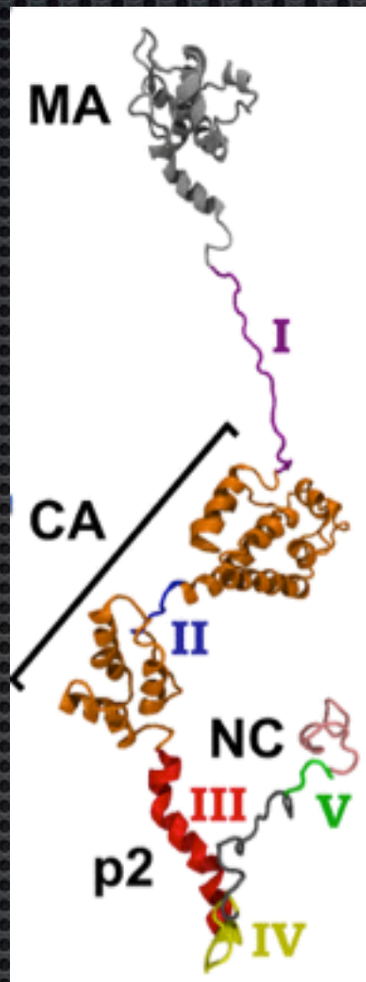
Monomer Monte Carlo

Single chain IDP / ID-NA
simple N -> C or 5’ – 3’
backbone torsion sampling

“What if” questions and
ensembles for further analysis

Configurations are correlated
Not usable with internal loops
Not usable for ds NA moves



Domain	Flexible Region	Residues
MA		1 - 122
linker	I	123 - 144
CA		145 - 276
	II	277 - 282
		283 - 353
p2	III	354 - 377
linker	IV	378 - 389
NC		390 - 407
	V	408 - 412
		413 - 432

Generate Ensemble

Energy Minimize & Calculate I(q)

Compare to Exp.: Chi-square Filter Density Plot

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Monomer Monte Carlo II

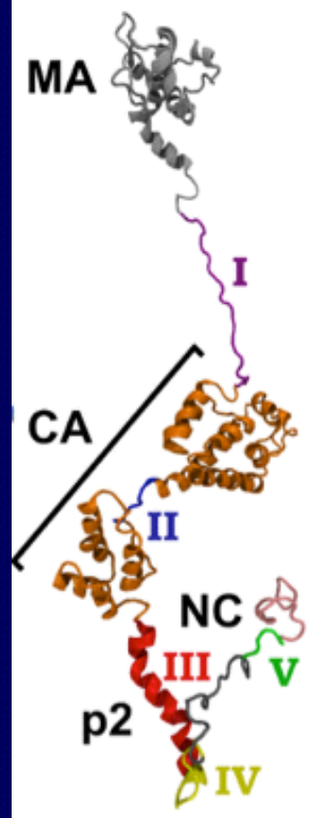
Monomer Monte Carlo

run name	run_0
reference pdb	Choose File hiv1_gag.pdb or Browse server *Local*: hiv1_gag.pdb
output file name (dcd)	hiv1_gag_monte_carlo.d
number of trial attempts	10000
return to previous structure	20
temperature (K)	300.0
molecule type	protein
number of flexible regions to vary	5
maximum angle sampled for each region	30.0,30.0,30.0,30.0,30.0
residue range for each flexible region	123-144,277-282,354-374,378-389,408-412
structure alignment: low residue	284
structure alignment: high residue	350
overlap basis	heavy atoms

Advanced Input

Check Box for Advanced Input

Submit Reset to default values



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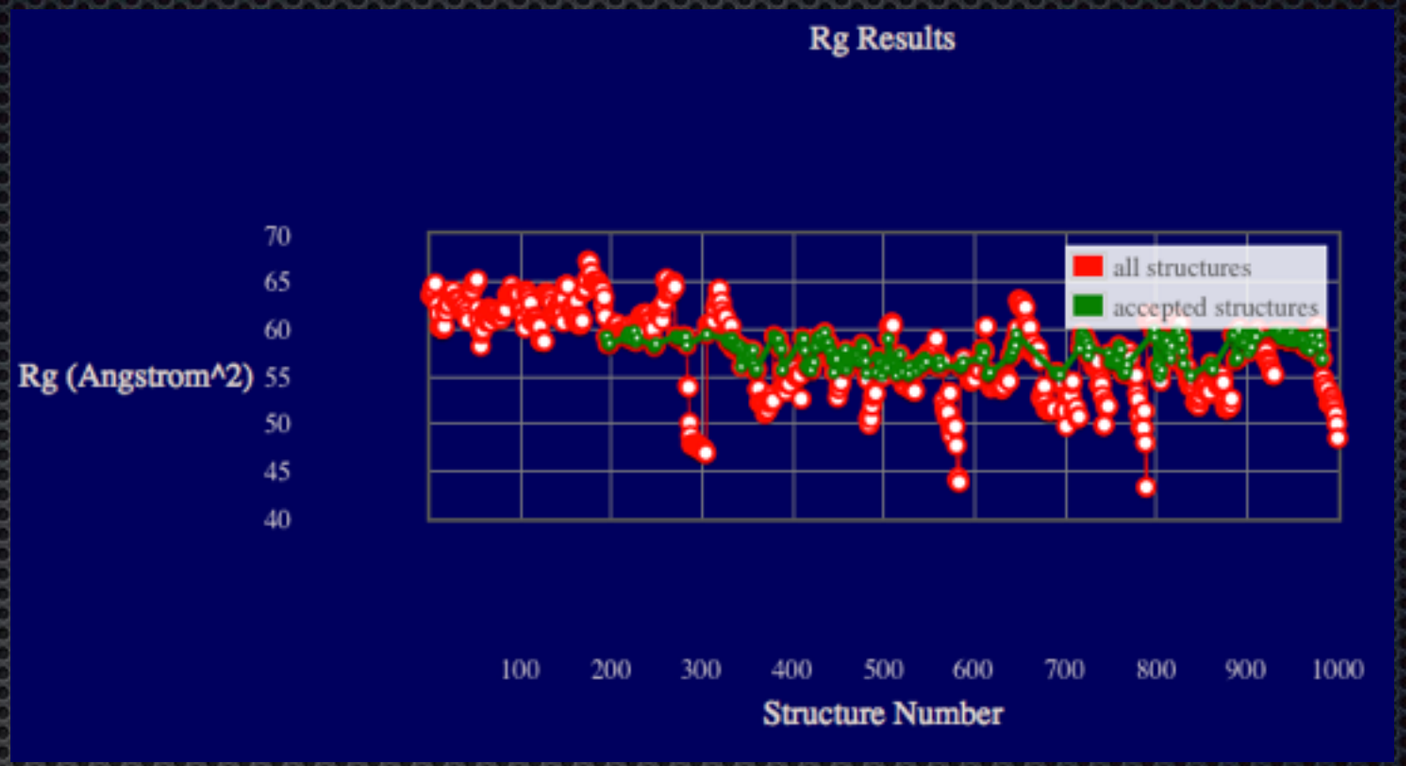
		413 - 432

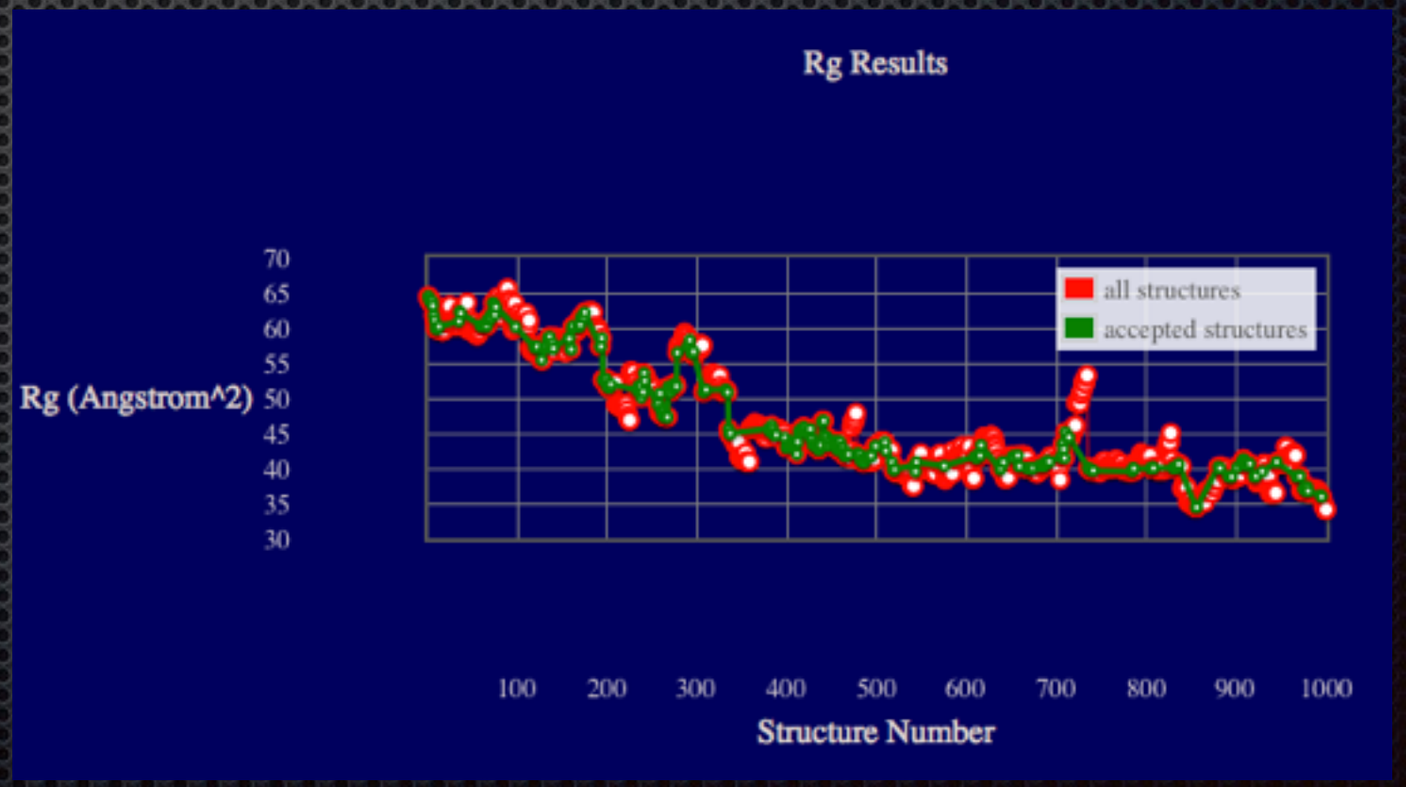
Monomer Monte Carlo III

Rg filter(s)

(eg. 55 < Rg < 60)



Directed Monte Carlo
(bias to an Rg value)

