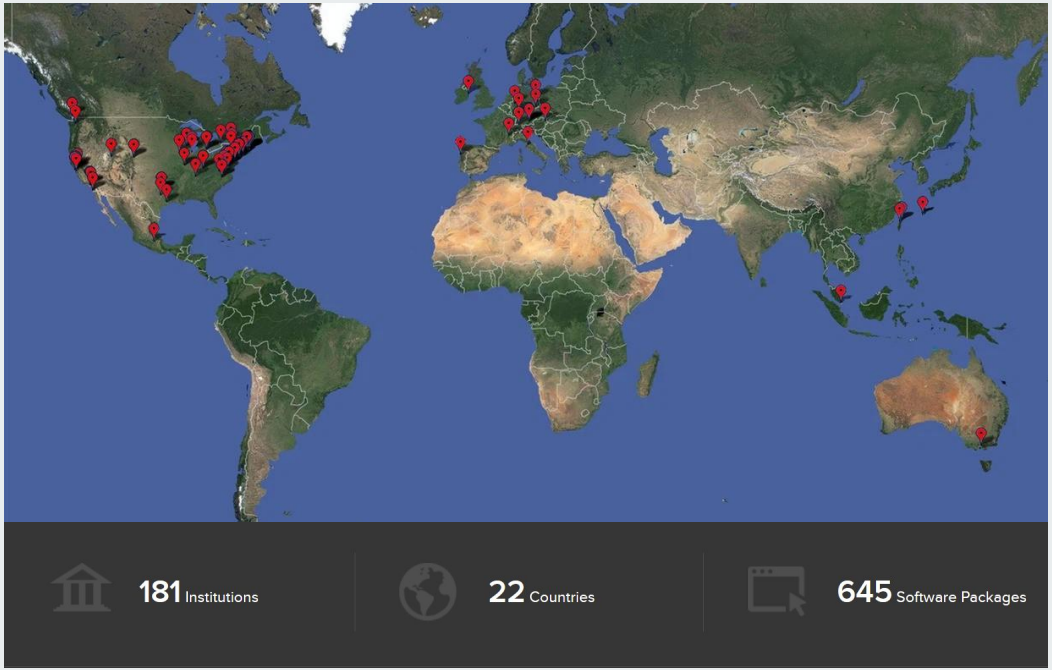
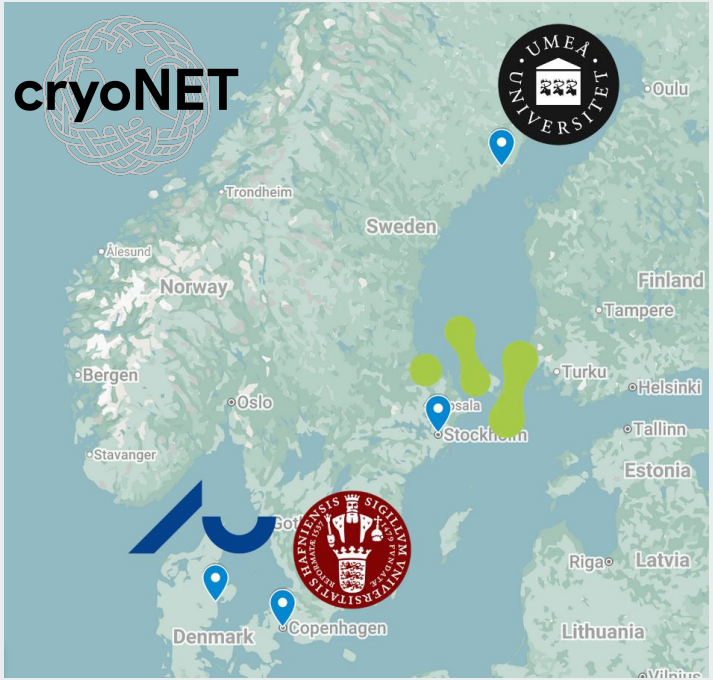
Cryo-EM Data at Scale:

