

# 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)

## 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

## 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