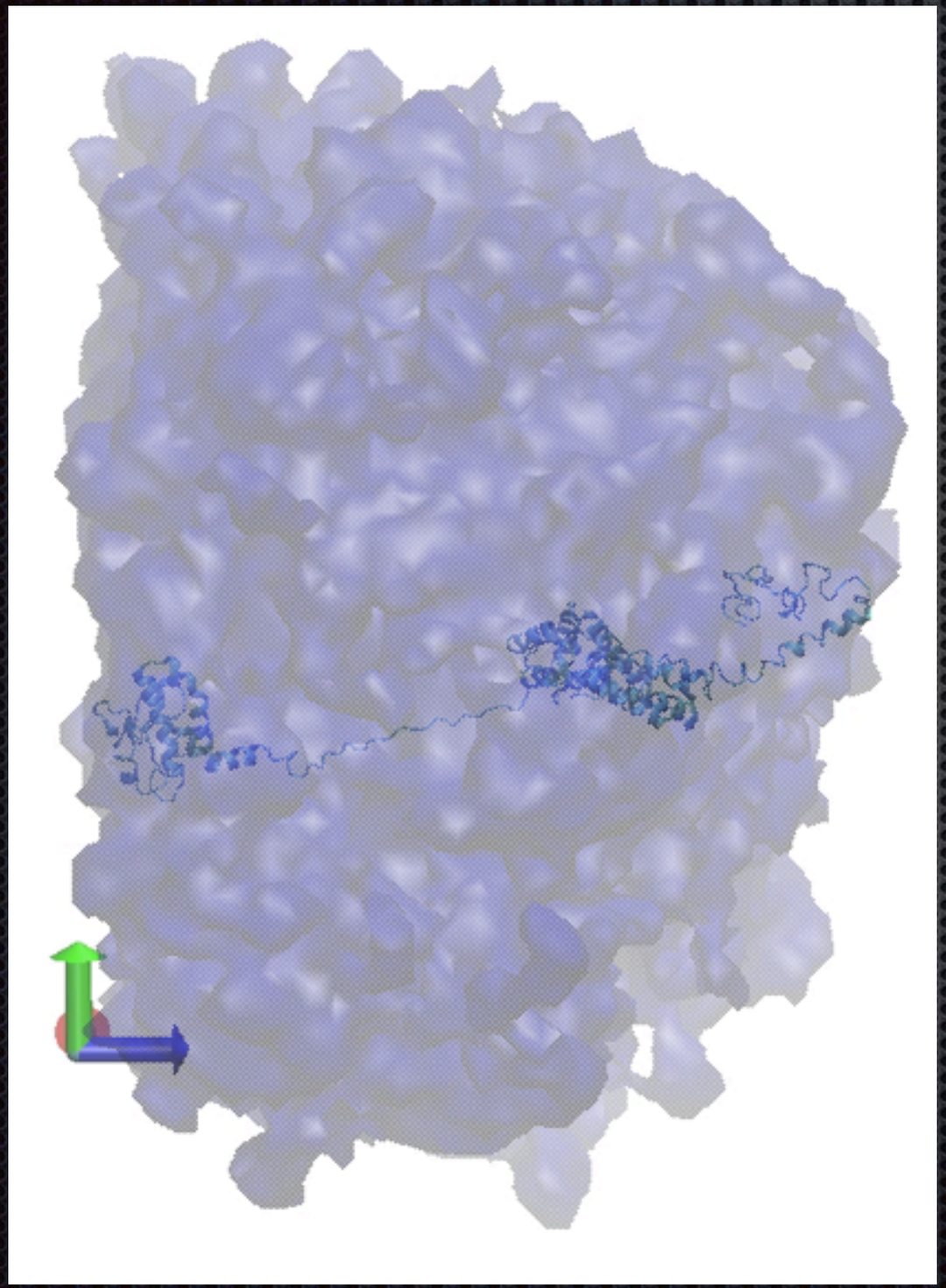


Monomer Monte Carlo IV

Z filter

check box to use Z coordinate filter ☑

Z cutoff (angstroms) 0.0



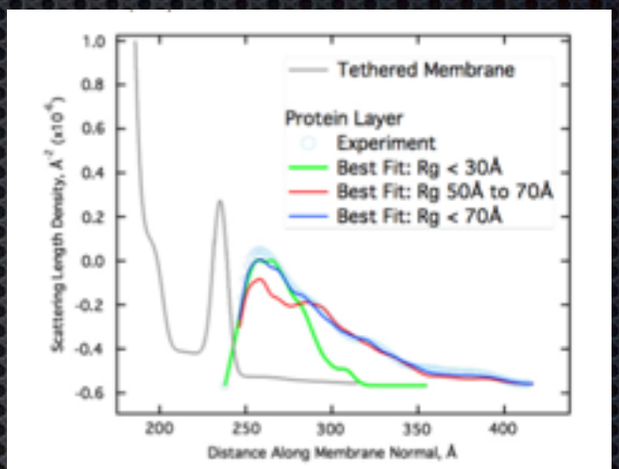


Fig. 2. Molecular modeling of Gag protein structure on the membrane using SLDMOL to fit experimentally derived SLD profiles. The experimentally derived SLD profiles for Gag, light blue circles, are shown in the compact conformational state, panel A, and the extended state, panel B. Using the SASSIE software package 100,000 independent conformations of the Gag protein were generated and subsequently filtered based on Rg values. An average SLD profile using a Monte-Carlo optimization to weight the structures provided a best fit for each Rg range and can be seen as solid lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Monomer Monte Carlo IV

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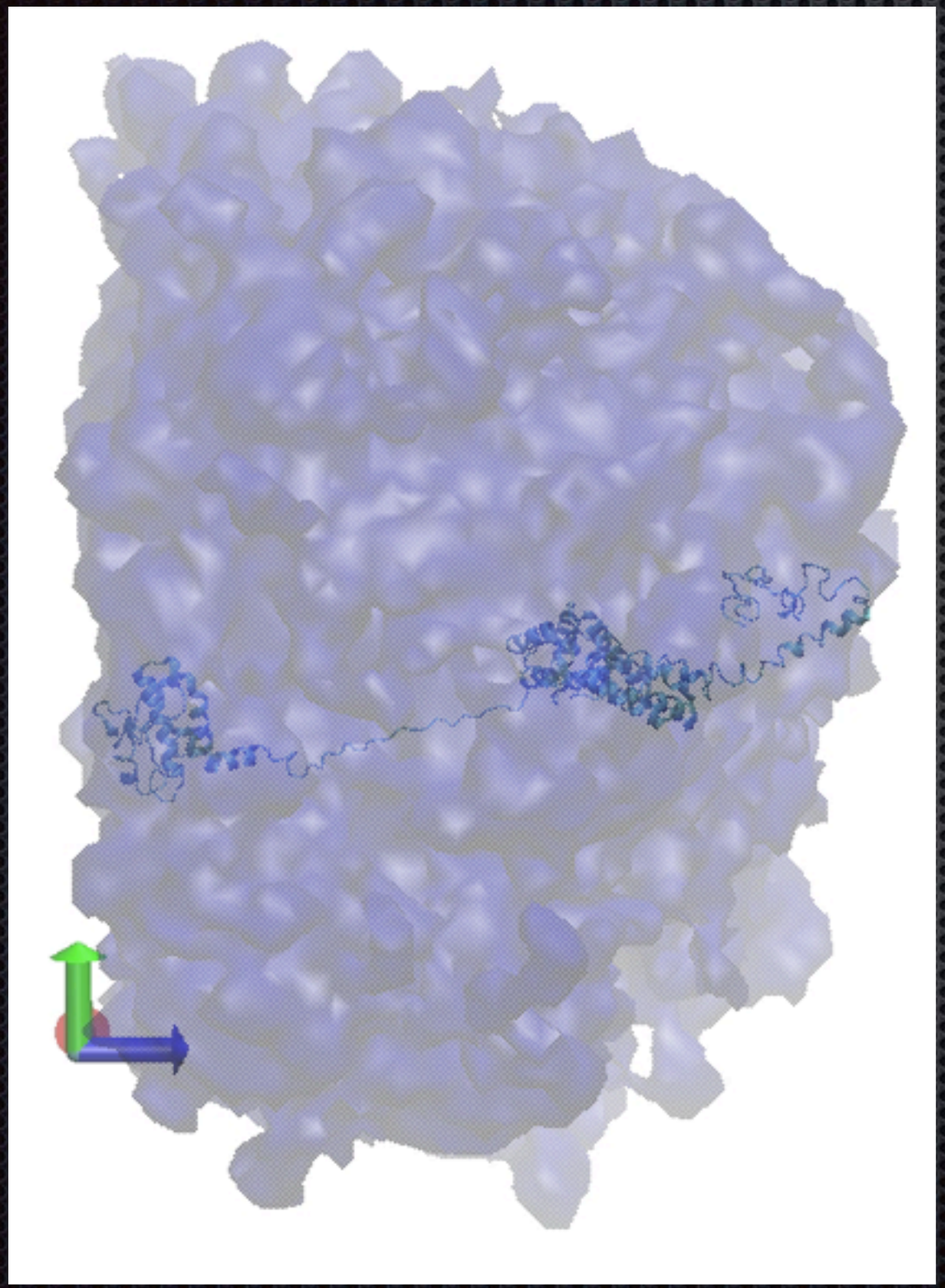

