Gromacs - Feature #1054
Feature # 1292 (Closed): mdrun features to deprecate for 5.0
Feature # 1500 (New): Post-5.0 feature clean-up plan

Improve implicit solvent parallelization
12/02/2012 04:53 PM - Justin Lemkul

| Status:   | New    |
| Priority: | Normal |
| Assignee: | Erik Lindahl |
| Category: | mdrun |
| Target version: | future |

Description
Currently, all implicit solvent simulations are restricted to a maximum of 2 processors when run on CPU. If OpenMM support is dropped (as mentioned by Szilard on the mailing list), the implicit code is largely useless since simulations are very slow on only 1-2 CPU, while their explicit solvent counterparts run orders of magnitude faster on a moderate number of processors. The 2-processor limitation was introduced to solve #777, but greater flexibility would be a significant improvement.

History
#1 - 12/04/2012 05:44 PM - Berk Hess
- Assignee changed from Berk Hess to Erik Lindahl

#2 - 08/21/2013 09:57 AM - Mark Abraham
- Parent task set to #1292

#3 - 05/13/2014 10:07 AM - Mark Abraham
- Target version changed from 5.0 to future
- Parent task changed from #1292 to #1500