Orientations, Rotation, and Symmetry

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Largely work with Wah, Steve Ludtke, Pawel Penczek

Phil and Pawel, The Transform Class in SPARX and EMAN2
Journal of Structural Biology Volume 157, Issue 1, January 2007, Pages 250–261

Phil and Pawel, Estimating alignment errors in sets of 2-D images
Journal of Structural Biology Volume 150, Issue 2, May 2005, Pages 211-225

Goal today (Very top down, Pointers to other sources):

A rotation is:

1. A coordinate, describing the current orientation of that object
2. Something that creates a motion of an object
3. Something that helps us align objects (Lie).

Conventions:

1. ZYZ, ZXZ,XYZ, spin axis (quaternionic)
2. When to use one convention over another
3. Numerically, what different ways to achieve a rotation?

Metric Structure:

1. Difference between two rotations
2. Topology of Euler Angles

Symmetries

1. Zoology of symmetries in cryo-EM
2. Pointer to more details (description of asymmetric unit, how to convert between conventions)
3. How to use symmetries to make algebra as simple as possible

“Apology”:

No references

Everything here, calculated by hand,
checked many ways, exists in EMAN/Sparx

Certainly nothing here is unique/new.
Probably (but not certainly) quite old.

Inputs from many directions celestial dynamics, computer vision, …

A rotation may mean either the present orientation (rotated from a given reference)
or … an entity which may be used to move a rigid body

think "adjective" vs "verb"

Euler: any motion of a rigid body in 2 or 3 dimensions (that is not pure translation) may be regarded as some amount of rotation of the body around some axis passing through some origin.

Rotations add a new twist (to pure translation) in describing the state of a rigid body. This is because the way that the rotation was applied is crucial in understanding the new state. The order of operations becomes important.

Orientations, Rotations: some of the basics

Fixed axes: Euler Angles

ZYZ SPIDER (Ψ,θ,φ

ZXZ EMAN (φ, alt, az)

ZYZ MRC (ω,θ,φ

ZYZ Imagic (α,β,γ

Will always be
direction perp to grid

Z Y Z

Can label point
on sphere

Does not change
information content
of a z-projection

Spin axes: Sgi, quaternionic

Any rotation can be described by an axis ($\hat{n}$) through the origin,
about which a rotation, Ω , is performed

See “The Transform Class in SPARX and EMAN2”, Baldwin and Penczek, JSB (2007) 250-261

ZYZ (in full glory)

$$\begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1}$$

$$= \begin{bmatrix} \cos\psi\cos\theta\cos\phi - \sin\psi\sin\phi & \cos\psi\cos\theta\sin\phi + \sin\psi\cos\phi & -\cos\psi\sin\theta \\ -\sin\psi\cos\theta\cos\phi - \cos\psi\sin\phi & -\sin\psi\cos\theta\sin\phi + \cos\psi\cos\phi & \sin\psi\sin\theta \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix}.$$

Spin axis, quaternionic

$$\overline{R} = \cos\Omega(\bar{I} - \hat{n}\hat{n}) - \sin\Omega\hat{n}\times + \hat{n}\hat{n},$$

$$\phi_n = \frac{\phi - \psi + \pi}{2},$$

$$\cos\frac{\Omega}{2} = \cos\frac{\phi+\psi}{2}\cos\frac{\theta}{2},$$

$$\cot\theta_n = \sin\frac{\phi+\psi}{2}\cot\frac{\theta}{2}.$$

How to Rotate an object (numerically)

Can rotate in Real Space, using naïve interpolation
Fourier Space, using naïve interpolation

Can go to polar coordinates in real space. Apply phase
polar coordinates in Fourier space. Apply phase

Reversible transformations using (3) *shears* in 2D! (FFTs and phase shifts)

Reversible transformations using *shears* in 3D!
www.ai.mit.edu/projects/im/broch/she1.html
Rotation of 3D Volumes by Fourier Interpolated Shears, Welling et al 2005

Using mirror operations

Principles Of Symmetry, Dynamics and Spectroscopy, Harter (1993, Wiley)
Quaternions and Rotation Sequences, Kuipers (2002, Princeton)

Differential Version of Movement

$$e^{a\partial_x + b\partial_y} f(x,y) = f(x+a, y+b)$$

Differential form of a translation

$$e^{t(a\partial_x + b\partial_y + \partial_\phi)} f(x,y) = f((x+b)\cos(t) - (y-a)\sin(t) - b, (x+b)\sin(t) + (y-a)\cos(t) + a)$$

Flow of a differential 2D alignment:
rotation by t about the point (–b,a)

$$e^{\Omega(n_x\partial_{\phi_x} + n_y\partial_{\phi_y} + n_z\partial_{\phi_z})} f(\vec{r}) = f(R_{\hat{n}}(\Omega)\vec{r})$$

Flow of a differential 3D rotation
(rotation by Omega about the spin-axis n)

A Fundamental Difficulty about Alignments (involving Rotations)

?

Point 1:
2D rotational/translational alignment and 3D rotational alignment are intrinsically more difficult than pure translational alignments.
There is no Fourier Transform trick.
(Go to reciprocal space, multiply, inverse transform, peak search)

Point 2:
There is no Fourier Transform trick, because the differential operators corresponding to the motions cannot be swapped out for scalar phases.

Point 3:
The operators can never be swapped out for scalars, because the order of the operations must be preserved (3D rotations, rigid body motions in the plane: non commutative group).

