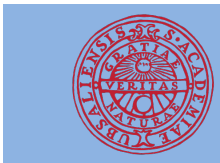

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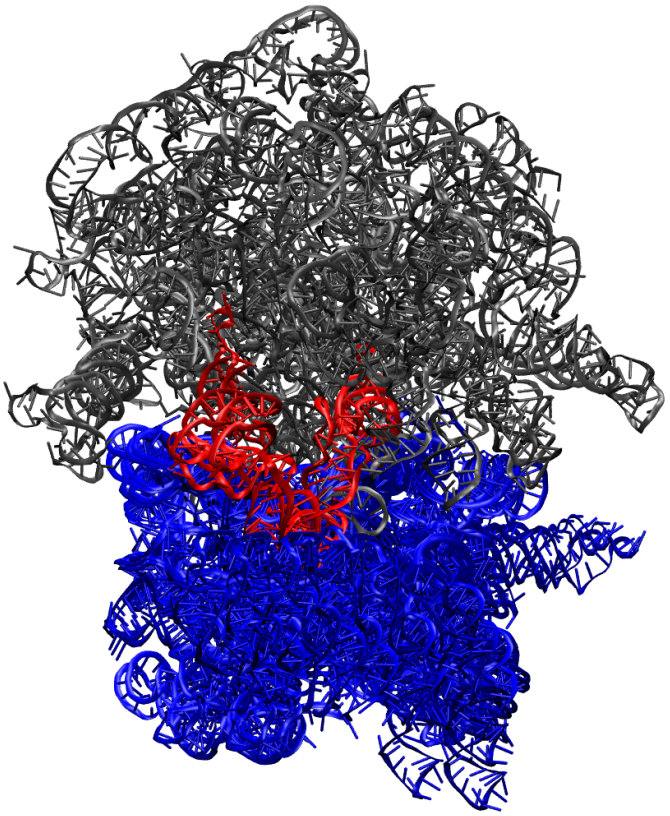

Reference guide

April 23, 2013

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Table of Contents

1 What's new?

In release 2.12 I enabled long chain ID's. This means you can make arbitrarily long chain ID's for biopolymers (RNA, DNA, protein) as long as you instantiate them explicitly (you may NOT use the loadSequencesFromPdb command with this).

In release 2.11 I changed the length units from Ångströms to nanometers, consistent with molmodel's conventions. This makes it easier to relate various stiffnesses, energies, and other physical quantities. I have created the `rootMobilizer` command, which for the first time allows you to connect a chain to ground using a Weld mobilizer (rather than the default Free) – this reduces the degrees of freedom of the system and saves compute time, for the often-found situation in which one or more chains are fixed to ground. There is also now a `constrainChainRigidSegments` command, which constrains all rigid segments in a chain either to ground or to a specified residue in the same chain (permitting center of mass motions). One application of this is to flexibilize an interface and allow (or not allow) center of mass motions, e.g. to equilibrate clashes on that interface. Lastly, we dealt with the five-character limitation on atom numbers in the PDB record format by switching to hexadecimal atom numbers after atom 99999 (thanks Mike Kuiper!) Now you can write out extremely long chains, subject to memory limitations.

For any published work which uses MMB, please cite one or more of the following:

Turning limited experimental information intio 3D models of RNA, by Samuel C Flores and Russ B Altman, *RNA* 16(9):1769-78 (2010).

Predicting RNA structure by multiple template homology modeling, by Samuel C. Flores, Yaqi Wan, Rick Russell, and Russ B. Altman (2010) *Proceedings of the Pacific Symposium on Biocomputing.*

Fast flexible modeling of RNA structure using internal coordinates, by Samuel C. Flores, Michael Sherman, Chris Bruns, Peter Eastman, Russ Altman (2011) *Transactions in Computational Biology and Bioinformatics* 8(5): 1247-57 .

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2 Biopolymers and monoAtoms

In this Appendix, we describe how to instantiate biopolymers (RNA, protein), as well as single atoms such as counterions. Note that the number of biopolymers and series of single atoms is limited by the number of characters available as chain identifiers.

2.1 Biopolymer sequences and first residue numbers

MMB can instantiate RNA chains using the following syntax:

```
RNA <chain ID> <first residue #>  <sequence in single letter code>
```

The RNA sequence uses the single letter code (A,U,G,C). Similarly, you can instantiate DNA chains like this:

```
DNA <chain ID> <first residue #>  <sequence in single letter code>
```

The DNA sequence uses the single letter code (A,T,G,C). You can instantiate a protein chain as:

```
protein <chain ID> <first residue #> <sequence in single letter code>
```

The protein chains use the 20 canonical amino acid alphabet for specifying the sequence.

