

2D Fast Rotational Matching

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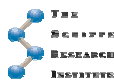


2D Image Alignment Methods

CSB Group

- **2D alignment:** 3 transformation parameters for matching two 2D images
- **Application in single particle analysis of EM data:**
 - 2D classification → 3D reconstruction
- **Efficiency:** a limiting factor in image processing
- **Commonly used 2D alignment methods:**
 - Direct alignment using 2D FFT
 - Indirect alignment using autocorrelation function (ACF)
 - Alignment using resampling to polar coordinates
- **Current state of the art:**

Resampling to polar coordinates (1D FFT on concentric rings), rated *most accurate & most efficient* method (Pawel Penczek et al., Ultramicroscopy, 2002).



FRM2D Description

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Simultaneous search of 2 angular and 1 linear parameters.

The correlation function is:

$$c(\phi, \phi'; \rho) = \int_{\mathbf{R}^2} f(\phi) \cdot g(\phi'; \rho)$$

Expand f and g in Fourier series:

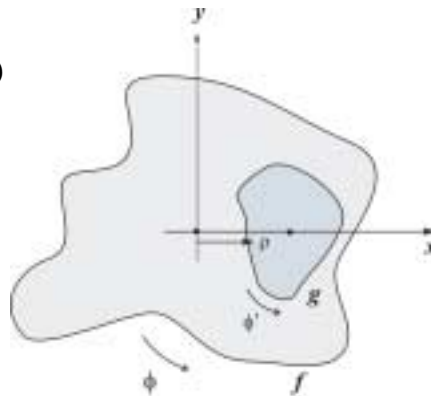
$$f(r, \beta) = \sum_m \hat{f}_m(r) e^{im\beta}$$

$$g(r, \beta) = \sum_n \hat{g}_n(r) e^{in\beta}$$

Therefore:

$$f(\phi)(r, \beta) = \sum_m \hat{f}_m(r) e^{im(\beta-\phi)}$$

$$g(\phi'; \rho)(r, \beta) = \sum_n \hat{g}_n(r') e^{in(\beta'-\phi')}$$



The correlation function becomes:

$$c(\phi, \phi'; \rho) = \sum_{m,n} e^{i(m\phi+n\phi')} I_{mn}(\rho)$$

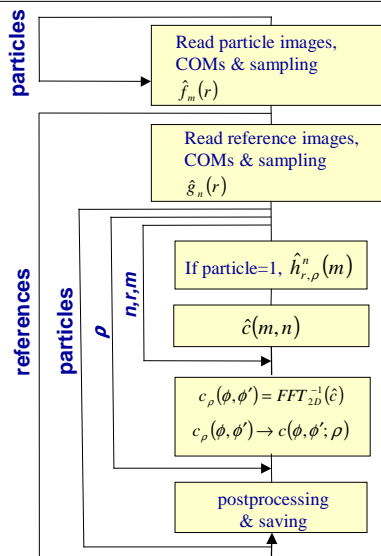
Where:

$$I_{mn}(\rho) = \int_0^\infty \left[\int_0^{2\pi} e^{-im\beta} \underbrace{\left(e^{-in\beta'} \hat{g}_n(r') \right)}_{h_{r,\rho}^n(\beta)} d\beta \right] \cdot \overline{\hat{f}_m(r)} \cdot r dr$$

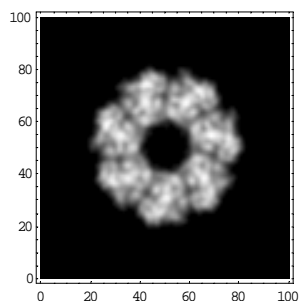
The 2D Fourier transform of correlation function:

$$\hat{c}(m, n; \rho) = I_{mn}(\rho) = 2\pi \int_0^\infty (\hat{h}_{r,\rho}^n)_m \overline{\hat{f}_m(r)} r dr$$

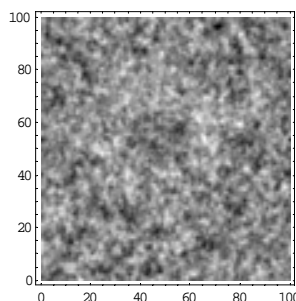
$$\hat{c}(m, n; \rho) = 2\pi \int_0^\infty (\hat{h}_{r,\rho}^n)_m \overline{\hat{f}_m(r)} r dr$$



Accuracy test (GroEL)



(a) Reference image (after applying a Gaussian low-pass filter with half-width $1/10 \text{ \AA}^{-1}$)



(b) Particle image (a) corrupted by Gaussian noise, SNR=0.95)