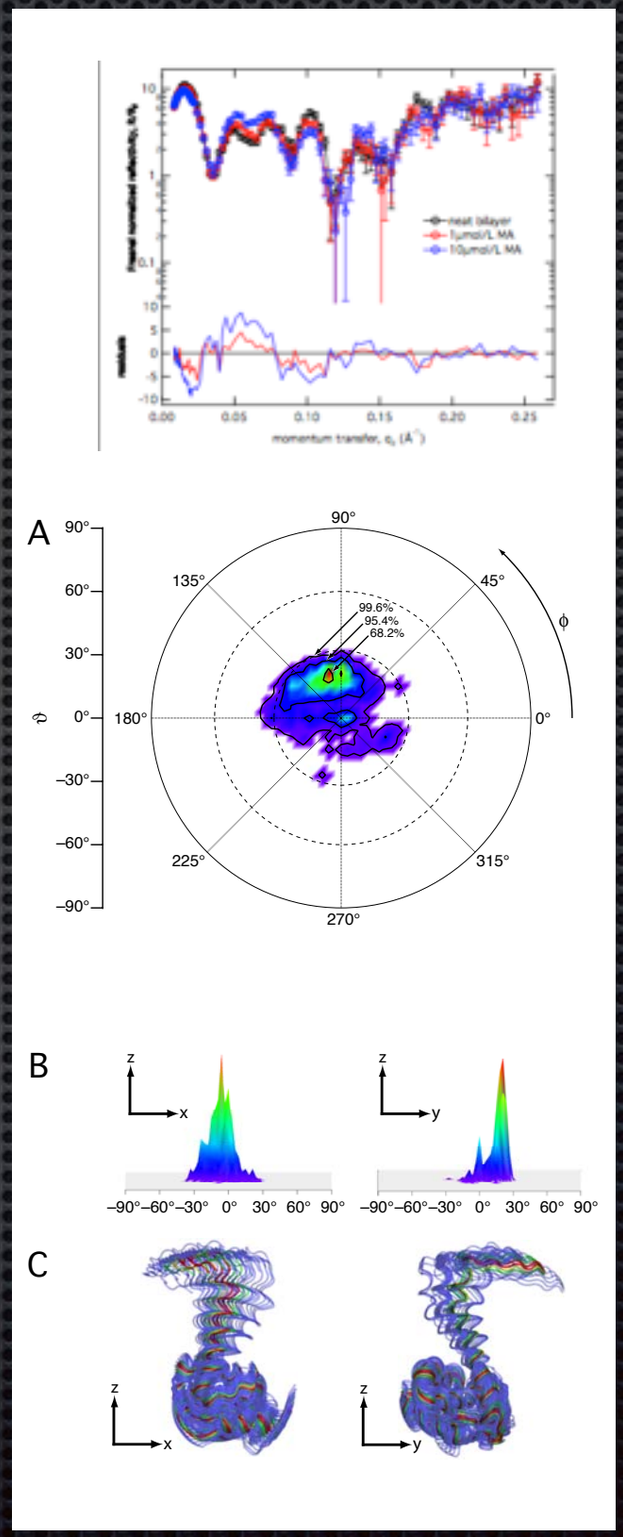

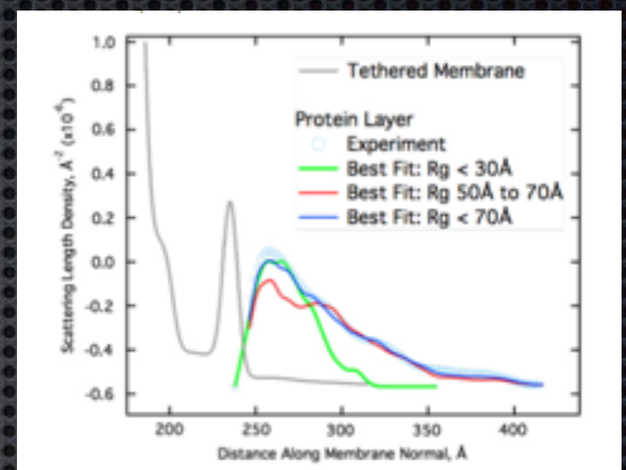

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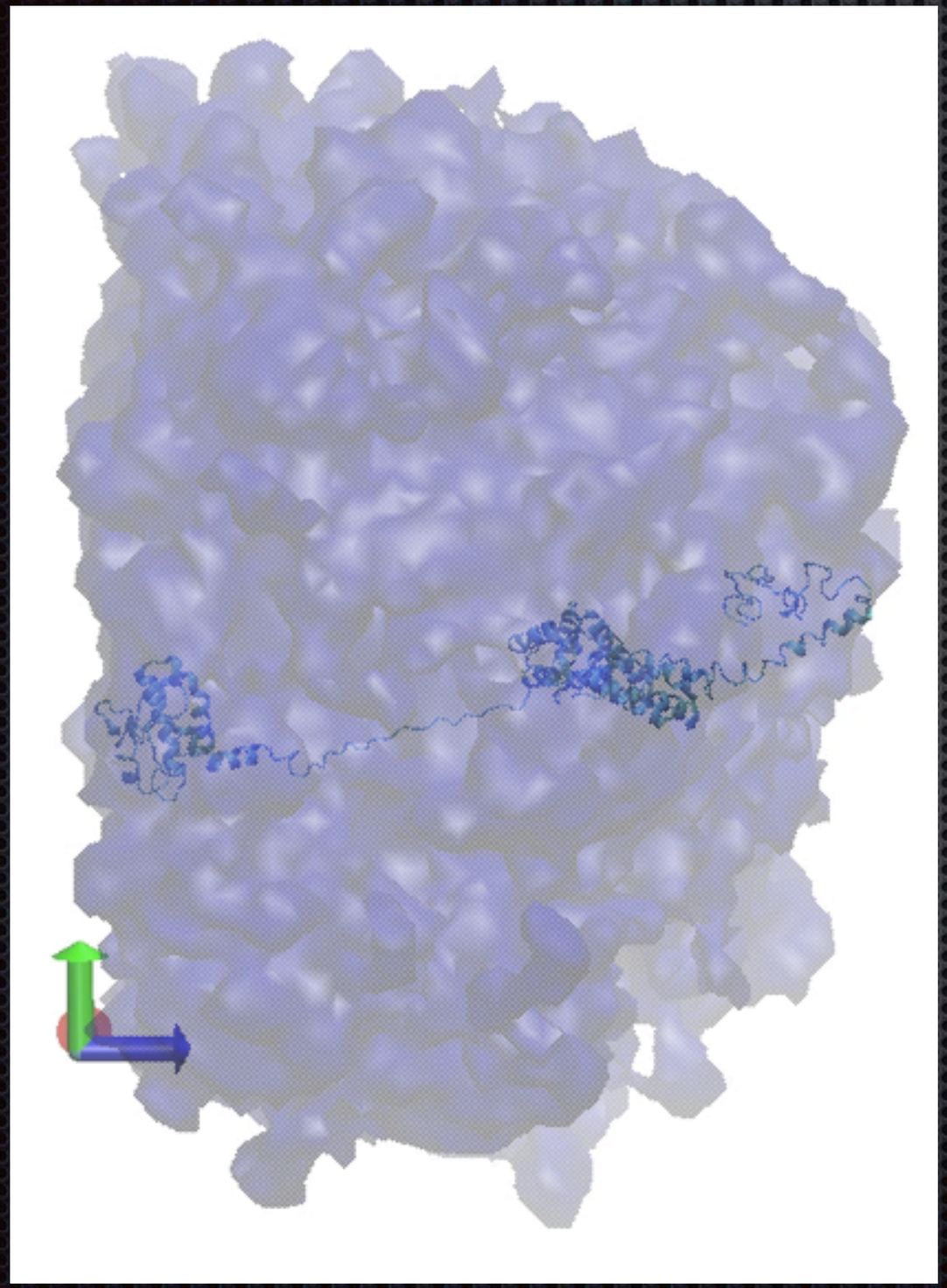
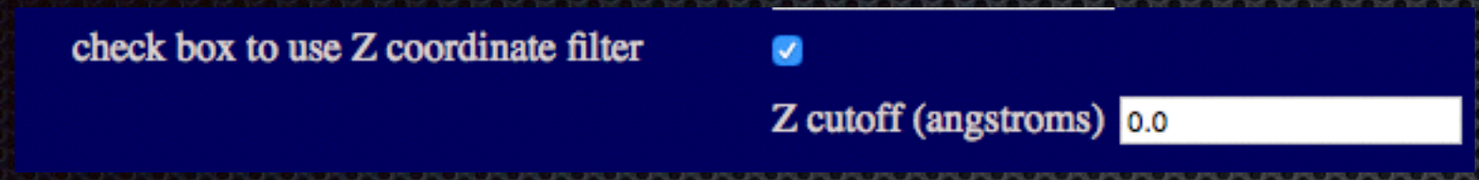
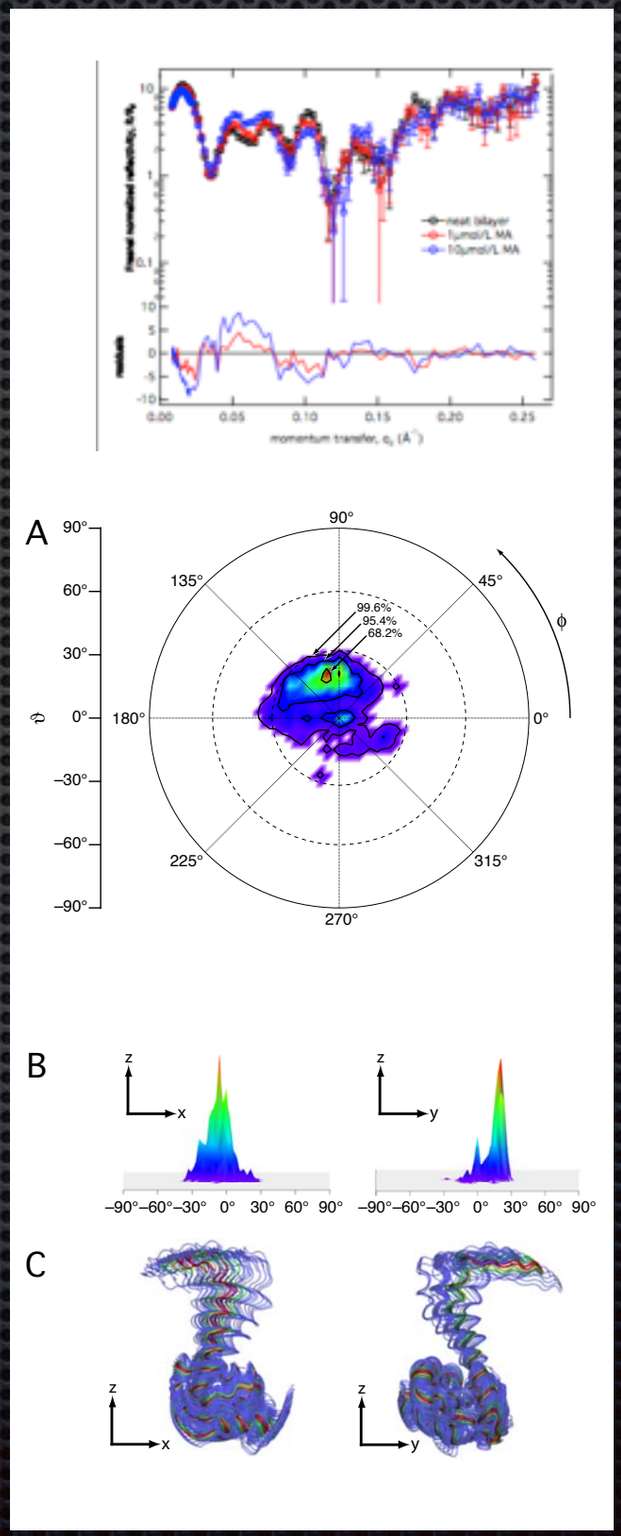






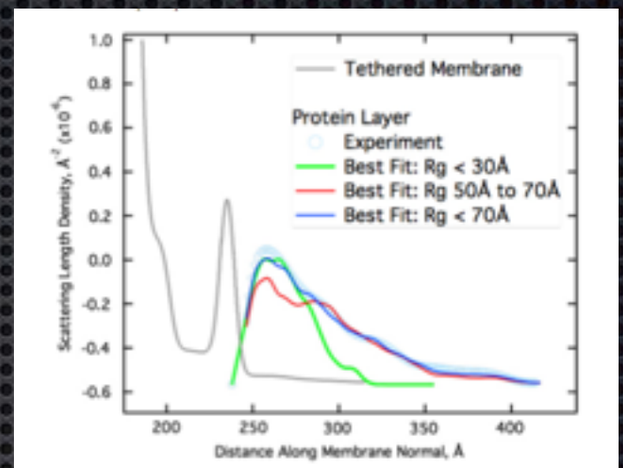
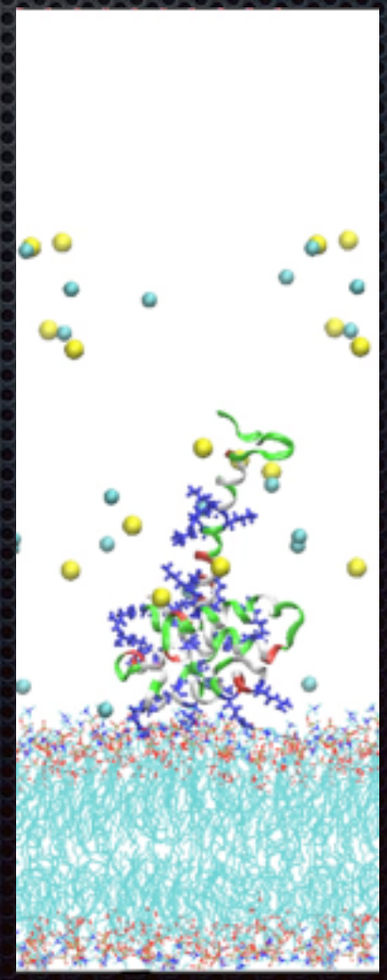
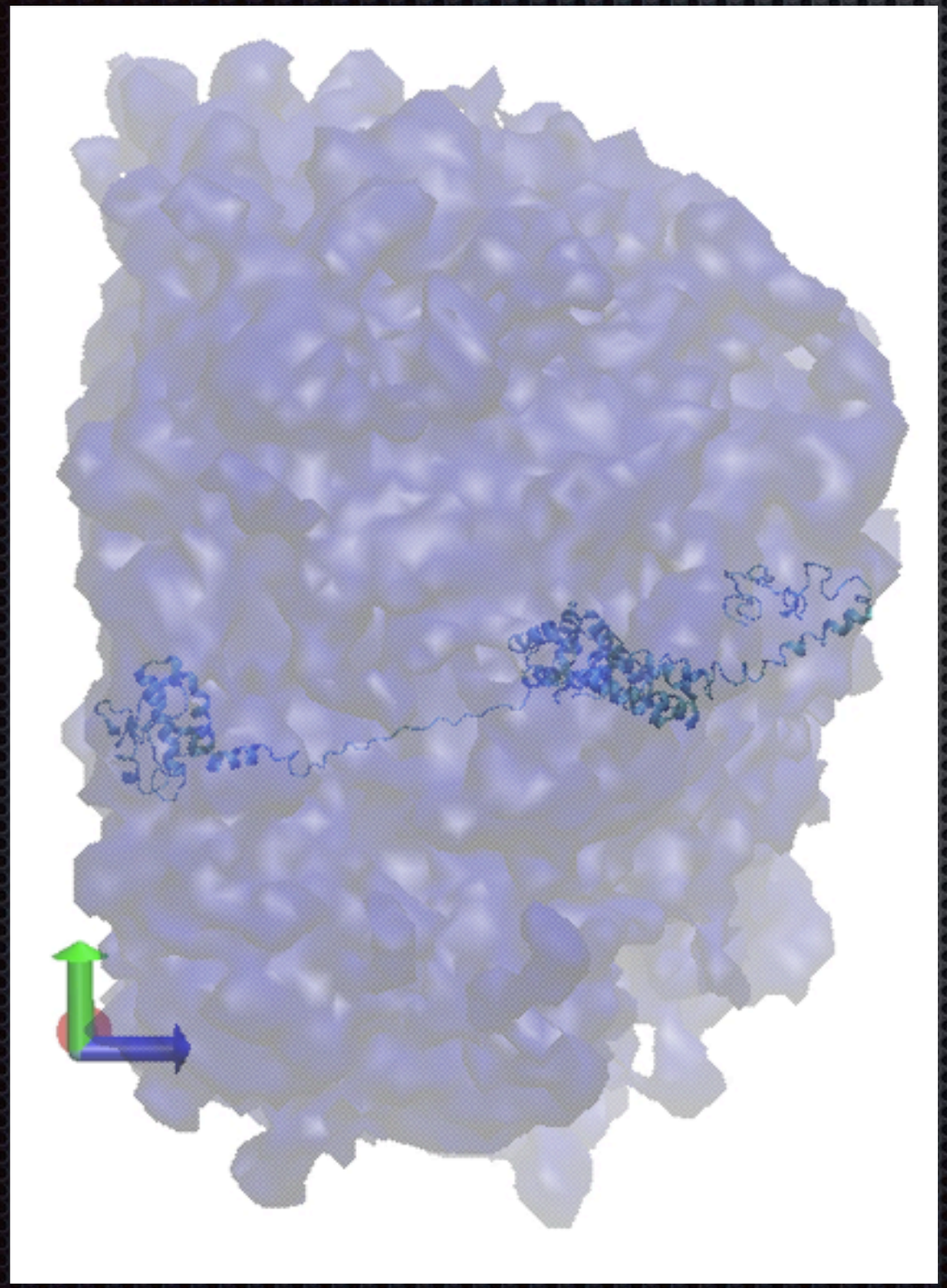


