

HPC for cryo-EM structure determination

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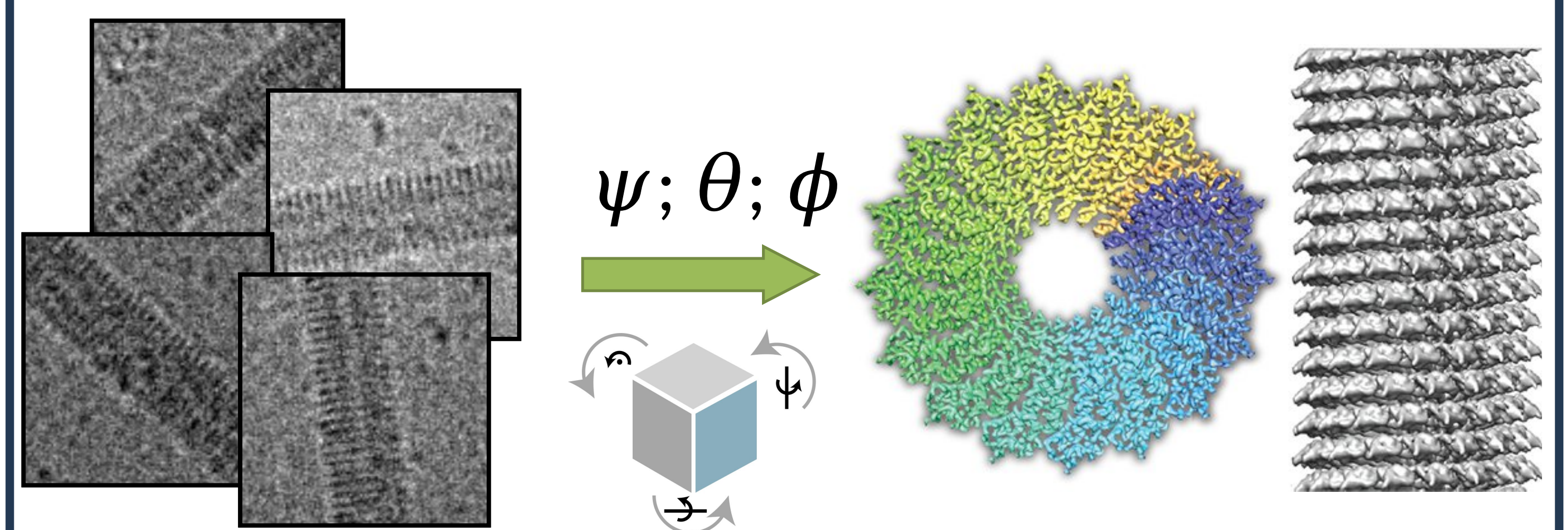
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Abstract

- Cryo-electron microscopy (cryo-EM) is a highly productive method in **structural biology**
- ER-C-3 operates several state-of-the-art cryo microscopes (Talos120, Talos Arctica, Titan Krios)
- Structure elucidation **by single particle analysis** requires large amounts of data for image processing on HPC
- Our research is focused on CryoEM **method development, autophagy and membrane remodeling**

The orientation problem

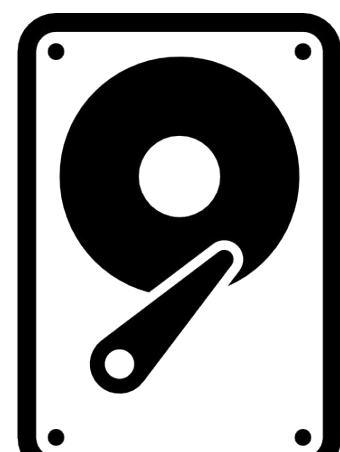
Find Euler angles that connect 2D projections with 3D volumes



