The MLZ Scientific Computing Group

Grenoble, 24 October 2013 | Joachim Wuttke, Jülich Centre for Neutron Science
Heinz Maier-Leibnitz Zentrum Garching

founded 2011

joint scientific use of FRM II

- TU München (and other universities, MPG)
- Helmholtz-Gemeinschaft (Jülich, Geesthacht)

common project and support groups

- User office (JCNS)
- Gas detectors (TUM)
- Scintillation detectors (FZJ)
- Administrative software (TUM)
- Scientific software (JCNS)

http://www.mlz-garching.de
The MLZ Scientific Computing Group

operative since January 2012

duties
- contribute software for data reduction and analysis
  - for all scattering instruments
  - regardless of affiliation
- coordinate data formats
  - represent TUM and FZJ in NIAC
- *support complementary simulations*

funding
- mostly from JCNS core budget
- 0.7 positions from HGF–HDRI

http://apps.jcns.fz-juelich.de
The MLZ Scientific Computing Group

Céline Durniak  Marina Ganeva  Gennady Pospelov  Antti Soininen  Walter Van Herck  Joachim Wuttke
Current Projects

- grazing-incidence small-angle scattering (GISAS)
- inelastic scattering
  - consolidate software at TOFTOF
  - multiple scattering simulation
  - forthcoming: DNS, TOPAS
- instrument development SPHERES
- data catalogue
- generic open-source libraries
Talks and Topics

- **introduction**
  - overview (Joachim)
  - presentation of team members (all)
  - agile development methods and tools (Walter)

- **projects**
  - GISAS (seminar Walter)
  - data catalogue (Joachim)
  - data reduction (Joachim, Céline)
  - multiple-scattering simulation (Antti)
  - generic open-source libraries (Joachim)

- **for technical discussion**
  - data treatment in HEP, CERN ROOT (Gennady)
  - interfacing Python and C++ (Gennady)
Dr. Marina Ganeva
Group member since 9/13

Projects:
- Data reduction

Research history:
- Neutron scattering
- Plasma physics
- Nano-size clusters
- Space weather

Programming experience:
- Python
- C, C++
- Labview
Dr. Antti Soininen
Group member since 5/13

Projects:
- multiple scattering simulation MSca3
- water in confined geometries

Research history:
- Soft nanomaterials
- Polymer physics
- Dynamics of confined water
- Neutron scattering

Programming experience:
- Python
- C, C++
- Labview
- Java
Dr. Céline Durniak
Group member since 1/13

Projects:
- Data reduction
- BornAgain

Research history:
- Neutron scattering
- Complex plasmas
- Photonics, optics
- Nonlinear dynamics

Programming experience:
- C, C++
- IDL
Dr. Walter Van Herck  
Group member since 1/12

Projects:
- BornAgain

Research history:
- High performance computing
- Neutron scattering
- Condensed matter physics
- String theory

Programming experience:
- C, C++, C#
- Python
- Agile development
Dr. Gennady Pospelov
Group member since 1/12

Projects:
- BornAgain

Research history:
- High performance computing
- Neutron scattering
- Particle detectors
- High energy particle physics

Programming experience:
- Fortran, C++, Python
- Cross platform and cross language programming
- Data reconstruction and analysis.
- Monte Carlo simulation
Dr. Joachim Wuttke
Head of the group

Projects:
- too many left from SPHERES

Research history:
- Neutron and light scattering
- Liquids dynamics, proteins, confined water
- Instrumentation (SPHERES)

Programming experience:
- Fortran77 -> C++
- Perl -> Python -> Ruby -> Python