There is a natural sense of magnitude for rotations

Magnitude should be the total amount of rotation that took place (using the unique spin axis). That is, Ω.

The difference between two rotations can be calculated from

$$\cos\frac{\Omega_3}{2} = \cos\frac{\Omega_2}{2}\cos\frac{\Omega_1}{2} - \sin\frac{\Omega_2}{2}\sin\frac{\Omega_1}{2}(\hat{n}_1\cdot\hat{n}_2),$$

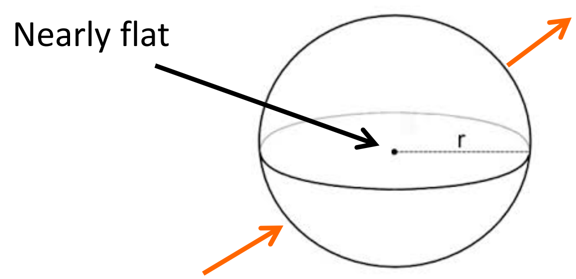
Differentially,

$$(\mathrm{d}s)^2 = \mathrm{d}\Omega^2 + 4\sin^2\left(\frac{\Omega}{2}\right)(\mathrm{d}\hat{n})^2$$

$$(\mathrm{d}\hat{n})^2 = (\mathrm{d}\theta_n)^2 + \sin^2\theta_n(\mathrm{d}\phi_n)^2$$

Solid angle between unit vectors

Topologically, let Ω be the "radius"



The surface is where Ω.=180. Identify antipodal points.

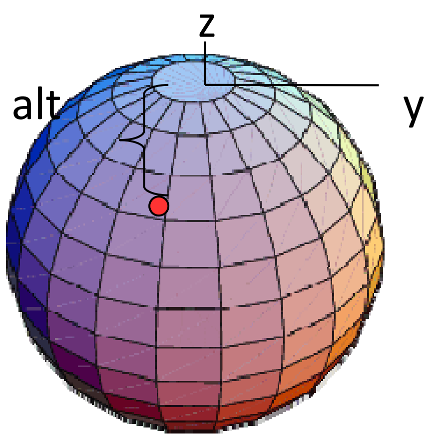
Euler Angles

$R = Z_{phi}\ X_{alt}\ Z_{az}$

$$\overline{R} = \cos\Omega(\overline{I} - \hat{n}\hat{n}) - \sin\Omega\hat{n}\times + \hat{n}\hat{n},$$

Euler angles for projections

$X_{alt}\ Z_{az}$



Why? The last in plane rotation does not change info in the projection.

If projections are rotated by -az, then the distance between them is given by the geodesic (tilt) on the sphere.

"Normal Form"

Euler Angles to use for Docking

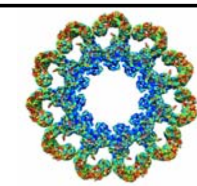
What is the total "magnitude" of a rotation?

It is the total spin, Ω

cos(Ω/2) = cos(az+phi) cos(alt/2)

Cryo EM Symmetries: $f(S\vec{r}) = f(\vec{r})$

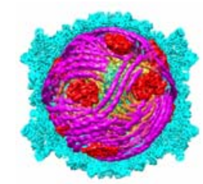
C symmetry: axial symmetry (z in EMAN)



Inflammasome, C12

D symmetry: C and additional 2 fold

Cypovirus, D3

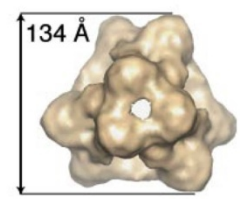


Symmetries of Platonic Solids: faces regular polygons assembled in the same way around each vertex.

Schläfli symbol {sym around face, sym around vertex}

(http://www.mathsisfun.com/platonic_solids.html)

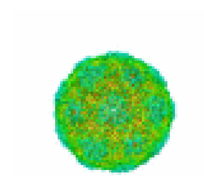
tetrahedron (self dual) F=V=4, E=6, {3,3} archaeal peptidase



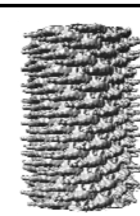
octahedral (cubic) F=8, V=6, E=12 {3,4}

DNA/AuNP

icosahedral (dodecahedral) F=20, V=12, E=30 {3,5} Ljungan virus



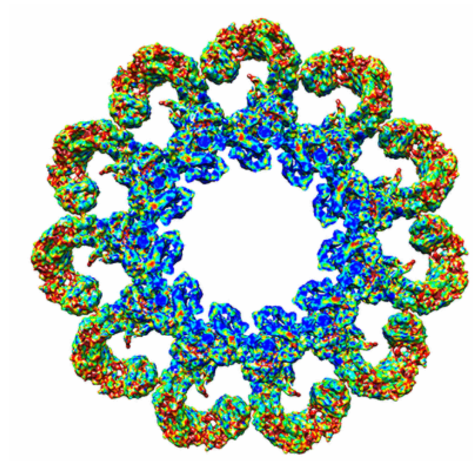
Helical symmetry (not part of core EMAN package):