How collaborative models arose around the world



Cutting Edge: Collaboration gets the most out of software, *eLife* **2**:e01456. **(2013)**
sbgrid.org



novo nordisk foundation

cryonet.nu

Knut and Alice Wallenberg Foundation

Sharing is caring

"The Mark Wainwright Analytical Centre (MWAC) is the largest shared facility in Australia." [Emph. mine / PVC RI]

MICROSCOPY AUSTRALIA

RESEARCH TECHNOLOGY SERVICES

Structural Biology Facility

COMPUTE DATA COMMUNITY

400+ Major scientific instruments

130+ Academic & technical staff

3,500+ Users per year

Australian Government
Australian Research Council

UNSW SYDNEY

NCRIS National Research Infrastructure for Australia
An Australian Government Initiative

NSW GOVERNMENT Cancer Institute NSW

NSW GOVERNMENT

Systems administration & design process

Trust & Respect

Gained

- Demonstrations
- Co-working
- Translation
- Mental models
- Progress updates
- Advocacy
- Expertise
- Collaboration with others
- Valuing other technical fields
- Learning their problems
- Turning up
- Planning

Eroded

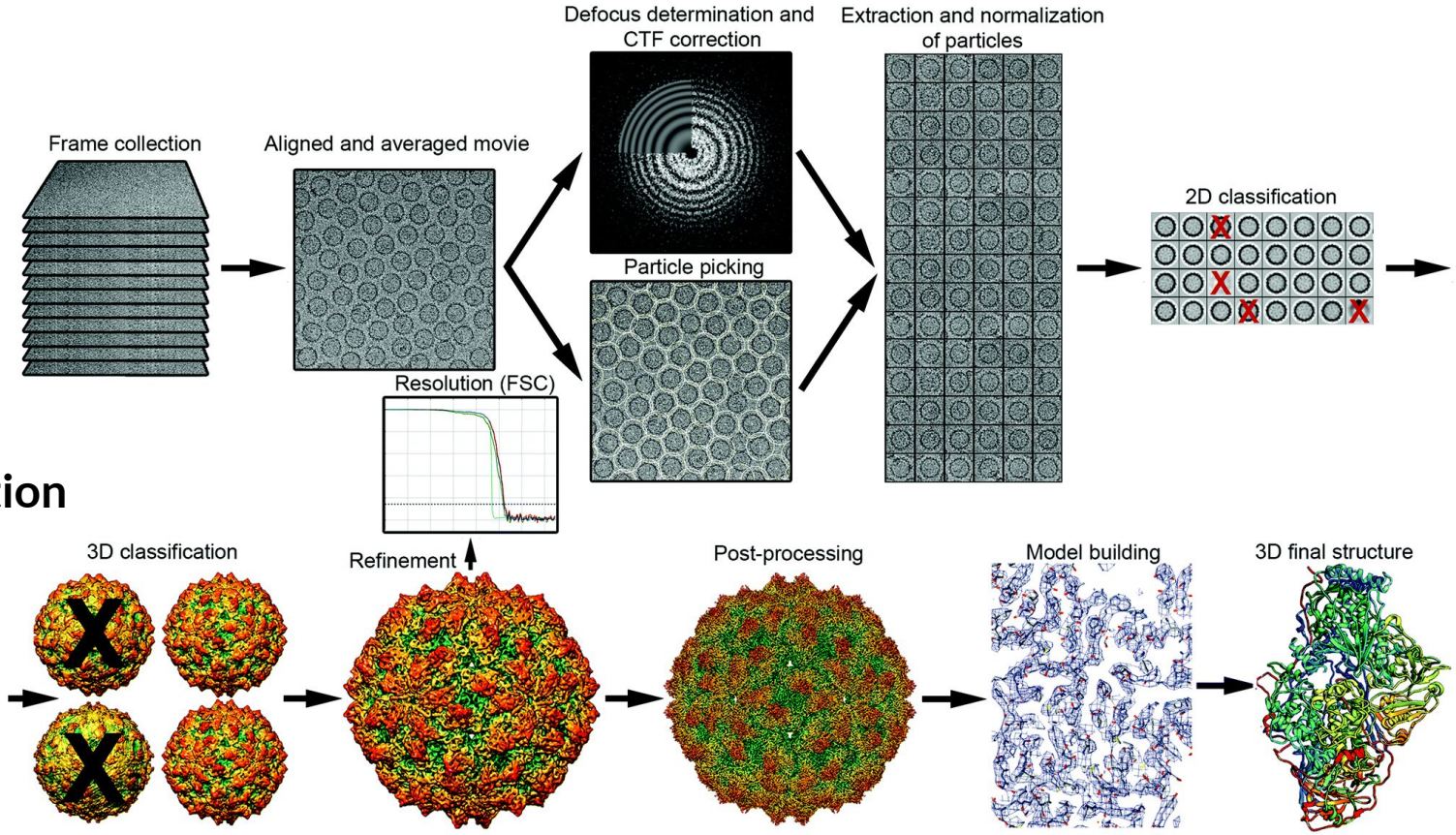
- Resource hoarding
- Outages
- Dismissiveness
- Jargon
- Solving the wrong problems
- Frustrations
- Puritanism
- Ego