Note that as of release 2.12, you can make the chain ID as long as you wish. This means that you are not limited to the 144 printable ASCII characters. In the output PDB file, the following tag will indicate the long chain ID:

```
REMARK-SimTK-long-ChainID mySuperLongNameForThisChain
```

.. where of course "`mySuperLongNameForThisChain`" will be replaced by whatever chain ID you specified. This will be followed by the corresponding ATOM records. The ATOM records will have a blank (" ") in column 22 (the chain ID column). Finally, after all the ATOM records for that chain have been printed, there will be another tag, like this:

```
REMARK-SimTK-long-ChainID
```

.. followed by nothing. This "turns off" the long chain ID specification. The next chain may be a normal chain (single-character chain ID in column 22) or there may be another chain with a long ID bracketed by "`REMARK-SimTK-long-ChainID`" tags as before.

There is one more way to instantiate sequences, which works for protein, RNA, and DNA. You can issue the command:

```
loadSequencesFromPdb
```

And MMB will go to your input structure file (last.??.pdb) and look for RNA and protein chains. It will extract the chain ID's, residue numbers, insertion codes, and residue types from there. It will also match the internal coordinates to the Cartesian coordinates it finds there, as usual. You will then be able to issue commands that involve residues in those chains, as before. Please note that you CANNOT use this command with long chain IDs, it just won't work. If you have long chain IDs, just instantiate the chains explicitly.

In addition to removing the need for you to specify these chains manually, this command also has the advantage of handling insertion codes and gaps in the numbering. You will be able to append an insertion code to the right of the residue number in *any* command, e.g. `constrainToGround A 32B` (where B is an insertion code).

The residue numbers and insertion codes do need to be increasing from the top to the bottom of the input structure file, though. Before using this command, you should clean up the input structure file, removing anything that is not RNA or protein – including DNA, water, ions, or other molecules.

Whether you use `loadSequencesFromPdb` or specify the sequences manually, it is possible to use the '+' operator to increment or decrement a residue ID by some number of residues. For instance,

```
constrainToGround A 32B+2
constrainToGround A 32B+-3
```

will constrain residues two residues to the C-terminus and three residues to the N-terminus of 32B. Do not insert any spaces between the the '+' operator and either of its arguments. You can use the '+' operator with *any* command that takes residue numbers as an argument.

2.2 monoAtoms

The `monoAtoms` command specifies single atoms (e.g. monatomic ions) The syntax follows:

```
monoAtoms <chain ID> <first residue #> <# of atoms> <name of atom>
```

Currently only the following atom names are supported:

```
Mg+2, Cl-, Na+, K+, Li+, Ca+2, Cs+, Rb+
```

The single atoms created with this command support the `atomSpring, atomTether, springToGround, constrainToGround,` and `constraint` commands, just like the biopolymers. They do not support the `mobilizer` command.

3 A word about units

I am making a special, very short chapter on units. In MMB 2.10 and earlier, some forces such as atomSpring, springToGround, atomTether, etc. took Å as the unit for dead lengths and ground locations. For consistency, we are going back to nm for the length unit. This is because internally all the math is done in nm, kJ/mol, ps, and daltons (g/mol). This implies that spring constants are in kJ/mol/nm^2. For example, if you want to make a spring which in Amber99 units (Å, kcal/mol, ps) would be 310 kcal/mol/Å^2, the equivalent spring in our choice of units would be 129790.8 kJ/mol/nm^2.

Please note that if you have any dead lengths or ground locations in your MMB 2.10 or earlier script which you are using with MMB 2.11, you will need to manually change them from Å to nm.

4 Forces

In this Appendix, we describe options for using the `baseInteraction, aromatic` two-residue forces, the `atomSpring, atomTether,` and `springToGround forces`, and the `contact` steric forces. Note that since forces are additive, there is no hard limit on how many forces can exist in the system or even acting on a single residue, base, or atom.

4.1 baseInteraction

The syntax for this command is:

```
baseInteraction <chain identifier for first residue>
           <residue number for first residue>
           <interacting edge for first residue>
           <chain identifier for second residue>
           <residue number for second residue>
           <interacting edge for second residue>
           <glycosidic bond orientation>
```

The following combinations of first base pairing edge, second base pairing edge, and glycosidic bond orientation are permitted:

```
WatsonCrick WatsonCrick Cis
WatsonCrick WatsonCrick Trans

WatsonCrick Hoogsteen Cis
WatsonCrick Hoogsteen Trans

WatsonCrick SugarEdge Cis
WatsonCrick SugarEdge Trans

Hoogsteen Hoogsteen Cis
Hoogsteen Hoogsteen Trans

Hoogsteen SugarEdge Cis
Hoogsteen SugarEdge Trans

SugarEdge SugarEdge Cis
SugarEdge SugarEdge Trans

WatsonCrick Bifurcated Cis
Stacking3 Stacking5 Cis
Stacking5 Stacking5 Trans
Stacking3 Stacking3 Trans
HelicalStackingA3 HelicalStackingA5 Cis
Superimpose Superimpose Cis
```

You might notice that some of these are actually not in the Leontis and Westhof classification. These are explained below:

- Stacking* simply specifies a stacking interaction between consecutive residues on a chain. The numbers indicate which face is interacting on each base. For example:
  `baseInteraction A 120 Stacking3 A 121 Stacking5 Cis`

  Means that the face of base 120 which would ordinarily point towards the 3' end of the strand in a helix, will be stacked on the face of base 121 which would ordinarily point to the 5' end of the helix.

