Fast Rotational Matching

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FRM: Fast *Rotational* Matching

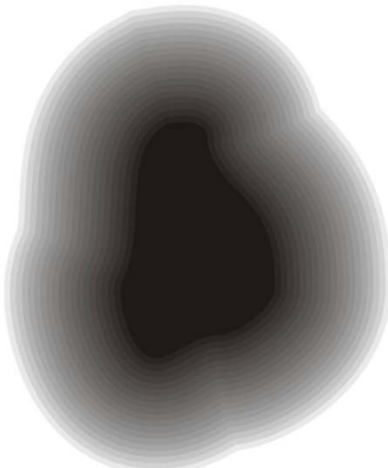
Euler angle search is expensive!

9º angular sampling (30481 rotations) requires > 10 minutes on standard workstation for rotations only.
Rotations + translations: 10-20 hours.

Our Goal: We seek to FFT-accelerate rotational search in addition to translational search.

To do this, we need to do the math in rotational space and take advantage of expressions similar to convolution theorem that are best described by group theory.

Expansion in Spherical Harmonics



Target map

f

$$f(su) = \sum_{l=0}^{B-1} \sum_{m=-l}^{l} \hat{f}_{lm}(s) Y_{lm}(u)$$

Y_{lm} are the *spherical harmonic functions*

Probe map

g

$$g(su) = \sum_{l=0}^{B-1} \sum_{m=-l}^{l} \hat{g}_{lm}(s) Y_{lm}(u)$$

FRM$_{3D}$ Method

The correlation function is:

$$c(R) = \int_{\mathbf{R}^3} f \cdot g(R) = c(\alpha, \beta, \gamma)$$

α,β,γ are specially chosen Euler angles (origin shift).

Expanding f and g in spherical harmonics as before we arrive at:

$$\hat{c}(p, q, r) = \sum_l d^l_{pq}(\tfrac{\pi}{2})\ d^l_{qr}(\tfrac{\pi}{2})\ \ I^l_{pr}$$

where:

$$I^l_{pr} = \int_0^\infty \hat{f}_{lp}(s)\,\overline{\hat{g}_{lr}(s)}\, s^2 ds$$

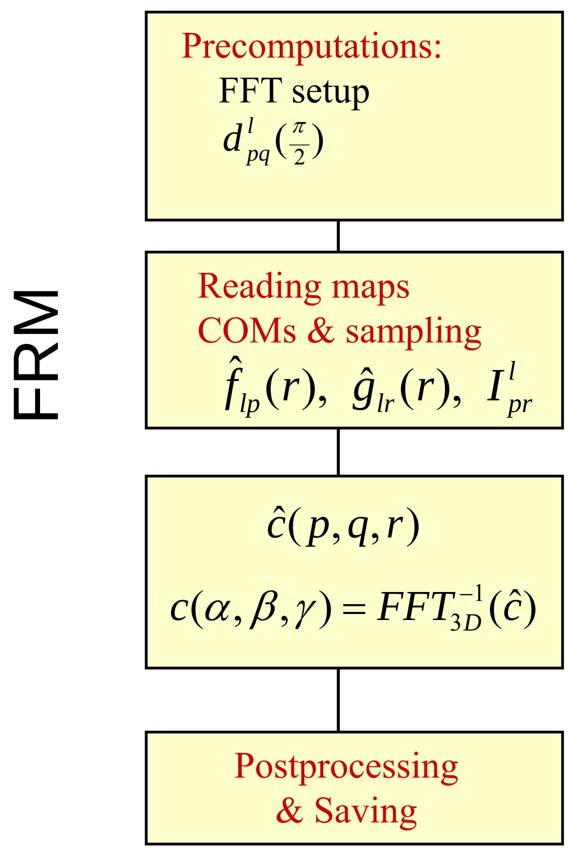
$$c(\alpha, \beta, \gamma) = FFT^{-1}_{3D}(\hat{c})$$

The quantities $d^l_{pq}(\frac{\pi}{2})$ (which come from rotation group theory) are precomputed using a recursive procedure.