Structural nanotechnology: three-dimensional cryo-EM and its use in the development of nanoplatforms for in vitro catalysis
Nanoscale, (**2019**), **11**, 4130-4146

Raw data explosion

Compute needs

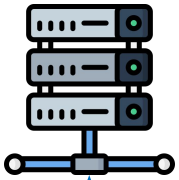
- 2-10 TB/day
- 10+ GbE
- Months retention
- Worker SSD
- Low/no queue



TFS Arctica **Cryo-EM**

5 TB
0.25–5 M particles

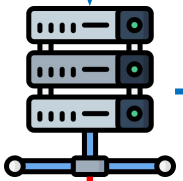
On-the-fly processing

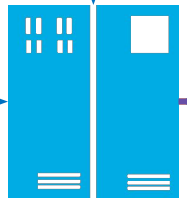


Electron Microscopy Unit Staff
QA, movie averaging, tomo., model building, *etc.*

Job files cached on SSD

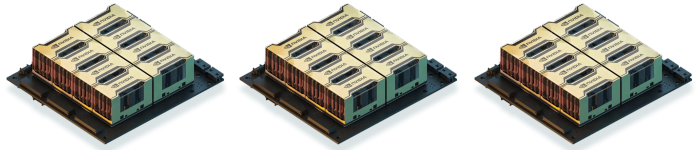
Direct detector
pass-through
storage



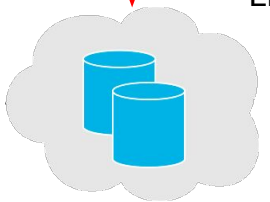


IBM
Elastic Storage System
10–20 TB
Total project files

Structural Biology Facility Users
Single particle reconstruction, AlphaFold, *etc.*



DDN (old)



DDN (newer)