amphiphysin

C12, 6458, 2015

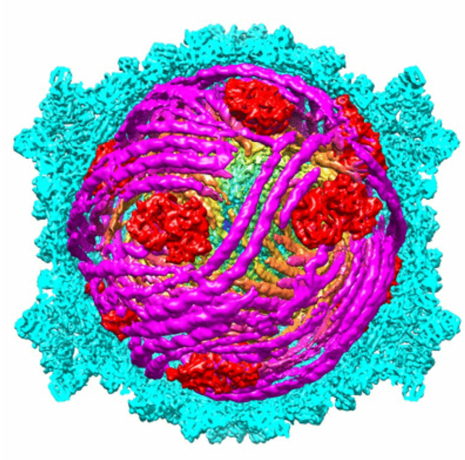
Title: Cryo-EM Structure of the Activated NAIP2/NLRC4 Inflammasome Reveals Nucleated Polymerization
Authors: Zhang L, Chen S, Ruan J, Wu J, Tong AB, Yin Q, Li Y, David L, Lu A, Wang WL, Marks C, Ouyang Q, Zhang X, Mao Y, Wu H
Sample: NAIP2/NLRC4 inflammasome, 11-fold disk
Method: Single particle reconstruction (4.7 angstroms resolution)



Protocol: Maximum-likelihood based projection matching
Software: Spider, EMAN2, Relion
CTF correction: Wiener-type filter
Number of particles: 75114
Imposed symmetry: C12
Resolution by author: 4.7 Å
Resolution method: FSC 0.143, gold-standard
Other details 9113 images 5 μm/

D3 2015-10-28

Title: **Genome and RdRp structure within the capsid of non-transcribing cypovirus**
Authors: **Liu H, Cheng L**
Sample: **non-transcribing cypovirus**
Method: **Single particle reconstruction (12 angstroms resolution)**

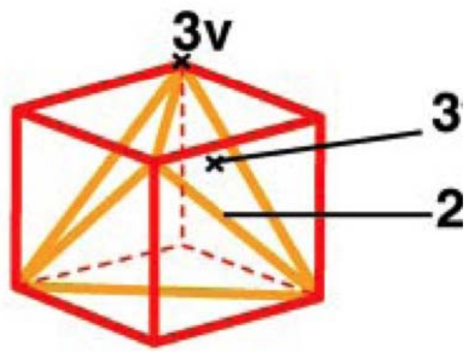


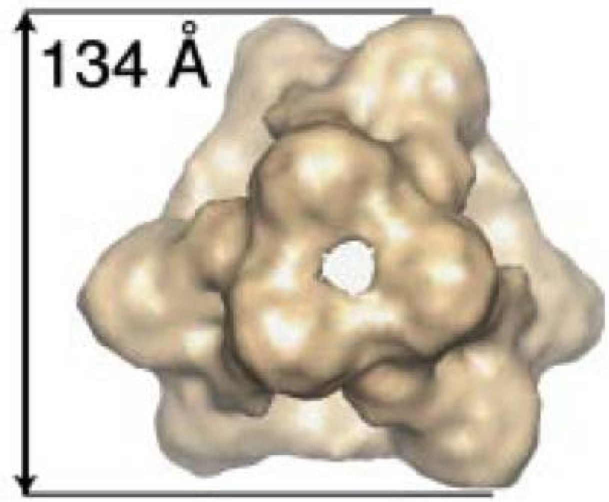
Protocol:	**cross-correlation coefficient**
Software:	**MRC**
CTF correction:	**Each particle**
Number of particles:	**28000**
Imposed symmetry:	**D3**
Resolution by author:	**12 Å**
Resolution method:	**FSC 0.143, gold-standard**
Processing details:	**Symmetry-mismatch reconstruction of icosahedral with D3 symmetry imposed.**

Tetrahedron, 1188

Title: An archaeal peptidase assembles into two different quaternary structures: A tetrahedron and a giant octahedron.
Authors: Schoehn G, Vellieux FM, … , Ruigrok RW, Ebel C, Roussel A, Franzetti B

Sample: TET1 metallopeptidase from Pyrococcus horikoshii
Method: Single particle reconstruction (15 angstroms) Updated: 2011-05-26 (2006)





Protocol: projection matching
Software: spider
CTF correction: ctfmix
Number of particles: 6000
Number of class averages: 58
Imposed symmetry: O
Resolution by author: 15 Å
Resolution method: FSC at 0.3 and X-ray filtering
Processing details: 6000 particles in 58 class average.

Octahedral, 6367, 2015

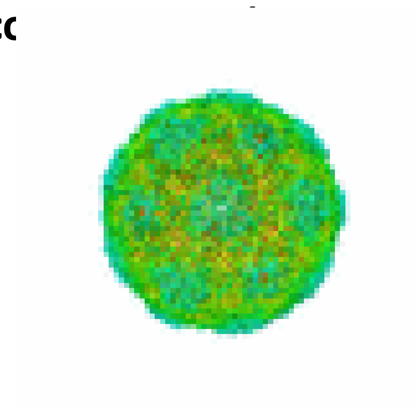
Title: Electron cryo-microscopy 3D reconstruction of an octahedral DNA/AuNP hybrid nanoparticle
Authors: Yu G, Yan R, Zhang C, Mao C, Jiang W
Sample: Hybrid nanoparticle of octahedral DNA cage encapsulating a gold nanoparticle
Method: Single particle reconstruction (24 angstroms resolution)