Comparison between FRM$_{3D}$ and Crowther

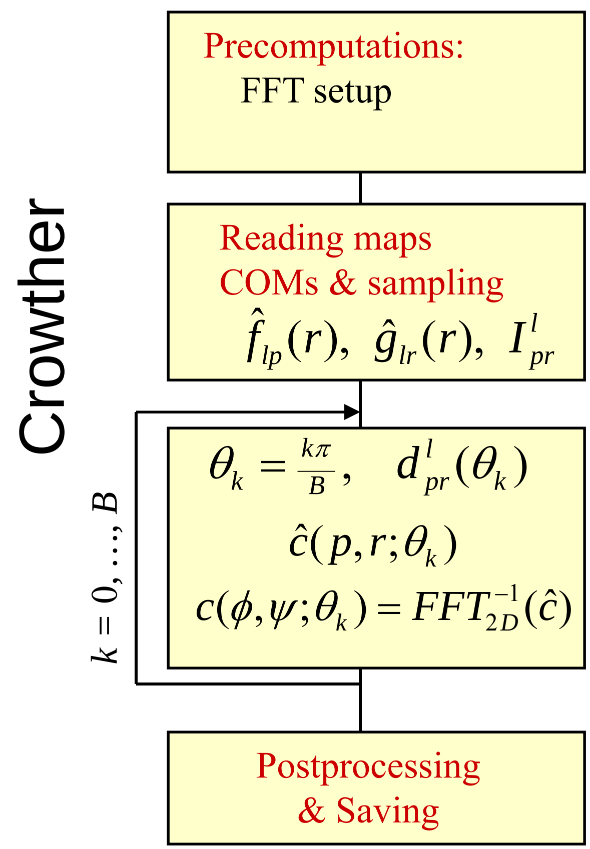
$$c(R) = c(\alpha, \beta, \gamma)$$

$$\hat{c}(p,q,r) = \sum_l d^l_{pq}(\tfrac{\pi}{2}) d^l_{qr}(\tfrac{\pi}{2}) I^l_{pr}$$



$$c(R) = c(\phi, \psi; \theta)$$

$$\hat{c}(p,r;\theta) = \sum_l d^l_{pr}(\theta) I^l_{pr}$$



Timings of FRM_{3D} and Crowther

(seconds)

angular sampling	Crowther	FRM
6°	1.66	0.97
3°	19.3	3.75
1.4°	337	37.4

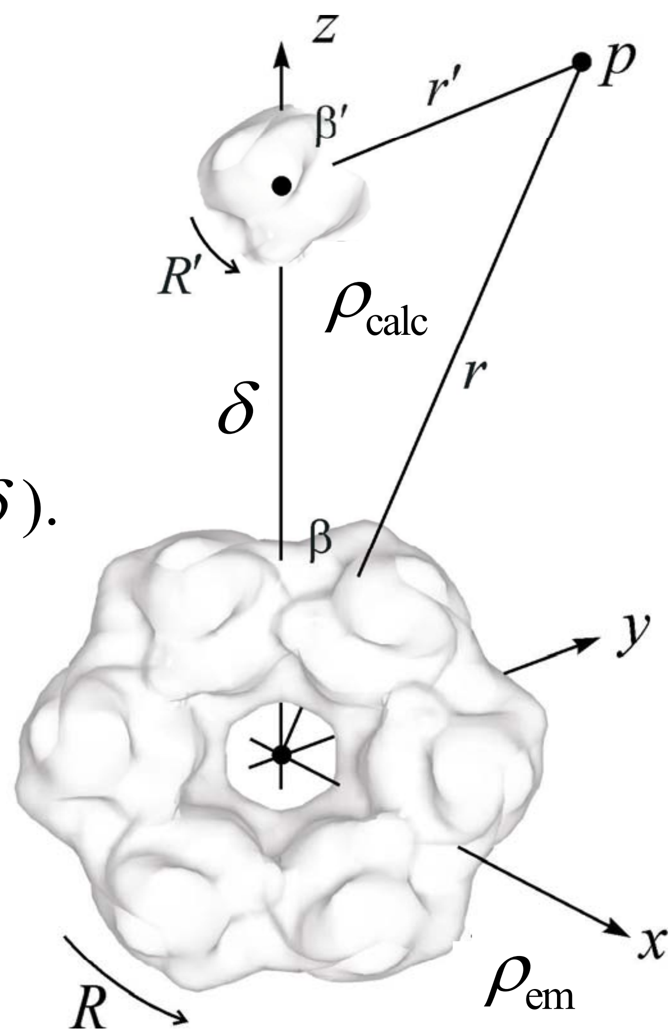
FRM_{6D} (Rigid-Body Matching)

5 angular parameters.

The correlation function is now:

$$c(R, R'; \delta) = \int_{\mathbf{R}^3} (e \otimes \rho_{em})(R) \cdot (e \otimes \rho_{calc})(R'; \delta).$$

1 linear parameter remains, distance δ of movement along the z axis.



