

Implementing the 3DEM Image Conventions

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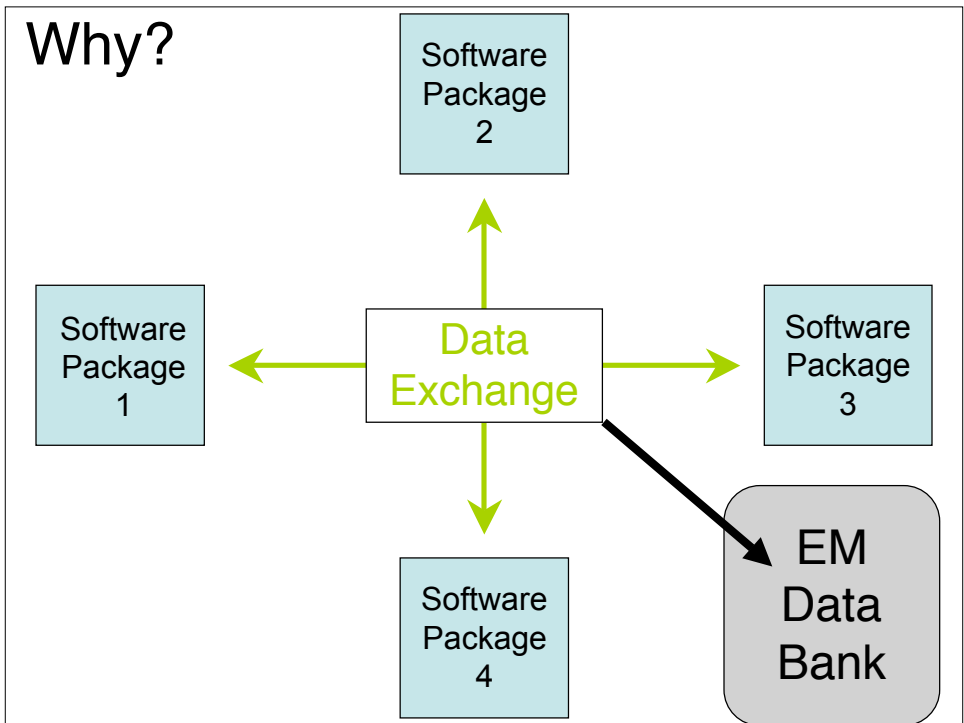
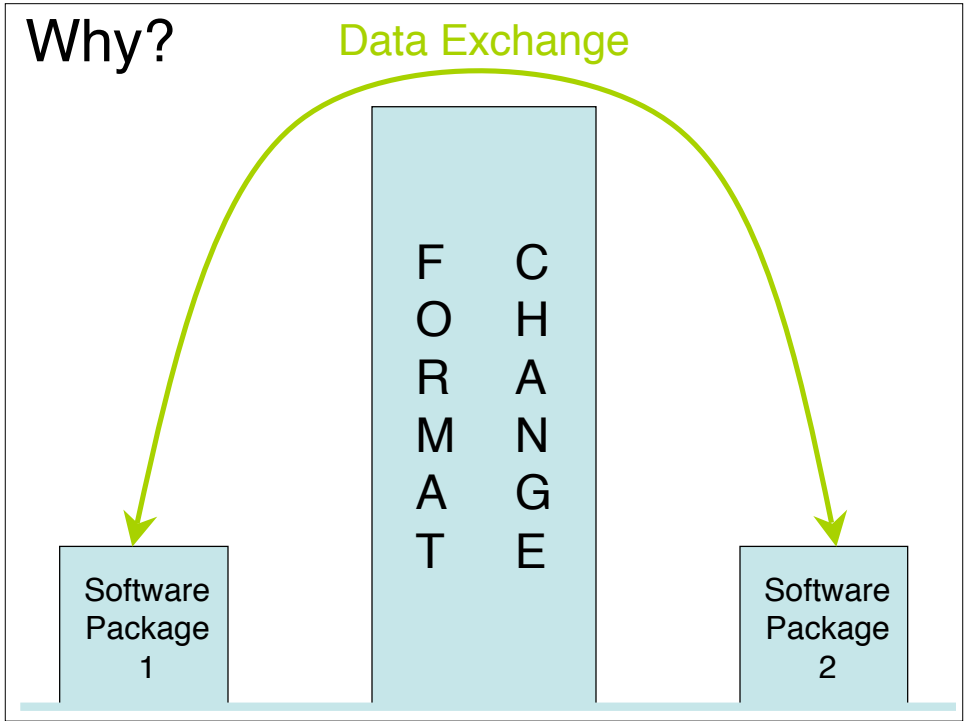
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Journal of
**Structural
Biology**

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Common conventions for interchange and archiving
of three-dimensional electron microscopy information
in structural biology

J. Bernard Heymann^{a,b}, Mónica Chagoyen^c, David M. Belnap^{a,*}



Diagnosis

1. Interpackage incompatibility
2. Too much time learning conventions
3. Inconsistent archiving in EM Data Bank
4. Incompatibility with other structural data