Software: jspr
CTF correction: each particle
Number of particles: 300
Imposed symmetry: O
Resolution by author: 24 Å
Resolution method: FSC 0.143, gold-standard
Processing details: Particles were selected using e2boxer.py in EMAN2. Contrast transfer function (CTF) estimation was performed using fitctf2.py. After preprocessing (i.e., particle picking, determination of CTF parameters, and phase correction), hybrid particles were masked using maskGold.py, resulting in two sets of particles: normalized particles (.norm, with the nongold pixels normalized to mean=0 and sigma=1) and masked particles (.masked) derived from the normalized images (.norm) with gold pixels masked. The entire data set of masked images was then halved into even and odd subsets from which initial models were derived and iterative refinements were performed independently using the random initial model method. Using the initial models as references, 2D alignment was performed using projection matching and 3D models were reconstructed using the direct Fourier inversion approach. The resolution of the reconstruction was estimated based on the 0.143 cutoff of the Fourier shell correlation between models from even and odd subsets. A final map of the hybrid particle was obtained by pooling the two half data sets and applying the refinement parameters for masked particles (.masked) to the corresponding normalized particles (.norm).

Icosahedron, 6394, 2015ß

Title: Structure of Ljungan virus: insight into picornavirus packaging
Authors: Zhu L, Wang XX, Ren JS, Porta C, Wenham H, Ekstrom J-O, Panjwani A, Knowles NJ, Kotecha A, Siebert A, Lindberg M, Fry EE, Rao ZH, Tuthill TJ, Stuart DI

Sample: Ljungan virus (type: 87-012)
Method: Single particle reco troms resolution)



Software: RELION
Number of particles: 5558
Number of class averages: 20
Imposed symmetry: I
Resolution by author: 3.8 Å
Resolution method: FSC 0.143, gold-standard

Helical, EMD-3192, 2015

Title: Helical reconstruction of amphiphysin N-BAR with a membrane tube radius of 140 Angstrom by cryo-electron microscopy

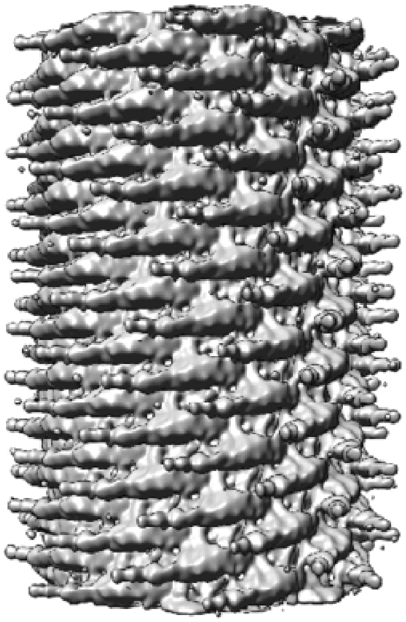
Authors: Adam J, Basnet N, Mizuno N

Sample: Amphiphysin N-BAR with a membrane tube radius of 140 Angstrom

Method: Helical reconstruction (10.3 angstroms resolution)

Map released: 2015-10-28

Amphiphysin, 0.06MDa



Protocol: IHRSR

Software: BSOFT, EMAN2, Relion, SPIDER, IHRSR

CTF correction: Phases of individual images are flipped

Resolution by author: 10.3 Å

Resolution method: FSC 0.5, gold-standard

Processing details: For the reconstruction 1948 segmented particles were used. The particles were 2D classified by Relion and for the reconstruction the helical symmetry was applied using IHRSR. Helix handedness is not confirmed by sub-tomogram averaging. Used programs: BSOFT software package, particle picking by EMAN2 with e2helixboxer, 2D classification by Relion, 3D helical reconstruction by IHRSR implemented into SPIDER.

Keep In Mind

Different packages have different conventions for arranging symmetric objects.

EMAN always uses high symmetry along z.

Construction of the asymetric unit for Platonic solid; Baldwin, Penczek, Transform Class, 2007

3.2. Angular description of an asymmetric unit of a platonic solid

Consider the three Platonic solids that are comprised of faces that are triangles: the tetrahedron ($m = 3$), the octahedron ($m = 4$) or the icosahedron ($m = 5$). In order to discuss proper sampling of the asymmetric unit, we need these boundaries in polar coordinates. Consider, therefore, the solid arranged such that it inscribes the unit sphere with one vertex b along the z-axis, a second vertex aligned in the xz plane denoted by c, and a third vertex a at the same altitude as c such that abc form the vertices of an elementary face of the Platonic solid in question (Fig. 2).

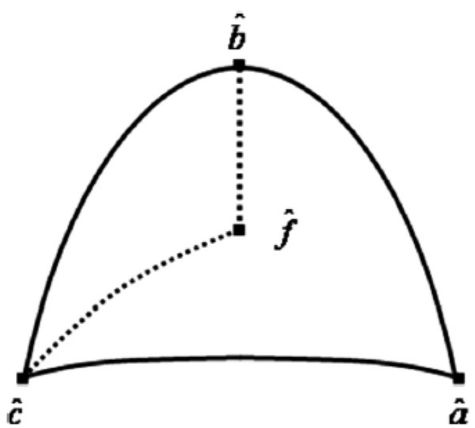


Fig. 2. A triangular subunit of some Platonic solid: either tetrahedron ($m = 3$), octahedron ($m = 4$), or icosahedron ($m = 5$): that has been projected onto a sphere (thus all the lines shown are arcs on the surface of the unit sphere). The angle $\Omega = \frac{2\pi}{m}$ is the smallest rotation such that applied to a vertex leaves the solid unchanged. The vertex $\hat{b}$ is oriented along the z axis and $\hat{c}$ is oriented in the xz plane at an angle $\theta_c = \mathrm{acos}(\frac{\cos\Omega}{1-\cos\Omega})$ to $\hat{b}$. The expression for the unit vector $\hat{f}$ normal to the face is given by (44). The asymmetric unit is demarcated by the segments bc, bf, and cf. The expressions for the first two segments are given by (47) and (48), respectively. The expression for cf is given by (50) together with (51).

