

GROMACS - Task #2976

Basic math for Multidimensional arrays

06/13/2019 12:37 AM - Kevin Boyd

Status:	New
Priority:	Normal
Assignee:	
Category:	core library
Target version:	2020
Difficulty:	uncategorized
Description	
<p>To use BasicMatrix3x3 as a drop in for the c-style tensor, we need to support the addition, subtraction, and several multiplication functionality found in math/vec.h. A lot of these functions are used in the main MD code, each of which will need to be supported before the matrices can be replaced.</p>	
<p>Functions to replace:</p> <ul style="list-style-type: none">copy_matclear_matmmul_ur0mmultransposetmmulmtmuldetm_addm_submismulmvmulmvmul_ur0tmvmul_ur0trace	

Associated revisions

Revision f3c2e710 - 07/02/2019 09:14 AM - Kevin Boyd

Add mdspan basic elementwise math

BasicMatrix3x3 provides a replacement for the c-style tensors, but has yet to replicate the tensor operations in math/vec.h. This provides a subset of that functionality for mdspan in general, which can be used for MultiDimArray trivially

Refs #2976

Change-Id: I17b77df032dbbfde0ff87108215edcec07fef6c4

Revision 6941eb5a - 07/25/2019 10:15 AM - Kevin Boyd

Add transpose operation to Matrix3x3

refs #2976

Change-Id: I8f0ce04b18be1e8b119de02cb6b52b3314cd67eb

Revision 0060f37a - 08/05/2019 08:26 PM - Paul Bauer

Add free function to convert matrix type

New free function that allows generation of a Matrix3x3 type from the legacy matrix type. Prepares for replacing the old matrix types.

Refs #2976

Change-Id: I5f17bef75d666b5221519c38abfa05a2ccd89cb0

Revision 4625c43c - 08/09/2019 06:58 PM - Paul Bauer

Add conversion from legacy to modern matrix type

Refs #2976

Change-Id: Iddf400bbb688a00c9de60e33d9c9a05f7c146f66

History

#1 - 06/13/2019 12:37 AM - Kevin Boyd

It's not clear to me whether these should be free functions or operator overloads.

#2 - 07/22/2019 09:09 PM - Kevin Boyd

- Description updated

#3 - 07/25/2019 05:56 AM - Kevin Boyd

There are a few composite functions which are used once or twice that I'm not sure are worth reimplementing for matrices.

For example, `tmul(a,b)` is `transpose(a) * b`, and vice versa for `mtmul`

#4 - 07/25/2019 04:23 PM - Eric Irrgang

Kevin Boyd wrote:

It's not clear to me whether these should be free functions or operator overloads.

In general, free functions are clean and clear.

#5 - 07/26/2019 06:24 PM - Kevin Boyd

- Description updated

#6 - 08/04/2019 09:33 PM - Mark Abraham

We would also want to think about the consequences on compilation time. Anecdotally, the density fitting code that Christian has been landing is rather slow to compile, presumably because of the cost of compiling code based on `mdspan`. Before Kevin gets too committed to the project, we should probably try replacing matrix type with `Matrix3x3` in a whole source file and getting a feel for the cost, in release and debug mode.

#7 - 08/04/2019 09:44 PM - Mark Abraham

Also <https://github.com/kokkos/mdspan> is of interest if we ever decide something needs improving. They're aware we depend on an earlier `mdspan` implementation, and would welcome feedback!