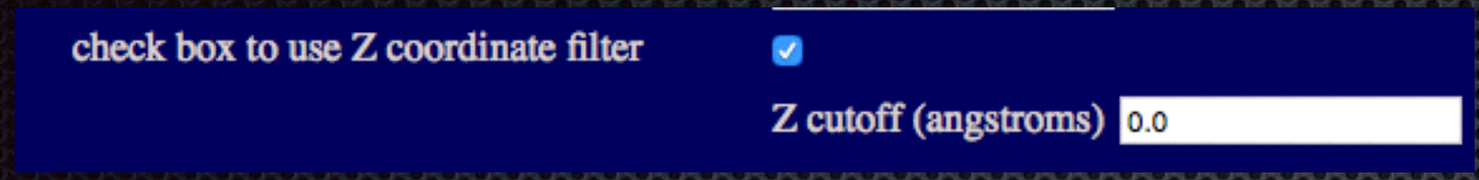
Fig. 2. Molecular modeling of Gag protein structure on the membrane using SLDMOL to fit experimentally derived SLD profiles. The experimentally derived SLD profiles for Gag, light blue circles, are shown in the compact conformational state, panel A, and the extended state, panel B. Using the SASSIE software package 100,000 independent conformations of the Gag protein were generated and subsequently filtered based on Rg values. An average SLD profile using a Monte-Carlo optimization to weight the structures provided a best fit for each Rg range and can be seen as solid lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

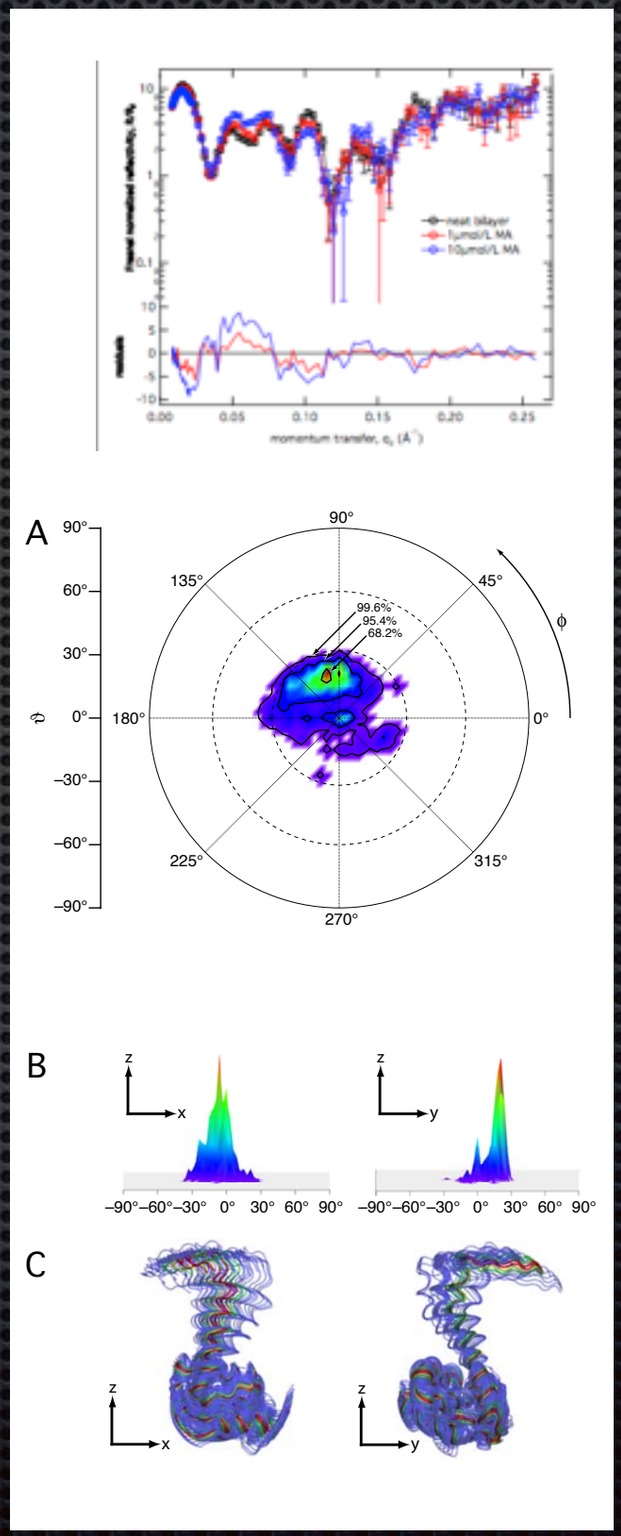


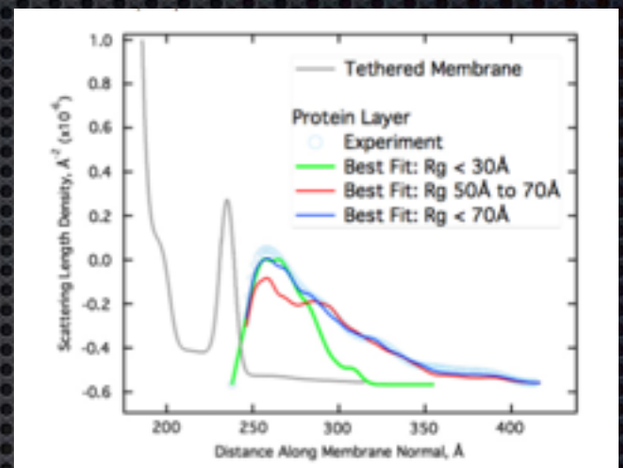
Monomer Monte Carlo IV

Z filter









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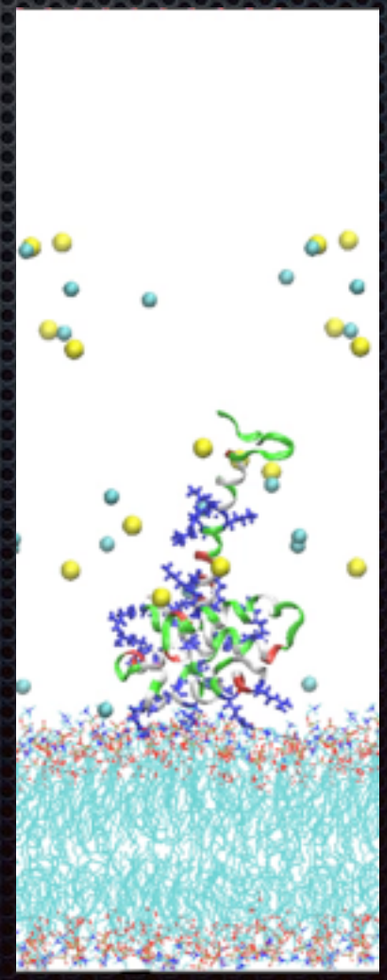
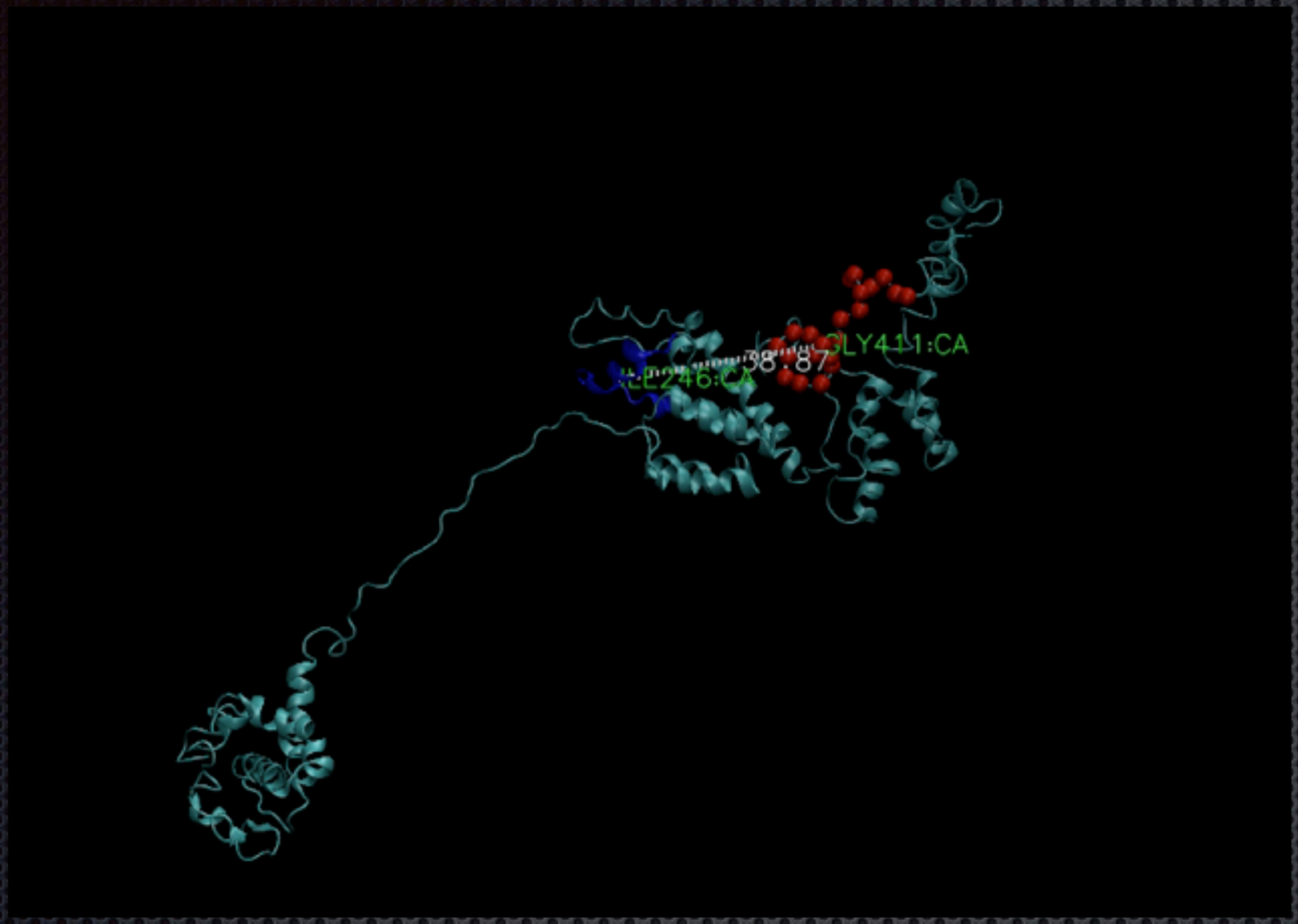
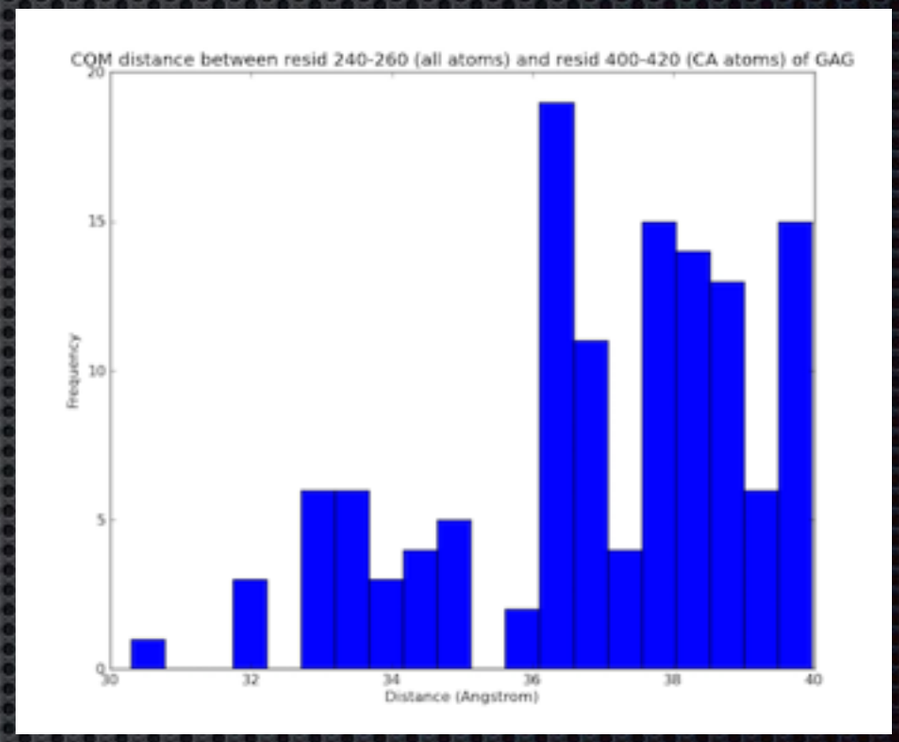