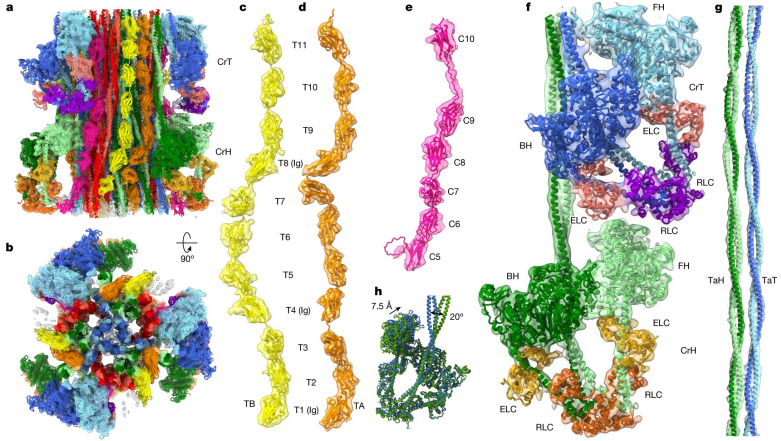
5–20 GB
Final map

cryosparc.analytical.unsw.edu.au

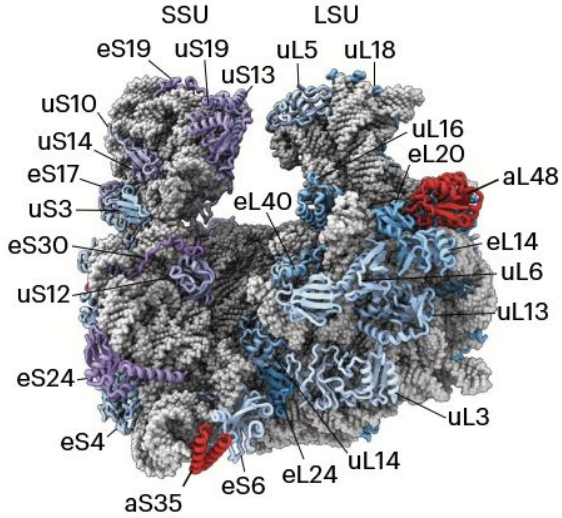
EMU ↔ **SBF** pipeline in development - **Orig. Credit:** A/Dir. Dr Daniel Luque

1. Cryo-EM structure of the human cardiac myosin filament, *Nature*, **623**, 853–862 (**2023**)
2. Structure of an archaeal ribosome reveals a divergent active site and hibernation factor, *Nature Micro.*, (**2025**)
3. In situ structure of a bacterial flagellar motor…, *Nature Micro.*, (**2025**)
4. Spliceosome activated for step 2 of splicing, *Nature*, **542**, 318–323 (**2017**)

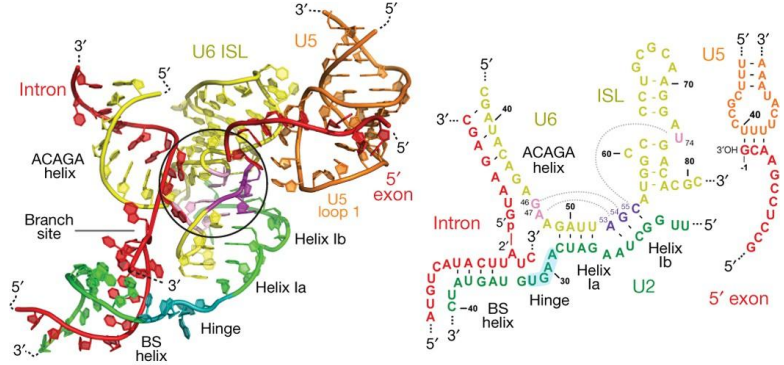
CryoEM is scientifically worth the pain



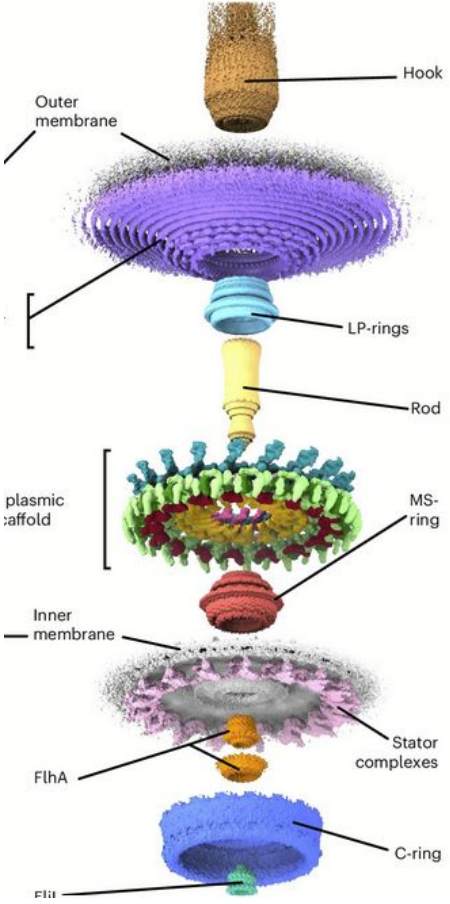
1. The solved structure of titin, the longest human protein