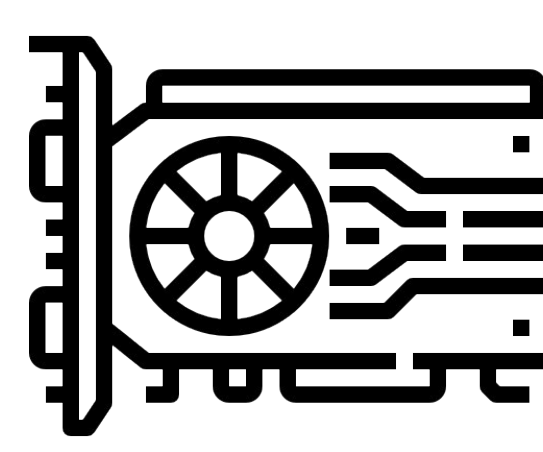
One dataset



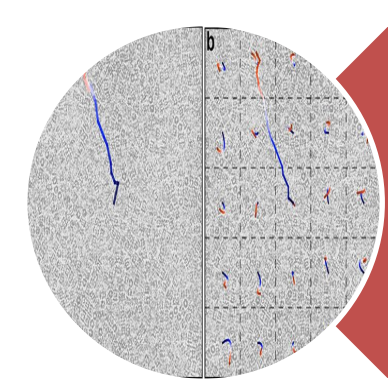
5000
images
(daily)



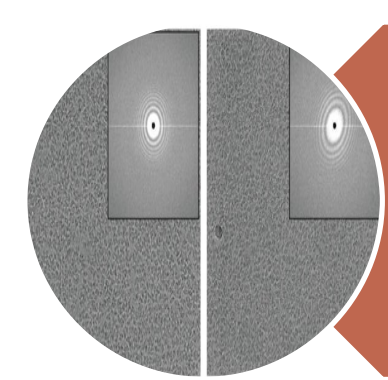
2.5 TB
raw data



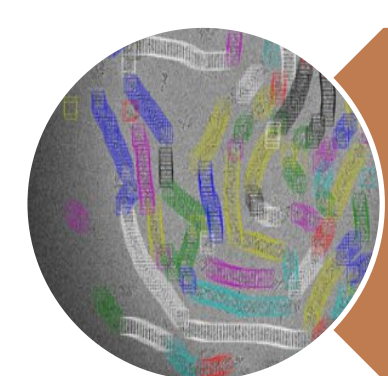
1 day
4x A100
node



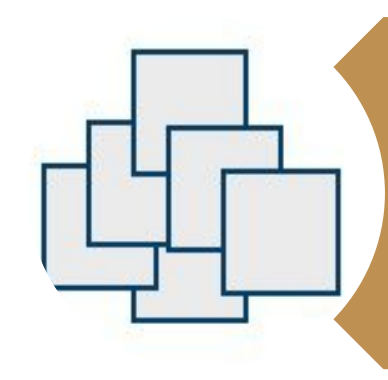
Motion correction (MotionCor2)



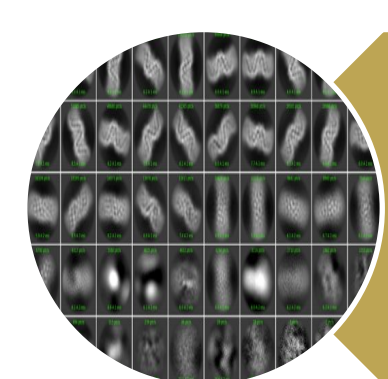
Correction of optical aberrations
/ CTF (CTFFIND4)



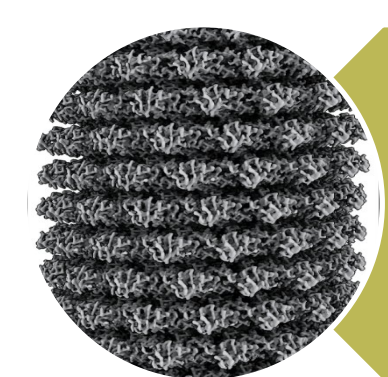
Find particle positions (CNNs)