Monomer Monte Carlo V





constraint file name Choose File constraints.txt or Browse server *Local*: constraints.txt

GAG 240-260 : GAG 400-420 CA : 40.0 : COM : COM

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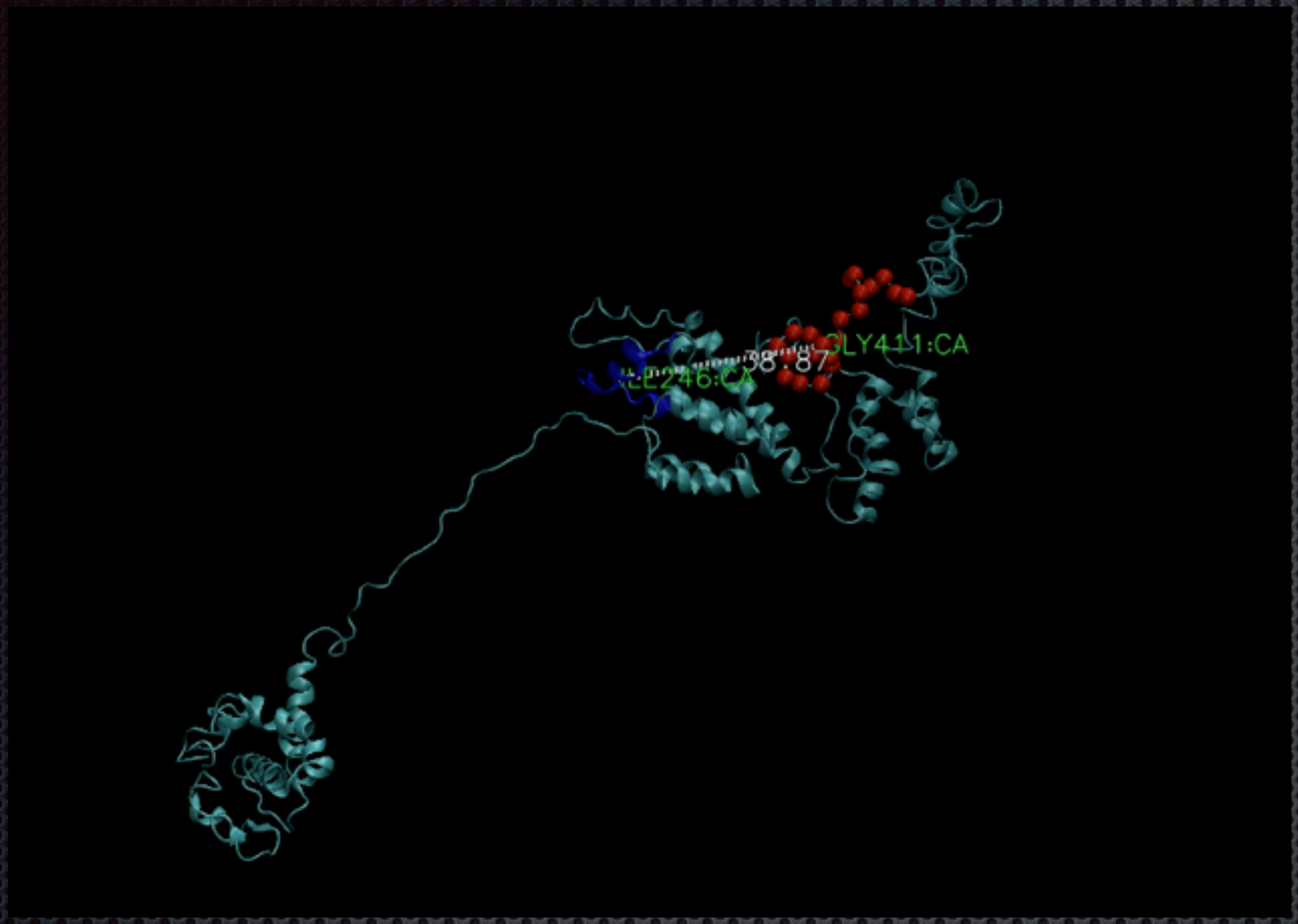
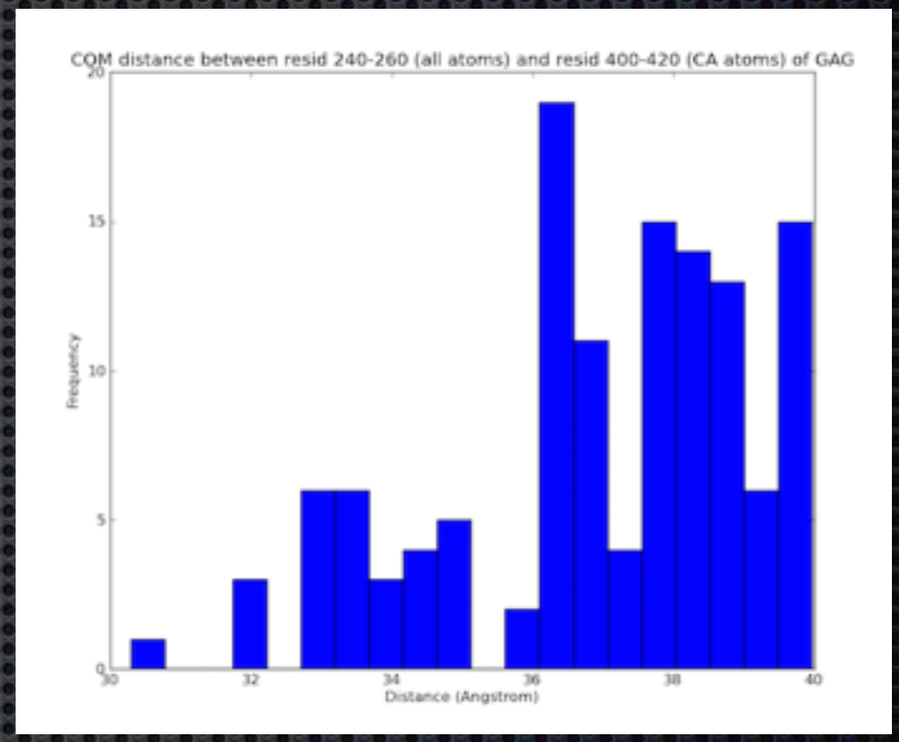
How to Use Atomic Constraints

NSF

Monomer Monte Carlo V





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GAG 240-260 : GAG 400-420 CA : 40.0 : COM : COM

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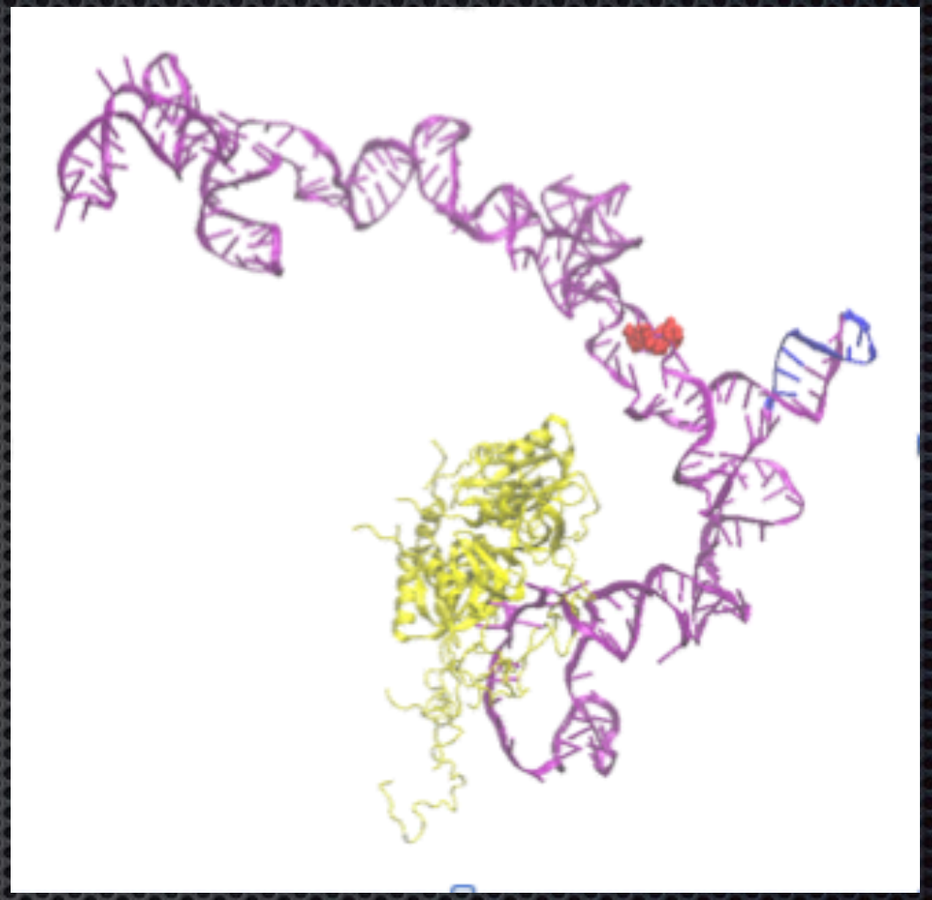
How to Use Atomic Constraints

NSF

Complex Monte Carlo

Mutiple, single chain IDP / ID-NA
simple N -> C or 5’ – 3’
backbone torsion sampling

“What if” questions and
ensembles for further analysis
Not all chains need to be flexible
(ds DNA etc. can be present)
Configurations are correlated
Not usable with internal loops
Not usable for ds NA moves



Generate Ensemble

Energy Minimize
&
Calculate I(q)