2. The archeal ribosome with unique archeal proteins coloured red



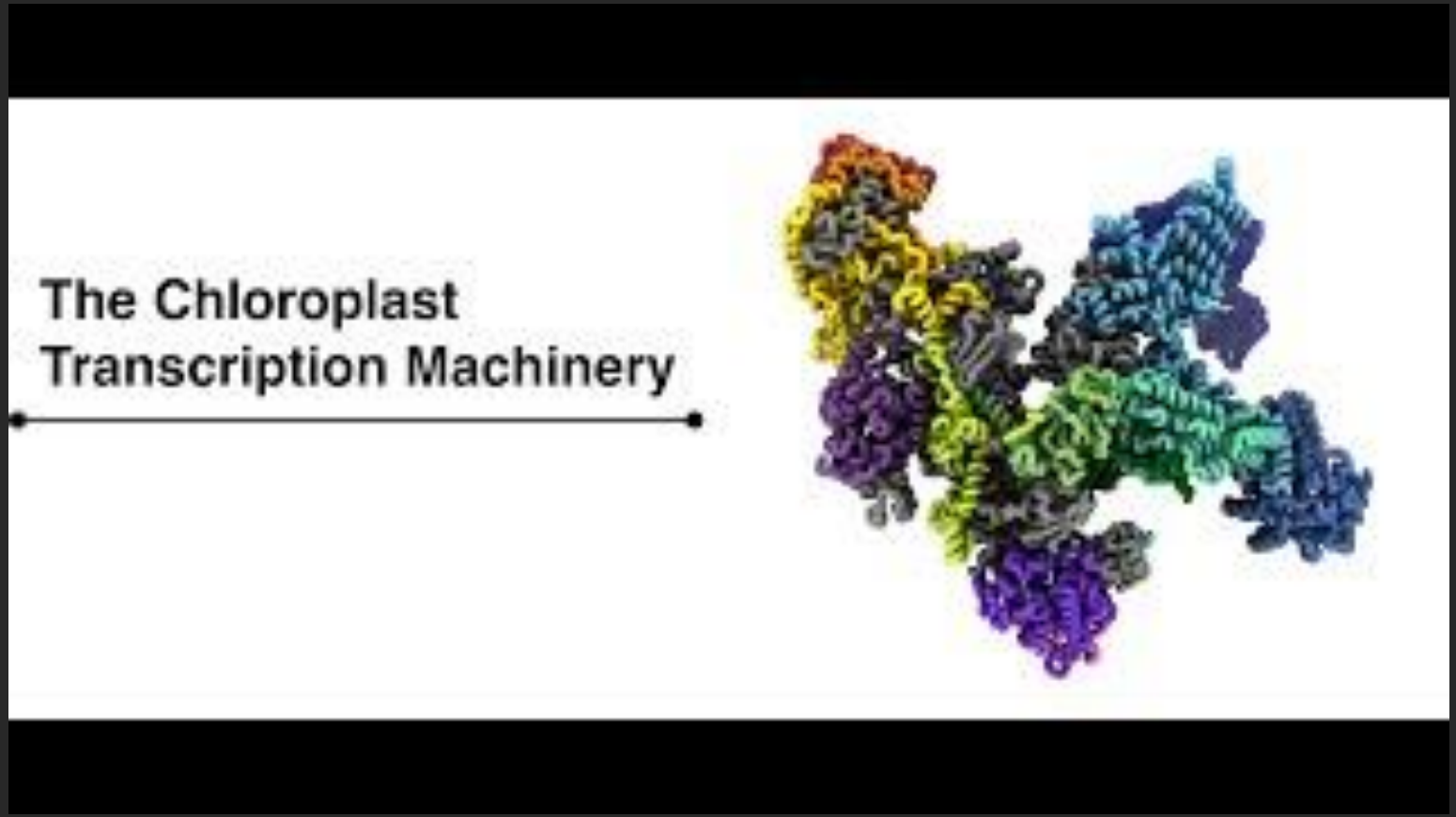
4. The intricate RNA network in the human spliceosome which ‘cuts’ mRNA into different forms of a protein



3. The entire bacterial flagella motor at fractions of a nm resolution

Structure of the plant plastid-encoded RNA polymerase, *Cell*, Volume 187, Issue 5, p1145-1159.e21, February 29, **2024**
"The Chloroplast Transcription Machinery" [video], Webster Lab, John Innes Centre for plant science

I mean really groundbreaking



Cryo TEM | Cryo Transmission Electron Microscopes | Thermo Fisher Scientific - AU **- Accessed:** 20/07/2025

Electron microscopes are expensive

Tundra (~$1M)

Glacios 2 (~$3M)

Krios 5 (~$6M)

They're organised I tell you!

