

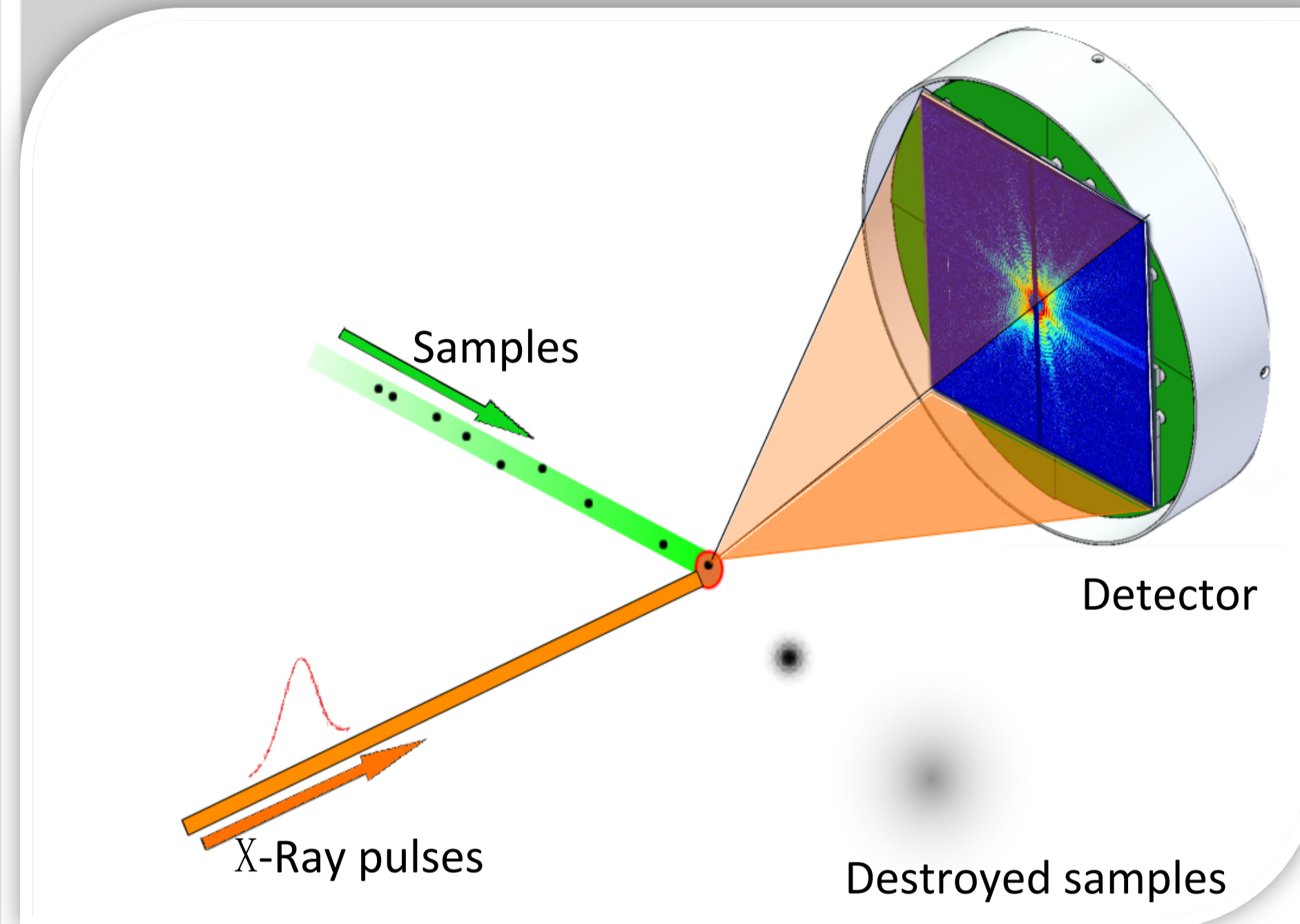


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1. Most atomic structures of particles (such as proteins) were solved by crystallography. What if particles cannot be crystallized?

Single particle Imaging in femtoseconds: Small objects at nanometer scale form diffraction patterns when hit by very intense and short X-rays. The following figure shows a typical single particle imaging setup.



3. Large datasets and Large computations.

20 min single particle experiments will generate > 800G raw data, given successful hit ratio 0.2, it will generate more than 10 000 diffraction patterns. Use CUDA/MPI to parallelize.