Compare to Exp.:
Chi-square Filter
Density Plot

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sassie-web -- Complex MC II

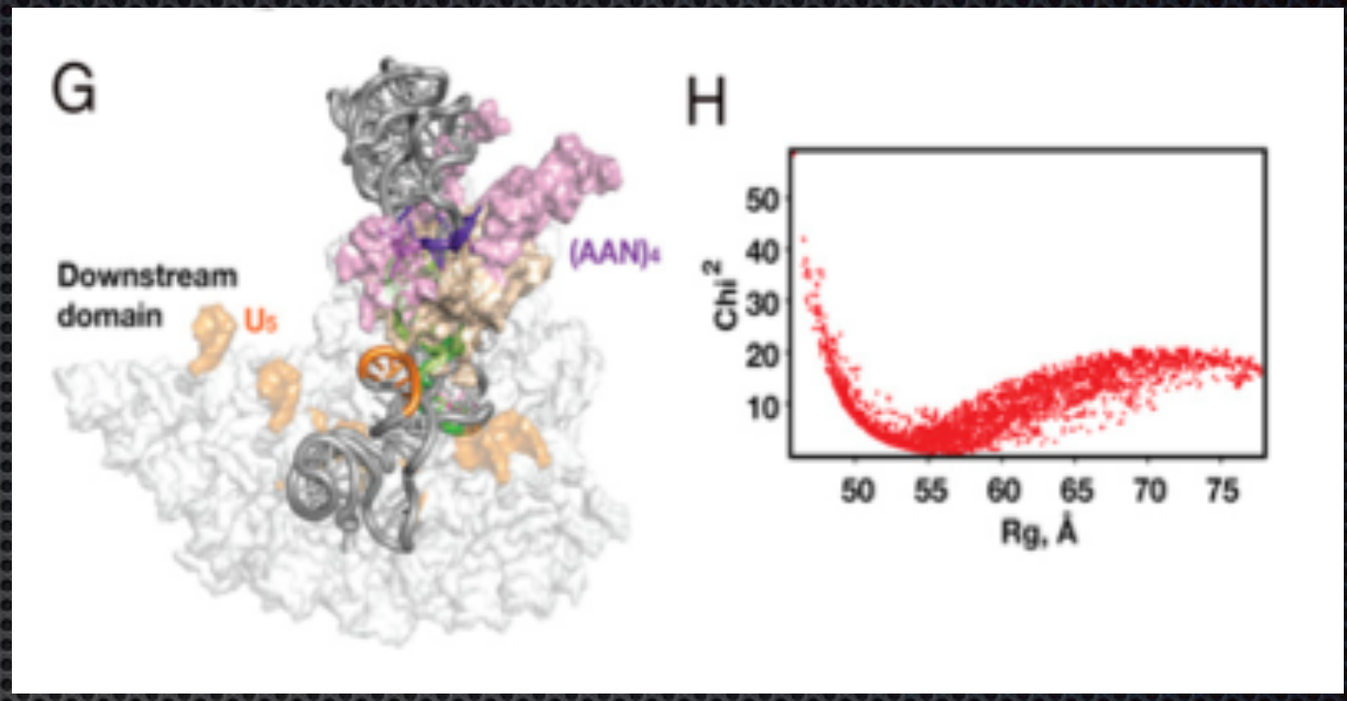
Rg filter(s)

Monte Carlo

Z-filter

Constraints etc.

Example: RNA – protein complex



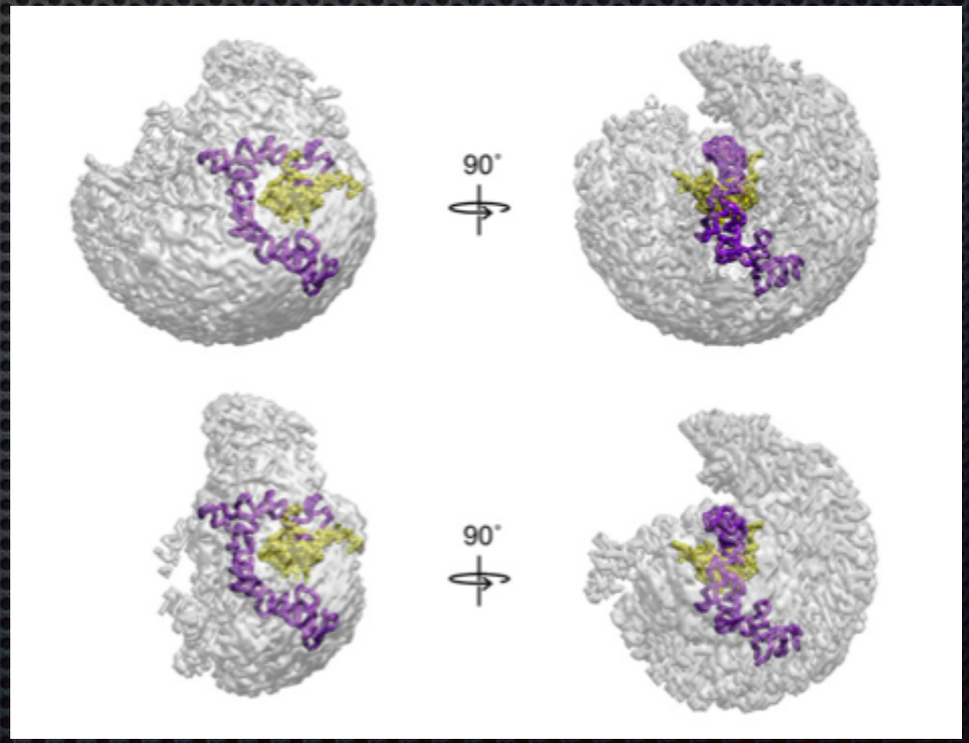
→ many experimental constraints (SHAPE)

→ 12 flexible regions in 6 protein segments (tails)

→ several RNA torsions sampled (systematically)

→ best fitting structures indicated a restricted range of motion:

opening and closing

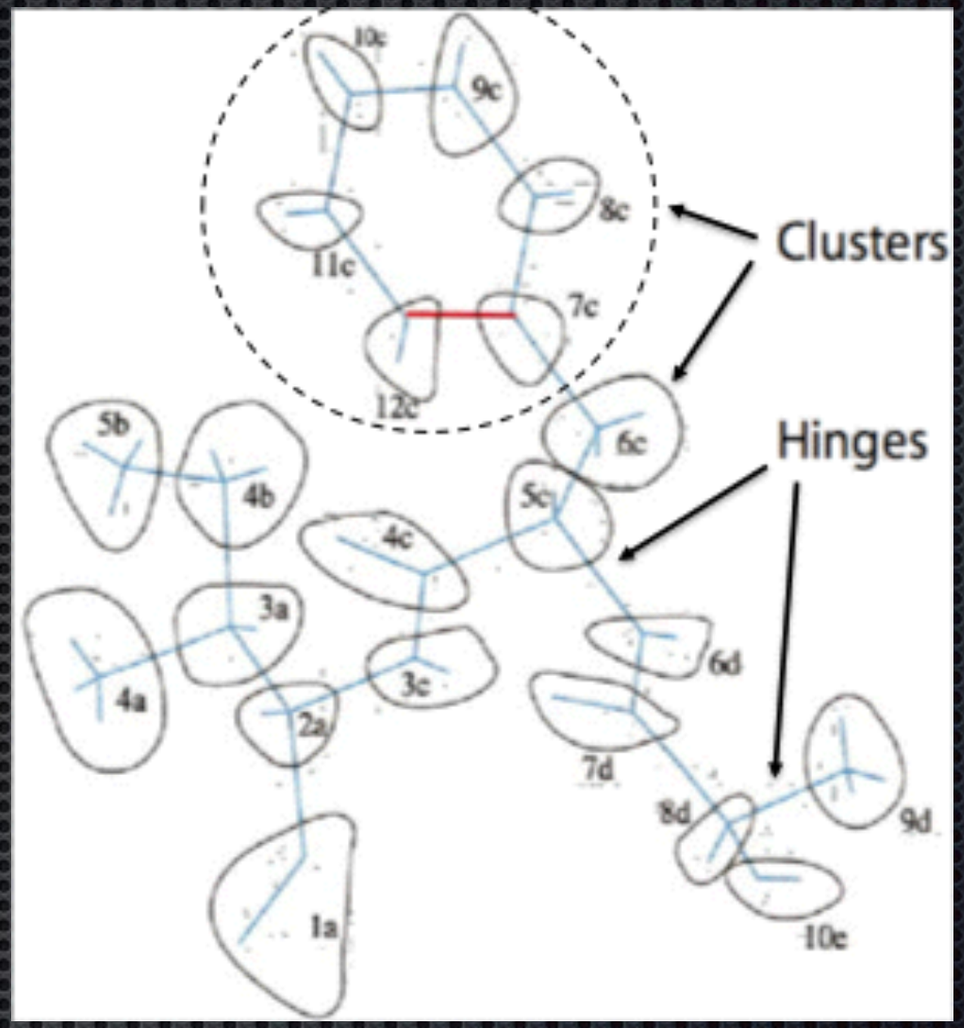


Y. Peng, et al. Proc. Nat. Acad. Sci. 111 (48), 17134-17139 (2014).

Torsion Angle MD

Much more robust than Cartesian MD (no high-frequency bond/ angle vibrations)
Larger MD time steps
Sample the most relevant degrees of freedom (dihedrals)
Convenient classification of rigid and flexible regions
Can handle internal loops

Requires extensive energy minimization to start



Run MC then TAMD: multi-scale sampling use SAS as a guide

J. Chen, W. Im, C. Brookes, JCC 26, 1565 (2005), Zhang et al. (in preparation)

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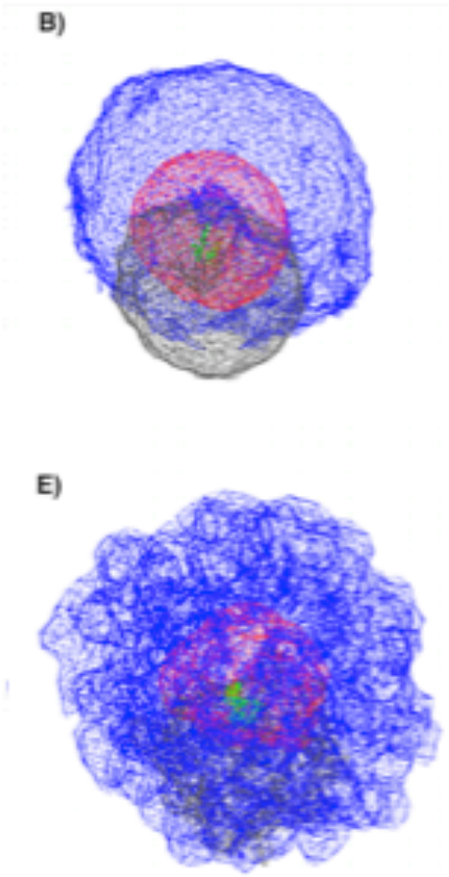
sassie-web -- Torsion Angle MD

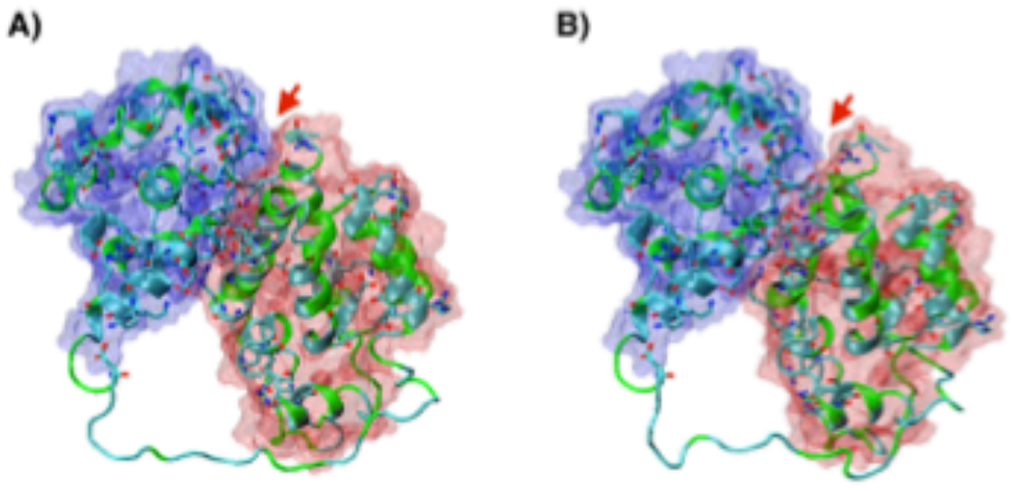
TAMD : combine MC w/ fast MD

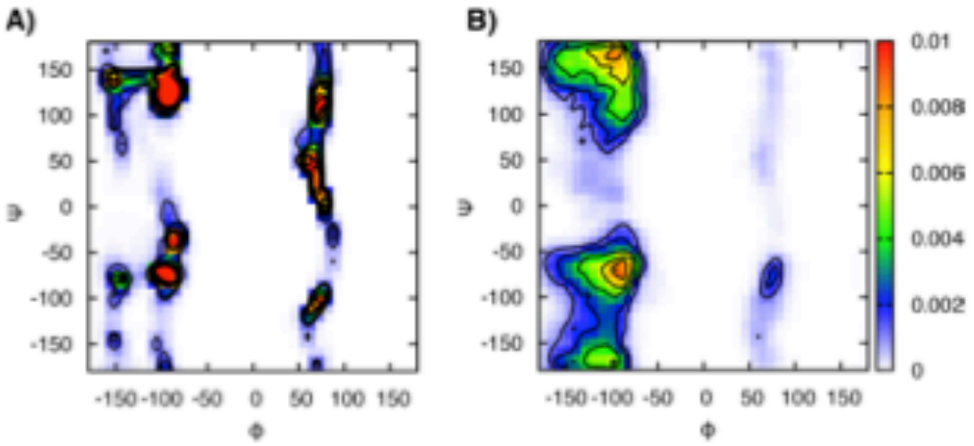
MC (50000)

