

GROMACS - Task #2834

C++ matrix classes

01/16/2019 10:41 AM - Christian Blau

Status:	In Progress
Priority:	Normal
Assignee:	Christian Blau
Category:	core library
Target version:	2021
Difficulty:	uncategorized
Description	
Similar to RVec, we want a C++ matrix class to replace C-style matrices.	
General requirements are	
<ul style="list-style-type: none">• member access operator (can be (x,y) or [x][y])• copy-able• movable• enables efficient algebra operations• implicit conversions between const and non-const matrices• constraint matrix implementation• implicit conversion from constraint to non-constraint matrices	
For a feasible transition period from the C-style matrices,	
<ul style="list-style-type: none">• implicit conversion operator to matrix type• member access with bracket notation [x][y]	
Previous discussion about C++ style vectors/matrices led to RVec implementation at #1017	
Subtasks:	
Task # 2835: Matrix class constraint to upper or lower triangle	New

Associated revisions

Revision a543a74f - 02/11/2019 05:30 PM - Christian Blau

view on MultiDimArray

Access the view and a const view on a MultiDimArray.

refs #2834

Change-Id: Ia82983ac9e3bc8edebc53a1c9f3335101ad4c704

Revision 27711dc3 - 02/12/2019 10:17 AM - Christian Blau

3x3 matrices

Matrices with contiguous, aligned memory as C-style "matrix" replacement

Matrix elements are accessed efficiently with bracket notation m(x,y) or, for compability reasons, with m[x][y] (though deprecated)

Matrices manage their own memory, but provide an implicit conversion to views and const views on their data which should be used instead of a copy.

Arithmetic operations will follow in a later patch.

refs #2834

Change-Id: Ia96037384d2e1d774559bcac97f420c58106625

History

#1 - 01/16/2019 10:42 AM - Gerrit Code Review Bot

Gerrit received a related patchset '16' for Issue [#2834](#).
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~lda9dd28d27e2b17bac05a17eb1110a900a7701bd
Gerrit URL: <https://gerrit.gromacs.org/6309>

#2 - 01/16/2019 10:42 AM - Gerrit Code Review Bot

Gerrit received a related patchset '7' for Issue [#2834](#).
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~l4d3eab9073e23afb752cc0f15d09acd9824b6e93
Gerrit URL: <https://gerrit.gromacs.org/6312>

#3 - 01/16/2019 10:43 AM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue [#2834](#).
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~la96037384d2e1d774559fbcac97f420c58106625
Gerrit URL: <https://gerrit.gromacs.org/8981>

#4 - 01/16/2019 08:34 PM - Roland Schulz

We can add [] bracket notation to mdspan.

#5 - 01/22/2019 03:07 PM - Mark Abraham

From src/gromacs/math/vec.h, we probably want ways to access most of the following functionality:

```
matrix (3x3) operations:
! indicates that dest should not be the same as a, b or src
the _ur0 varieties work on matrices that have only zeros
in the upper right part, such as box matrices, these varieties
could produce less rounding errors, not due to the operations themselves,
but because the compiler can easier recombine the operations
void copy_mat(matrix a, matrix b)           b = a
void clear_mat(matrix a)                   a = 0
void mmul(matrix a, matrix b, matrix dest) ! dest = a . b
void mmul_ur0(matrix a, matrix b, matrix dest) dest = a . b
void transpose(matrix src, matrix dest)    ! dest = src*
void tmmul(matrix a, matrix b, matrix dest) ! dest = a* . b
void mtmul(matrix a, matrix b, matrix dest) ! dest = a . b*
real det(matrix a)                         = det(a)
void m_add(matrix a, matrix b, matrix dest) dest = a + b
void m_sub(matrix a, matrix b, matrix dest) dest = a - b
void msmul(matrix m1, real r1, matrix dest) dest = r1 * m1
void mvmul(matrix a, rvec src, rvec dest)  ! dest = a . src
void mvmul_ur0(matrix a, rvec src, rvec dest) dest = a . src
void tmvmul_ur0(matrix a, rvec src, rvec dest) dest = a* . src
real trace(matrix m)                       = trace(m)
```

There's probably some useful operations (or implementation details) to copy from BasicVector in vectypes.h

#6 - 01/22/2019 04:09 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2834](#).
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~lf2c1d8f05bba95318f3fe725599e91392cd1869a
Gerrit URL: <https://gerrit.gromacs.org/9018>

#7 - 01/23/2019 12:19 PM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue [#2834](#).
Uploader: Christian Blau (cblau@gwdg.de)
Change-Id: gromacs~master~la82983ac9e3bc8edebc53a1c9f3335101ad4c704
Gerrit URL: <https://gerrit.gromacs.org/9016>

#8 - 12/28/2019 10:40 AM - Paul Bauer

- Status changed from New to Resolved

I think this is resolved

#9 - 12/29/2019 10:32 AM - Paul Bauer

- *Status changed from Resolved to In Progress*
- *Target version changed from 2020 to 2021*

not resolved, bumped