# of GTX680 GPUs	$M_{\text{pix}} = 64 \times 64$		$M_{\text{pix}} = 128 \times 128$	
	Time	GFLOPS/GPU	Time	GFLOPS/GPU
16	164.6	36.3	552.2	43.3
32	83.5	35.8	281.2	42.5
64	42.3	35.3	141.6	42.3
96	28.3	35.2	95.4	41.8
100	27.2	35.2	91.6	41.8

5. Future work.

Automatic online 3D reconstruction in atomic resolution and with a quantitative evaluation of confidence measurement.

→ Pattern selection and 3D reconstructions .

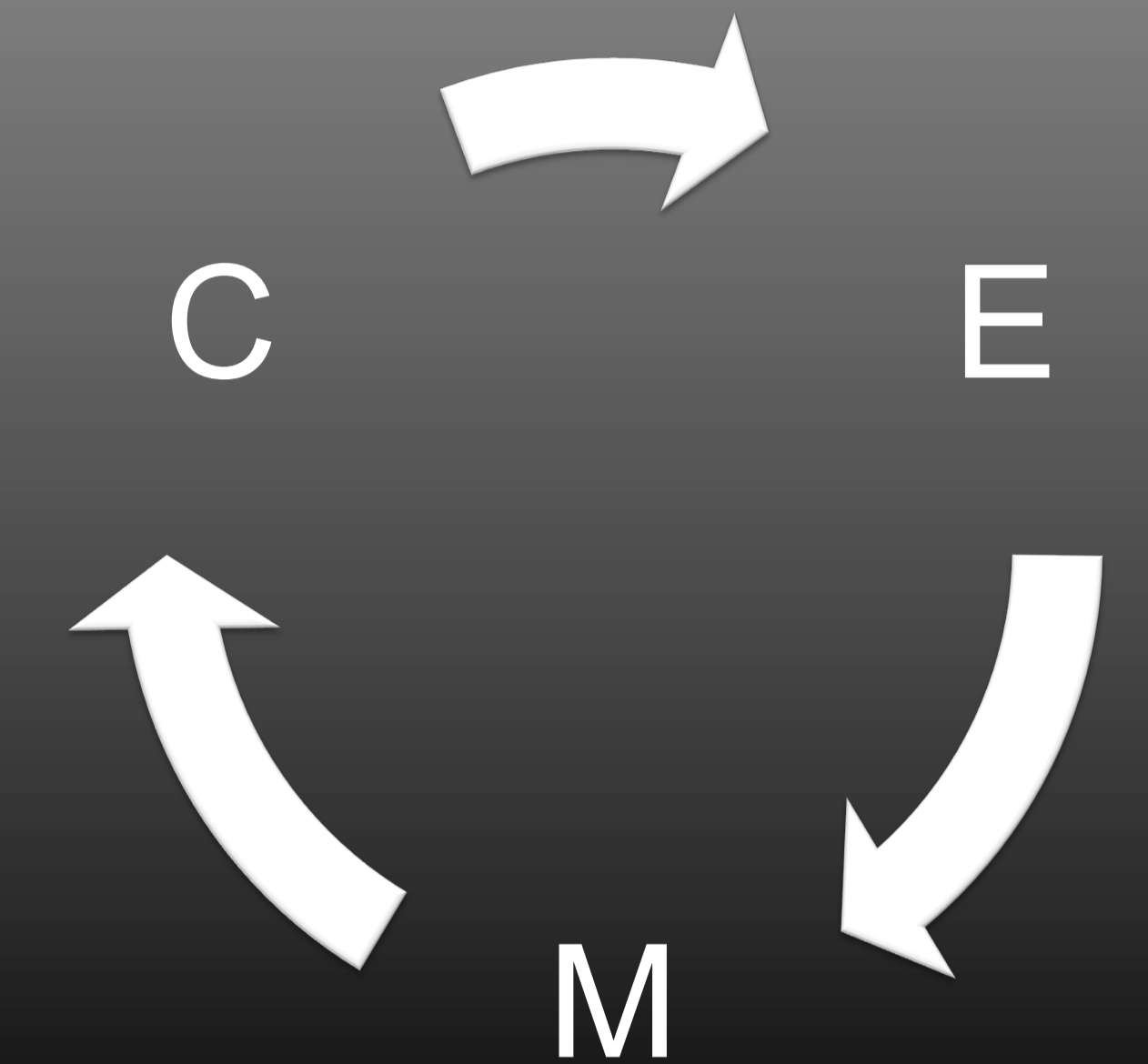
2. Particle Reconstruction: from 2D to 3D