Rigid-Body Search by 5D FFT

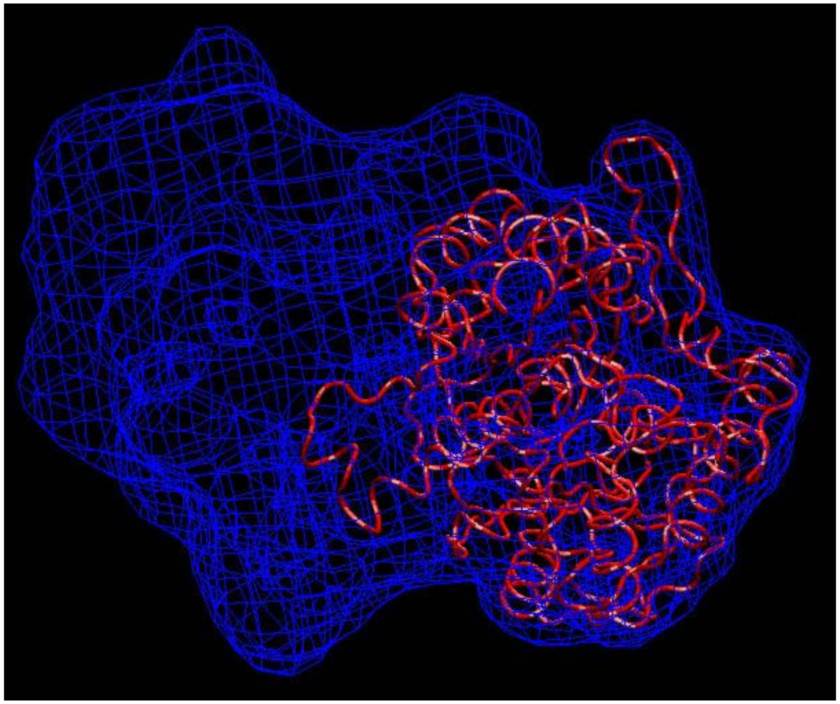
The 5D Fourier transform of the correlation function turns out to be:

$$\hat{c}(n,h,m,h',m';\delta) = (-1)^n \sum_{l,l'} d^l_{nh} d^l_{hm} d^{l'}_{-nh'} d^{l'}_{h'm'} I^{ll'}_{mnm'}(\delta).$$

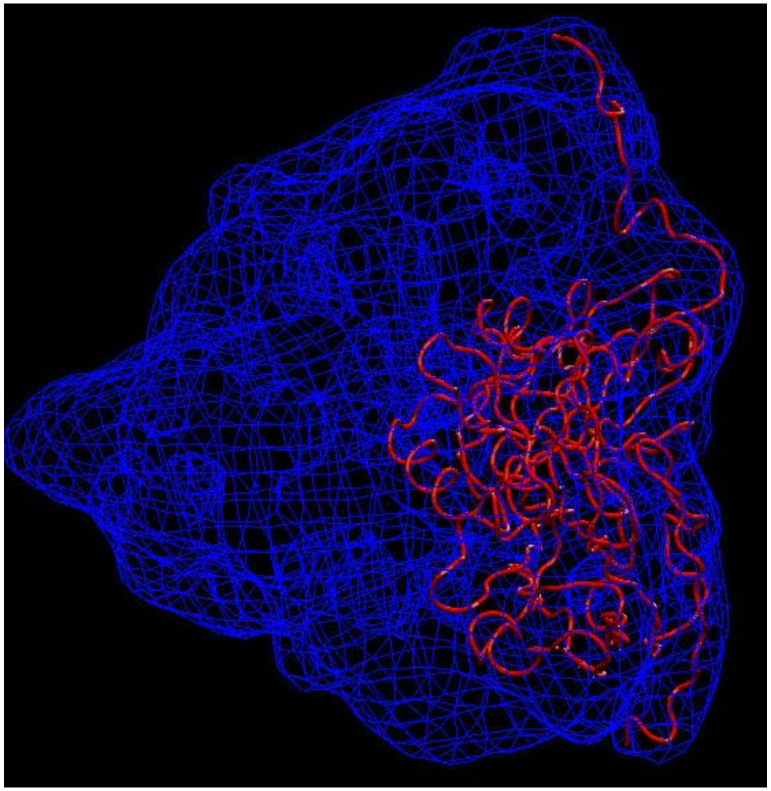
The quantities $I^{ll'}_{mnm'}(\delta)$ are the so called *two-center integrals*, corresponding to the spherical harmonic transforms of the two maps, at a distance δ of one another:

$$I^{ll'}_{mnm'}(\delta) = \sqrt{(l+\tfrac{1}{2})(l'+\tfrac{1}{2})} \int_0^{\pi} \left[\int_0^{\infty} \overline{\hat{\rho}^{lm}_{em}(r)\hat{\rho}^{l'm'}_{calc}(r')} \quad d^{l'}_{n0}(\beta') r^2 dr \right] d^{l}_{n0}(\beta) \sin\beta \quad d\beta$$

