Advanced techniques with SMOG model

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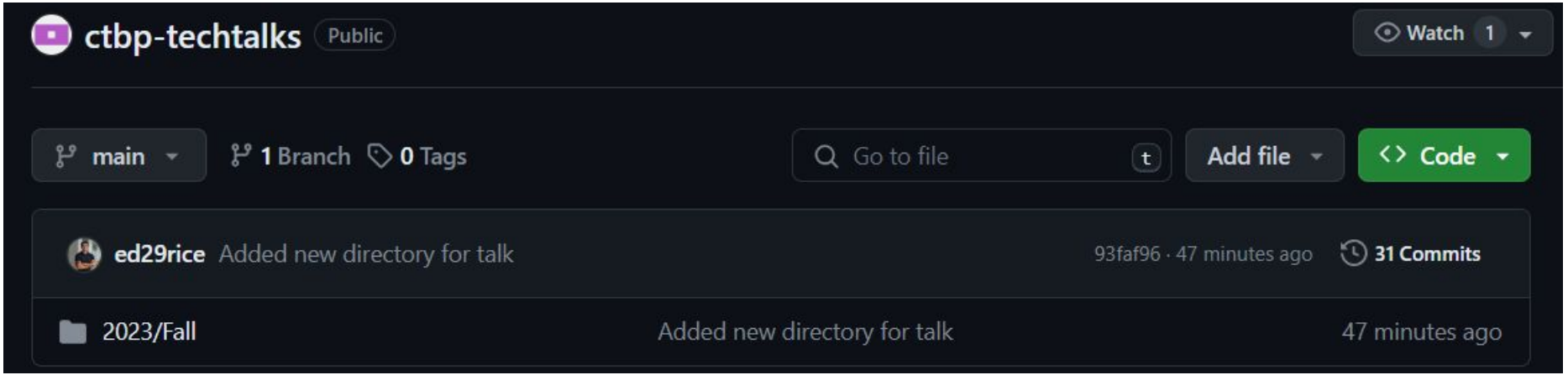
Topics for today

- Create a custom template
- Include new/custom residues
- Format PDB for custom templates
- Use other smog tools

Clone the repo

git clone https://github.com/Whitford/ctbp-techtalks.git



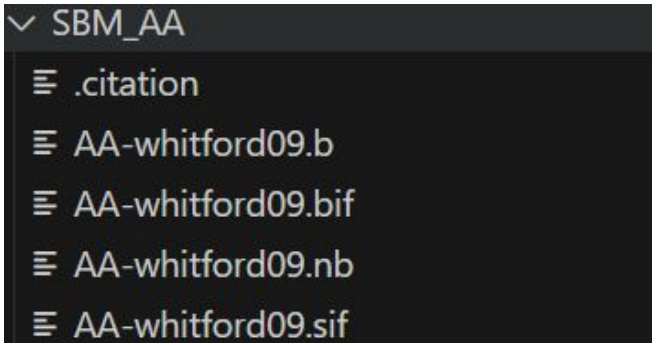
Meet the template files

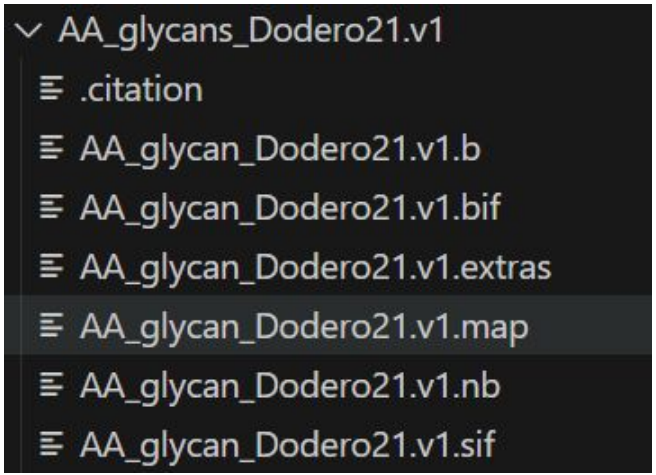
Biomolecular Information File (.bif)
Defines the structure of biomolecules to be supported

