

The newly established interdisciplinary Collaborative Research Center CRC 1114 „Scaling Cascades in Complex Systems - Across-Scale Modeling and Simulation Paradigms” offers the following 4 open project positions for

- PhD Students (part time 75%, except B05-b with 65%) and
- PostDocs (full time 100%)

with fixed term contracts, limited to 30.06.2018 (except A04b)
and salary according to E13 TV-L FU/ TVöD Bund.

CRC 1114 aims at methodological developments for the modelling and computational simulation of complex processes involving many (more than two) interacting scales, driven by real-life applications from the bio-, geo-, and material sciences. In its individual projects, mathematicians cooperate with colleagues from the natural sciences to advance both their modelling capabilities and their insight into concrete multiscale phenomena.

Project A04b	<p>Efficient calculation of slow and stationary scales in molecular dynamics Dr. Thomas Weigl, 1 PhD student, part time 75%, at Max Planck Institute of Colloids and Interfaces, Potsdam</p> <p>In this project, we will investigate the conformational changes of proteins during binding to ligand molecules with molecular dynamics (MD) simulations and Markov state modeling. A challenge for MD simulations of protein binding is that the typical timescales of the conformational transitions and binding events are in the microsecond and millisecond range, while the timesteps of these simulations are in the femtosecond range. This challenge is addressed by a combination of enhanced sampling and Markov state modeling techniques that allows the key molecular processes occurring on slow timescales to be characterized.</p>
Project B01a	<p>Fault networks and scaling properties of deformation accumulation Prof. Dr. Ralf Kornhuber, 1 PhD student, part time 75%, at Freie Universität Berlin</p> <p>Project B01a is characterized by the interplay of advanced concepts from Numerical Analysis, Applied Analysis, and Scientific Computing with concrete applications in the geosciences.</p>
Project B05b	<p>Origin of the scaling cascades in protein dynamics Institute of Theoretical Physics Prof. Dr. Petra Imhof, 1 PhD student, part time 65%, at Freie Universität Berlin</p> <p>This interdisciplinary project is located at the interface of chemistry, physics and mathematics. By performing first principles simulations of linear and 2D-IR spectra we aim at analysing the coupling between local vibrations and conformational dynamics. Our molecular simulations help in bridging experimental and mathematical methods so as to reveal the origin of scaling cascades in protein dynamics.</p>

Project C05	<p>Effective models for interfaces with many scales Prof. Dr. Alexander Mielke, 1 PostDoc, full time 100%, at Weierstraß-Institut Berlin</p> <p>The goal of the project C05 is the mathematical study of multiscale effects arising at interfaces or surfaces of bulk materials taking into account the interactions of bulk and interface phenomena, such as e.g. diffusion and reactions of chemical species, elastic deformations, delamination, and dry friction. Relevant mathematical concepts are:</p> <p>Hamiltonian and gradient systems and their coupling via GENERIC, weak convergence methods, such as Gamma-convergence, homogenization, multiscale convergence, discrete-to-continuum limits.</p>
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More detailed information on the areas of responsibility, requirements and desired qualifications are provided under <http://jobs.sfb1114.de> as well as <http://www.fu-berlin.de/service/stellen/>. Applications are to be submitted no later than **September 28, 2014**, electronically only, via the project website <http://jobs.sfb1114.de>.