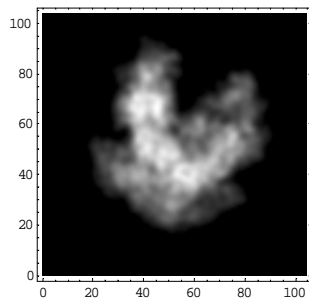
Accuracy (angular sampling: 1.4°):

- FRM2D: 0.72 pixels
- Resampling to polar coordinates^a: 1.55 pixels

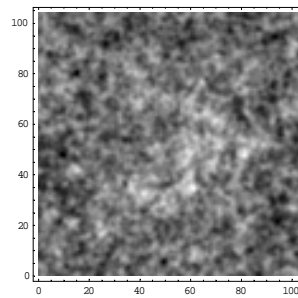
$$e_{\max} = d \left| \sin \frac{\Delta\theta}{2} \right| + \sqrt{\Delta x^2 + \Delta y^2}$$

^aL. Joyeux, P. A. Penczek, Ultramicroscopy 92(2002) 33

Accuracy test (RNA polymerase)



(a) Reference image (after applying a Gaussian low-pass filter with half-width $1/10 \text{ \AA}^{-1}$)

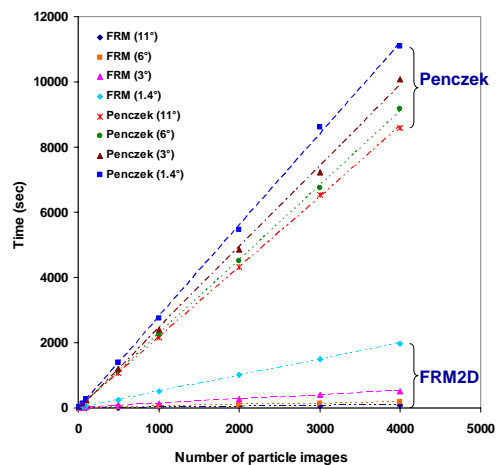


(b) Particle image (a) corrupted by Gaussian noise, SNR=1.07)

Accuracy (angular sampling: 1.4°):

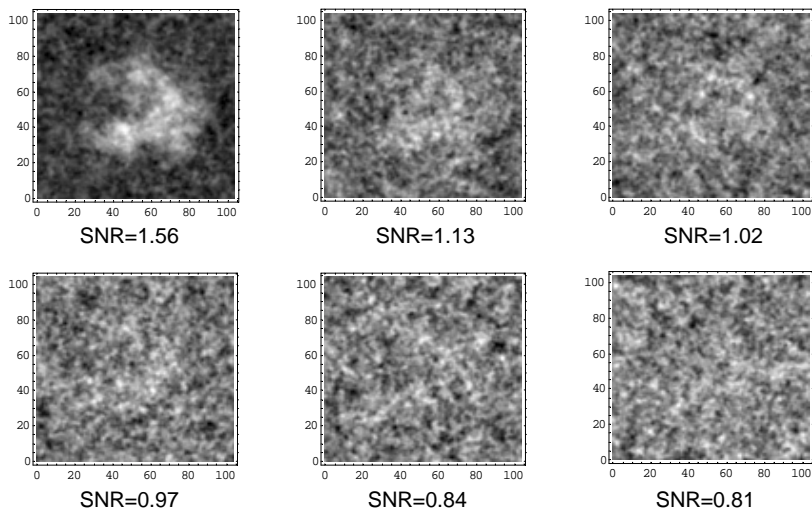
- FRM2D: 1.53 pixels
- Resampling to polar coordinates^a: 1.41 pixels

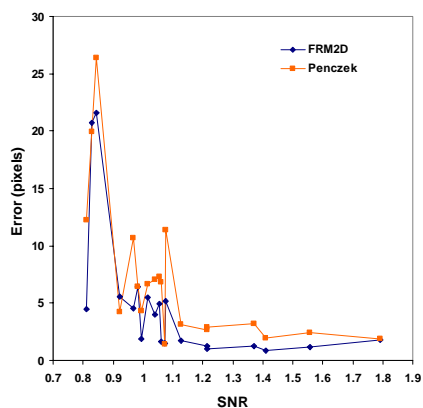
Timing comparison (RNA polymerase)



Comparison with Penczek's resampling to polar coordinates method

Testing noise images (RNA polymerase)





Comparison with Penczek's resampling to polar coordinates method

- Use 2D FFT to accelerate the search for 2D rotational space
- Several times faster than current state of the art
- Comparable accuracy
- Situs is 3D package, so 2D FRM will be disseminated in collaboration with SPIDER (Penczek) and EMAN (Ludtke) developers in Houston