Tinker-HP 1.1 : Release Notes

June 14, 2018

Several new methods and models have been included in Tinker-HP version 1.1, they can be listed as follows:

1 New Models

- possibility to have fixed charge terms for electrostatics
- possibility to have Lennard-Jones potential for van der Waals interactions

These updates make Tinker-HP compatible with classical force fields such as AMBER, CHARMM or OPLS.

- extra.f, extra1.f and extra3.f files have been added with explanations about the data structure of Tinker-HP for those wanting to add new energy and forces terms to Tinker-HP. As such a method may require additional information about neighboring atoms when run in parallel within the spatial decomposition framework, an additional keyword: **DD-CUTOFF x** x being a distance in Angstroms has been added. It makes sure that each core has information (positions and parameters) about all the atoms within a x radius around its local domain before each force calculation and that forces are communicated back to the corresponding neighboring cores afterward. For large values, each core has all the information about all the system.

2 New Methods

- DC/JI-DIIS of Nocito and Beran iterative method to solve the polarization equation (ref: https://doi.org/10.1063/1.4977981). It accelerates the previously implemented solvers by about 20% and is the new default polarization solver in Tinker-HP. It is set by using the line **polar-alg 5** in the *.key file
- The rattle algorithm for constrained molecular dynamics has been implemented. It can be used similarly in Tinker-HP as in Tinker 8.4 by using the keyword **rattle** and by adding information about the degrees of freedom that has to be constrained (angles, bonds, distances...). Additional information about how to use it can be found in the Tinker user guide
- Langevin integrators have been added: bbk, baoab of Leimkulher and Matthews (ref: https://doi.org/10.1098/rspa.2016.0138) and a baoab-respa integrator (similar to the default respa integrator but with the baoab scheme for the inner and the outer loop).
- the Monte-Carlo barostat has been added, as well as the andersen thermostat
- Faster linked-cell method to compute neighbor lists
- Faster I/O for big system at a high number of cores (less communications)

Furthermore, changes have been made to the structure of the code as it uses modules for global variables and not common blocks any more. Every variable in these modules is now succintly described within the code.