Define the angle $\Omega \equiv \frac{2\pi}{m}$ to be the amount of rotation such that when applied to a vertex leaves the solid unchanged. The situation may be described as

$$\hat{b} = (0, 0, 1), \tag{39}$$

$$\hat{c} = (\sin\theta_c, 0, \cos\theta_c), \tag{40}$$

$$\hat{a} = (\sin\theta_c \cos\Omega, \sin\theta_c \sin\Omega, \cos\theta_c), \tag{41}$$

$$\hat{f} \equiv \frac{\hat{b} + \hat{c} + \hat{a}}{|\hat{b} + \hat{c} + \hat{a}|}. \tag{42}$$

The points $\hat{b}$, $\hat{c}$, and $\hat{f}$, the vector through the center of the triangle, bca, form the boundary of the asymmetric unit. The altitude, θ_c, of the vertex $\hat{c}$ can be found directly from the right hand side of (37) with $n = 3$, and $\Omega \equiv \frac{2\pi}{m}$:

$$\cos\theta_c = \frac{\cos\Omega}{1 - \cos\Omega}, \tag{43}$$

so

$$\hat{f} = \frac{1}{\sqrt{3}\sin\frac{\Omega}{2}} \left(\hat{z}\cos\frac{\Omega}{2} + \sqrt{1 - 2\cos\Omega} \left(\cos\frac{\Omega}{2}\hat{x} + \hat{y}\sin\frac{\Omega}{2} \right) \right). \tag{44}$$

At this point, all of the 4 unit vectors, $\hat{a}$, $\hat{b}$, $\hat{c}$, and $\hat{f}$, of Fig. 2 are described.

A segment $\hat{n}(t)$ of the great circle with starting point $\hat{\imath}$ and final point $\hat{\omega}$ spanning an angular distance β (that is $\hat{\imath} \cdot \hat{\omega} = \cos\beta$) is given by

$$\hat{n}(t) = \frac{\sin(\beta - t)\hat{\imath} + \sin t\hat{\omega}}{\sin\beta}, 0 \leqslant t \leqslant \beta, \tag{45}$$

where $\hat{n}$ is a vector to a point on the unit sphere. The arc described by (45) is mapped out uniformly, meaning $|\frac{d\hat{n}(t)}{dt}| = 1$. We use the formula to demarcate the asymmetric unit below.

3.2.1. The asymmetric unit

The three line segments joining $\hat{b}$ to $\hat{c}$, $\hat{b}$ to $\hat{f}$ and $\hat{c}$ to $\hat{f}$ (see Fig. 2) define the asymmetric unit of the Platonic solid. In order to use (45), we need the vertex-face angle, α, given by (38) above

$$\cos\alpha = \hat{f}\cdot\hat{b} = \frac{1}{\tan(\pi/3)\tan(\Omega/2)} = \frac{1}{\sqrt{3}\tan(\Omega/2)}, \tag{46}$$

Using (45) with $(\hat{i}\hat{\omega},\beta) = (\hat{b},\hat{c},\theta_c)$ or $(\hat{b},\hat{f},\alpha)$ or $(\hat{c},\hat{f},\alpha)$ yields

$$\hat{n}_{bc}(t) = (\sin t, 0, \cos t), \qquad 0 \leqslant t \leqslant \theta_c, \tag{47}$$

$$\hat{n}_{bf}(t) = \left(\sin t\cos\frac{\Omega}{2}, \sin t\sin\frac{\Omega}{2}, \cos t\right), \qquad 0 \leqslant t \leqslant \alpha, \tag{48}$$

$$\hat{n}_{cf}(t) = \frac{\hat{c}\sin(\alpha - t) + \hat{f}\sin t}{\sin\alpha}, \qquad 0 \leqslant t \leqslant \alpha. \tag{49}$$

We use (49) together with (40), (43), (44) and (46) to map out the difficult boundary of the symmetric unit. To understand the segment $\hat{n}_{cf}$ as altitude versus azimuth, however, we write

$$\hat{n}_{cf} \equiv (\sin\theta_{cf}\cos\phi_{cf}, \sin\theta_{cf}\sin\phi_{cf}, \cos\theta_{cf}). \tag{50}$$

One may calculate the quantities, $\hat{y}\cdot\hat{n}_{cf}$ and $\hat{y}\cdot(\hat{n}_{cf}\times\hat{c})$ from (49) and (50). Taking the ratio between these quantities eliminates the parameterization variable, t, yielding:

$$\cot\theta_{cf} = \frac{\sin\left(\frac{\Omega}{2} - \phi_{cf}\right)}{\sin\frac{\Omega}{2}}\cot\theta_c + \frac{\sin\phi_{cf}}{\sin\frac{\Omega}{2}}\cot\alpha,$$
$$= \frac{\cos(\Omega - \phi_{cf})}{\sqrt{1 - 2\cos(\Omega)}}, \quad 0 \leqslant \phi_{cf} \leqslant \frac{\Omega}{2} \tag{51}$$

This allows θ_{cf} to interpolate between θ_c (which is the altitude of the starting vertex $\hat{c}$, where $\phi_{cf} = 0$) and α, which is the altitude of the center of the triangle, where $\phi_{cf} = \frac{\Omega}{2}$. The Eqs. (47), (48) and (51) are the expressions for the boundaries of the asymmetric unit for T, O, and I symmetries, with $\Omega = \frac{2\pi}{m}$.