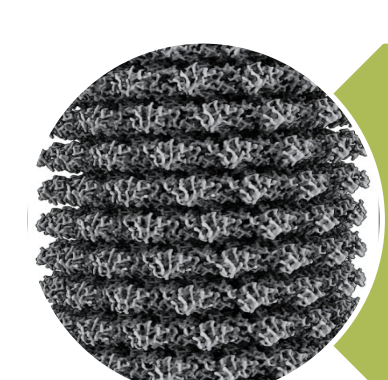
Particle extraction



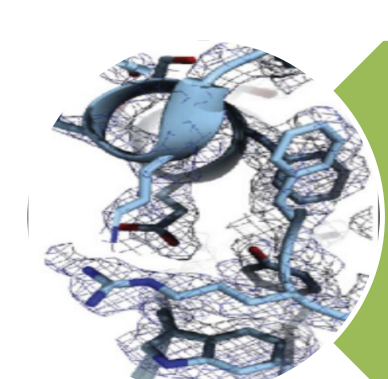
2D classification (maximum
likelihood, Relion5)



Ab initio 3D model (Relion5)



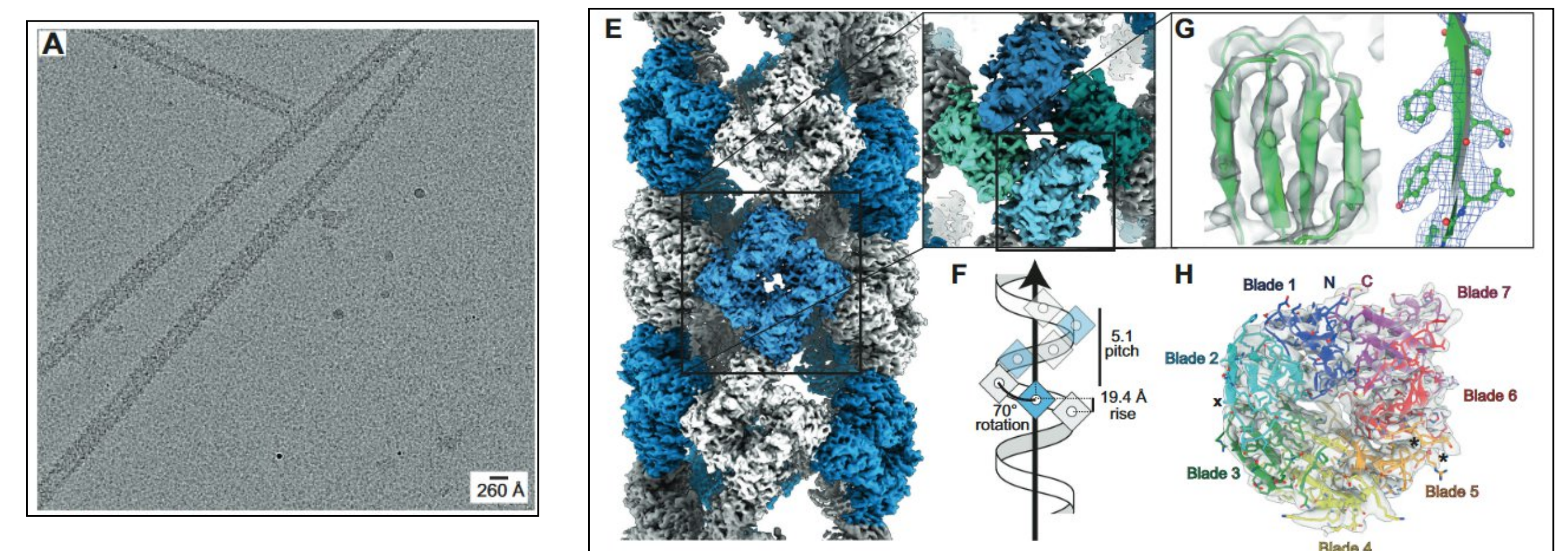
High resolution 3D refinement
(Relion5)