Test Cases

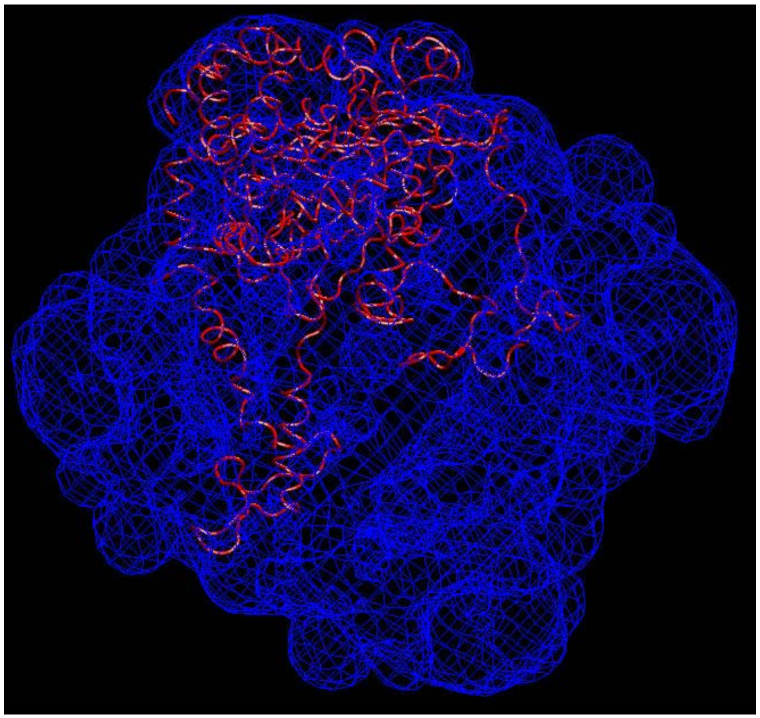


1afw
(peroxisomal thiolase)

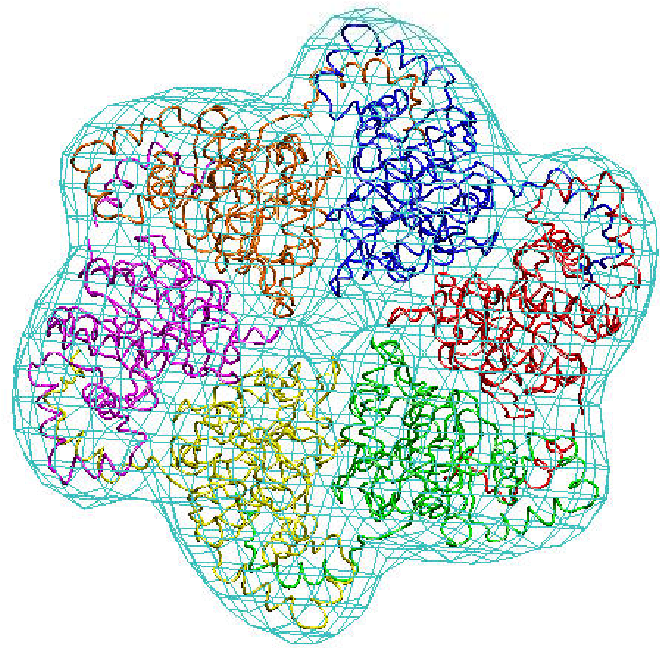


1nic (copper-
nitrite reductase)

