Bartender

Automated CG bonded parameters for small molecules

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Small molecules in CG simulations

Drug discovery[1]

Allosteric regulation[2]

Hydrophilicity determination

(1) Souza, P. C. T., et al., Front Mol Biosci 2021, 8, 657222. (10.3389/fmolb.2021.657222)
(2) Souza, P. C. T., et al. J. Phys. Chem. Lett. 2019, 7740 (10.1021/acs.jpclett.9b02868)

But, the parameters?

“Standard” molecules are supported

A growing set of small molecules

But, of course, you will not find your new molecules

Parameters for small molecules

Run an atomistic MD for the molecule

Fit your parameters to the equivalent distribution for your trajectory

See the problem?

The idea behind Bartender

Basically, knowing about the existence of the GFN-xTB family of methods[1]

The GFN methods are accurate and fast enough

So, we can skip the atomistic parametrization!

(1) Bannwarth, C. et al. Wiley Interdiscip. Rev. Comput. Mol. Sci. 2021, 11, e1493 (10.1002/wcms.1493)

What Bartender does

Set up a GFN (semiempirical or classical) MD for your system

Run the simulation on the xtb program[1]

Obtain bonded parameters as usual

    Different alternatives

Write Gromacs topology

(1) github.com/grimme-lab/xtb

Under the hood or Bartender

Written in Go

- Basically, the best from compiled and scripting worlds
- Small, minimalistic language (Bell Labs tradition)

Uses the Gonum and goChem libraries[1]

Not run-time dependencies (other than xtb)

(1) gonum.org
gochem.org

Under the hood or Bartender

Attention to usability

- Atomistic geometry (Gro, PDB, XYZ)
- Input file
- Several flags available, but OK defaults

But wait, there is more

Replica-exchange MD implementation

- Pure Go
- Can be used without Bartender

You can also read in your own trajectory

- DCD
- XTC (requires library)
- Multi-PDB
- Multi-XYZ

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And you!