GROMACS - Feature #2137

Preliminary refactoring of constraints and update machinery.

03/11/2017 08:32 AM - Michael Shirts

Status:	New
Priority:	Normal
Assignee:	Michael Shirts
Category:	mdrun
Target version:	future
Difficulty:	uncategorized

Description

As per Mark Abraham, preliminary refactoring of the constraints or update machinery, with a view to evolving a more consistent C API for the various pieces that will make a more manageable transition to some kind of C++ interface e.g. IConstraintAlgorithm.

Setting up even a C-style object that has all the data that's currently passed on the command line would be a useful improvement, so that the calls to shake, settle and lincs can have the same signature.

To be updated with more details over the next bit.