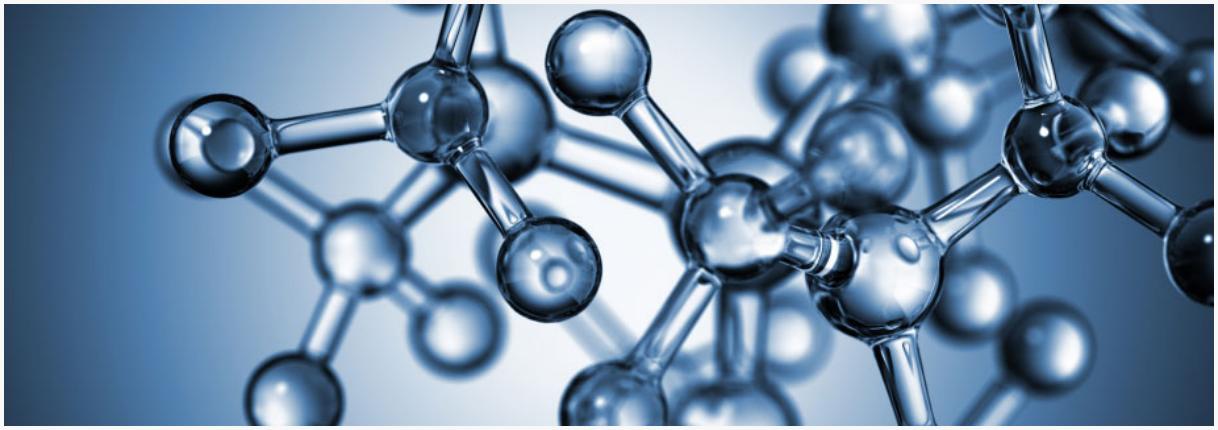
TAMC: Torision Angle Monte Carlo



This document describes the components and syntax to define a TAMC move-set.

> draft 0.1 by JEC 12/15/2014

Pivots

There are two types of pivots. They can be sampled at the same or different frequency. Pivots are assigned to specific residues by their residue number.

Pivots are defined by four atoms. The atoms can be in the same residue or in different residues.

Pivots can be defined for subsets of the complete system and syntax defined here can be used to manage the torsional sampling between flexible and rigid units in the complete system.

main pivots
These pivots are used to describe the main chain in the molecule from beginning to end. *secondary pivots* can branch off of a *main pivot*. An example of a *main pivot* is the backbone of a bio-polymer.

secondary pivots
These pivots are used to describe atoms that are attached to a *main pivot* but are not part of the main chain of the molecule. An example of *secondary pivot* is the side-chain of an amino acid. *secondary pivot(s)* can be collected into a single group, that we will call a *tree*.

Components

Each pivot type has components that help define the individual properties of pivots.

"outside"
Used to define atoms required to define a torsion angle outside the current residue that the pivot is assigned. This component has several available keywords: *"previous"*, *"next"*, and *"selection"*.

"terminals"
Used to define the active pivot(s) when residue is at the end of the main chain (defined by a set of main pivots) or a secondary chain.

"post"
Used to define the atoms within the current residue and beyond that move when the torsion is sampled. An example would be secondary pivot(s) assigned to the residue, such as an amino acid sidechain.

Example Usage

To illustrate the usage of pivots and pivot components we will describe the code used to define a move set for protein backbone torsions. **Note that numbering is zero-based as found in Python/C/C++** The coded examples are shown in Python syntax.

First, main pivots should be defined through a dictionary.

```
main_pivots = {}
```

Since protein backbone torsion angles are described by two dihedral angles per residue, we define and add the *"basis"* keyword to the dictionary.

```
main_pivots["basis"] = [["C", "N", "CA", "C"], ["N", "CA", "C", "N"]]
```

Note that this is done using specific atom naming. There are two main pivots defined. One for atoms

```
["C", "N", "CA", "C"]
```

and one for atoms

```
["N", "CA", "C", "N"]
```

While arbitrary, *main pivot* atoms may exist outside of the current residue. This is described by defining and adding the *"outside"* keyword to the dictionary.

```
main_pivots["outside"] = { 0: ["previous", [0]], 1: ["next", [3]] }
```

The syntax is broken down as follows. There are two keyword:value pairs in the "outside" entry.

```
0: ["previous",[0]]
```

and

```
1: ["next", [3]]
```

The first is defined to be associated with *main pivot* "basis" 0 with a description that atom [0] is found in the "previous" residue. Therefore atom "C" in the first *main pivot* basis described above is in the previous residue.

Therefore the second entry is defined to be associated with *main pivot* basis 1 with a description that atom [3] is found in the "next" residue. Therefore atom "N" in the second *main pivot* basis described above is in the next residue.

Note: the atom numbers are shown as a one-element list. This is done since more than one atom can be assigned to belong to another residue. For example, for nucleic acids defined with a *main_pivots* basis such as:

```
       main_pivots["basis"] = [["O3'", "P", "O5'", "C5'"], ["P", "O5'", "C5'
", "C4'"], ["O5'", "C5'", "C4'", "C3'"], ["C5'", "C4'", "C3'", "O3'"], ["C4'"
, "C3'", "O3'", "P"], ["C3'", "O3'", "P", "O5'"]]
```

the appropriate "outside" definition would be

```
       main_pivots["outside"] = { 0: ["previous", [0,1]], 1: ["previous", [0
]], 4: ["next", [3]], 5: ["next", [2,3]] }
```

where multiple atoms are found in the "previous" residue for *main pivot* 0, one atom is found in the "previous" residue for *main pivot* 1, one atom is found in the "next" residue for *main pivot* 4, and two atoms are found in the "next" residue for *main pivot* 5.

Note: the keyword "selection" is also valid to define the position of the atom in your system when it is not located in either the "previous" or "next" residue. For example,

```
       main_pivots["outside"] = { 0: ["selection", ["segname[i] == 'DNA1' an
d resid[i] == 23 and name[i] == 'C5\'' "], 0]}
```

would define the atom C5' in residue 23 of the segment DNA1 to be the source of atom 0 for *main pivot* 0.

> the "selection" bit above has not yet been implemented

The next item to define are the allowed *main pivots* for the ends of the chain. For the protein backbone torsion move set one defines the "terminals" keyword to the *main pivot* dictionary

```
main_pivots["terminals"] = { "nter": 1, "cter": 0 }
```

which tells us that the amino terminus ("nter") only allows *main pivot* 1 to be active, while the carboxy terminus ("cter") only allows *main pivot* 0 to be active.

The final definition adds the keyword "post" to the *main_pivots* dictionary to describe what atoms both within the residue and outside the residue using the direction of the move set to be used as a keyword to indicate resiudes in the main chain either after (for a "forward" directional move) or preceding (for a "backward" directional move). This is defined in a if/else block

```
        if direction == 'forward':
            main_pivots["post"] = [0, "sidechain", "forward"]
        else:
            main_pivots["post"] = [1, "sidechain", "backward"]
```

> TODO: need to define atoms that move explicitly ... i.e. carbonyl oxygen etc.

where the first option defines that for a *main pivot* move for pivot 0 that the residue "sidechain" and all atoms in the flexible group "forward" are acted upon my the sampling of the 0 torsion.

The second option defines that for a *main pivot* move for pivot 1 that the residue "sidechain" and all atoms in the flexible group "backward" are acted upon by the sampling of the 1 torsion.

Subsequent atom selection definitions can be added to "post" in order to specify the movement of the *main pivot* torsions on other atomistic components in your system.