Spatial Clusters (~100)



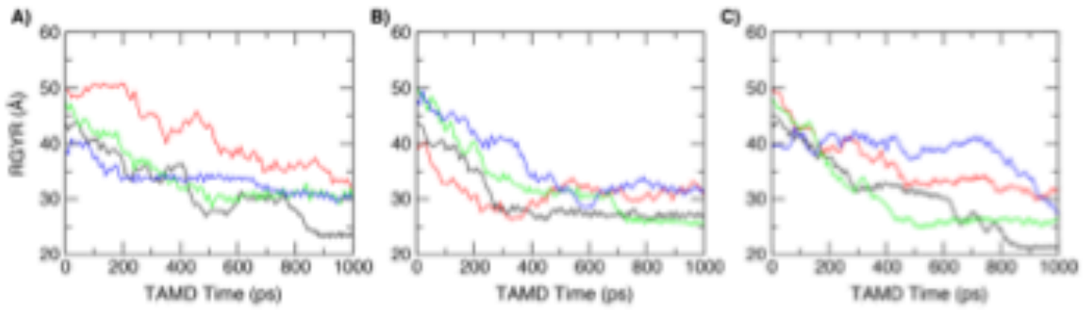
Protein, DNA, RNA, carbohydrates . . . and complexes





Zhang et al. (in preparation)

Implicit solvent effects



EFF1, SASA, GB, ACE

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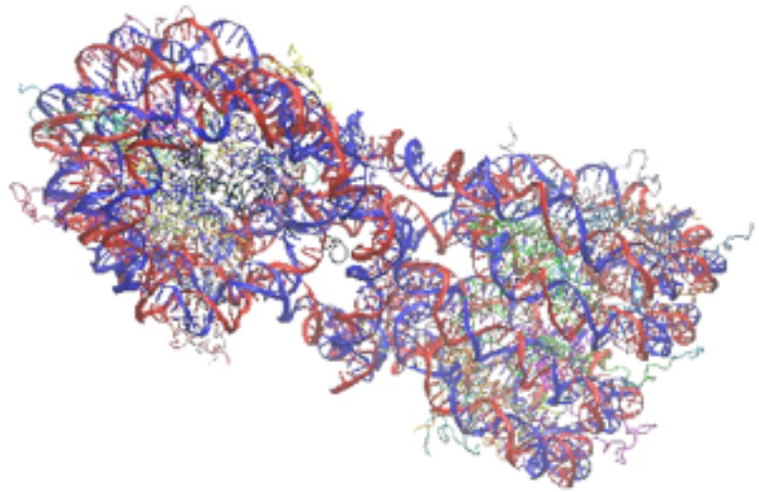
Torsion Angle MC

Multiple, multi-chain species: ds-DNA, proteins, RNA, carbohydrates, etc.

Group based rotations … can handle odd topologies (mAb) natively.

User defined torsion sampling backbone, concerted motions, side-chains, carbohydrates, iso-peptide bonds, etc.



Beta testers are needed ;)

Howell et al. (in press: JCC) & Curtis et al. (in preparation)

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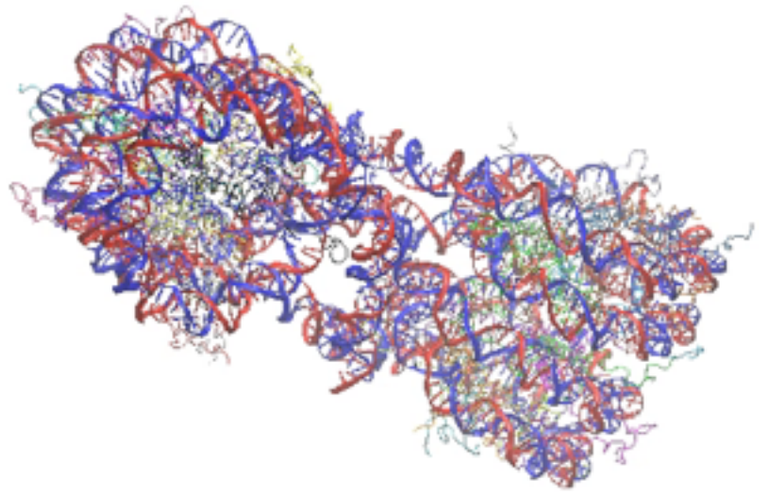

Beta testers are needed ;)

Howell et al. (in press: JCC) & Curtis et al. (in preparation)

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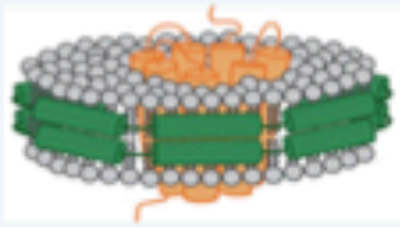
CG Sim. For Chem.

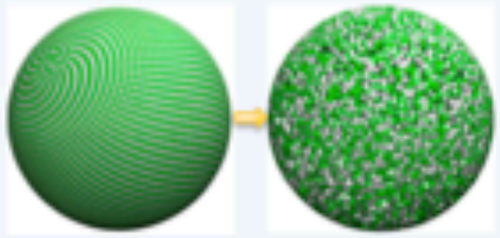
- Martini / LAMPPS etc. accessible *now* via SASCALC (contrast coming soon)
- But some systems are even bigger and may benefit from specialized CG Methods

Coarse-grain model systems

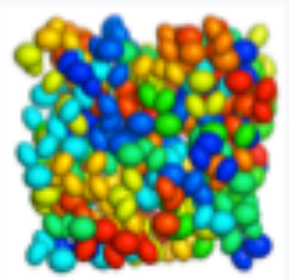
Lipid rafts



Nanodiscs

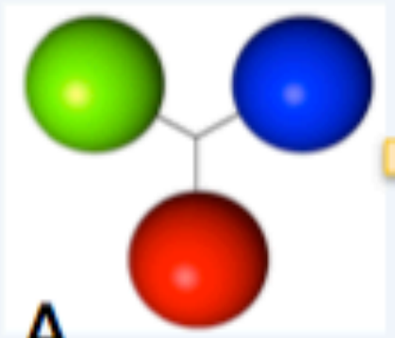


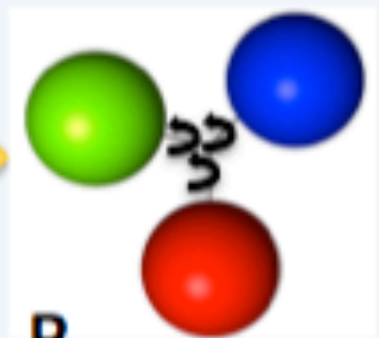
Lipid rafts on sphere surfaces

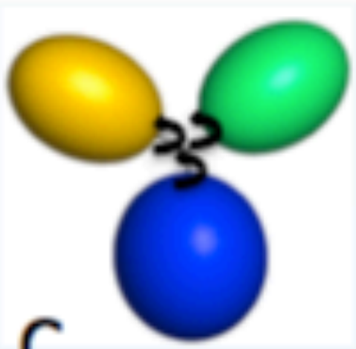


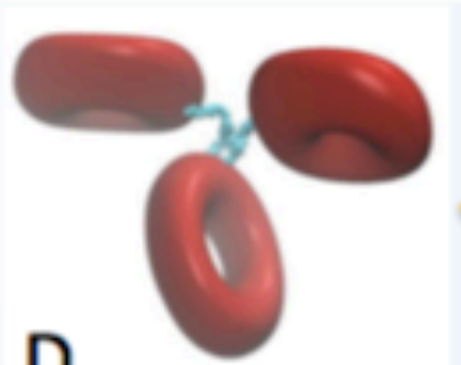
High-density protein systems

Apply the level of detail required by experiment









Zhang & Curtis (in preparation)

$$S(\mathbf{q}) = 1 + \rho \int_V \mathrm{d}\mathbf{r}\, \mathrm{e}^{-i\mathbf{q}\mathbf{r}} g(\mathbf{r})$$

sassie-web -- Calculate

Input a TRAJECTORY and get an ensemble of scattering profiles

Calculate -- generate theoretical scattering data from structures

SasCalc Calculates neutron and X-ray scattering profiles from input structures. Will replace xtal2sas once completed.

SasCalc-MD Calculates neutron and X-ray scattering profiles from MD trajectories with explicit water.

Xtal2sas Calculates neutron scattering profiles from input structures.

Cryson Calculates neutron scattering profiles from input structures.

Crysol Calculates X-ray scattering profiles from input structures.

SCT Calculate Calculates neutron and X-ray scattering profiles from input structures.

SLD MOL Calculates neutron and X-ray reflectivity scattering length density from user supplied structures. Utilities for experimental planning and isotopic labeling and optimization of ensemble populations are supplied.

EM to SANS Calculates neutron scattering profile from user supplied electron density map.

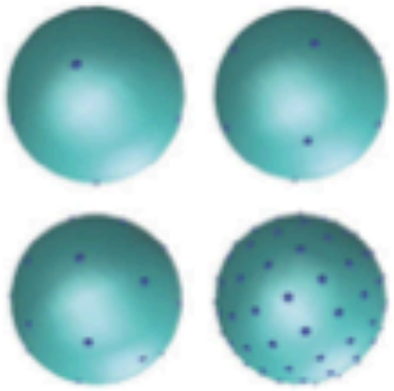
calculate scattering

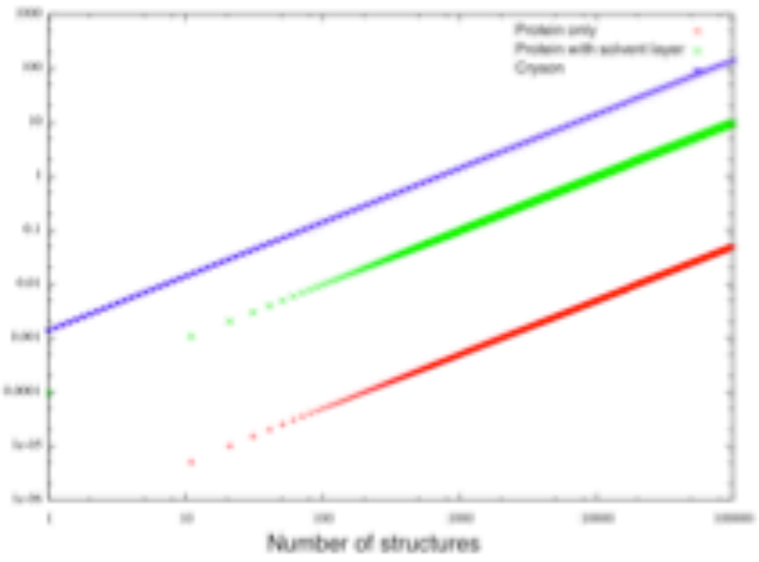
SASCALC (gpu – golden vector method)

J. Appl . Cryst 46, 1171 (2013) & somewhere (2015)

$$I(\mathbf{q}) = \left[\sum_j^N b_j \cos(\mathbf{q}\cdot\mathbf{r}_j)\right]^2 + \left[\sum_j^N b_j \sin(\mathbf{q}\cdot\mathbf{r}_j)\right]^2.$$

$$I(q) = \frac{1}{n}\left\{\sum_{k=(1-n)/2}^{(n-1)/2} I[\mathbf{q}^{(k)}]\right\}$$