Test Cases



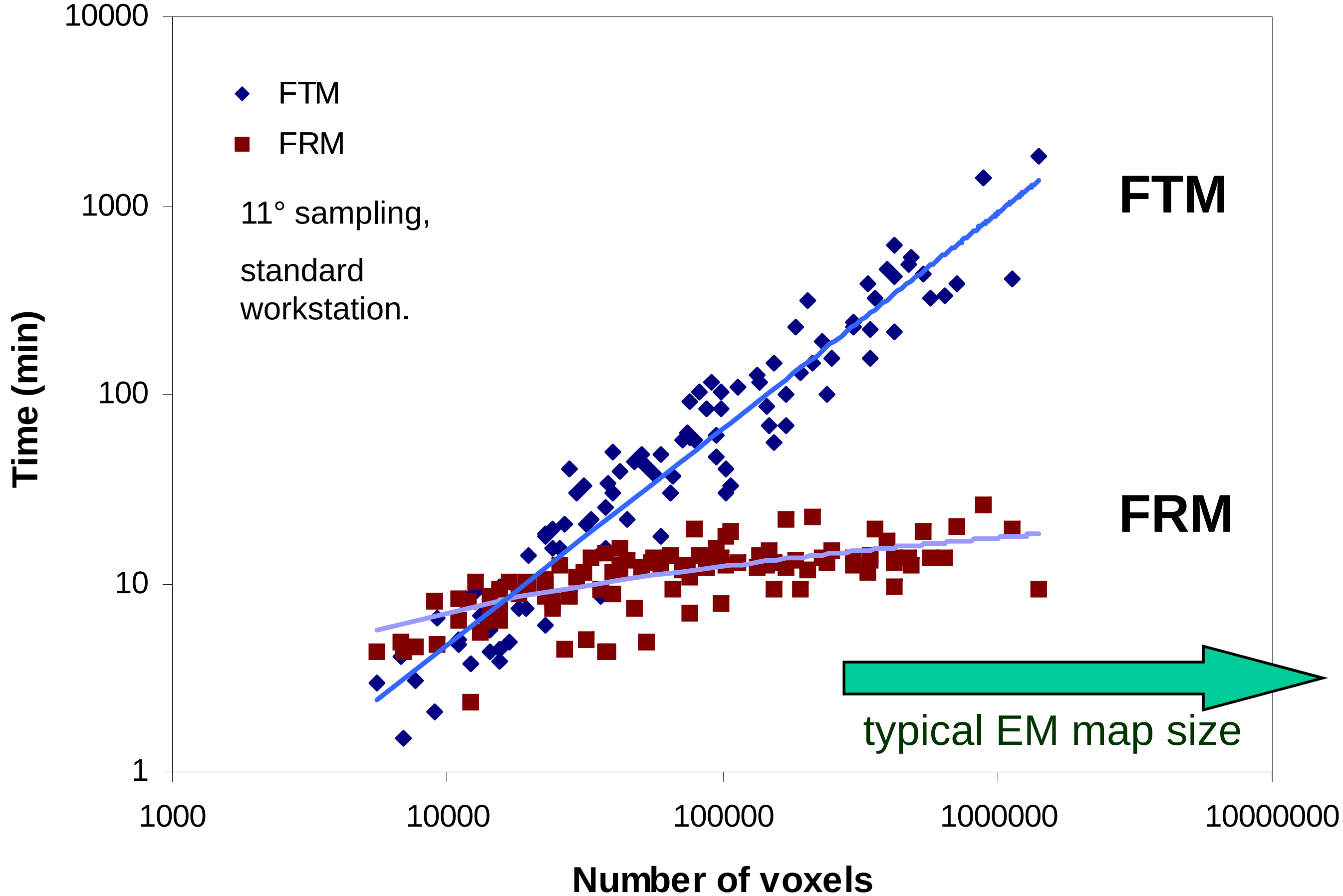
7cat
(catalase)



1e0j
(Gp4D helicase)

Efficiency: FRM vs. FTM

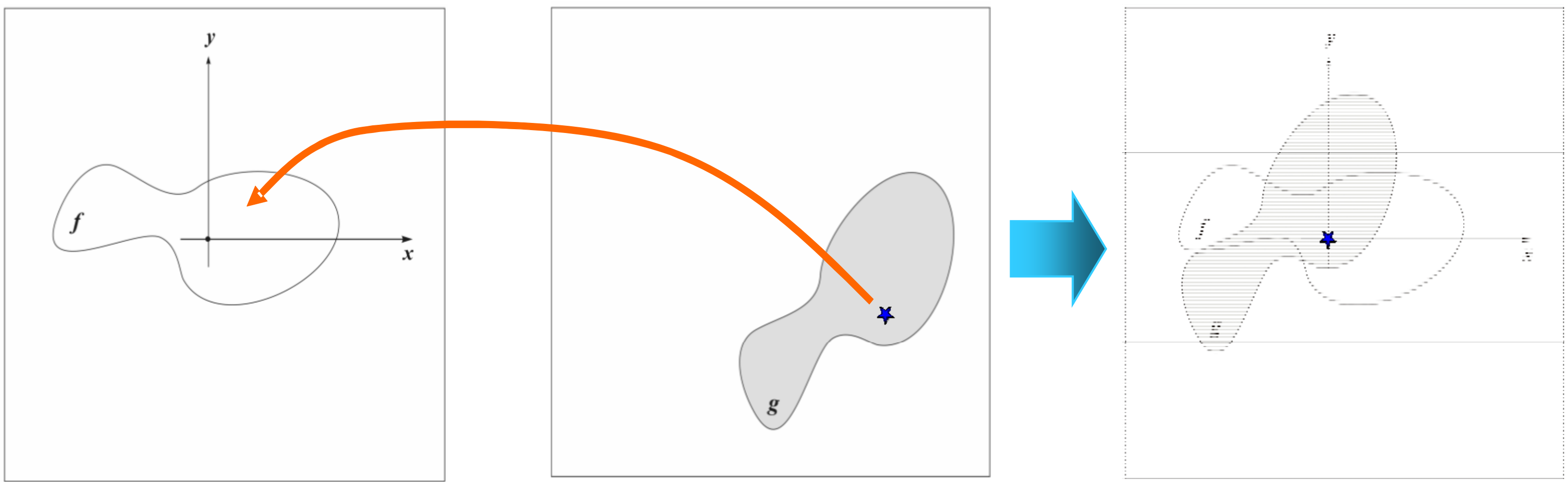
FTM: 3D FFT + 3D rot. search
FRM: 5D FFT + 1D trans. search