- HelicalStacking* works the same as Stacking, but adds the offset appropriate for consecutive bases in a helix. HelicalStackingA3/HelicalStackingA5 is automatically applied to all consecutive bases in helices, unless you specify `setHelicalStacking FALSE`. MMB assumes an A-form helix exists whenever it finds three consecutively numbered RNA residues on a single strand Watson-Crick base paired with three consecutively numbered residues on the same or another

single RNA strand. If you want to generate a helix where this is not the case, you should manually apply HelicalStackingA3 / HelicalStackingA5 interactions.

4.2 nucleicAcidDuplex

This command generates WatsonCrick/WatsonCrick/Cis interactions between two specified segments on the same or different RNA chains. It is a shortcut for manually specifying each such interaction for every pair of canonically interacting residues in the duplex. The syntax is:

```
nucleicAcidDuplex     <chain identifier A>
                      <first residue on A>
                      <last residue on A>
                      <chain identifier B>
                      <first residue on B>
                      <last residue on B>
```

Recalling that the duplex is antiparallel, we require that:

`(first residue on A) < (last residue on A)`

and

`(first residue on B) > (last residue on B)`

For example:

```
nucleicAcidDuplex A 1 3 A 10 8
```

Makes the segments between residues 1 and 3 (inclusive) and between 10 and 8 (inclusive) into two halves of a duplex, by applying a base pairing interaction between 1 and 10, 2 and 9, and 3 and 8.

4.3 Units

Before we describe the various variants of user-applied springs, let's clarify the units. MMB and molmodel use nm, kJ/mol, ps, and daltons (a.k.a. atomic mass units = u, or g/mol). The Amber99 force field, on the other hand, uses nm, kcal/mol, and ps, and u. The user

4.4 atomSpring

The `atomSpring` command creates a linear spring connecting two atoms. Two optional parameters (square braces []) specify the dead length and spring force constant.

```
atomSpring  <first chain ID>
            <first residue number>
            <first atom name>
            <second chain ID>
            <second residue number>
            <second atom name>
            [<dead length>
            [<spring constant>]]
```

4.5 atomTether

The `atomTether` command, as the name implies, applies no force if the distance between atoms is less than a certain `<dead length>`, and applies an attractive force with Hookean `<spring constant>` when the distance exceeds the former. Default values for the last two parameters are 0.0 and 3.0, respectively, as they are for `atomSpring`. Make `<spring constant>` large for a strict "dog leash" or small for a permissive restraint.

```
atomTether  <first chain ID>
            <first residue number>
            <first atom name>
            <second chain ID>
            <second residue number>
            <second atom name>
            [<dead length>
            [<spring constant>]]
```

4.6 springToGround

The `springToGround` command creates a linear spring connecting a specified atom and a specified location in Ground. Two optional parameters (square braces []) specify the dead length and spring force constant.

```
springToGround   <atom chain ID>
```

```
<atom residue number>
<atom name>
<X location in Ground>
<Y location in Ground>
<Z location in Ground>
[<dead length>]
```

4.7 threading

The `threading` command applies `atomSpring`'s between pairs of atoms with the same name, on corresponding residues. The result is that the atoms of a given stretch of residues in a given chain 1 are aligned to the like-named atoms of a corresponding stretch in a second chain 2. For release 2.6.2 and higher, this command works with any biopolymer; its predecessor only worked for protein. The optional parameter (square braces []) specifies the spring force constant.

```
threading   <chain 1 ID>
                  <first residue number of chain 1>
                  <last  residue number of chain 1>
                  <chain 2 ID>
                  <first residue number of chain 2>
                  <last  residue number of chain 2>
                  [<spring constant (default = 3.0)>]
```

If you are trying to align just the backbone of a protein, you can use the `proteinBackboneThreading` command, which has the same syntax as above, but only applies springs between corresponding N, CA, and C atoms.

4.8 contact

You can also apply space-filling Contact spheres to a range of residues using the `contact` command. (The idea is similar to that of the parameters `addSelectedAtoms` and `addAllHeavyAtomSterics`)

```
contact    <contact type>
           <chain identifier>
           <residue number for first residue>
```

```
            <residue number for last residue>
```

The first residue should be lower numbered than the second, and both residues should be on the same chain. You can also issue:

```
contact     <contact type>
            <chain identifier>
```

And the contact spheres will be applied to every residue on the specified chain.