Setting Information File (.sif)
Defines interaction function declarations

Bond File (.b)
Defines bonded interactions between atoms

Nonbond File (.nb)
Defines non-bonded interactions between atoms





extras file (.extra file; optional) used to add static content to force fields
ions file (.ions.def file; optional) used to by smog ions when adding ions
Map file (.map) used to map the particles of the residues

Meet the template files - Definition of interactions

SMOG 2 input		Gromacs .top		OpenSMOG
Name	**Args.**	**declaration**	**ftype**	**supported?**
bond_harmonic	r_0 (nm), ϵ_r (ϵ/nm^2)	[bonds]	1	yes
bond_type6[a]	r_0 (nm), ϵ_r (ϵ/nm^2)	[bonds]	6	yes
angle_harmonic	θ_0 (deg), ϵ_θ (ϵ/rad^2)	[angles]	1	yes
angle_free	don't assign potential to specific bond angles			yes
dihedral_harmonic	ϕ_0 (deg), ϵ_χ (ϵ/rad^2)	[dihedrals]	2	yes
dihedral_cosine[b]	ϕ_0 (deg), ϵ_D (ϵ), multiplicity	[dihedrals]	1	yes
dihedral_cosine4[b]	ϕ_0 (deg), ϵ_D (ϵ), multiplicity	[dihedrals]	4	yes
dihedral_free	don't assign potential to specific dihedral angles			yes
contact_1[c]	N, M, σ (nm), ϵ_C (ϵ)	[pairs]	1	yes
contact_2[d]	f(σ), g(σ), σ (nm), ϵ_C (ϵ)	[pairs]	1	no
contact_gaussian[e]	ϵ_C (ϵ), r_{NC}^{12} (nm^{12}), σ (nm), r_0 (nm)	[pairs]	6	yes
contact_free	don't assign contacts between specific sets of atoms			yes
User-defined name[f]	User-defined contact potential	N/A	N/A	only

Meet the template files - Modify strength interactions

Standard strength of contacts and dihedrals depends on several parameters adjusted automatically by SMOG2

Let’s rebel and change those parameters!

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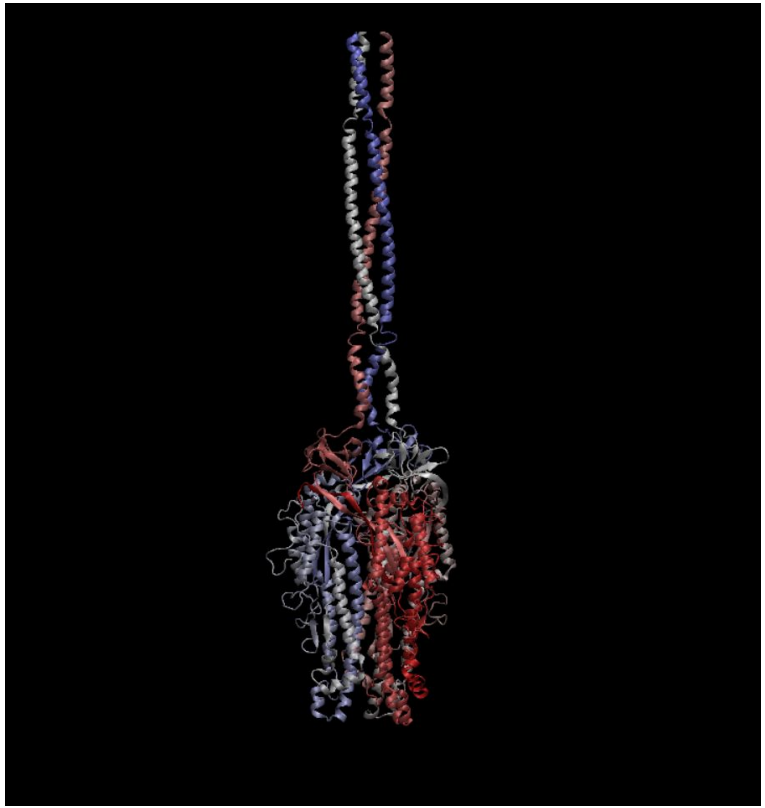
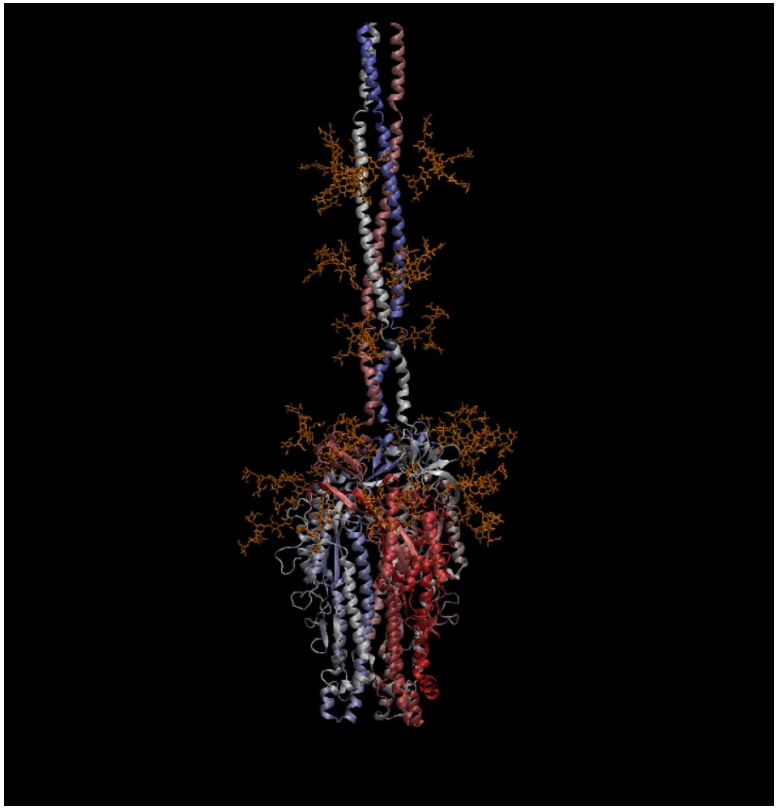
```
<!-- CONTACTS -->
<contact func="contact_1(6,12,?,energynorm)" contactGroup="c">
  <pairType>*</pairType>
  <pairType>*</pairType>
</contact>
```

