

PAUL SCHERRER INSTITUT



Dr. Greta Assmann :: Paul Scherrer Institute

BIO HPCE computing

30. 04. 24

- BIO (~170 members)
 - LBR, LNB, CRS
- Research: (cell signaling, structural biology, genomics, imaging)
- Facilities: SwissFEL, SLS, EMF (Electron Microscopy Facility)
- Computing: mainly Merlin6 GPU cluster (EM), RA (Crystallography)

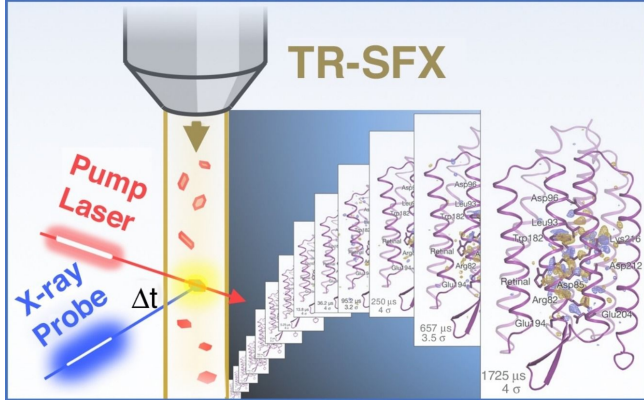
My position:

- “Liaison between AWI and BIO” - successor of Spencer
- BIO user support
- Software maintenance (EM, MX (partially))
- EM-Facility networking support
- Project - based work related to BIO (MX)

SwissFEL - Project: CLARA

CristaLlina AlvRA TR-SX Data Processing

- Idea: (New/Improved) data processing pipeline at Cristallina (Alvra) for time-resolved crystallography : **CLARA**
-> Automate & Facilitate TR-SX Crystallography

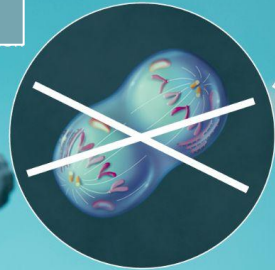


Standfuss (2019)

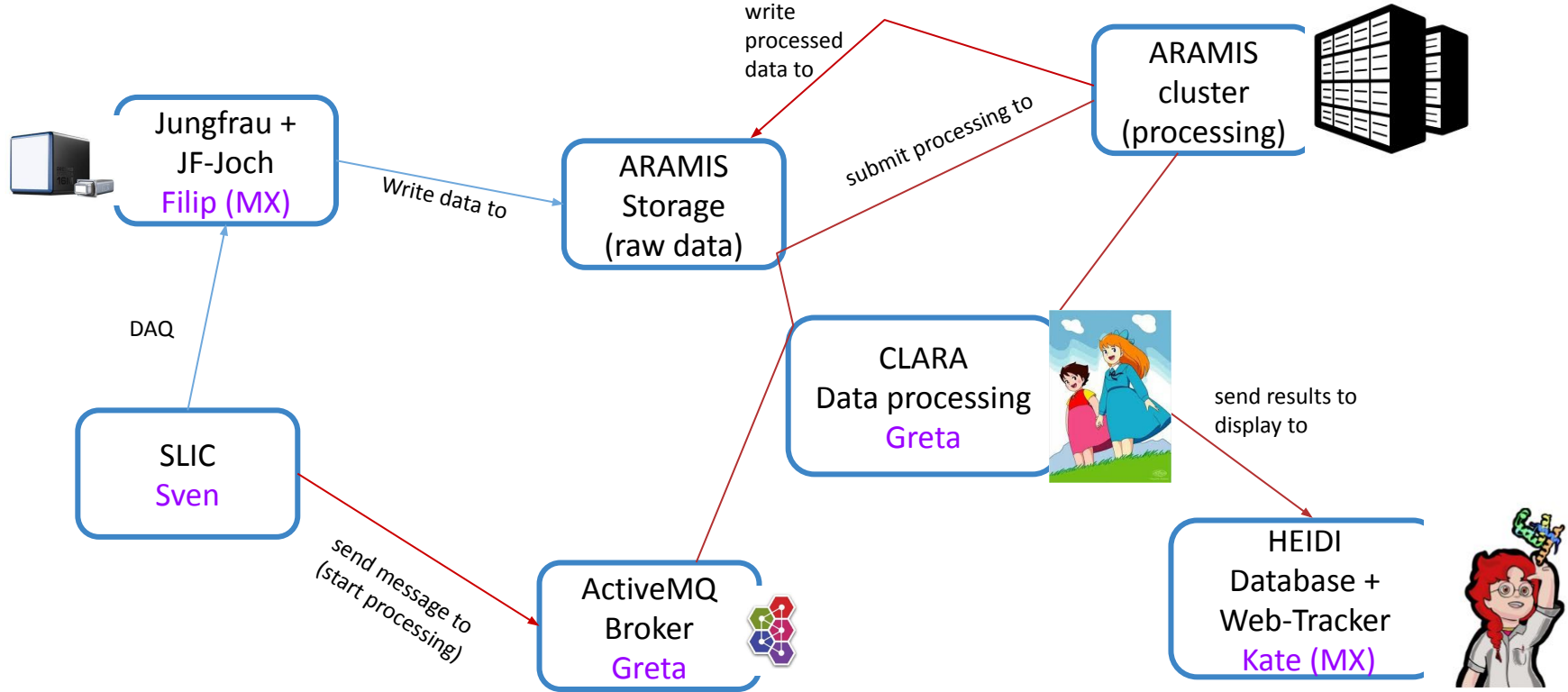
- Setup (ideal):
 - In combination with Jungfrau and real-time indexing (recent TORO project) (MX, Filip L.)
 - In combination with the HEIDI web-tracker/database (MX, Kate S.)
 - User interaction possible (processing parameters)
 - Usable without admin rights (<-> current setup at Cristallina)

