Represent data on regularly spaced N-dimensional grids.

The accelerated histogram method (awh), PME summation, fourier-transform and experimental input from crystallography and cryo-EM make extensive use of data on regular grids.

A common data structure should simplify accessing grid points in space and iterating over lattices and parts of them.

Further related to em-core development, a library for cryo-EM refinement, see here

[https://drive.google.com/drive/folders/0BwBKE-uRQnTzQ1AxY0pTWURPeliJ]

Related issues:
Related to GROMACS - Feature #2282: Density map toolset

Associated revisions
Revision 7156e73a - 11/22/2018 12:29 PM - Christian Blau
mdspan - basic infrastructure
Setting up directory to contain a stripped-down and modified-for-GROMACS version of a reference implementation of the LEWG P0009 proposal, revision 8:
"mdspan: A Non-Owning Multidimensional Array Reference"

Original code is available at
https://github.com/ORNL/cpp-proposals-pub/tree/master/P0009/reference-implementation/include/experimental

Refers to #2281
Change-Id: I4b8dee54e923d269d38e1f71c4e8956768ef42e

Revision b65cb880 - 12/04/2018 04:50 PM - Christian Blau
mdspan - extents of multidimensional arrays.

Extents describe the number of elements along a certain dimension, a multidimensional index space of rank R. This is equivalent to the Cartesian product space of integer intervals [0, N_0) x [0, N_1) x ... x [0,N_{(R-1)}) 

The extents class distinguishes between extents known at compile time (static) or at run time (dynamic). Static extents are templated to allow compile time indexing evaluation (part of later patch).

Confer to P0009r8 of the Library Evolution Working Group and mdspan.extents

Source code copied and modified from Oakridge National Labs repository.

https://github.com/ORNL/cpp-proposals-pub/tree/master/P0009/reference-implementation/include/experimental/bits

Refers #2281
Change-Id: I5301f172fa1d891bc929a70e3765a2c52b3d8b8

History
#1 - 10/25/2017 10:52 AM - Christian Blau
- Related to Feature #2282: Density map toolset added

#2 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~Ic0363d9b4808fd9c372250ed380cf710d6653b65
Gerrit URL: https://gerrit.gromacs.org/7081

#3 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~Ie68c4e1013efc27b5d0e707b66f66bda327d6b
Gerrit URL: https://gerrit.gromacs.org/7082

#4 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~I9ea250d26f60b68041f16912798ec4cb45a07b1d
Gerrit URL: https://gerrit.gromacs.org/7083

#5 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~I3245821b969e8c97d0380fc96bd695dc7e3eed68
Gerrit URL: https://gerrit.gromacs.org/7084

#6 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~I7c87419b399eb890ba25b712779f1815c8a84c
Gerrit URL: https://gerrit.gromacs.org/7085

#7 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~I2a5eb4f9555ea6bf582cd51d91e380b5889e486
Gerrit URL: https://gerrit.gromacs.org/7086

#8 - 10/25/2017 01:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2281.
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~Ia5eb4f9555eb682cd51d91e380b5889e486
Gerrit URL: https://gerrit.gromacs.org/7087

#9 - 10/25/2017 05:05 PM - Gerrit Code Review Bot
Gerrit received a related patchset '11' for Issue #2281.
Uploader: Carsten Kutzner (ckutzne@gwdg.de)
Change-Id: gromacs~master~I5f18c33e777db55445bebc55c6edde6a16d7b3ff0
Gerrit URL: https://gerrit.gromacs.org/6970

#10 - 10/30/2017 01:33 PM - Christian Blau
For proposals for the C++ standard where the grid is a non-owning special case of an arrayRef (mdspan) see here:

- Multidimensional Array Reference
- A Minimal mdspan
- Multidimensional bounds, offset and array_view
- Additions to Array View for Performance
- Span: bounds-safe views for sequences of objects
- Multidimensional bounds, index and array_view

Implementations:

- Microsoft GSL multi_span
- N-D array-view

#11 - 11/14/2017 03:56 PM - Berk Hess
- Status changed from New to In Progress

#12 - 10/08/2018 06:52 PM - Mark Abraham
I figure there are two different questions to address:
1. How do represent multidimensional arrays, optimally with arbitrary strides, padding and without performance overhead?
2. How do we translate multidimensional coordinates to lattice-point?

For 1. I concluded in https://gerrit.gromacs.org/#/c/7081/:
"Then I would put P0009 [1] from github.com/ORNL/cpp-proposals-pub/ in utilities once we bump to C++14."

For 2:
Build our own, trying to use as much of P0009 infrastructure as possible. Add the iterator back into P0009.

My code built onto N3851, but I planned to rebase onto P0009 once we're through with the beta release.

My hope would be that P0009 would make the Thomas 2d irreg array patch a bit smaller as well; looking at the very good tests there at least.

I would like to gather the relevant use cases that already exist in GROMACS, and start to use new concepts there as much as possible rather than implementing for use in future modules.

Find related data structures in other tools here:
https://docs.scipy.org/doc/numpy-1.15.0/reference/c-api.types-and-structures.html#c.PyArrayObject
https://docs.python.org/3/c-api/buffer.html#buffer-structure
https://eigen.tuxfamily.org/dox/classEigen_1_1Matrix.html
https://eigen.tuxfamily.org/dox/classEigen_1_1Array.html

The mdspan in P0009 mirrors most of the aspects of matrices in the Eigen library and allows to extract the information needed to build CPyArrayObjects without copying data, so I would argue that this strengthens the case for mdspan even more.
Ongoing mdspan development has moved to
https://github.com/kokkos/mdspan

#22 - 12/20/2019 12:11 PM - Paul Bauer
@Christian can this be marked as resolved?

#23 - 12/20/2019 01:03 PM - Christian Blau
Yes, though we would like to keep up to date with mdspan developments
I'll open a new task for this, so that this very issue can be closed

#24 - 12/28/2019 10:53 AM - Paul Bauer
- Status changed from In Progress to Resolved

#25 - 12/28/2019 10:53 AM - Paul Bauer
- Status changed from Resolved to Closed