There are two kinds of permitted values of `contact type`. In the fixed type, the atom identities are hard-coded and can't be modified by the user, but the contact sphere radii and stiffness (both of which are the same for all atoms regardless of atom name) correspond to the `excludedVolumeRadius` and `excludedVolumeStiffness` parameters which are set in the MMB input file (e.g. commands.dat). These include:

`AllAtomSterics` : Puts one sphere on each atom of the chain, except for the end caps on proteins (when used).
`AllHeavyAtomSterics` : Puts one sphere on each atom of the chain EXCEPT hydroges, and again except for the end caps on proteins.
`RNABackboneSterics` : Puts one sphere on each of the following atoms: P, O5*, C5*, C4*, C3*, and O3*. An error will result from attempting to apply this to proteins, as anytime when you attempt to put sterics on an atom which doesn't exist on a given residue.

The second type of sterics are user configurable, in the parameter file (e.g. parameters.csv). Here the user can choose on which atoms to put the spheres, with a maximum of four atoms. The radii and stiffness can be controlled separately for each atom name. A different choice of zero to four atom names can be chosen for each residue type (4 residue types for RNA, 20 for protein). The user can add as many steric schemes to the parameter file as he/she wishes; as supplied the `parameters.csv` file has two: `SelectedAtoms` and `ProteinBackboneSterics`. For the first one, the parameters look like:

RECORD	A		SelectedAtoms	SelectedAtoms	X	P	C4*	N9
RECORD	C		SelectedAtoms	SelectedAtoms	X	P	C4*	N1
RECORD	G		SelectedAtoms	SelectedAtoms	X	P	C4*	N9
RECORD	U		SelectedAtoms	SelectedAtoms	X	P	C4*	N1

The second column is the residue type, and columns 7,8, and 9 are the atom names. Note that the glycosidic nitrogen is named differently for purines vs. pyrimidines. Subsequent columns give the sphere radii, stiffnesses, and information to identify these as `contact parameter` entries. Parameters become available for use immediately upon being entered in the parameter file, much as for MD force field parameter files.

It is also possible to apply a specified steric scheme to all residues within a certain distance of a specified residue. The distance is measured by between representative atoms – Cα for proteins, C4* for RNA and DNA. The syntax is:

```
applyContactsWithin <radius (nm)> <contact scheme> <chain> <residue>
```

4.9 Restraining to ground

Much as residues can be constrained to each other (see next chapter), any residue of any chain can also be restrained to ground, meaning that a force can be applied to pull all six translational-rotational degrees of freedom to an equilibrium position and orientation in Ground:

```
restrainToGround <chain ID> <residue number>
```

Keep in mind that unlike a constraint, a restraint acts as a spring and thus allows some displacement with respect to ground. Any displacement at the end of a stage is carried over to the next stage, potentially leading to a "creeping" effect. Two parameters which are relevant to this command are `restrainingForceConstant` and `restrainingTorqueConstant`. These set the translational and angular restitution force constants.

4.10 Density based force field

As explained in the tutorial, MMB's density based force field is formulated following Klaus Schulten's MDFF as follows:

$\vec{f}_i = A \cdot m_i \vec{\nabla} D(x_i, y_i, z_i)$

Where *i* is the atom index, m_i is the mass of atom *i*, $D(x_i, y_i, z_i)$ is the electronic density at the nuclear position of atom *i*, A is a user-adjusted scaling factor, and $\vec{\nabla}$ is the gradient operator. Accordingly, $\vec{f}_i$ is the density-derived force vector applied to atom *i*. This is computed for and applied to every atom *i* in the system.

To turn on the density based force field on or off, you just need to specify which chains you want to be subjected to such forces. For instance:

```
fitToDensity
```

Specifes that all chains in the system should be fitted to the map. If you only want certain chains to be fitted, with the remaining chains not subjected to these forces, just specify each chain to be fitted like this:

```
fitToDensity <chain ID>
```

Lastly, if you only want certain stretches of residues to be fitted, you can issue:

```
fitToDensity <chain ID> <start residue> <end residue>
```

.. and only the residues starting at `<start residue>` and ending at `<end residue>` of chain `<chain ID>` will be fitted.

Your density map must be in XPLOR format. To specify the location of the density map, file, use:

```
densityFileName <density file name>
```

The scaling factor (A in the equation above) defaults to unity, but you can set it to any floating point number (including negative numbers) as follows:

```
densityForceConstant <scale factor>
```

4.11 Physics where you want it

"Physics where you want it," introduced in release 2.4, allows you to turn on the all-atoms force field only for certain regions of your system, referred to as the "physics zone."

To specify a range of residues to be added to the physics zone, use:

```
includeAllNonBondAtomsInResidues <chain ID> <first residue in range>
<last residue in range>
```

Sometimes it will be convenient to include all residues within a certain radius of a specified residue. For this you would use:

```
includeAllResiduesWithin <distance> <chain ID> <residue number>
```

The `distance` (in Å) is measured between key atoms, CA for protein and C4* for RNA and DNA.

Default behavior is for all atoms to be subjected to the non-bonded force field terms. If that is what you want, just don't specify either of the above commands.

