For 5.0, I will move the expected place for table input to be grompp, so that we write a .tp that actually does contain all the physics. We'd have to retain table-reading code and command-line options in mdrun for backward compatibility, but deprecate that in 5.0.

We would also like table support for the Verlet kernels for 5.0, as part of the scheme to provide a version where group and Verlet kernels are notionally equivalently fully-featured, so that we can deprecate the group kernels at some point over the next year or two.

Also, the day of the cubic-spline potential table for MD is over. Erik has various plans for using only quadratic-spline force tables, so probably cubic spline table energy input will be deprecated in 5.0, unless we decide that we still want it for MC.

Related issues:
Related to Gromacs - Feature #1192: Add support for Verlet scheme with Buckingham added

History
#1 - 10/01/2013 01:15 PM - Mark Abraham
- Description updated

#2 - 10/22/2013 04:30 PM - Berk Hess
One complication is that user supplied tables per energy group pair will be problematic (complex code and bad performance, since several tables will compete for cash).
For 5.0 I don't see a strong need for tables in the Verlet scheme, but we need to resolve this before the group scheme is retired.

#3 - 10/22/2013 09:13 PM - Mark Abraham
One point arising from the Virginia workshop was that it would be good to provide a version that offers interoperability of old features with both Verlet and group kernels, so that a validation version exists before the group kernels are retired. Ideally, that version would be 5.0, but if need be, that would be a good reason for a 5.1 or something around June 2014.

#4 - 05/13/2014 10:39 AM - Mark Abraham
- Target version changed from 5.0 to 5.x

#5 - 10/14/2015 06:14 PM - Mark Abraham
- Related to Feature #1192: Add support for Verlet scheme with Buckingham added