We will write down in more detail the case of greatest interest: the icosahedron (I) where $m = 5$, $\Omega = 72.0°$, θ_c (vertex-vertex angle given by (43)) $= 63.43°$, α (face-vertex angle given by (46)) $= 37.38°$. Then

$$\hat{n}_{bc}(t) = (\sin t, 0, \cos t), \qquad 0 \leqslant t \leqslant 63.43°, \tag{52}$$

$$\hat{n}_{bf}(t) = (0.809\sin t, 0.5878\sin t, \cos t), \qquad 0 \leqslant t \leqslant 37.38°$$

Finally if we parameterize altitude versus azimuth of the non-trivial segment *cf*

$$\cot\theta_{cf} = 1.6180\cos\left(\frac{2\pi}{5} - \phi_{cf}\right), \qquad 0 \leqslant \phi_{cf} \leqslant 36°, \tag{54}$$

which is to be used with (50).

In this section we have given parameterizations of the boundaries of the asymmetric units of those Platonic solids, that have triangles as faces (T, O, I). It is imperative to establish these parameterizations before one can consider the uniform sampling of Eulerian angles that might be used to create projections of symmetric objects such as these (the quasi-uniform distribution of Eulerian angles for asymmetric objects was covered in Section 2.3).

3.3. Symmetry elements, vertices, faces in the Transformation Class

The ability to retrieve symmetry elements in SPARX/EMAN2 has been significantly extended to allow the user to specify orientations of symmetry axes. For the case of C and D symmetries, it is often the case that one wishes to use the axis as the axial symmetry axis and the following sequence of function calls in SPARX

```
RA = Transform3D();
RA.get_sym(''c3'',2);
```

sets RA to a rotation around the z axis of 120°, which corresponds to the second element (hence the 2 above) generated by SPARX for C3 symmetry (the first element is the identity). However, particularly for I symmetry, we have obliged users who have wished orientations other than the default.

For example, originally there existed, and still exists, the function get_sym

```
RA = Transform3D();
RA.get_sym(''icos'',3, ''orientation'');
```

which allows one to systematically access symmetry elements of the icosahedron positioned in a specified orientation with respect of the system of coordinates. In the above case, one has set RA to the 3rd of the possible 60 symmetry elements of the icosahedron. The capacity to call symmetry elements has been extended so that one is able to specify symmetry elements defined with respect to arbitrary axes. For example, consider the sequence of calls

```
vertex = Vec3f(0,0,1);
face = Vec3f(sin(mu),0, cos(mu));
RA = Transform3D();
RA.get_sym(''icos'',3,vertex,face);
```

where mu is the face-vertex angle of the icosahedron (37.3°). This orients an icosahedron in such a manner that "vertex" is in the direction of the 5-fold axis of the icosahedron and "face" is in the direction of the 3-fold, then sets RA to the third symmetry element. The first vector, of the pair of vectors that appear, denotes the placement of the symmetry axis corresponding to the higher symmetry. This variant of the get_sym function uses internally the set_rotation function described in Section 2.4.1 to find the rotation that maps the default orientation of face and vertex to that specified by the user. Then this rotation is applied to each default symmetry element before being returned to the user.

We realize that it would be unnecessary effort for the SPARX user to calculate positions of face and vertex that the user may wish to use as reference orientations; we have therefore provided a large number of commonly used options from which the user may simply select. For example,

```
RA = Transform3D();
RA.get_sym(''icos'',3,''mrc'');
```

would assign to RA the 3rd symmetry icosahedral symmetry element for the icosahedron as oriented in the MRC convention: with 2-fold symmetry axes along each of the coordinate system axes (see (Heymann et al., 2005a)). An example of another option is "5fz3fx" that places the icosahedron with a 5-fold axis along *z*, and one of the five nearest 3-fold axes placed such that it has no y component. A list of the possible conventions can be accessed *via*

```
icos_poss = get_sym_poss(''icos'');
```

Now "icos_poss" has been sent to an array of strings, including "mrc" and "5fz3fx".

Finally, faces and vertices of the Platonic solids can be accessed with options similar to just described via "get_-face" and "get_vertex". For example,

```
Top_face = get_face(''icos'',3, ''mrc'');
```

returns to Top_face an array of Vec3f objects which represent the vertices of one of the faces of the icosahedron. The options "mrc" and 3 affect which particular face, and in which order the vertices are returned; these options will be amply documented.

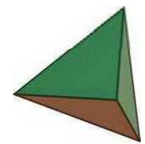
How to move between different symmetry conventions

How to efficiently write down symmetries in EMAN2:

Platonic Solids

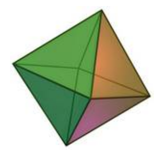
p number of Edges at each face
q number of edges meeting at each vertex

Tetrahedron: (F=4, V=4, E=6)
(p=q=3)



pF=2E
qV = 2E

Octahedral (Cubic)
(F=8, V=6, E=12) (p=4, q=3)



V-E+F=2

Icosahedral: (Dodecahedral)
(F=20, V=12) (p=3, q=5)

Either q or p must be 3

V=4p/ Denominator
E= 2pq/ Denominator
F =4q/Denomniator

Denominator =4 – (p-2)(q-2)

Exercise:

Symmetries as word problem (Baldwin and Penczek)

2E is the number of symmetry elements
Symmetry maps an edge into some other edge in one of two orientations.