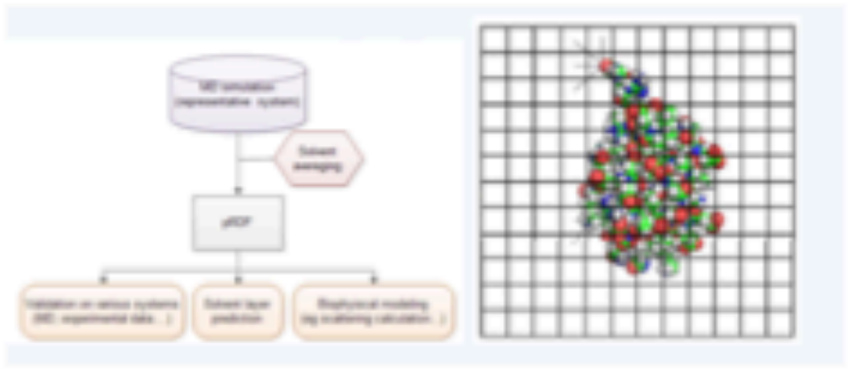


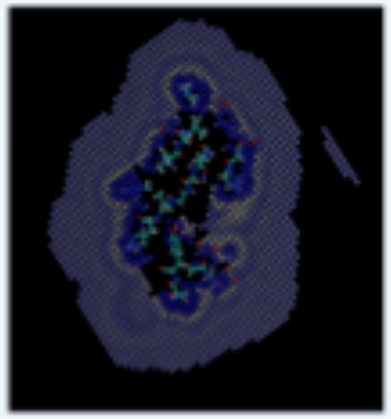
10^5 structures in 3 mins versus 159 hours ;
Implicit solvent -> ~ 11 hours

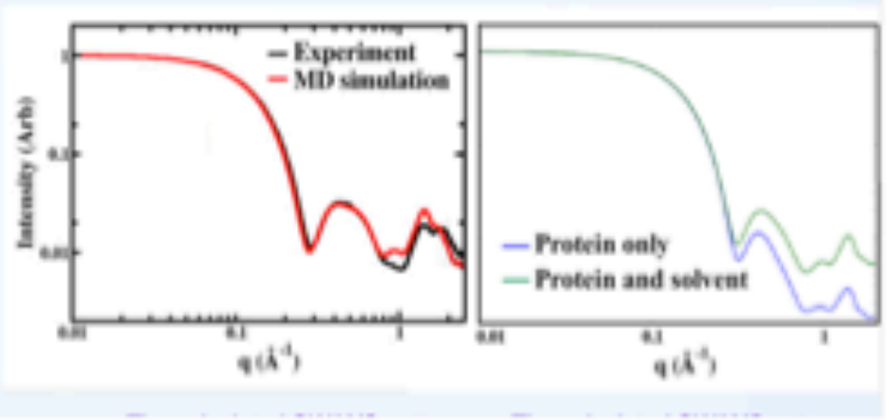
Chemical RDF Library

Implicit: HyPred BPJ 99, 1611 (2010)

"library of pRDFs" for chemical systems / co-solutes



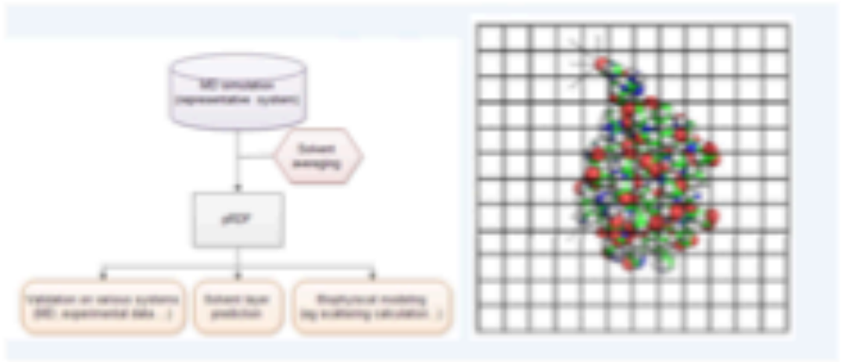




Now, w/ K. Freed U. Chicago

calculate scattering

Chemical RDF Library



Documentation, MD requirements, code, and API

→ so LIBRARY can be built for new chemical systems (formatted)

→ SasCalc will read formatted LIBRARY

→ vacuum scattering already covers X-ray / neutron for periodic table

→ Initial LIBRARY : proteins, NA, carbohydrates in water

Krueger, Koefinger, Grishev, Stanley
→ high Q validation data

SasCalc – MD

Code to calculate scattering from MD trajectories

All-atom: J. Koefinger PRE 87 (2013)

sassie-web -- Analyze

Analyze -- compare theoretical data to experimental data and advanced analysis methods

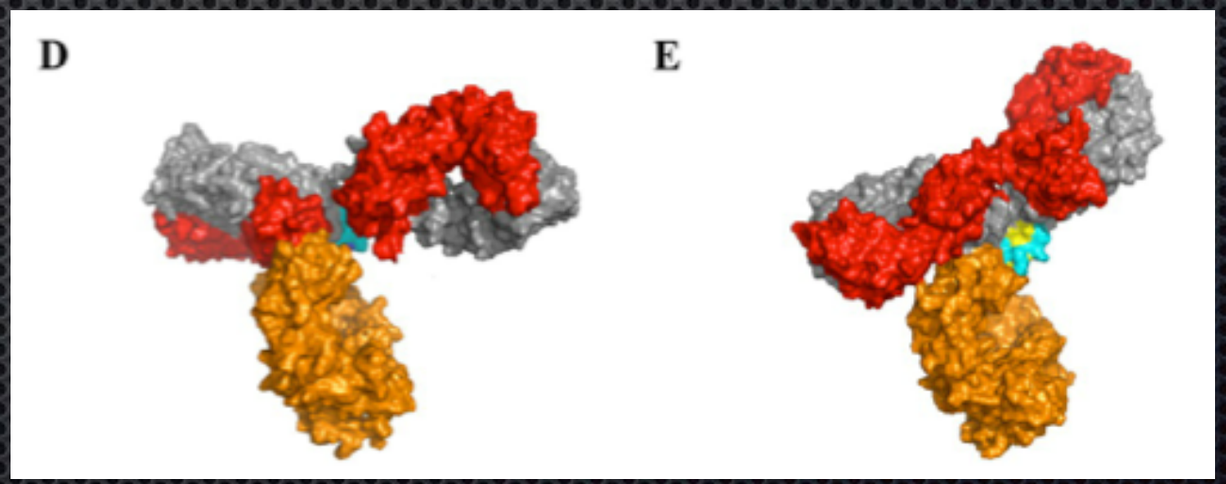
Chi-Square Filter Compares calculated scattering profiles to user supplied interpolated scattering profiles. No fitting.

SCT Analyze Compares calculated scattering profiles to user supplied interpolated scattering profiles. No fitting.

Density Plot Calculates volumetric gaussian cube files from user supplied structures. These files can be rendered in VMD and Pymol.

APBS Calculates non-polar solvation energy using adaptive Poisson-Boltzman solver from user supplied structures.

Both X^2 ~ 1



Free Energy differs by > 400 kCal/mol

Clark et al. J. Phys. Chem. B 2013, 117, 14029–14038, 2013

sassie-web -- Tools

Tools -- general utilities

Contrast Calculator Experimental planning to predict scattering length density and I(0) from input PDB file, Fasta sequence file, or chemical formula.

Align Moves structures from input structure file so that they overlap with a reference input structure.

Data Interpolation Creates a new data file that is spaced in a uniform grid from input experimental data file.

Extract Utilities Allows user to extract individual structures and/or SAS profiles from a larger input structure file and/or folder containing SAS profiles.

Merge Utilities Allows user to combine user supplied structures and calculated scattering profiles into a single set of new files.

Small-Angle Scattering Contrast Calculator for Protein and Nucleic Acid Complexes in Solution, J. Appl. Cryst. 46, 1889-1893 (2013).

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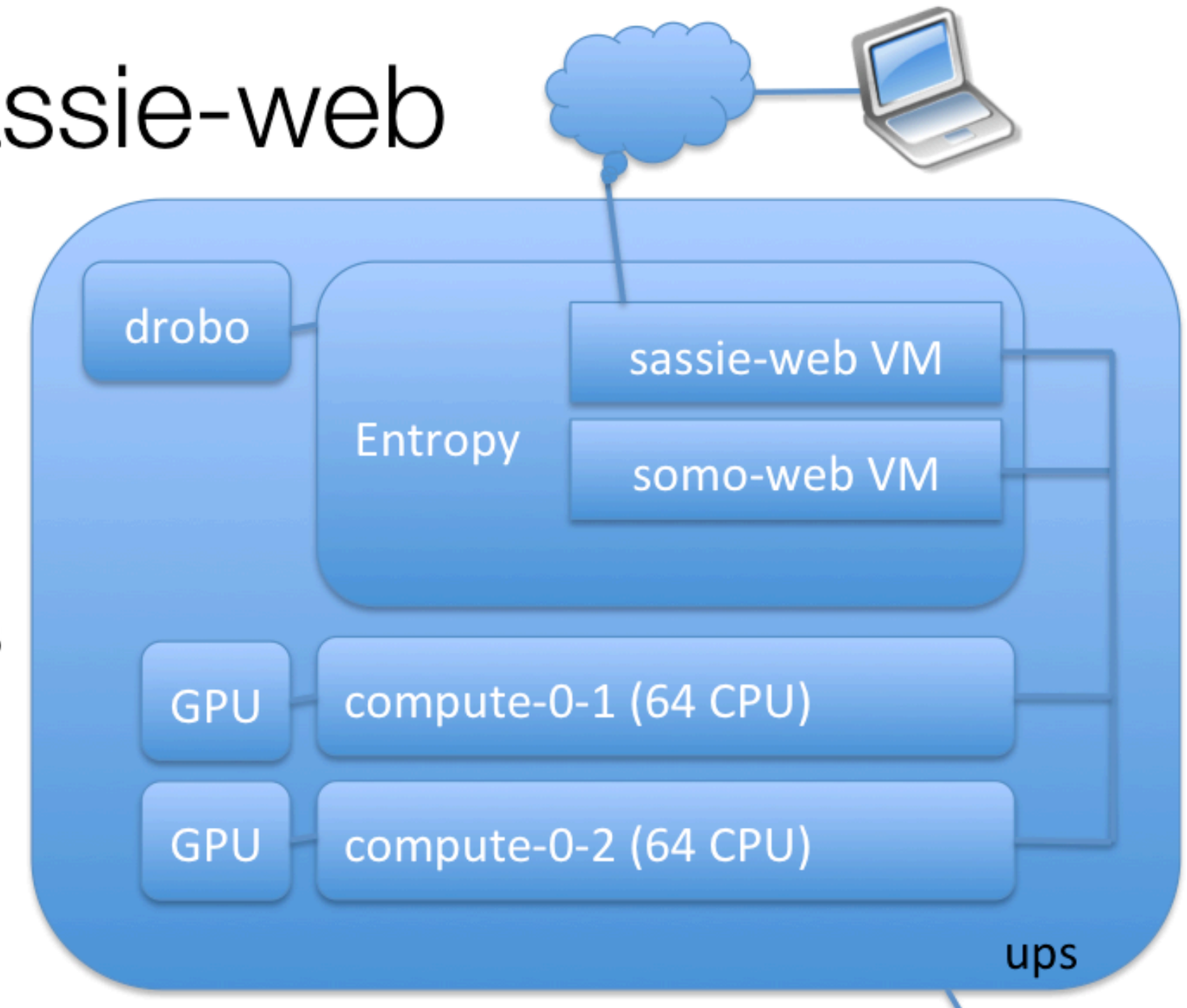
sassie-web



20+ modules ported using GenApp

sassie-web.chem.utk.edu/sassie2

User persistent data structure

128 CPU / ~20,000 GPU cluster / 30 TB

beta testers Google Group:

CCP-SAS SASSIE

https://groups.google.com/forum/#!forum/madscatt

Remote web-monitoring & control

Allows fewer stand-alone roll-outs && potential GenApp stand-alone GUI version(s) && iOS & Android Apps.

Please contribute feedback to Group!

HPC is relative

Basic server: mobile-entropy

Prototype server: Entropy → sassie-web

Google Summer of Code 2015

The Apache Software Foundation

Enable advanced MD & APBS

Langan & Smith

HPC is relative

-web

2015

Enable advanced MD & APBS

Langan & Smith

sassie-web -- work in progress

https://sassie-web.chem.utk.edu/sassie2

Ease of use, then HPC and advanced simulation tools