Lastly, we have found that small chemical groups such as methyl or alcohol can spin out of control in the absence of viscous forces, leading to small time steps and excessive computational expense. To deal with this, you can scale the inertia of such small groups with:

```
smallGroupInertiaMultiplier <inertia scale factor>
```

Any nonnegative floating point number can be used here; we suggest 11.0.

5 Mobilizers and constraints

In this Appendix we describe `mobilizer` commands, which define or modify the internal coordinate topology of the molecule as well as `constraint` commands, which add constraint equations that reduce the degrees of freedom of the system.

It is important to keep in mind the crucial difference between these two in Internal Coordinate Mechanics. A `mobilizer` command can reduce or increase the number of bodies that exist in a system; in the former case you will always save computer time. On the other hand a `constraint` command adds constraint equations which must then be solved; while the net effect depends on masses and forces, computational cost typically increases. Mobilizers control bond mobilities, which here can `be Free, Torsion,` or `Rigid`.

`Free` means that the bond can change its length, angle, and dihedral.
`Torsion` means it can change only its dihedral angle.
`Rigid` means it has no degrees of freedom.

One must also avoid overconstraining the system. For example, if two rigid molecules are already `Weld`'ed (see below) to each other, do not put additional constraints on this pair of molecules, even if they are nominally applied to different residues. While this is easy to keep track of for two bodies, watch out for more insidious ways of overconstraining. For example, if A is `Weld`'ed to B, and B is `Weld`'ed to C, do not then `Weld` C to A.

5.1 mobilizer

The `mobilizer` keyword is used for specifying the bond mobilities for a stretch of residues. This command is overloaded. The first variant has the following syntax:

```
mobilizer  <bond mobility>
           <chain identifier>
           <first residue number>
           <last residue number>
```

The first residue should be lower numbered than the second, and both residues should be on the same chain. Bond mobility can be set to `Free, Torsion, Rigid,` or `Default`. The "`Default`" bond mobility is special, as we'll explain in a moment. Don't forget you can use the keywords `FirstResidue` or `LastResidue`, or do arithmetic on the residue numbers using the "+" operator, as described earlier.

You can also simply say:

```
mobilizer  <bond mobility>
           <chain identifier>
```

... and this will set ALL residues in chain `<chain identifier>` to `<bond mobility>`.

Lastly, you can say:

```
mobilizer  <bond mobility>
```

... and this will set all residues in ALL chains to `<bond mobility>`.

5.2 applyMobilizersWithin

The `applyMobilizersWithin` command is used to specifying the bond mobilities for all biopolymer residues within a certain radius of a specified residue. It has the following syntax:

```
applyMobilizersWithin <bond mobility>
                      <radius>
                      <chain identifier>
                      <residue ID>
```

The `radius` is measured between representative atoms (Cα for protein, C4* for nucleic acids) and (like always) in Å. The acceptable values of `<bond mobility>` are as listed above.

5.3 mobilizeInterfaces

The `mobilizeInterfaces` command is used to specifying the bond mobilities for all biopolymer residues within a certain distance of all interfaces of a given biopolymer chain. The syntax is:

```
mobilizeInterfaces    <interface depth>
                      <bond mobility>
                      <chain identifier>
```

The `<interface depth>` is measured as the minimum distance between representative atoms (Cα for protein, C4* for nucleic acids) on different chains across an interface. `<chain identifier>` is the chain whose interfaces you are interested in.

As an example, if you have a trimer of chains A,B, and C, and issue :

```
mobilizeInterfaces 6.0 Torsion C
```

Then all residues at all interfaces between chain C and A, and between C and B (but not between A and B), to a depth of 6.0Å, will get bond mobility `Torsion.`

5.4 singleBondMobility

The `singleBondMobility` command is used for specifying the bond mobility for a single bond:

```
singleBondMobility    <chain identifier for first atom>
           <residue number for first atom>
           <atom name for first atom>
           <bond mobility>
           <chain identifier for second atom >
           <residue number for second atom >
           <atom name for second atom>
```

The two atoms should be covalently bonded to each other, of course.

5.5 Default mobilizers

It is important to understand what is the default setting for the mobilizers in your system.

The default bond mobility leaves most bonds set to `Torsion,` but there are also some `Rigid` bonds, depending on the residue type and atoms it connects. For instance, the bond mobilities for an RNA residue look like this:

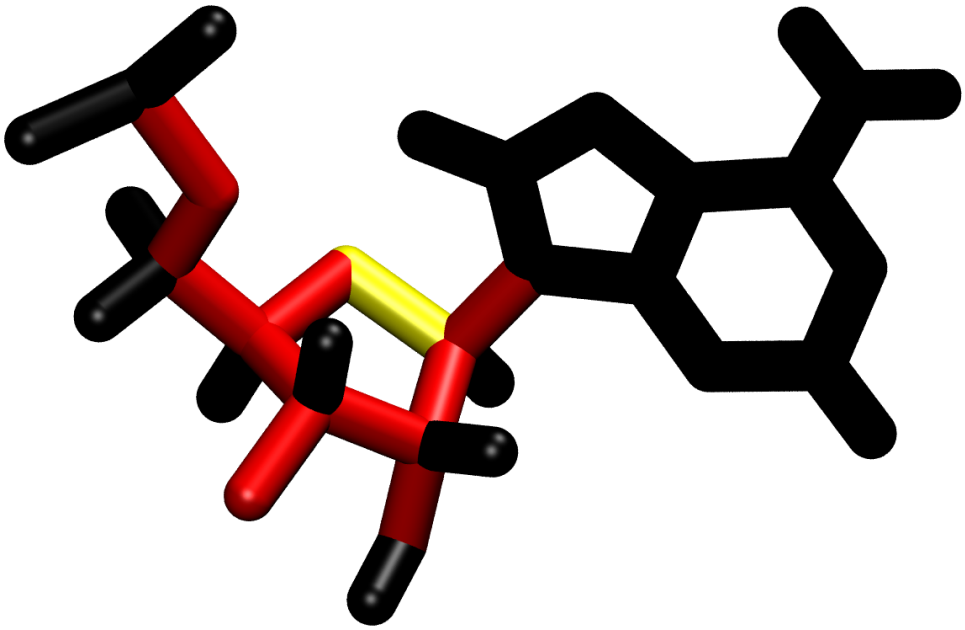

Figure 1 : Default bond mobilities for an RNA residue

Black: `Rigid`; **Red:** `Torsion`; **Yellow:** `Free`.

Similarly for a protein residue, most bonds are also `Torsion`, but the peptide bond is `Rigid`, as are some cyclic side chain groups.

5.6 Order of application of mobilizers

In order to get the desired result out of MMB, you should understand the order in which these commands are applied. They go like this:

1. `mobilizer` (for `Rigid`, `Free`, and `Torsion`)
2. `applyMobilizersWithin` (for `Rigid`, `Free`, and `Torsion`)
3. `mobilizeInterfaces` (for `Rigid`, `Free`, and `Torsion`)
4. `mobilizer`, `applyMobilizersWithin`, and `mobilizeInterfaces` (for `Default`)
5. `singleBondMobility`

A common mistake is to forget that before any commands are applied, all chains have a default bond mobility, as described above. Note also that the "`Default`" bond mobility isn't actively applied to residues – instead when you specify this, all *other* modifications to the residue bond mobility are removed, so it is simply never changed from its original bond mobility.

Here is a simple example:

```
protein A 1 AAAAAA
mobilizer Rigid A 1 6
mobilizer Default A 3 4
```

Results in two `Rigid` stretches (1 to 2 and 5 to 6) – the output looks something like this:

```
/Users/Sam/svn/RNAToolbox/trunk/src/MobilizerContainer.cpp:44
Mobilizer stretch 0 BondMobility = Rigid
/Users/Sam/svn/RNAToolbox/trunk/src/MobilizerContainer.cpp:45 chain=
A from residue 1 to 2
/Users/Sam/svn/RNAToolbox/trunk/src/MobilizerContainer.cpp:44
Mobilizer stretch 1 BondMobility = Rigid
/Users/Sam/svn/RNAToolbox/trunk/src/MobilizerContainer.cpp:45 chain=
A from residue 5 to 6
```

5.7 constraint

The `constraint` command is used for specifying constraints to weld two residues together:

```
constraint      <chain identifier for first residue>
                <residue number for first residue>
                Weld
                <chain identifier for second residue>
                <residue number for second residue>
```

The two welded residues can be on different chains; in fact either or both residues can be in RNA or protein chains. The weld is applied on C3* atoms of RNA residues and on C atom s of protein residues. There is no preference for residue number ordering.

You can also specify which atoms you want welded, as follows:

```
constraint      <first atom chain identifier>
                <first atom residue>
                <first atom name>
                Weld
                <second atom chain identifier>
                <second atom residue number>
                <second atom name>
```

Lastly, you can weld to ground, either specifying the atom to be welded or using the default:

```
constraint      <chain identifier>
                <residue number >
                <atom name>
                Weld Ground
```

or:

```
constraint      <chain identifier>
                <residue number >
                Weld Ground
```

5.8 Constraining to ground

Just as residues can be constrained to each other, any residue of any chain can also be constrained (rigidly attached) to ground:

```
constrainToGround <chain ID> <residue number>
```

See *Appendix: Parameters* for an explanation of the `constraintTolerance` parameter, relevant to this command.

Much more efficient are a couple of variants of this command. For example:

```
constrainToGround
```

(with no parameters) attaches each chain to ground using a Weld rather than a Free mobilizer. Thus rather than granting 6 DOFs and then removing them with constrain equations, the DOFs never exist to begin with.

