

UPPSALA UNIVERSITET

Jing Liu jing.liu@it.uu.se jing.liu@icm.uu.se

Scientific Computing, Dept. of IT,

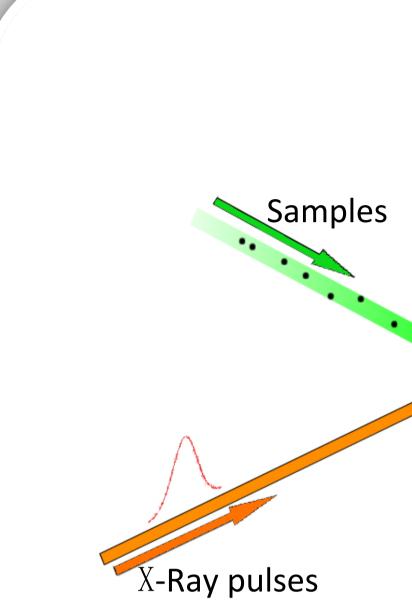
Lab of Molecular Biophysics, **Dept. of Cell and Molecular** Biology,

Uppsala University,

Uppsala, Sweden

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.



Detector **3D** Reconstructions Destroyed samples of **Biomolecules 3.Large datasets and Large** using GPU cluster 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. $_{\rm pix} = 64 \times 64$ $M_{\mathrm{pix}} = 128 \times 128$ GFLOPS/GPU GFLOPS/GPU Time 36.3552.243.3

42.5

42.3

41.8

41.8

# of GTX680 GPUs	$M_{ m p}$
	Time
16	164.6
32	83.5
64	42.3
96	28.3
100	27.2

5. Future work.

Automatic online 3D reconstruction in atomic resolution and with a quantitative evaluation of confidence mearsurement. Pattern selection and 3D reconstructions.

281.2

141.6

95.4

91.6

35.8

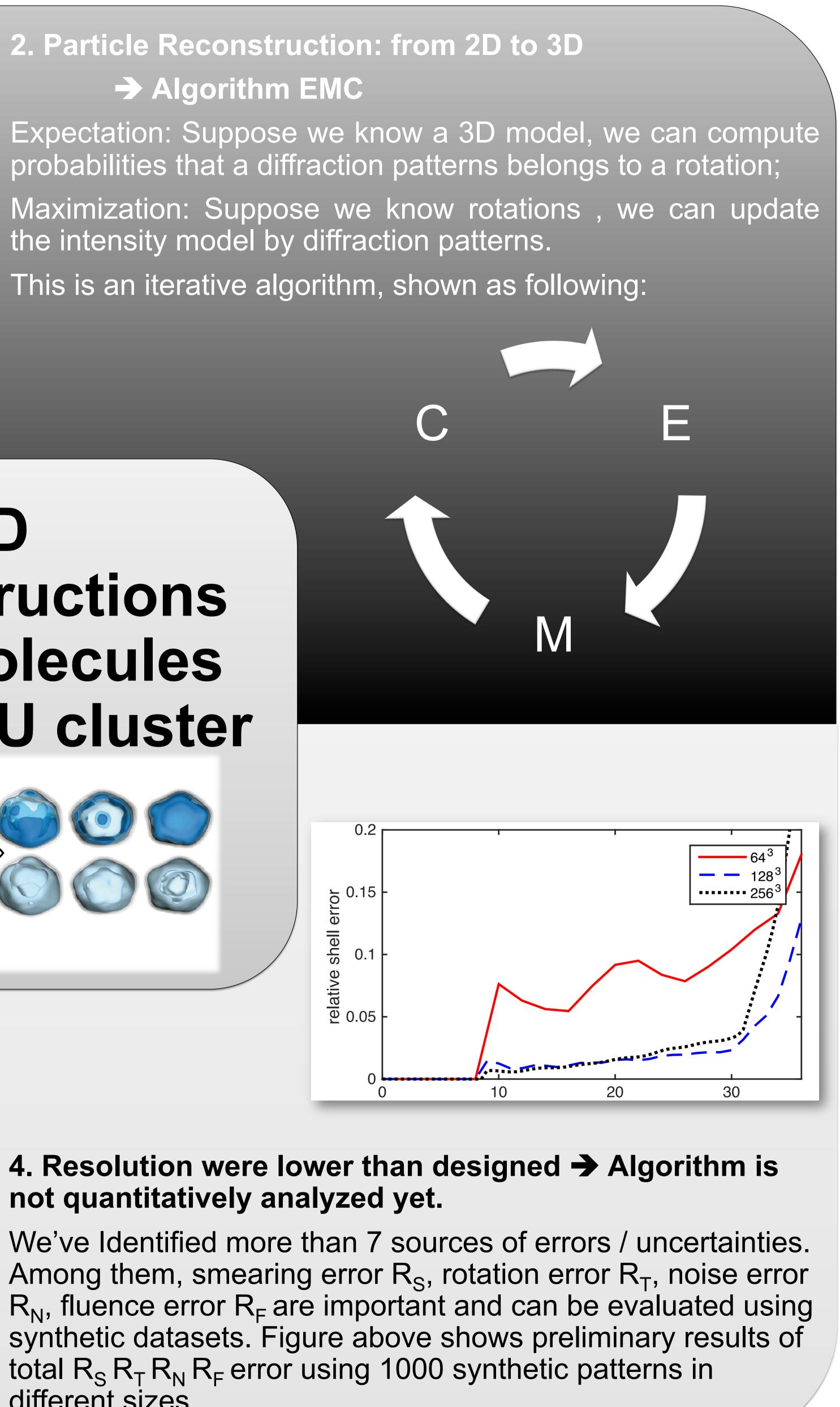
35.3

35.2

35.2

Algorithm EMC

- the intensity model by diffraction patterns.



different sizes.