modernize constraints code

02/26/2018 04:02 PM - Mark Abraham

Status: New
Priority: Normal
Assignee: Mark Abraham
Category: core library
Target version: future
Difficulty: uncategorized

Description
This touches several strategic objectives:

- modularize the code better
- use proper C++ classes
- minimize run-time work passing lots of maybe-unused parameters to do-it-all functions
- minimize development overhead from unrelated changes to types and names of variables that happen to be textually adjacent
- support transition to better auto-tuning
- provide a framework in which a task can be separated from its execution on piece(s) of hardware
- support evolution of integrator framework
- evolve towards the integrator loop building a task graph for subsequent execution, rather than itself being the point of execution

Pieces of work needed in the checklist below, roughly in order of what makes sensible git commits. (NB the checklist will be similar to lists for other code needing modernization - what else should go on this checklist?):

Related issues:
Related to GROMACS - Bug #2434: wrong values accumulated to dvdlambda in SHAK...
Closed

Associated revisions
Revision f1ea683f - 02/28/2018 03:38 PM - Mark Abraham
Reorganized constraint code

Renamed constraints files after just their algorithm, not the original programming language, which matches the test file that they have. Separated header files for each algorithm with matching names. Removed extern C. Minimized header dependencies. Removed excessive use of struct keyword.

Removed some header declarations of functions declared static.

Refs #2423
Change-Id: If60ab052ae73ad981fa031c2db6b3e206b380f4c

Revision 21b21524 - 02/28/2018 06:04 PM - Mark Abraham
Moved and removed constraint code

No functionality changes here.

Removed code that was formerly called by the now-removed combination of Andersen T coupling and constraints.

Removed crattle declaration from header, and moved its definition to before the point of use, as normal for functions with file static linkage.

Moved constr_r_max and support functions to constraintrange.cpp, because conceptually the functionality is independent of which algorithm implements the constraints. The current implementation only works with LINCS, but that's because SHAKE and DD can't be used together.
Add more const to uses of t_commrec and t_inputrec.

Also removed some pointless struct keywords.

Create gromacs/mdrun module and move code there

Improving how we dispatch the work for do_md and friends requires that they all compile as part of libgromacs (or all outside of it). The code currently in src/programs/mdrun is there simply because it hasn't been moved from the old src/kernel layout, rather than through any clear design, so we should move it now that we have a reason.

Other code from src/programs/mdrun now needs to move into libgromacs also, but we currently don't have a module for miscellaneous mdrun features, so we're adding to the abuse of mdlib for now.

Reorganize energy evaluation for EM

Used aggregate initialized structs to simplify future refactoring.

Remove use of where(), if DEBUG etc.

The where() debugging function causes run-time branches in release-mode builds, and replaces functionality for which one should use a debugger.

Other such preprocessing clutter should also go away. Since we don't check whether any of it compiles or produces useful data, we may as well delete it.

This coincidentally simplifies the call sigatures of some functionality, too.

Retained some useful essentialdynamics debug code, which is now always compiled, and written from setup code only at debug level 2.

Clean up constraints code

Moved constraint code into gmx namespace.

Used more forward declarations in both the old and new headers.

Removed typedef from type declarations.
Removed `gmx_` prefix from some names, since it is no longer required and we may as well avoid verbiage.

Renamed some types more consistently with newer coding styles, and called them class now where they will be one shortly.

Added some const correctness.

Apparently this inspires uncrustify to change positions of some comments. Go figure.

Replaced all `gmx_bool` in constraints code with `bool`.

Maths functions from `vec.h` (which are not in the top-level namespace) now need namespace qualifications.

Added and fixed various Doxygen, which is primitive in some cases where the code was particularly cryptic.

Noted policy on multiple authors within Doxygen comments.

Refs #2423

Change-Id: I41bf3a4b9a4fbbcb3a3a7a27dc922d563abedbc

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**Revision acc3940a - 04/17/2018 10:03 AM - Mark Abraham**

Break apart update_constraints

There are four distinct kinds of work being done, and never was any call to update_constraints doing all of them, so it's better to have a group of functions, each of which do one thing, and the relevant ones called. This also makes it simpler to express by returning fast that when we don't have constraints, we do nothing.

Made the logic for whether this is a log or energy step match that of the main MD loop. The old implementation may not have prepared for the last step correctly when it was triggered by something other than the `nsteps inputrec` value.

Removed a comment mentioning iteration, which is a feature that was removed a while ago.

Removed some ancient debug dump output.

Refs #2423, #1793

Change-Id: I21c10826721ddc9a79a33b1dc79971a20d0855d9

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**Revision 5ae5bf42 - 04/25/2018 02:12 PM - Mark Abraham**

Refactor SD update

The former use of multiple boolean control variables made the logic hard to follow. Without constraints, the two parts of the integrator are fused, which is now expressed explicitly.

This means it is now clear that the second half of the sd update does not compute anything from the forces.

Removed some of the vestiges of the way we once had two SD integrators.

Refs #2423, #1793

Change-Id: I39d4cd0b8568859220b3a592b138f3f4405f8991

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**Revision e384d530 - 06/05/2018 03:05 AM - Mark Abraham**

Make Constraints a proper class

Converted the opaque C struct to a pimpl-ed C++ class.

Numerous callers of constraint routines now don't have to pass parameters that are embedded within the class at setup time.
e.g. for logging, communication, per-atom information, performance counters.

Some of those parameters have been converted to use const references per style, which requires various callers and callees to be modified accordingly. In particular, the mttop utility functions that take const pointers have been deprecated, and some temporary wrapper functions used so that we can defer the update of code completely unrelated to constraints until another time. Similarly, t_comrec is retained as a pointer, since it also makes sense to change globally.