Prescription

1. No exotic treatment
2. You can understand the instructions
3. No Favorites
4. Doesn't need to be taken internally
5. Long-term treatment
6. Long shelve life (e.g. EMDB)

Another Standard Convention

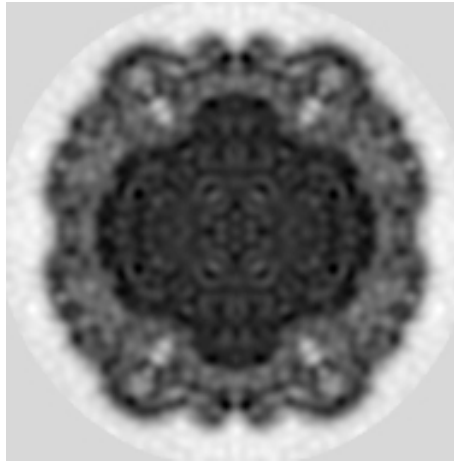
Royal Observatory,
Greenwich, UK



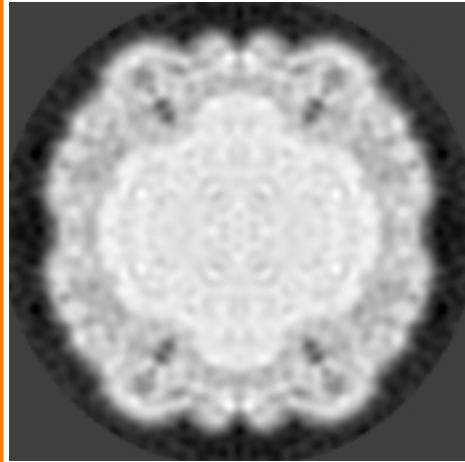
Fairness

- Not based on any one software package
- Evolution through public forum, EMDB
- No change of internal convention
- Read and write standard file
- A change for everyone is most fair way

Density Convention



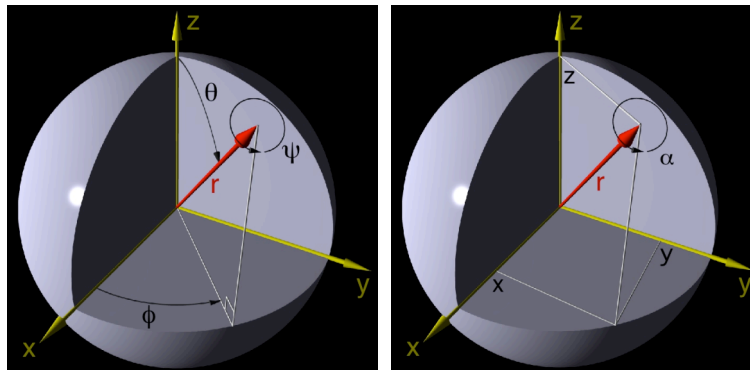
Density negative



Density positive

Orientation Convention

- Many ways to describe orientation, e.g. quaternions
- Euler angles and View vector and angle are easier to understand



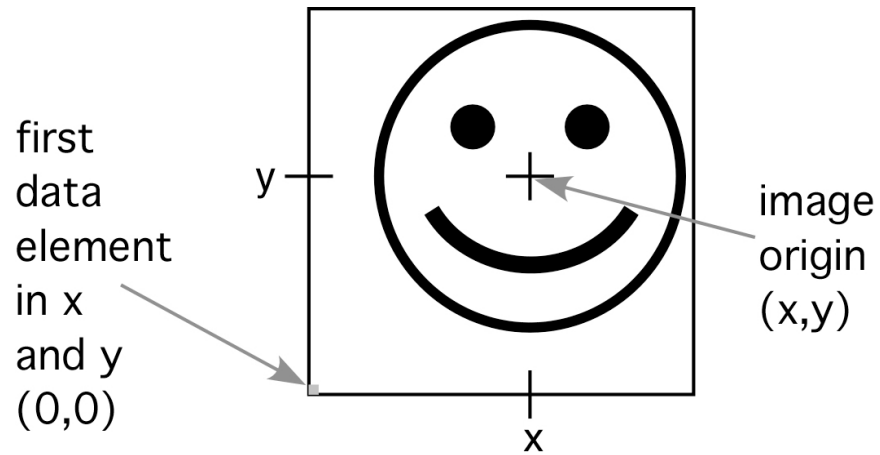
Fairness: Orientation Convention a Change for Every Package

- Tim Baker, MRC? (ϕ , θ , ω)
- ω , left-handed rotation
- $\psi = -\omega$
 - * Convention: positive rotations right-handed

Fairness: Orientation Convention Is a Change for Everyone

- EMAN (Az, Alt, Phi)
 - * Rotations about z, x', and z''
- Convention is z, y', z''