Similiarly, you can choose the mobilizer type (`Free` vs. `Weld`) for all chains by issuing:

```
rootMobilizer <"Free" | "Weld">
```

Or, you can choose the mobilizer type for a specific chain by issuing:

```
rootMobilizer <Chain> <"Free" | "Weld">
```

5.9 Constraining rigid segments to each other or to ground

In the antibody design example (see Tutorial), we have a protein which has two rigid segments and one flexible segment. To prevent the two rigid segments from moving with respect to ground, we welded them to ground. Alternatively, maybe we could have welded the rigid segments to each other, so the protein as a whole could move with respect to its binding partner (or ground, for that matter). Sometimes you may want a chain to have many rigid segments, all welded either to ground or to a specified residue. MMB has a convenient command for this.

If you want to weld all rigid segments of all chains to ground, just issue:

```
constrainChainRigidSegments
```

If you want to weld the rigid segments of a specified chain to ground, issue:

```
constrainChainRigidSegments <chain ID> Ground
```

where `<chain ID>` refers to the chain in question.

Lastly, if you want to weld the rigid segments of a specified chain to a specified residue (on the same chain), issue:

```
constrainChainRigidSegments <chain ID> <residue ID>
```

In this latter case, all the rigid segments in chain `<chain ID>` will be welded to the same residue `<residue ID>`. This means that the rigid segments will move together, allowing rigid body motions of the entire chain. If you want several chains to move together, just add a `constraint` command.

6 Global parameters

This appendix, describes global parameters available to users. It does not cover *commands* such as `baseInteraction, aromatic, contact, mobilizer,` and `constraint.` The simplest difference between a *parameter* and a *command* is the following. A *command* can be issued an unbounded number of times, subject only to memory and computer time limitations. The major caveat is that in the case of `constraint` commands, one must not overconstrain the system. In contrast a *parameter* can only be set once (at least for a given stage); if a parameter is set multiple times for a given stage, only the last value of that parameter will be used. A listing of all user-configurable global parameters and their current values is printed at the beginning of every stage of an MMB run. Some additional parameters are available but rarely used or not recommended; contact the author with questions on these.

This chapter does not describe *staged* parameters. These are parameters for which not only the *value,* but also the *stage* at which they first take effect is specified, for example `temperature` and `dutyCycle`.

addAllAtomSterics	Bool	FALSE	Add steric contact spheres to all atoms. This is more expensive and more prone to kinetic trapping than addSelectedAtoms.
addAllHeavyAtomSterics	Bool	FALSE	Add steric contact spheres to all atoms EXCEPT hydrogens.
checkSatisfied	Bool	FALSE	At each reporting interval, list all the baseInteraction's and determine which were satisfied.
constraintTolerance	float	0.05	This determines the tolerance of the Weld constraint. If Weld'ed pieces are moving relative to each other, reduce this number.
cutoffRadius	float	0.1	This is the range of the MMB potential. See our Multiple-template homology modeling paper.
densityFileName	String		Name of file for fitting based on electron density, in .xplor format. If you need to convert from some other format, we recommend using mapman (e.g. rave_osx for mac). Instructions are here: http://xray.bmc.uu.se/usf/mapman_man.html#S10
densityForceConstant	Float	1	Scale factor for the density based forces
firstStage	int	1	Stage at which simulation should begin.
globalAmberImproperTorsionScaleFactor	float	0	These eight parameters set scaling factors for terms in the Amber99 potential. Most default to 0 for economy.
globalBondBendScaleFactor	float	1.0	
globalBondStretchScaleFactor	float	1.0	
globalBondTorsionScaleFactor	float	0	
globalCoulombScaleFactor	float	0	

globalGbsaScaleFactor	float	0	
globalVdwScaleFactor	float	0	
initialSeparation	float	20.0	Sets the separation between chains at stage 1, or whenever readPreviousFrameFile = false.
integratorAccuracy	int	0.001	Integrator tolerance, applies for variable step size time integrators.
integratorStepSize	int	0.001	Step size in ps, for fixed step size integrators.
integratorType	string	Verlet	Choose between Verlet, RungeKuttaMerson
integratorUseFixedStepSize	Bool	FALSE	self explanatory
lastStage	int	1	Stage at which simulation will end
leontisWesthofInFileName	string	./parameters.csv	MMB parameter file
loadTinkerParameterFile	Bool	FALSE	If FALSE, uses hard-wired Tinker parameters. If 1, reads parameters from tinkerParameterFileName
numReportingIntervals *alias* maxReportingIntervals	int	100	Number of reporting intervals per stage.
nastGlobalBondTorsionScaleFactor	int	10	Scale factor for NAST torsional potential
randomizeInitialVelocities	Bool	FALSE	Adds a random velocity to each body at the beginning of the simulation stage. Note that if you are have any non-interacting bodies (e.g. free ions with charges turned off) you may wish to apply initial velocities, otherwise the Nose-Hoover thermostat will leave them in their zero kinetic energy state.
reportingInterval	float	1.0	Duration of reporting intervals, in ps.
removeRigidBodyMomentum	Bool	FALSE	When True, periodically sets overall translational and rotational momentum to zero.
rigidifyFormedHelices	Bool	FALSE	
scrubberPeriod	float	4	Duration of one cycle of potential rescaling (ON time + OFF time) in ps.
safeParameters	Bool	TRUE	When TRUE, checks for syntax errors as well as some potentially dangerous parameter values.
setForceAndStericScrubber	Bool	FALSE	No longer user configurable. When dutyCycle < 1.0, this is automatically set to TRUE. It turns ALL forces (including baseInteraction's, sterics, Amber force field, springToGround's, etc.) off for (dutyCycle -1) fraction of each scrubberPeriod.
setHelicalStacking	Bool	TRUE	if TRUE, identifies three consecutive WatsonCrick/WatsonCrick/Cis base pairs as a helix and applies HelicalStackingA3/HelicalStackingA5/Cis baseInteraction's between the consecutive residues on each strand.
setTemperature	Bool	TRUE	Turns on thermostat.
thermostatType	string		Choices are NoseHoover and VelocityRescaling
tinkerParameterFileName	string		Name of the tinker-formatted parameter file. Only needed if the tinker force field is turned on.
baseInteractionForceMultiplier *alias* twoTransformForceMultiplier *alias* forceMultiplier	float	100	Scale factor applied to all baseInteraction and aromatic forces. 100 or 1000 is recommended to speed up modeling.
useFixedStepSize	Bool	FALSE	Specifies fixed-step-size time integration.