$B^p=1$
$A^q=1$

BABA=1 (try it; Vertex belongs to the face.)

This is how symmetries are formulated in code of EMAN2:

Unique Symmetries ⇔ Unique words

For tetrahedron: $A^3= B^3=1$, BABA=1

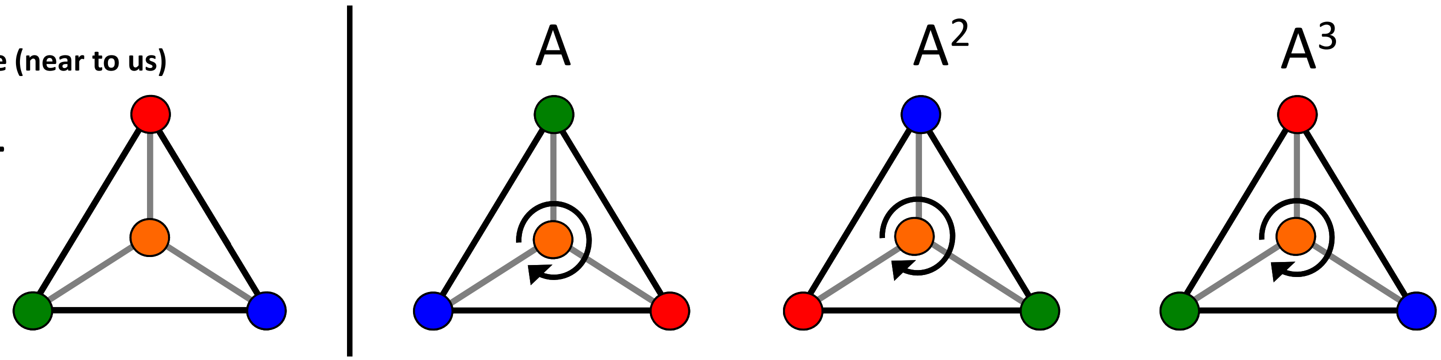
Only need to use at most one A
1, A, B, BA, AB , BB, ABB,BAB, BBA,
BABB, BBAB, BBABB (only 12 "words")

The 12 symmetry operations of the tetrahedron

(Proof AA = BABAAA= BAB; ABA= BBBABA=BB; ABBA= ABA A ABA=BBABB

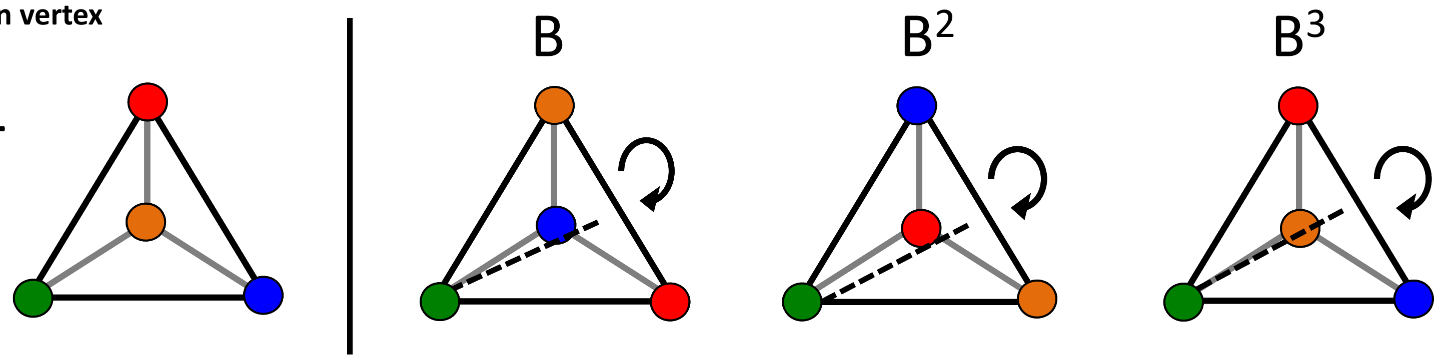
Symmetry around face (near to us)