SBGrid (2000)

electron Bio-Imaging Centre Diamond light source (2018)

National Electron Cryo-Microscopy Facility (2017)

LNNano (2018)

PReSTO (2013)

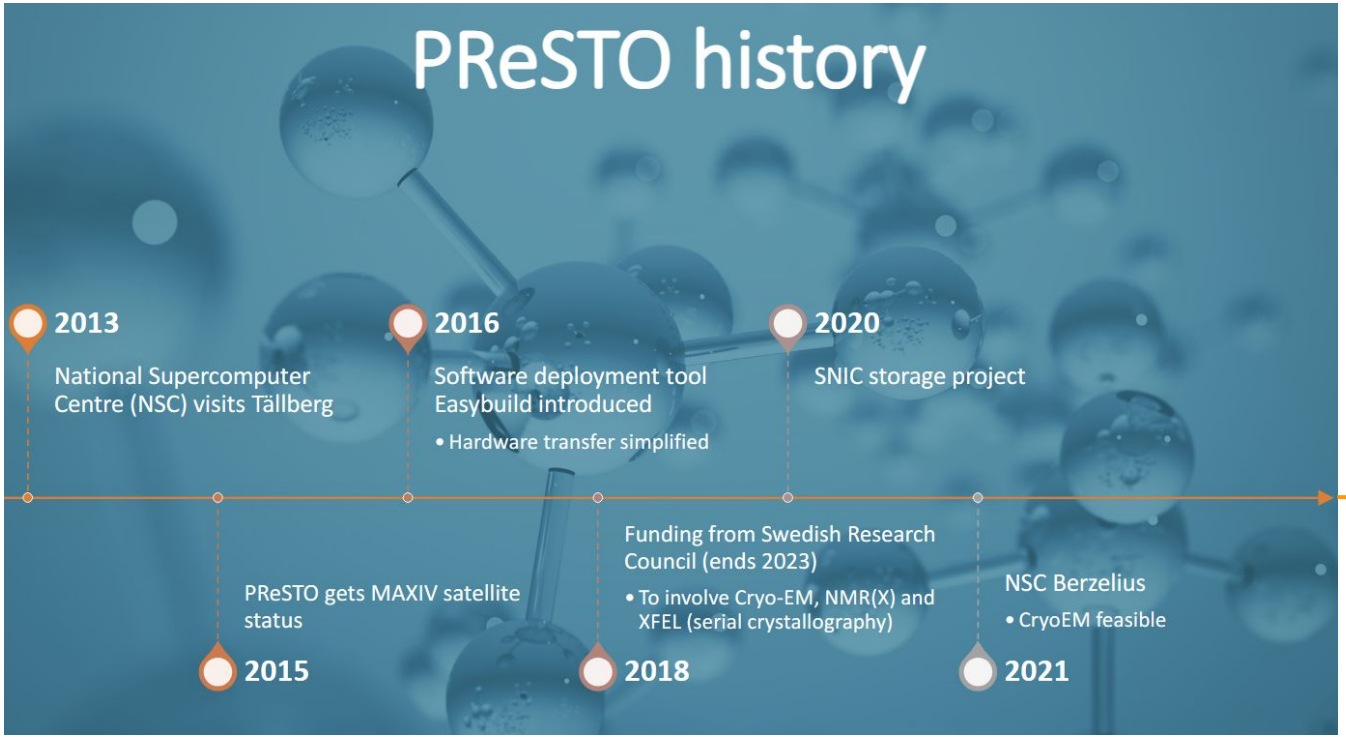
cryoNET (2018)

iNEXT-Discovery (2020)

BINDS CryoEM network (2018)

Beijing Frontier Research Centre for Biological Structure (2007)