7 Macros

This appendix describes macros available to users. These macros set parameters on the user's behalf. These are provided in cases where the corresponding commands might be confusing to the user, or simply not under user control.

matchFast	See the chapter, "Matching to the input structure file." This sets matchExact TRUE, matchIdealized FALSE, and matchOptimize FALSE. It is very economical. It is now the ONLY matching parameter setting macro, and only reinstates the defaults, so is effectively vestigial
setDefaultMDParameters	Equivalent to issuing: globalBondTorsionScaleFactor 1.0 globalAmberImproperTorsionScaleFactor 1.0 globalBondBendScaleFactor 1.0 globalBondStretchScaleFactor 1.0 globalBondTorsionScaleFactor 1.0 globalCoulombScaleFactor 1.0 globalVdwScaleFactor 1.0 globalAmberImproperTorsionScaleFactor 1.0

8 User defined variables, parameter arithmetic, and conditional blocks

In this Appendix, we describe how to define numerical variables, and various ways to specify sections of the input file which are to be read or ignored at certain stages.

8.1 Comment marker

The comment marker is #, e.g.:

```
# Don't read this, it's just a comment
```

8.2 User defined variables

User variables are defined with the following syntax:

```
@<variable-name> <float or integer value>
```

The variable `@<variable-name>` can then be used wherever a literal integer or float is expected. If a float is assigned to the variable, and the variable is later used where an integer is expected, MMB will return an error. The definition of the variable should precede its first use in the input file. For example:

```
#declare @myStage variable and set to 3
@myIntervals 3
# now use it where a number (in this case an integer) is expected:
numReportingIntervals @myIntervals
```

Don't use any punctuation or whitespace in `<variable-name>`.
Don't try to set `firstStage` or `lastStage` with a user variable.

8.3 Parameter arithmetic

User variables are pretty handy, and start to make the command file more like a programming language. In the same vein, MMB allows the '+' and '–' operators. This means that any integer or floating-point (double-precision) parameter value can be set using a combination of literals, user variables, and the above operators. There is no limit to the number of operators and operands. Here are a couple of examples:

```
@DUMMY 40
numReportingIntervals  @DUMMY+10-@DUMMY
@MYFLOAT 0.35
reportingInterval  4+@MYFLOAT-0
```

This is equivalent, of course, to:

```
numReportingIntervals  10
reportingInterval  4.35
```

Don't use any whitespace or additional punctuation (such as parentheses, commas, etc.) in an arithmetic expression. Note also that residue ID's are special (they're not integers), and their '+' operator follows different rules (see Chapter 2).

8.4 Conditional blocks

In many cases we will want to issue different commands and make different choices of parameter values at different stages of a job. For this purpose we can enclose a block of the input file in a conditional block, which is opened as follows:

`readFromStage <stage-number>` Read only if the current stage is equal to or GREATER than `<stage-number>`.

`readToStage` Read only if the current stage is equal to or LESS than `<stage-number>`.

`readAtStage` Read only if the current stage is EQUAL to `<stage-number>`.

`readExceptAtStage` Read only if the current stage is NOT EQUAL to `<stage-number>`.

The commands and parameters to be conditionally read follow, and the end of the block is indicated with a `readBlockEnd` statement, e.g.:

```
# start conditional block:
readAtStage 3
# read the following lines only at stage 3:
sequence C CCUAAGGCAAACGCUAUGG
firstResidueNumber C 146
baseInteraction A 2658 WatsonCrick A 2663 WatsonCrick Cis
contact C 146 SelectedAtoms C 164
# end conditional block:
readBlockEnd
# continue with the rest of the input file
```