Made ConstraintVariable an enum class. This generates some compiler warnings to force us to cover potential bug cases with fatal errors. Used more complete names for some of the enum members.

Introduced a factory function to continue the design that constr is nullptr when we're not using constraints.

Added some const correctness where it now became necessary.

Refs #2423

Change-Id: I7a383489b67f30863ca37c0359cd3e950b5494

Revision 143ab3d6 - 06/05/2018 09:30 AM - Mark Abraham

Separate flexible constraint counting

Functions should do one thing, particularly when the thing is only needed some of the time and complicates returning multiple things.

Minimized scope of some variables, avoiding risky re-use of variables with the same name.

Refs #2423

Change-Id: I1860447b4780e76c20a53964a2a946512689b872

Revision ddc3dd50 - 06/13/2018 04:11 PM - Mark Abraham

Use more containers and views for constraints code

Lifetime and usage is clearer if we don't use raw pointers.

Refs #2423

Change-Id: I7d76e30acfd209baf2256efbd3c40290ed38caab

Revision ec536ccf - 06/13/2018 05:41 PM - Mark Abraham

Use initializer lists for Lincs and Task

This permits us to have some constructors that work the same way that snew used to do (ie. calloc), so that future cleanup can use more vectors, etc.

Also made a destructor of Constraints::Impl so the Lincs object gets freed.

Refs #2423

Change-Id: Ie4a2001556d04f620a9d5241a9e1da9024cb9ce1

Revision dd0560e4 - 06/14/2018 12:18 AM - Mark Abraham

Call Constraints::setConstraints with other setup code

Refs #2423

Change-Id: lebee644a133f60778fe9b8030b7b7bf9656ba82
on the checklist - more will follow. I haven't tagged this redmine issue on them, yet

#2 - 02/26/2018 04:52 PM - Mark Abraham
- Description updated

#3 - 02/28/2018 03:39 PM - Gerrit Code Review Bot
Gerrit received a related patchset '3' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~If60ab052ae73ad981fa031c2db6b3e206b380f4c
Gerrit URL: https://gerrit.gromacs.org/7608

#4 - 02/28/2018 03:39 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I9e4fa14bb87119caca7c55f312103439b38190e3
Gerrit URL: https://gerrit.gromacs.org/7609

#5 - 03/02/2018 09:52 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~Iacc008fb11a31646e798364e253de322c16ccae
Gerrit URL: https://gerrit.gromacs.org/7646

#6 - 03/02/2018 11:34 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I4f9ad5d0bf6585675472b49b2d5654f588b7214e
Gerrit URL: https://gerrit.gromacs.org/7648

#7 - 03/06/2018 04:43 PM - Mark Abraham
- Description updated
- Assignee set to Mark Abraham
- Target version set to 2019

#8 - 03/06/2018 05:10 PM - Mark Abraham
- Related to Bug #2434: wrong values accumulated to dvdlambda in SHAKE with FE calcs added

#9 - 03/14/2018 01:34 PM - Gerrit Code Review Bot
Gerrit received a related DRAFT patchset '21' for Issue #2423.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~Ie9460963927249c7d713e76f166e687122c68de
Gerrit URL: https://gerrit.gromacs.org/6000

#10 - 03/14/2018 01:34 PM - Gerrit Code Review Bot
Gerrit received a related DRAFT patchset '1' for Issue #2423.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~Ic6e6e2a71f5c5c11e161fa26aafbed2764e014daa
Gerrit URL: https://gerrit.gromacs.org/7680

#11 - 04/05/2018 10:55 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~Iedbbbf3b4cb2d7f238c4b6774e459564a3f76a20
Gerrit URL: https://gerrit.gromacs.org/7745

#12 - 04/05/2018 11:04 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I2c60c162734f14c2ec1d56153853a36d28e6a66ff
Gerrit URL: https://gerrit.gromacs.org/7746

#13 - 04/09/2018 01:15 AM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I41bf3a4b9af4bbc3a3a7a27dc922d563abedbc
Gerrit URL: https://gerrit.gromacs.org/7611

#14 - 04/13/2018 12:53 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I21c10826721ddc9a79a33b1dc75971a20d0d55d9
Gerrit URL: https://gerrit.gromacs.org/7759

#15 - 04/16/2018 09:28 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I39d4cd0b85689220b3a592b1381f3f44558991
Gerrit URL: https://gerrit.gromacs.org/7764

#16 - 04/16/2018 09:29 AM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I7a3834889b75f3063ca37c0359ed3e950b5494
Gerrit URL: https://gerrit.gromacs.org/7762

#17 - 06/05/2018 03:33 AM - Gerrit Code Review Bot
Gerrit received a related patchset '3' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I4ebee644a133f0778fe9ab8030b7b7bf9656ba82
Gerrit URL: https://gerrit.gromacs.org/7970

#18 - 06/05/2018 03:34 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I1860447b4780e76c20a53964a2a946512589b872
Gerrit URL: https://gerrit.gromacs.org/7973

#19 - 06/11/2018 04:22 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I7d7e30a6f209ba1f2256efbd3c40290ed38caab
Gerrit URL: https://gerrit.gromacs.org/7988

#20 - 06/13/2018 12:31 AM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #2423.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~Ie4a2001556d04620a9d52a1a9e1da9024cb9ce1
Gerrit URL: https://gerrit.gromacs.org/7989

#21 - 09/19/2018 03:01 PM - Mark Abraham
- Target version changed from 2019 to future