Online Image Alignment using the EDNA Framework

Jérôme Kieffer
Data Analysis Unit
I. What is a Synchrotron?

II. Full Field XANES experiment
   • XANES and microscopy
   • Full-field XANES data analysis pipeline

III. EDNA Framework
   • Strength & weakness

IV. Results
   • Algorithms and implementations
   • Speed, memory footprints and visualization
What is a Synchrotron?

Linear Accelerator
Booster
Storage Ring
Optics Hutch
Experiment Hutch
Control Hutch

Answer: An X-ray source, a very bright and tunable one
Full-Field XANES microscopy

ESRF-ID21: X-ray microscopy Beamline
XANES & Microscopy

• X-ray Absorption Near Edge Structure:
  • X-Ray absorption spectroscopy
  • Chemically specific
  • Sensitive to oxidation state of elements

• Microscopy using XANES:
  • 3D dataset is composed by:
    • X horizontal positions
    • Y vertical positions
    • E points in energies

• Scanning microscopy
  • 2D spacial scan on the sample (X*Y datapoints: slow)
  • Pencil X-ray beam (sub-micron size)

• Full-field microscopy
  • Large beam that covers all the sample
  • 1D Scan in energy (faster)
Submicrometer Hyperspectral X-ray Imaging of Heterogeneous Rocks and Geomaterials: Applications at the Fe K-Edge
Vincent De Andrade, Jean Susini, Murielle Salome, Olivier Beraldin, Cecile Rigault, Thomas Heymes, Eric Lewin, and Olivier Vidal
dx.doi.org/10.1021/ac200559r | Analytical Chemistry 2011, 83, 4220–4227
Scan in energy with monochromator crystal around absorption edge of a given element (Fe, Ti, ...)

Sample size: 2 mm x 2 mm x 10 µm
Resolution: 1µm - 500nm (with optical zoom)

- Measure 2 flats at each energy to correct for scintillator & CCD pixel response, $I_0$
- Align the sample at each position to correct sub-micron position change
Full-Field data processing

Raw stack

Aligned stack

Each pixel is a XANES spectrum

Fit PCA NNMA

Fit PCA NNMA using PyMCA

Dif. along x
Accumulator

Shift

Measure

Offset

Shift Image

HDF5

Image stack

Make pairs of images

Calculate absolute offset

Stack images in HDF5

Align Stack

Normalize Image

\[
\frac{I - I_{\text{dark}}}{I_{\text{flat}} - I_{\text{flat}}_{\text{dark}}}
\]

Measure sub-pixel offset by 2D correlation (FFT)

Scipy.ndimage.shift

First pure python EDNA-pipeline

Pure SciPy Code

Full-Field XAS Pipeline
EDNA Framework

A pipeline tool for the development of robust on-line data analysis applications
Strength of EDNA

- EDNA is a robust pipe-lining tool for on-line data analysis
  - Written in (pure) python and fully open-source
  - It has been tested with thousands of tasks at once
- EDNA allows hi-performances
  - Multi-threaded implementation
- EDNA relies on data-models
  - Visual communication with scientists
  - Automatic bindings with the code
- EDNA has a strong testing framework
  - Unit & execution tests
  - Continuous integration with nightly builds
- EDNA is efficient to program
  - Plugin generator for execution plug-ins based on the data model
  - Re-use of plug-ins already written by others: EDNA-Toolbox
EDNA at a Glance

Collaboration

- ESRF (Grenoble),
- Diamond (Oxford),
- EMBL (Grenoble, Hamburg),
- MRC-LMB (Cambridge),
- CCP4 (UK mainly),
- Soleil (Paris), Bessy (Berlin),
- Max Lab (Sweden), SLS-PSI (Swiss),
- Univ Sidney, Univ York,
- Global Phasing (UK)

EDNA applications

- MX protein crystallography (ESRF, DLS, ...)
- SAXS (EMBL, ESRF, DLS)
- Darc Archiver (DLS)
- Diffraction Tomography (ESRF)
- Dimple molecular replacement (CCP4)
- Full-Field XANES (ESRF)
- Xncf EXAFS analysis (DLS)

EDNA tool box

- Modular Plugins
- Data Model / UML -> Code
- Workflow model
- Testing Framework
- Project Management

Many tools available:

- 86 Control plugins
- 106 Execution plugins
- 25 Others plugins

Easy to extend:

- Python code (v2)
- Tested daily on linux, mac, win & jython
- GPL or LGPL licence

http://www.edna-site.org
Weaknesses of EDNA

• Hard to install
  • No setup.py, no installer but a lot of documentation
  • Relies on many external programs
    • When proprietary: licensing issues
    • Integration within EDNA needs additional configuration
• Learning curve is very steep
  • Data-modelling, UML, EDML, data-binding
• Javaish style repels python developers
  • Code structure and coding convention
  • Inheritance model for all plugins
• Multi-threading limited by the GIL in CPython
  • No problem if the GIL is released
    • External programs, that's the standard way of EDNA
    • Do numpy and scipy calls always release the GIL?
• Few scientists develop with EDNA, mainly IT staff.
Results

Full-Field microscopy
Algorithms tested

• Offset Measurement:
  • By Convolution:
    • By FFT: $\text{iFFT(FFT(im1) * FFT(im2).conjugate())}$
      • Numpy and Scipy.fftpack are the same (1.7s)
      • Fftw3 is faster (0.8s) but “plan” generation is not thread-safe
      • scipy.signal.fftconvolve gave weird results
    • Offset image to place the max to the center
      • Shift by block is better than interpolation.shift(order=0, mode="wrap") (30 vs 130ms)
    • Measure maximum: Centre of mass after threshold
      • Precision: better than 0.1 pixel
  • Using “sift” (scale-invariant feature transform)
    • Patented algorithm (in the USA)
    • Free implementation in C and C#
    • They have been EDNA-ised, but still slow (5 seconds)
    • Keypoints matching not yet done … but very promising

• Image shift with cubic interpolation
  • scipy.ndimage.shift does the job but FFT works as well.
Full-Field XANES Results

- Tested online & offline; next experiment in September 2011
- Image alignment by FFT is pretty good
- Execution time is around 3 sec / 3 frames (flat – data – flat)

Issues remaining:
- Memory consumption for both EDNA & PyMca (dataset: 5GB)
- Limits of parallelism with the GIL & serialization in HDF5 (x1.5)
- Live normalization of oscillation of the blank signal
Acknowledgements

X-ray microscopy Beamline (ESRF ID21)
- Barbara Fayard
- Murielle Salomé
- Marine Cotte

Software Group

Data Analysis Unit
- Olof Svensson
- Vicente Armando Solé

Beamline Control Unit
- Gilles Berruyer
- Cyril Guilloud
→ COD (36 month) position available on PyQt
http://esrf.profilsearch.com/recrute/fo_annonce_voir.php?id=49