Introduce new residues - Glycans





Introduce new residues - Glycans

- Describe the new residue (.bif file)
  - Bonds
  - Dihedrals
  - Particle type
- Specify how the new residue interacts with everything (.sif, .nb, .b)
  - Contact type
  - Bond type
  - Angle type
  - Dihedral type

Introduce new residues - Glycans

Adding Ions - smog_ions

Generate common files

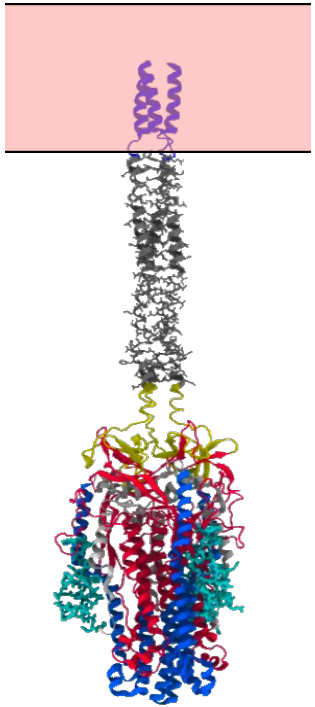
smog2 -t ../AA_ions_Wang22.v1 -i adjusted_ions.pdb -dname ions -OpenSMOG

Add ions

smog_ions -f ions.top -g ions.gro -OpenSMOG ions.xml -of sample_ions.top -og sample_ions.gro -OpenSMOGout sample_ions.xml -ionnm K -ionn 100 -t ../AA_ions_Wang22.v1/

Adding Ions - smog_scale

Scale energy - Changing manually the landscape



Sometimes rescaling the energy is needed

Generate simple SBM

smog2 -t ../SBM_AA/ -i prefusion_with_0_0_0_0_0_0_0_0_0.pdb -dname 2rescale

Change the strength of contacts for specific groups of atoms
smog_scale-energies -f ./2rescale.top -n index.ndx -rd 0.5 -rc 0

Acknowledgements - Paul :D

Paul Whitford,
Northeastern University