JÜLICH
FORSCHUNGSZENTRUM

HDRI — WP3

Hamburg, 27/28 feb 2012 | Joachim Wuttke, Jülich Centre for Neutron Science

The Scientific Computing Group at FRM II

Organization

- a joint group of HGF and TUM
- under leadership of JCNS

Scope of responsability

- supporting all scattering instruments
- regardless of affiliation
- not: data acquisition ($\rightarrow$ EDV, ZEL)
- but: data format

The Scientific Computing Group at FRM II

Staff

- Joachim Wuttke, nominated July 2011
- Christian Felder, since August 2011 (also admin duties)
- Gennadi Pospelov, since January 2012
- Walter Van Herck, since January 2012
- one more JCNS positions to be filled soon
- several TUM positions coming later

Funding

- mostly from core budget
- 0.7 positions from HFG-HDRI

Strategy

Service & Science

- responding to specific needs
- collaborating with instrument responsibles
- involved in scientific projects
- produce publishable software & documentation

Modular approach

- decouple physical modelling / data fitting / GUI
- publish libraries / plugins
- support multiple output formats

Use and produce open source code

- standard languages: C++, Python

Cooperations

HDRI

- observer/customer in WP 1 (data management)
- coordinator of WP 3 (data analysis, GISAS)

NeXus

- JWu representing FZJ and FRM II in NIAC

PaNdata–ODI

- participation since kick-off meeting at ISIS, November 2011

ILL

- informal contacts with scientific computing group

HDRI — WP3

Data Analysis, Modelling, and Simulation
Coordination: JCNS (Th. Brückel)
Partners: DESY, HZG, HZB

Project goals:

- visualization and standard analysis for SANS/SAXS
- simulation and modelling for off-specular scattering
- analysis software for GISANS/GISAXS

visualization and standard analysis for SAS

Available software

- SAS-modules in LAMP, DAVE, MANTID?
- QtiKWS (JCNS: V. Pippich)
- BERSANS (HZB: U. Keiderling?)
- SASFIT (PSI: J. Kohlbrecher)
- ? (ESRF: P. Boesecke)

HDRI project: DPDAK

- cooperation DESY (G. Benecke/S.Roth) & MPI Golm
- assured maintenance
- high throughput: $>$10’000 images
- taught at workshops, growing user community
- modular, users start contributing
- web site with free download available by March

off-specular scattering and GISAS

Open-source projects

- R. Lazzari, Paris: IsGisaxs
- D. Babonneau, Poitiers: FitGisaxs
- A. Glavic, FZJ

Other contacts

- L. Deàk, Budapest: next 4 weeks in Garching

Starting point IsGisaxs

Status

- R. Lazzari: cooperative, but no longer active
- 10’000 F90
- ported to Linux by G. Benecke
- ported to gfortran by J. Wuttke
- side result: SLATEC for gfortran by J. Wuttke
- code analysed and basically understood
- rewrite would be easy and fast

Todo

- understand limitations and possible extensions
- coordinate with interested parties (Poitiers, Budapest, ?)
- write mathematics before coding