Master-program **Computational Sciences**

- **starts** Wintersemester 2016/17
- **application**: July 1st - August 15th
- **admission**: 50% by grade, 50% by interview
- **contact**: info@compsci.fu-berlin.de
  - frank.noe@fu-berlin.de
- **infos**: compsci.fu-berlin.de
Master-program Computational Sciences

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Master-program Computational Sciences

- Starting WS 2016 @ FU Berlin
- Interdisciplinary Master program between natural sciences (Chemistry, Physics, Geosciences) and mathematics / computing.
- Open to all Bachelors from Mathematics, Computer Sciences, Physics, Chemistry, Geosciences

Synchronization Module:
- Computational Sciences: new lecture - from physical theory, across numerics, efficient algorithms and implementation. 4 SWS lecture plus software project
- 15 LP Synchronization modules to get up to speed with natural science applications or with maths+computing.

Scientific Computing Module:
- Selection of two modules from areas of statistics, numerics and informatics
- Each module: 4+2 lecture plus 1 research or project seminar.

Specialization Modules and MSc thesis:
Specialization in molecular sciences, geosciences or atmospheric sciences.

More information: Prof. Frank Noé / frank.noe@fu-berlin.de
Study plan MSc Computational Sciences

“LP” correspond to ECTS

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<th>15 LP</th>
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<td><strong>Computational Sciences</strong></td>
<td><strong>Scientific Computing A</strong> (not graded)</td>
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<td><strong>Specialization</strong> (Mol / Geo / Atmo)</td>
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<td><strong>MSc Thesis</strong> (Mol / Geo / Atmo)</td>
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**Synchronization Module:**
15 LP’s worth of Bachelor-modules from a Bachelor-program that the candidate has no degree in, and that prepare for a specialization in that area (e.g. physicist moving into geosciences), or build some basic formal training (e.g. math upgrade for chemists and geographers)

**Scientific Computing Module:**
Selection of 2 modules from the three scientific computing areas (statistics, numerics and informatics)
Each module consists generally of 1 large lecture from an existing program (math, CS, physics) and 1 seminar that is common to all MSc Comp. Sci. Students.

**Specialization Modules and MSc thesis:**
Specialization in molecular sciences, geosciences or atmospherical sciences.
Admission requirements
MSc Computational Sciences

Einer der folgenden Abschlüsse:
- BSc in Physics at FU (or similar)
- BSc in Chemistry at FU (or similar)
- BSc in Mathematics at FU (or similar)
- BSc in Computer Science at FU (or similar)
- BSc in Geological Sciences at FU (or similar)
- BSc in Geographical Sciences at FU (or similar)
- BSc in Meteorology at FU (or similar)
- BSc in an Engineering Science

Languages:
- **English**: The “red” module and part of the “green” modules are taught in English
- **German**: Needed for some modules and for the Atmospheric Sciences specialization
  - —> The study program is accessible without german, but with limited choices.
This is a common module and the starting module for all Comp. Sci students. It consists of:

- a 4 SWS lecture in which methods of the computational sciences (physical theory and equations, computational methods, numerics, implementation) are taught on one or two guiding examples.
- a 4 SWS software project in which implementations of the guiding examples are developed in teams using state-of-the-art software development practices.

Example:

**Theory:** Interaction of Charged Particles

**Efficient computation:** Fast multipole method, Ewald simulation

**Numerics:** Accurate and stable solution

**Software:** Software design implementation testing

**High-performance computing:** Parallelization Graphics card implementation

**Physics**

**Mathematics**

**Computer Science**
Implementation Sync Module (selected module):

Sync Module: 15 BSc LPs depending on BSc qualification
The aim of this module is to equip the candidate with yet missing qualifications that are essential to continue with Computational Sciences in general or to specialize into the area of interest. Clearly, a full synchronization of the various different candidates is impossible within 15 LP. To cope with that we have a lot of extra flexibility in the “green” and “red” modules.

