CyberInfrastructure Training and Education for Synchrotron X-Ray Science (X-CITE)

Hands-on Tutorial:
Data Analysis & Visualization

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Acknowledgements: Tutorial Authors

CHESS Analysis Pipeline (CHAP)

National Science Data Fabric (NSDF)

Keara Soloway Cornell Univ.
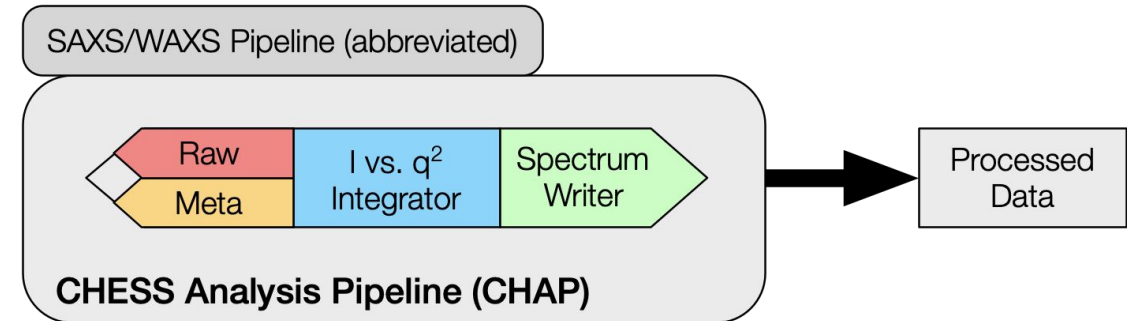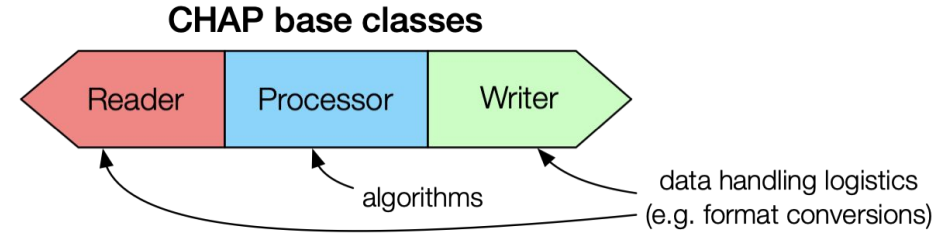
Rolf Verberg Cornell Univ.

Valerio Pascucci Univ. of Utah

Giorgio Scorzelli Univ. of Utah

CHESS Analysis Pipeline (CHAP)

- Object-oriented framework
- Data analysis code organized into reusable modules
  - Reader
  - Processor
  - Writer
- Multiple inputs
- User interface
  - Command line (expert)
  - Galaxy (non-expert)
  - CHAPBook (coding interface)

CHAP base classes

Reader | Processor | Writer

algorithms

data handling logistics (e.g. format conversions)

SAXS/WAXS Pipeline (abbreviated)

Raw / Meta | I vs. q^2 Integrator | Spectrum Writer → Processed Data

CHESS Analysis Pipeline (CHAP)

renci

USC Viterbi
School of Engineering
Information Sciences Institute

CHESS
CORNELL HIGH ENERGY
SYNCHROTRON SOURCE

Tutorial Outline

1. **CHAP + Jupyter:**
   - Azimuthal integration of 2D diffraction images

2. **CHAP + NeXpy:**
   - Tomographic reconstruction of 3D samples

3. **NSDF dashboards:**
   - On-the-fly data visualization

Instructions on Indico

https://indico.classe.cornell.edu/event/2440/page/39-hands-on-tutorial-instructions

X-CITE Workshop Agenda

Time	Content
8:30 - 8:50 am	**Introduction to X-CITE training program**
8:50 - 9:40 am	**Overview of CHESS research workflow and CI (data collection software, data analysis software, Compute Farm, preparing for beamtime)**
9:40 - 09:55 am	**Break**
9:55 - 10:55 am	**Programming modules (Python and Jupyter, packages/libraries Conda, numerical analysis with Python)**
10:55 - 11:20 am	**Systems Fundamentals (Linux, command line, scripting)**
11:20 - 11:40 am	**CI resources at CHESS and beyond (job submission, CHESS systems, other NSF resources (ACCESS))**
11:40 - 12:15 pm	**Town Hall on CHESS User Experiences and Challenges**
12:15 - 1:15 pm	**Lunch**
1:15 - 3:15 pm	**Hands-on session with complete end-to-end data analysis examples**
3:15 - 3:30 pm	**User survey and feedback**
3:30 - 4:30 pm	**Office hours**

Thanks

Project website: https://sites.google.com/view/x-cite-nsf/home

Training materials: https://xcitecourse.org

NSF Cybertraining Award # 2320373