Scientific fields adopt new techniques

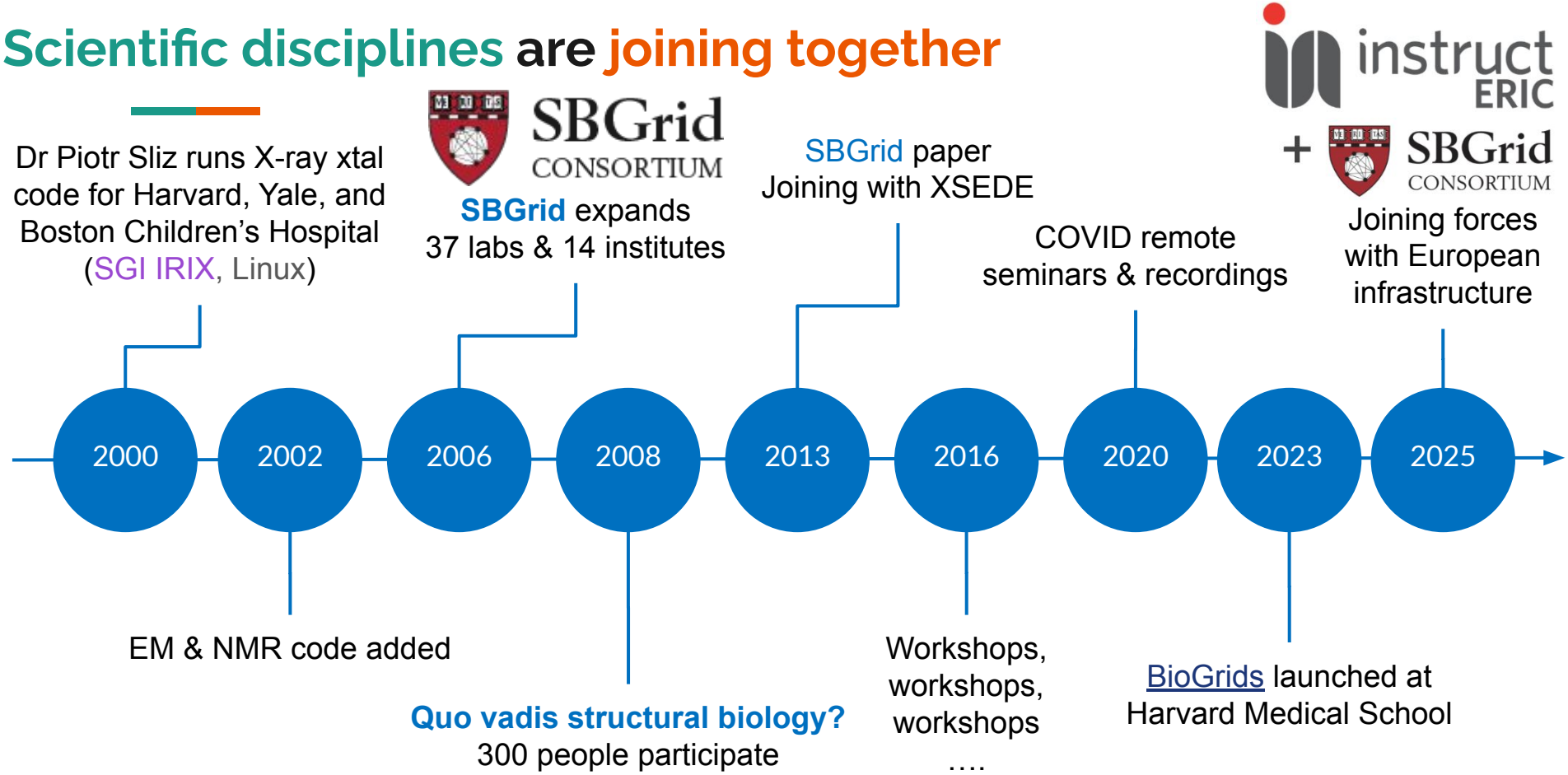


2022
PReSTO launches
3 training courses
in Struct. Bio.

2023
Lund Uni. adds
8,000 AMD cores
w/ 256 GB RAM,
12xA100+ 12xA40

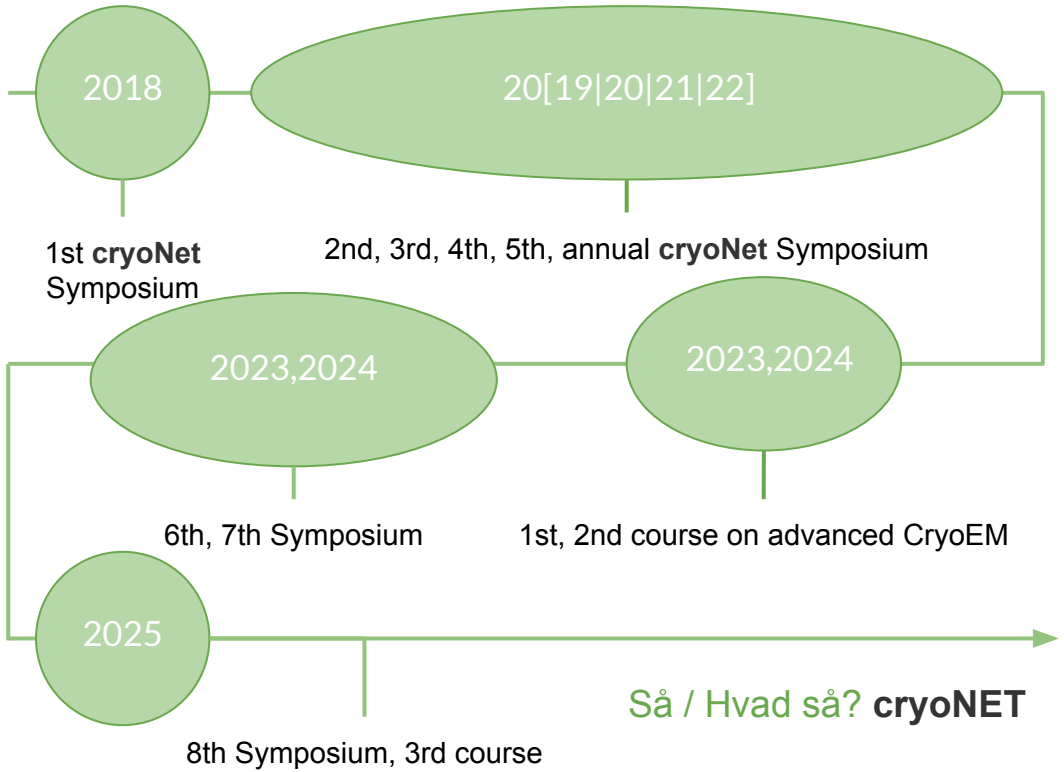
2024
Workshop at
Berzelius
SciLifeLab
supercomputer

Scientific disciplines are joining together



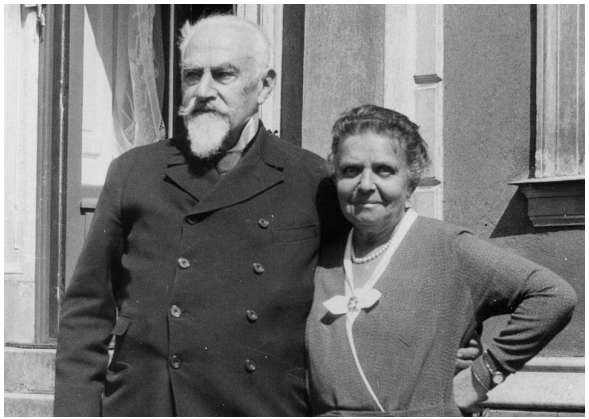
cryoNET, **Accessed -** 20/07/**2025**
1. A Nordic pyramid, *The Economist*, 10th March **2016**

Even countries are joining together



cryoNET

SciLifeLab



Knut & Alice Wallberg (**1917**) of Wallberg business family
Ericsson, Electrolux, AstraZeneca, SAS Airlines… (*i.e.* loaded)
in 1970s influenced 40% of stock market & workforce [**1.**]

Where ya goin' Australia?

Questions/Discussion

Facility: unsw.edu.au/research/facilities-and-infrastructure/find-a-facility/sbf

Web port: cryosparc.analytical.unsw.edu.au

My site: keiran-rowell.github.io/

Staff (thanks!): Nathan & Josh (Computational Systems Officers)

Collaborators: Drs Hasti Iranmanesh & Daniel Luque, Peilie Yang