

## GROMACS - Feature #1877

### Support reading 3d-grid data from cryo-electron microscopy tomography and X-ray crystallography

12/11/2015 04:34 PM - Christian Blau

<b>Status:</b>	Closed	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	Christian Blau	
<b>Category:</b>		
<b>Target version:</b>	future	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
<p>Comparison against experimental data within simulation or trajectory analysis requires reading from and writing to common experimental data formats.</p> <p>For cryo-electron microscopy and X-ray crystallography, the common vanilla data format is the ccp4/mrc format, even though the standard slightly diverged,</p> <p>I suggest implementation of the electron microscopy database (EMDB) ccp4/mrc format, documented here <a href="ftp://ftp.wwpdb.org/pub/emdb/doc/Map-format/current/EMDB_map_format.pdf">ftp://ftp.wwpdb.org/pub/emdb/doc/Map-format/current/EMDB_map_format.pdf</a></p> <p>Implementation of other standards should be straightforward from there, if needed.</p> <p>Other format specifications can be found here: <a href="http://www.ccp4.ac.uk/html/maplib.html#description">http://www.ccp4.ac.uk/html/maplib.html#description</a> <a href="http://www2.mrc-lmb.cam.ac.uk/research/locally-developed-software/image-processing-software/">http://www2.mrc-lmb.cam.ac.uk/research/locally-developed-software/image-processing-software/</a> <a href="http://bio3d.colorado.edu/imod/doc/mrc_format.txt">http://bio3d.colorado.edu/imod/doc/mrc_format.txt</a> <a href="http://www.ccpem.ac.uk/mrc_format/mrc_format.php">http://www.ccpem.ac.uk/mrc_format/mrc_format.php</a></p> <p>The ccp4/mrc density format should also be useful for any 3d-density output, e.g. from analysis tools, since it is agnostic to the source of the data.</p>		
<b>Related issues:</b>		
Related to GROMACS - Feature #2282: Density map toolset		<b>New</b>

#### Associated revisions

##### Revision c94c85dc - 03/19/2019 06:22 PM - Christian Blau

densityfitting - density file format (mrc) header.

Implements mrc/cc4/map format file headers as described in "EMDB Map Distribution Format Description Version 1.01 (c) emdatabank.org 2014"

Reading and writing is part of a follow-up patch.

refs #2282 and #1877

Change-Id: Ild43cedb137c0beeb320e1299df8bae9916c8ea8

##### Revision 582fc1fb - 03/19/2019 06:23 PM - Mark Abraham

Add support for serializing 32-bit integers

Some file formats explicitly require this size, which we should support explicitly. Note that C++ requires that int be at least 16 bits. In practice on current systems it is always 32 bits, but being explicit might help future portability if any architecture would use 64-bit int.

Also added some support for unsigned 32- and 64-bit integers where I saw it was missing and might be useful.

Added some test coverage where it already exists.

Refs #1877

## History

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### #1 - 12/11/2015 05:36 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#1877](#).  
Uploader: Christian Blau ([cblau@gwdg.de](mailto:cblau@gwdg.de))  
Change-Id: If36bdcc4c0dbc6dee8f3455f35a6501633f90661  
Gerrit URL: <https://gerrit.gromacs.org/5447>

### #2 - 10/25/2017 10:55 AM - Christian Blau

- Related to Feature #2282: Density map toolset added

### #3 - 02/05/2019 05:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1877](#).  
Uploader: Christian Blau ([cblau@gwdg.de](mailto:cblau@gwdg.de))  
Change-Id: gromacs~master~la4d63faadeb595d7a2eeb4ac4760c211c0d2aac6  
Gerrit URL: <https://gerrit.gromacs.org/9089>

### #4 - 03/08/2019 04:12 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#1877](#).  
Uploader: Christian Blau ([cblau@gwdg.de](mailto:cblau@gwdg.de))  
Change-Id: gromacs~master~lfd43cedb137c0beeb320e1299df8bae9916c8ea8  
Gerrit URL: <https://gerrit.gromacs.org/9281>

### #5 - 03/19/2019 05:09 AM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#1877](#).  
Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))  
Change-Id: gromacs~master~I05efd7d4ba07b695fc4ed7c9d9cac8738873a3a5  
Gerrit URL: <https://gerrit.gromacs.org/9330>

### #6 - 04/29/2019 09:23 AM - Christian Blau

- Status changed from New to Closed