- Gain: 2-4 orders of magnitude for typical EM map

FRM Matching in 2D

<u>Idea:</u> Rotate both objects around their own center of mass, while translate one object along the positive ***x*** axis, until find the best matching position.

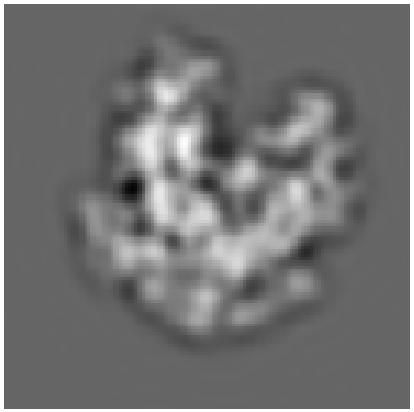


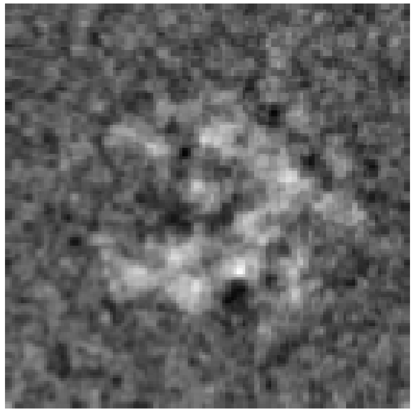
FRM2D: 2 rota.+1 trans.