Consider the following examples:

Chemistry, Geography, Geosciences with chemical-biological focus,

Aim of Sync: Achieve math upgrade
Algebra for Physicists (4 lecture + 2 tutorial hours)
Computer-oriented Mathematics (2 lec + 2 tut)

Physics

Aim of Sync: Insight into computer science / software-design or a new application area
15 LP from Sync modules from Computer Science, Chemistry, Geosciences, …

Mathematics, Computer Science

Aim of Sync: Become familiar with an application area
15 LP from Sync modules of Physics, Chemistry, or Geosciences

Meteorology, Geosciences with mathematical-physical focus

Aim of Sync: Computer science or numerics upgrade
15 LP from Physics, Computer Science or Mathematics
Numerics Module:

15 LP
Introduction to numerical mathematics

15 LP
Numerics for ODEs and linear algebra

15 LP
Numerics for PDEs

Content:

Numerics I (Mathe BSc)

Numerics II (Mathe MSc)

Numerics III (Mathe MSc)

Research-oriented seminar or software tutorial

10 LP

5 LP
Computational Statistical Physics Module:

- 15 LP Computational Statistical Physics A
- 15 LP Computational Statistical Physics B
- 10 LP Stat Mech I (Physik MSc)
- 5 LP Stat Mech II (Physik MSc)
- 5 LP Seminar or Software-Tutorial

Content:
Implementation Scientific Programming Module:

15 LP
Computer Science and Functional Programming

15 LP
Computer Science and Object-Oriented Programming

15 LP
Computer Science and Data Structures

15 LP
Complex Algorithms

Content:

15 LP
Algorithms and programming I (Inf BSc)

15 LP
Algorithms and programming II (Inf BSc)

15 LP
Algorithms and programming III (Inf BSc)

10 LP
Higher Algorithmics (Inf MSc)

For example:
HPC Seminar or Scientific Programming and Software design or small Software Project (5 LP)
Choose 30 LP’s from a list of modules in the specialisation

**Examples:**

### Specialization: Molecular Sciences
- Research project (5 or 10 LP),
- Molecular Simulation I (5 LP),
- Molecular Simulation II (5 LP),
- Markov Modeling (5 LP),
- Selected topics in theoretical computational sciences (5 LP),
- Selected topics in applied computational sciences (5 LP),
- Research seminar computational sciences (5 LP),
- Quantum chemistry (5 LP) (MSc program Chemie)
- Density functional theory (5 LP) (MSc program Chemie),
- Quantum chemical correlation methods (5 LP) (MSc program Chemie),
- Quantum reaction dynamics (5 LP) (MSc program Chemie),
- Selected Topics in Physics (5 LP) (MSc program Physik),
- Modern Methods in Theoretical Physics A (5 LP) (MSc program Physik)

### Specialization: Geosciences
- Research project (5, 6 or 10 LP),
- Physics of the earth I (5 LP) (MSc program Geosciences),
- Physics of the earth II (5 LP) (MSc program Geosciences),
- Seismsics II (5 LP) (MSc program Geologische Wissenschaften),
- Thermodynamics & kinetics of geological processes (5 LP) (MSc program Geosciences),
- Dynamics of the earth (5 LP) (MSc program Geosciences),
- Selected topics in theoretical computational sciences (5 LP),
- Selected topics in applied computational sciences (5 LP),
- Research seminar computational sciences (5 LP).

### Specialization: Atmospheric Sciences
- Research project (5, 6 or 10 LP),
- Theoretical meteorology I or II (8 LP) (choose only 1) (MSc program Meteorology),
- Models for weather and environment (8 LP) or climate variability and models (8 LP) (choose only 1) (MSc program Meteorology),
- Satellite meteorology (8 LP) (MSc program Meteorology),
- Weather & climate diagnosis (8 LP) (MSc program Meteorology),
- Selected topics in theoretical computational sciences (5 LP),
- Selected topics in applied computational sciences (5 LP),
- Research seminar computational sciences (5 LP).
Responsible

Molecular Sciences

Prof. Frank Noé
Prof. Bettina Keller
Prof. Petra Imhof

Atmospherical Sciences

Prof. Rupert Klein
Prof. Uwe Ulbrich

Geosciences

Prof. Georg Kaufmann