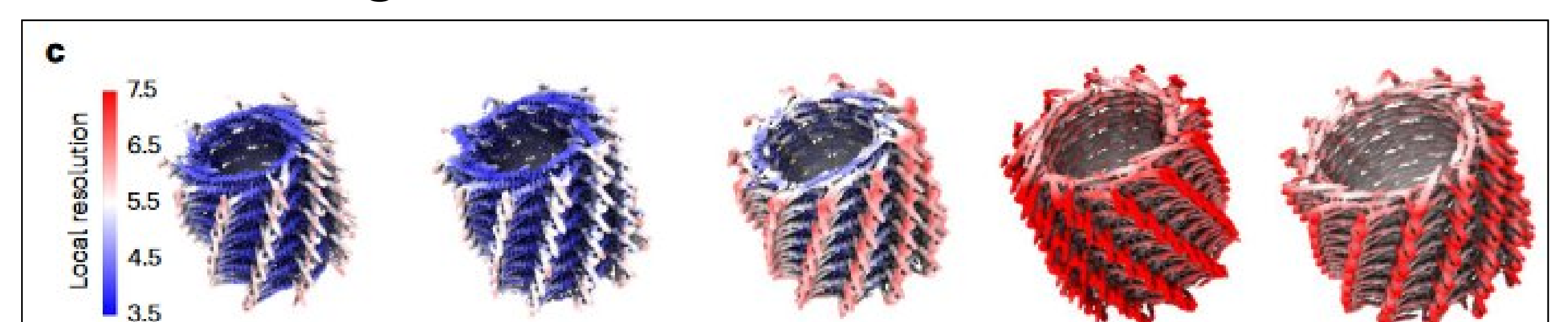
Build atomic model into density
map

Research

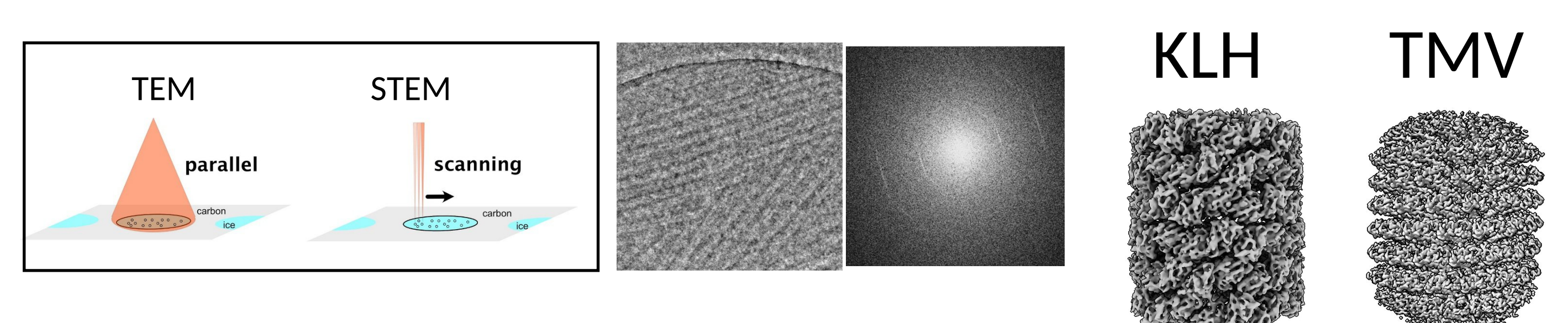
Atg18 (Mann...Sachse *Nat.Comm.* 2023)



ESCRT (Junglas...Mann...Sachse *Cell* 2022)



iDPC-STEM (Lazic...Mann...Sachse *Nat.Meth.* 2022)



More info: www.er-c.org