→ Algorithm EMC

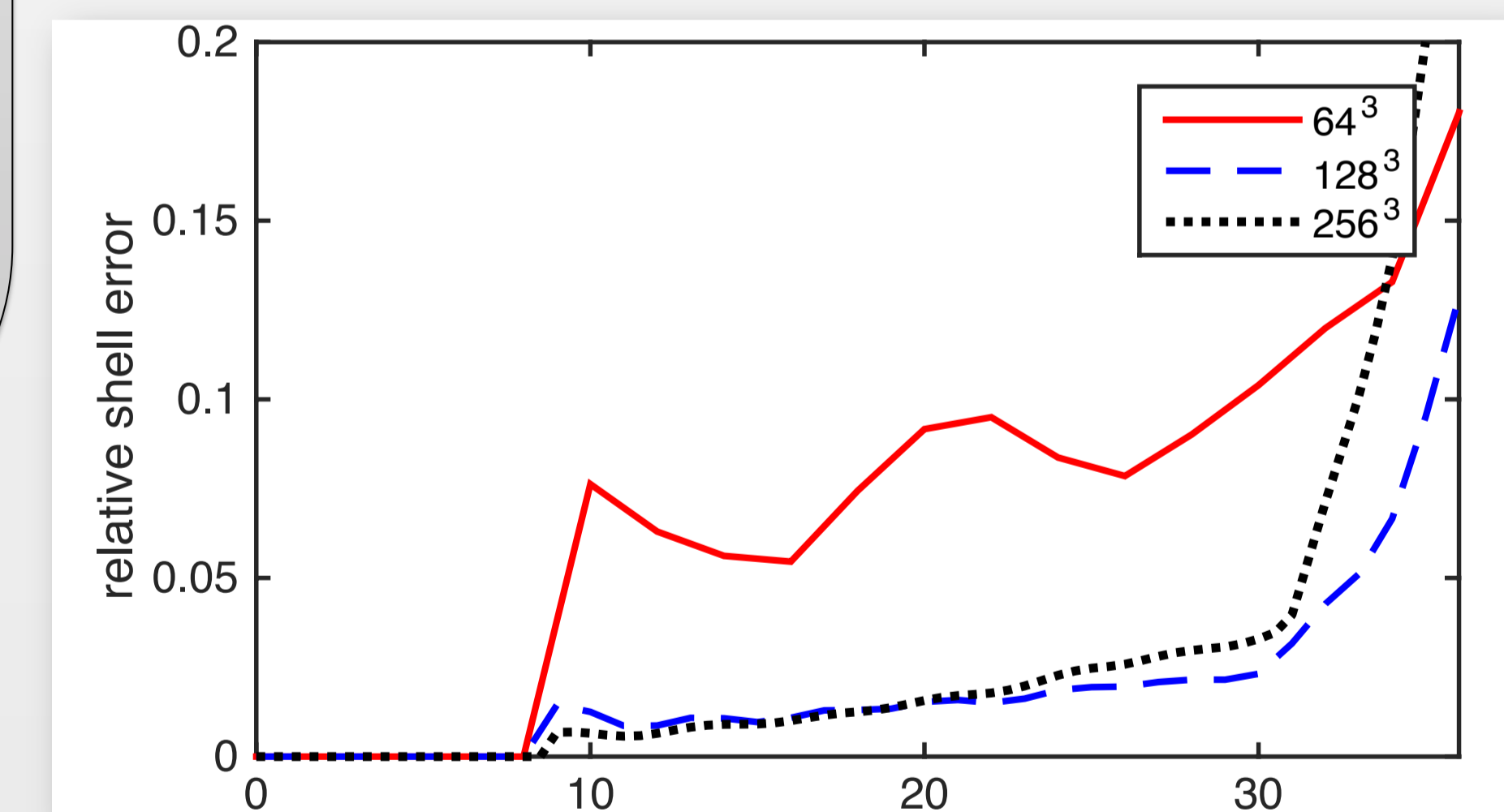
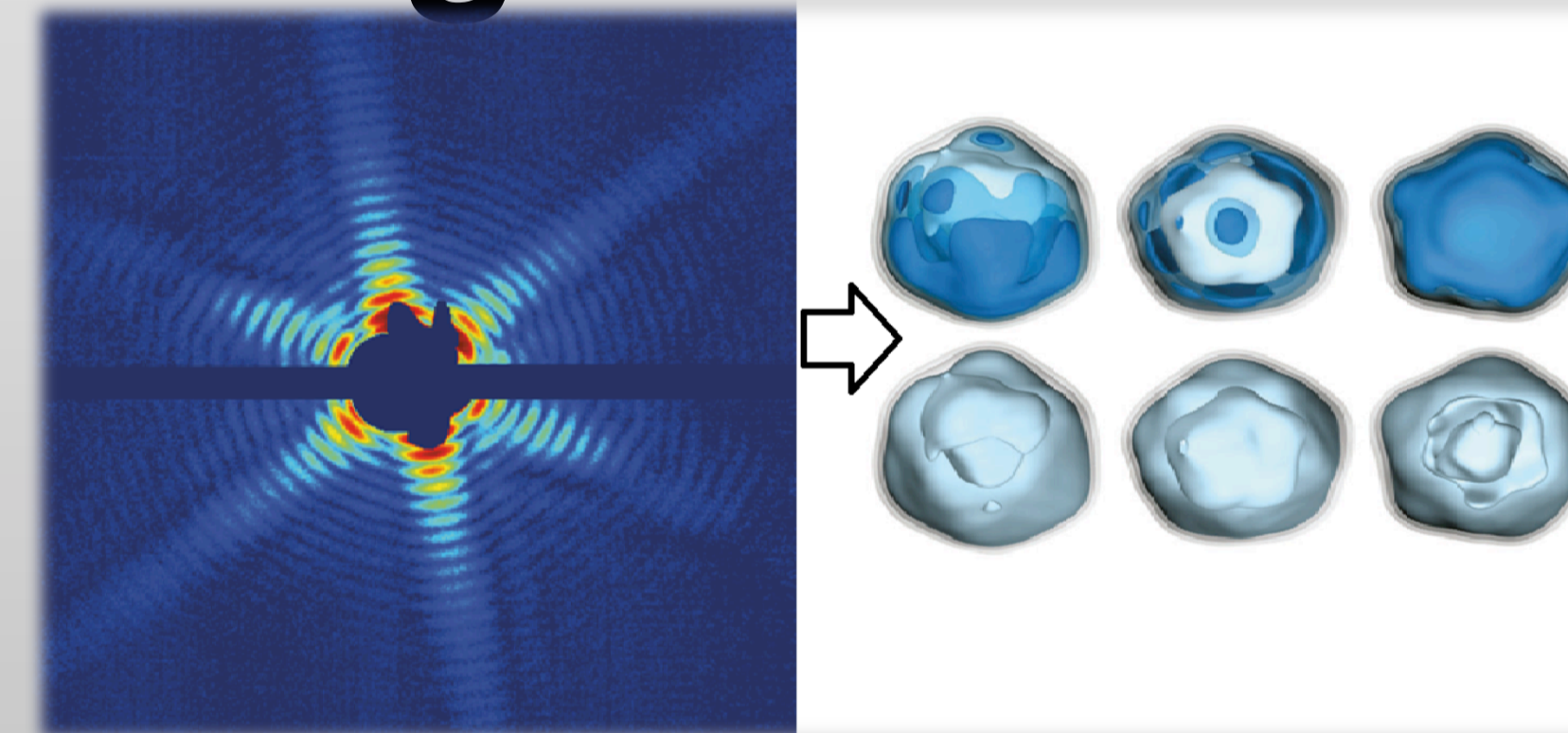
Expectation: Suppose we know a 3D model, we can compute probabilities that a diffraction patterns belongs to a rotation;

Maximization: Suppose we know rotations , we can update the intensity model by diffraction patterns.

This is an iterative algorithm, shown as following:



3D Reconstructions of Biomolecules using GPU cluster



4. Resolution were lower than designed → Algorithm is not quantitatively analyzed yet.

We've Identified more than 7 sources of errors / uncertainties. Among them, smearing error R_S , rotation error R_T , noise error R_N , fluence error R_F are important and can be evaluated using synthetic datasets. Figure above shows preliminary results of total $R_S R_T R_N R_F$ error using 1000 synthetic patterns in different sizes.