$A^{(p=3)}=1$



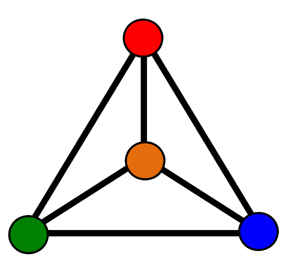
Symmetry around green vertex

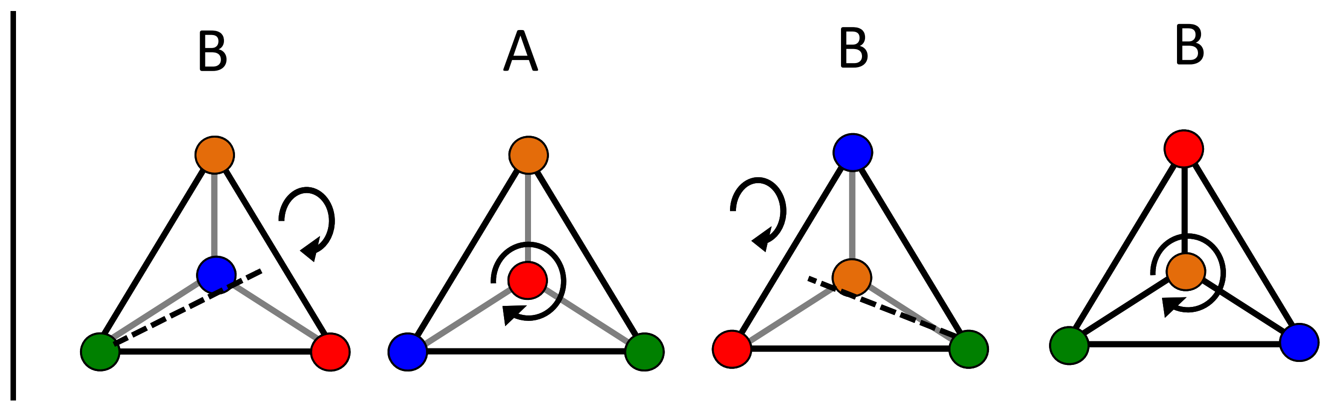
$B^{(q=3)}=1$



Green vertex belongs to near face

$ABAB=1$





Slide by Michael Bell

Platonic Symmetries in Other Dimensions

Footnote: Other dimensions

2 dimensions => N – gons

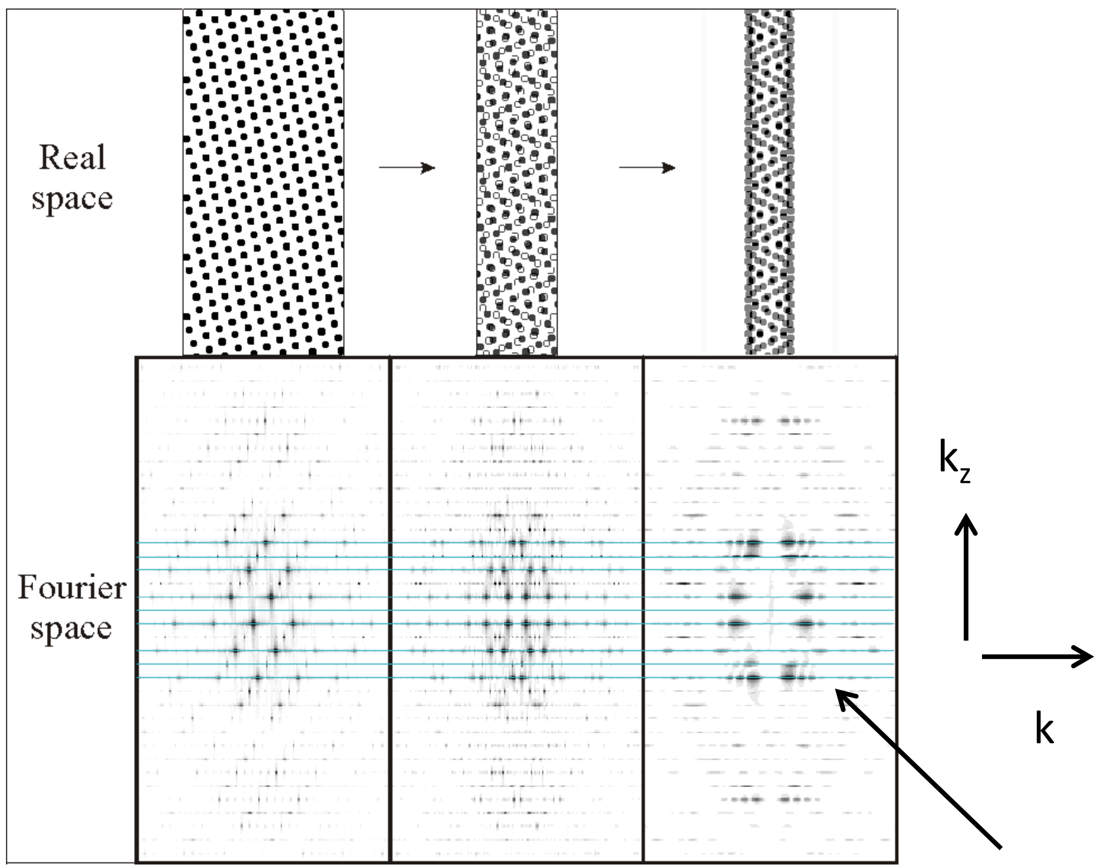
3 dimensions : tetrahedron, cube, icosahedraon

4 dimensions also 24 cell

5+ dimensions hyper tetrahedron, hypercube, (lost icosahedron)

http://math.ucr.edu/home/baez/platonic.html

Non-repeating helical symmetry: (rise over run)
The angle of rotation θ required to observe the symmetry is irrational.
θ never repeats exactly no matter how many times the helix is rotated.
DNA, approximately 10.5 base pairs per turn.



Modulated by Bessel across “layer line”

Conclusions, and Looking Forward

0. Rotations $\equiv$ Orientations

1. Almost Every Rigid Body Motion is Rotation
2. Think of Rotations as a single entity (point or member of a group), rather than product of three things.
3. Future Directions:
   Need to look at resharpening class sums from estimate of rotational alignments.
4. Look at rotational FSC.