- 2D FFT accelerate 2 rota. param. search
- Avoid expensive zero padding

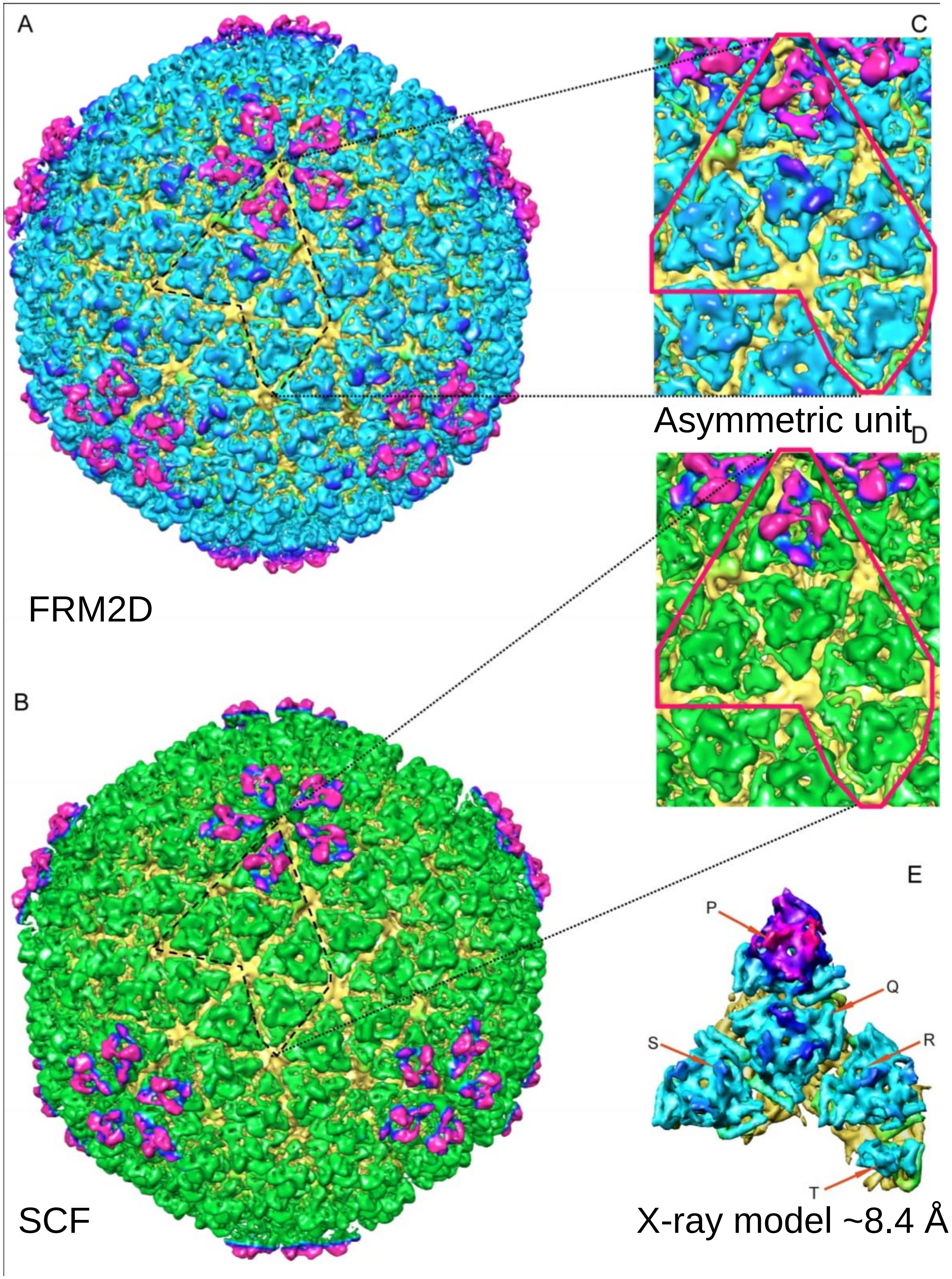
2D Image Alignment in EM

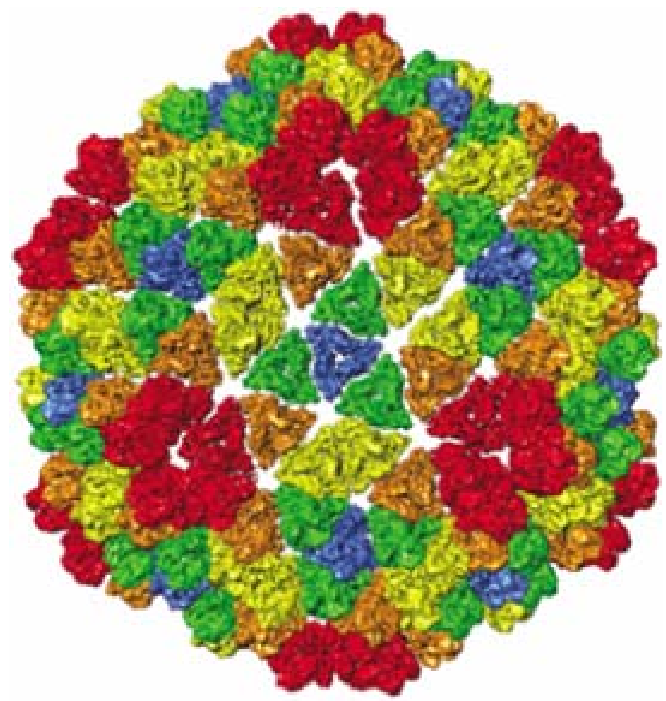
- **2D alignment**: determines the 3 relative transformation parameters of two images (1 rotat. & 2 trans.)