Origin Convention

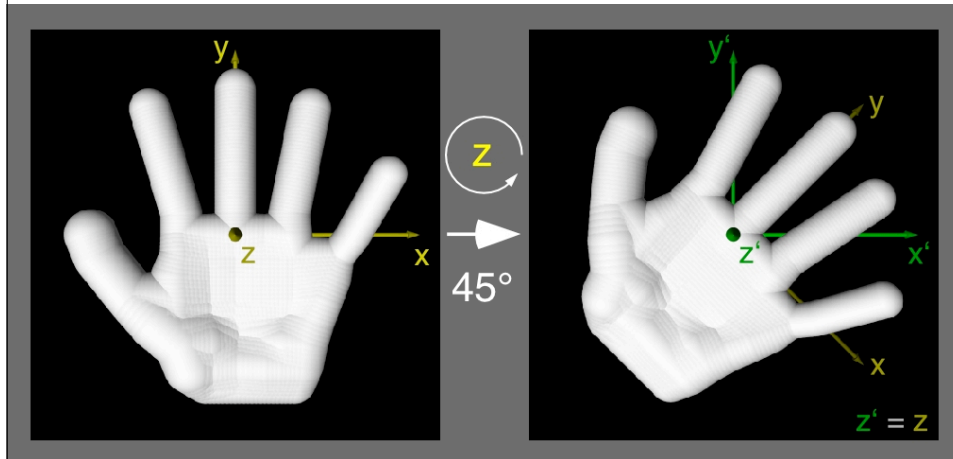


Rotation Convention

- Right-handed rotations are positive
- What is a right-handed rotation?

Right-Handed Rotation Convention

- Coordinates rotate anti-clockwise
- Object rotates clockwise



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Macromolecular Structure Database Group

Please Note: Wednesday 14th November 2007 -
Many services will be affected by essential maintenance on Wednesday 14th November 2007 from 15:00 to 18:00 GMT. We apologise for any inconvenience.

Welcome

Welcome to the EBI Macromolecular Structure Database - the European project for the collection, management and distribution of data about macromolecular structures, derived in part from the Protein Data Bank (PDB).

Submission	Documentation	Resources	Services
<ul style="list-style-type: none"> • PDB AutoDep • EMDep 	<ul style="list-style-type: none"> • MSDSD guide • MSDSD schema • Software • API • LIMS • mmCIF • XML • PDB • DB in tools • 3DEM Conventions 	<ul style="list-style-type: none"> • SIFTS @ EBI • SPINE @ EBI • RECOORD @ EBI • NMR @ EBI • Funding • Education • Projects • CAPRI • Publications • About MSD • Past Workshops • Future Events • News 	<ul style="list-style-type: none"> • MSDlite • MSDpro • MSDmotif • MSDtemplate • MSDpisa • MSDchem • MSDmine • MSDsite • MSDfold • MSDtarget • MSDanalysis • EMsearch • MSDbar • PDB

www.ebi.ac.uk/msd

3DEM Image Conventions Web Site at EBI

The 3DEM Image Conventions

The 3DEM Image Conventions

Reference
[-Heymann *et al.* \(2005\) "Common conventions for interchange and archiving of three-dimensional electron microscopy information in structural biology" *Journal of Structural Biology* 151, 196-207](#)
[-Corrigendum \(2006\) 153, 312](#)
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[Origin and Orientation Conventions](#)

by David Belnap, 9 Mar 2006
Comments, problems, questions? Please send to [David Belnap](#) and [Richard Newman](#)

3DEM Conventions Web - Home Page

CONVENTIONS FOR DATA INTERCHANGE IN 3DEM

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Aim:

Three-dimensional electron microscopy (EM) allows imaging of large biological macromolecules nearly in their native state. Different techniques have been developed within the last forty years to process the EM data and not surprisingly, success on EM particle analysis is highly correlated with the continuous development of various image processing packages. A significant development in the field was the establishment of the EM Data Bank (EMDB), a public repository that stores structural information. This Web Site addresses the main difficulties the EM community faces for interchanging and sharing both data and methodological developments: (i) inconsistency in the data submitted to the EMDB and (ii) lack of a clear, curated and centralized resource that stores the different conventions and assumptions made by each EM software package. Therefore, this web site has a double aim: check whether the map files produced in a particular package are consistent with the 3DEM conventions ([Heymann *et al.* \(2005\)](#)) and publish the conventions and assumptions followed by each EM package.

Select one of the following links:

- [Submit a new package convention](#)
- [Browse the different package conventions](#)
- [Conversion utilities archive](#)

SHOULD YOU NEED HELP, PLEASE CONTACT WITH [HELP-DESK](#)

Where do we go from here?

- **Standards and 3DEM Dictionary**
 - Meeting at PDB, Oct. 2004
 - Working group: PDB, EBI, and EM labs
- **Developers please input your conventions**
- **Medium of exchange between packages**
 - Develop a common parameter file
- **Standards Keeper and Enforcer, EMDB**

Standards Keeper and Enforcer

- **EMDB keeps conventions**
- **EMDB “enforces” standards upon submission**
- **3DEM Standards Committee**

3DEM Standards Committee

- Set policy
- Amend conventions
- Representatives from various labs and EMDB

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