Dear all,

this message is for everyone using the NOVA force field:

The NOVA force field was YASARA's very first force field developed in 1997 (with parameters optimized at the CMBI in 2001, published 2002). In the core, it uses assembler code optimized for Pentium I CPUs, which were the top CPUs back then (with clock frequencies up to 0.2 GHz). 14 years later, this code has reached the end of its lifetime, since it lacks support for all the new things invented since then: vector registers (3DNow!,SSE), parallelism (multi core CPUs) and 64bit instruction sets.

Consequently, this "clump at YASARA's leg" will be removed during the next weeks, since it hinders progress (like a 64bit YASARA version, which would be convenient to have especially in Linux).

Over summer, a new NOVA force field has been developed, which employs the (Y)AMBER/YASARA force field infrastructure to achieve the same thing as the old one:
protei*N* *O*ptimization in *VA*cuo.

The new NOVA force field keeps the simple recipe of the old one: reducing the net charges to ensure that it can be used in vacuo, without water molecules that would screen the electrostatic interactions.

To make sure that existing macros do not have to be changed, the new NOVA force field uses the same default parameters as the old one (10.48 A force cutoff, no longrange electrostatics).

In terms of accuracy, the new NOVA force field also does much better than the old one:

When energy-minimizing high-resolution X-ray structures, the old NOVA force field moved them on average 0.46 A RMSD (Calpha atoms) and 0.73 A RMSD (all heavy atoms) away from the starting structure (tested with a validation set of 25 structures that shares no sequence identity with structures used to optimize the force field parameters).

Using the new NOVA force field, the RMSDs are 0.31 A (Calpha atoms) and 0.49 A (heavy atoms).

This movement away from the experimentally determined coordinates normally corresponds to a reduction in structure quality, quantified using the three most sensible WHAT IF checks, but not for the new NOVA force field:

1) Ramachandran plot quality (WHATIF RAMCHK):

```
Force field | Z-score, more positive is better
============================================
None,X-ray  | 0.997729
Old NOVA    |-2.442835
New NOVA    | 1.534810 (scores better than X-ray)
```

2) Packing quality (WHATIF QUACHK):

```
Force field | Z-score, more positive is better
============================================
None,X-ray  | -0.447011
Old NOVA    | -0.535423
New NOVA    | -0.327706 (scores better than X-ray)
```

3) Backbone conformation (WHATIF BBCCHK):

```
Force field | Z-score, more positive is better
============================================
None,X-ray  | 1.161091
Old NOVA    | 0.607908
New NOVA    | 1.621363 (scores better than X-ray)
```

As a summary, the new NOVA force field..

- is much faster due to 3DNow!,SSE support
- is much faster due to multi core support
- has support for periodic boundaries and triclinic cells
- is much more accurate
- is much easier to use (ligands parameterized automatically via AutoSMILES)

I hope the above is enough to make up for any inconveniences caused by the removal of a long used force field. Please contact support if this plan gets you into trouble.

As of today, the new NOVA force field is available for beta testing, using force field name 'NOVABeta'. During the beta testing phase, the old NOVA force field is still available as 'NOVA'. Afterwards, 'NOVABeta' will become 'NOVA', and any macros using NOVA will use the new one.

Kind regards,
Elmar