Why? (5232)

Taxol (cancer drug)
inhibits formation of
the cytoskeleton
("tubes") and inhibits
cell division
→ kills cancer cells
→ can be "seen"
with TR-SX



(How?)



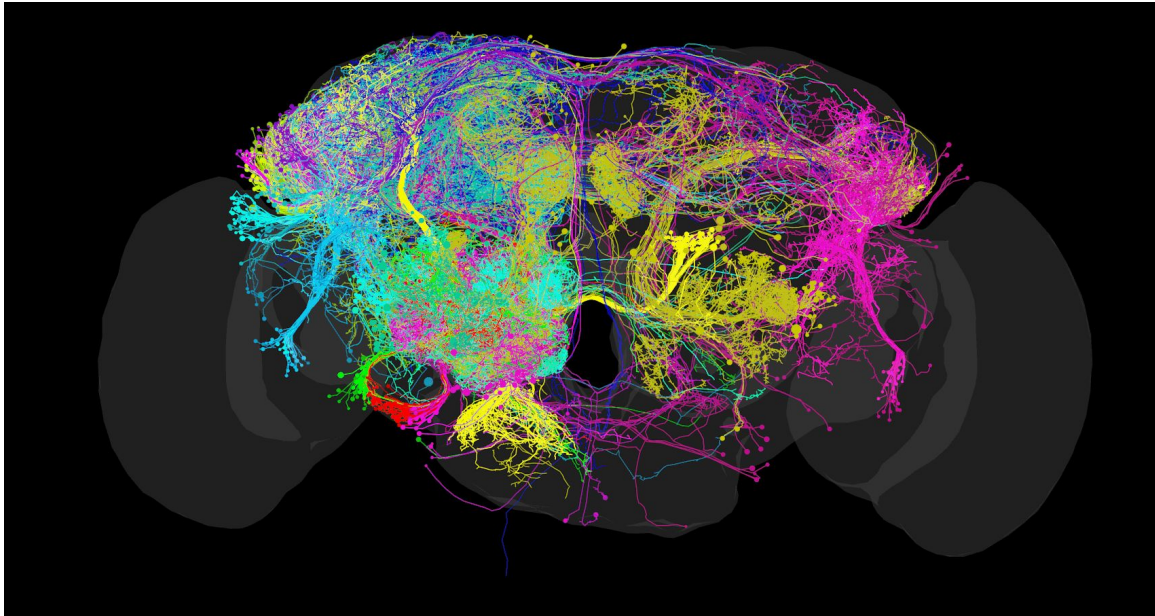
Other projects

1. Jungfrau for EM (Abrahams group):
 - a. JF + JFJ for electron diffraction experiments at EM
 - b. Involved in comp. setup with Leo, Filip (MX) - May/June

2. Microtubule (MT) data processing (Steinmetz group):
 - a. Cryo-EM datasets (processed with relion, cryosparc)
 - b. Need “special” treatment
 - c. Enabling the use of “special treatment” steps for MT data in combination with available software (relion, cryosparc)



3. Mouse-brain connectome (Wanner group):
 - a. Needs 10 Mio CPU hours + 1 Mio GPU hours for one dataset (500TB)
 - b. New microscope ~July
 - c. Currently processing on google → maybe a project for ALPS?



Thanks for helping
me!