RDV 3D Reconstruction Validation





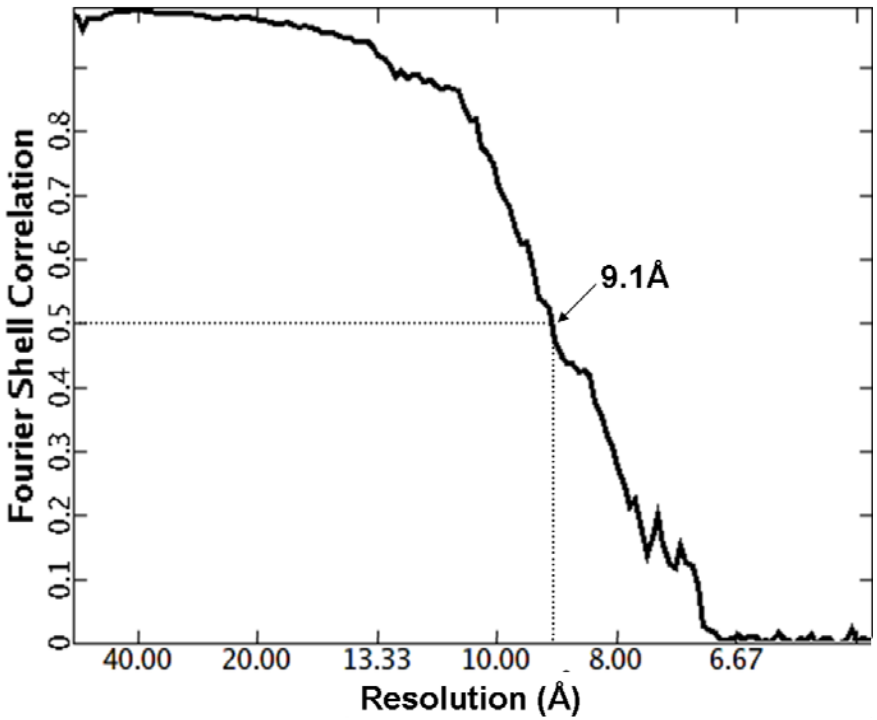
6.8 Å model (Zhou)

T=13/ icosahedral lattice

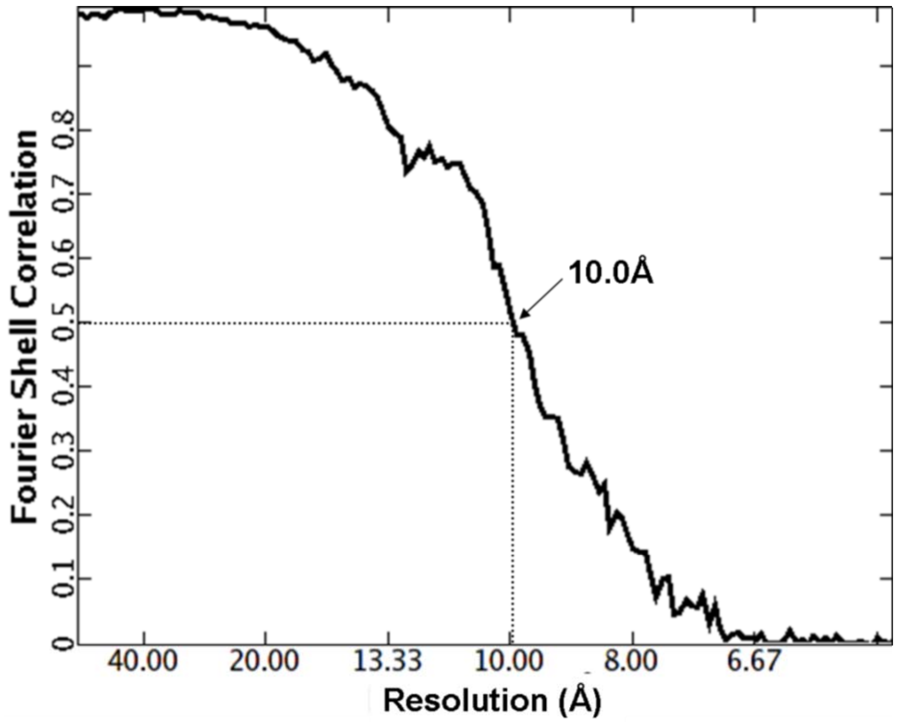
RDV 3D Reconstruction Validation

1.4º sampling

FRM2D+refine vs. 6.8Å map



SCF+refine vs. 6.8Å map



- Yao Cong now with Wah Chiu
- algorithm available in EMAN or as standalone download from *Situs Flavor* site

Cong, Jiang, Birmanns, Zhou, Chiu, Wriggers, J. Struct. Biol, 152 (2005) 104

Availability and Support

•No support, sorry.

•3D and 6D methods available for download as “Situs Flavors”.

•We decided against implementing FRM (3D or 6D) into colores (despite speed advantage) because (i) translation function from FTM can be visualized more easily and is useful for interactive peak selection with Sculptor; (ii) the off-lattice refinement step of colores is often slower than the exhaustive search, masking any gain in efficiency; (iii) potentially large memory requirements of FRM; (iv) more recent research has focused on peak selection and on multi-fragment docking which does not benefit from FRM 3D or 6D.

•2D method (particle picking) available for download as “Situs Flavors” and was implemented into EMAN.

•FRM remains a useful technique which we will keep in the arsenal for future applications.