

## Call for Proposals

## Information for Applicants 82a

# Computer Simulation of Molecular and Cellular Bio-systems as well as Complex Soft Matter

### I. Objectives

In 2003 the funding initiative **New Conceptual Approaches to Modeling and Simulation of Complex Systems** was established. It aims at mathematical modeling and computer simulations advancing a better understanding of complex systems. Equally, a strengthening of cooperations among theory, modeling, and simulation is intended. The initiative addresses suitably qualified theoreticians from all scientific disciplines.

Here, complexity is attributed to systems which consist of a large number of elements and which cannot be adequately described by studying their constituents. Characteristic features of such systems are the competition between autonomy and integration of the constituting elements, emergent phenomena across different hierarchical levels, and adaptation in response to the environment. In this context, the funding initiative aims at concepts which are systematically improvable and can be applied to broad classes of problems. The Foundation anticipates that joint concepts of experts employing complementary methods in theory, modeling, and simulation are particularly promising.

On the one hand, research projects with interdisciplinary or comprehensive methodological characteristics are funded after prior topical calls. Currently, the focus is again on complex

(bio-) macromolecules and dynamic processes in cells and soft matter as described in more detail below. Please note that the former call 'Complex networks as a phenomenon across disciplines' is closed. New topical calls are envisaged for 2008/2009.

On the other hand, postdoctoral researchers can apply for a Fellowship 'Computational Sciences' when moving to another laboratory (see 'Information for Applicants 82c'). There is an annual deadline for fellowship applications. Furthermore, teaching substitutions for additional sabbaticals, workshops and summer schools according to the Foundation's modalities (see 'Information for Applicants 1'), as well as projects tackling the fundamentals of complexity are supported.

### II. Topic of the call

The call **Computer Simulation of Molecular and Cellular Bio-systems as well as Complex Soft Matter** refers to research projects dealing with complex systems at the interface of theoretical physics, biophysics, chemistry, and biology, including soft matter. In December 2004 the Foundation granted twelve projects on the announced topic involving 20 research groups. A list of these projects can be found on the Foundation's homepage.

The analysis and prediction of experimental findings in the molecular biosciences relies on progress in theory and modeling. Appropriate methods for this task are still in their infancy. The situation with soft matter systems is similar. Accomplished methods reflecting the solid as well as fluid-like behavior are still missing. Computer simulations of these complex systems face a number of challenges which may be addressed in an application:

- connecting to experimental data and advancing model configurations accordingly
- bridging spatial scales
- expanding the temporal scale towards biologically relevant processes
- computing larger systems and reducing complexity
- identifying optimal problem-oriented methods
- making methods more applicable and accessible

A special emphasis of funding lies on novel methodological approaches, and their systematic improvement and generalization. For example, coarse-graining based on an atomic perspective or multi-scale approaches are conceivable. Innovative combinations of elements from quantum chemistry, electrostatics, hydrodynamics, molecular dynamics, and many-particle theory may be taken into account as well. (Semi-) empirical and stochastic approaches are eligible too in order to overcome existing limitations.

By any means, the proposed methodological development should apply to a well-defined scientific problem, and the simulation results should be connected to real data. Funding of experimental sub-projects is beyond the focus of this initiative. However, if indispensable, the determination of missing data is acceptable on a limited scale to allow for a validation of the simulation results.

### III. Delimitation

Proposals referring to routine application or re-parameterization of simulation software are not considered. The same applies for data analyses in genomics, proteomics, or bioinformatics.

Further, the Volkswagen Foundation excludes funding of topics which are covered by programs of other institutions, e. g. the priority areas of the Deutsche Forschungsgemeinschaft, or specific research calls of federal ministries and governmental agencies.

### IV. Funding

Research projects with interdisciplinary and/or methodologically comprehensive attributes can be funded. Projects involving groups with complementary expertise are preferentially considered. The project may initially last up to three years. A one-time renewal application is possible – again covering up to three years.

The research projects are supported with personnel, materials, and travel costs. Travel and subsistence costs for project-related temporary exchange of personnel of the contributing teams (up to one year) or for foreign guest researchers might be included. Non-scientific personnel (technicians, secretarial staff) and computing equipment will, as a rule, not be funded.

Highly qualified postdoctoral researchers can apply for their own salary. In international collaborations a grant for the benefit of a foreign partner is possible. However, the necessity for the international cooperation has to be substantiated, and the Foundation requires that the project is coordinated by the obligatory German partner.

## V. How to apply

Detailed information on the submission of a pre-proposal or a full application, respectively, can be found in the enclosed checklist. In view of the international peer review only proposals in English are accepted. The pre-proposals and full applications will be evaluated by an interdisciplinary peer review panel. The Foundation does not process applications which are pending with another funding institution, neither in the identical nor in a similar form.

Regarding new projects a two-step application procedure is in effect. First, three-page short proposals plus information on the applicant(s) and the costs may be submitted. The deadline for pre-proposals is **November 2, 2007** (date as postmarked). After completion of the peer review the Foundation will inform you whether your pre-proposal was selected and which additional information should be included in a full application.

Applicants already funded in the initiative may directly apply for a renewal of grant. The project continuation can last up to three years. A full application of approximately ten pages on the objectives and the work plan of the second project period as well as a report on the current status of the project are expected. Such renewal applications can be submitted either before **November 2, 2007** or before **August 1, 2008**.

The Volkswagen Foundation can award grants to scientific institutions only. Applicants outside of universities and well-known publicly-maintained research institutions are asked to provide details on the legal status, statutes, trustees and boards, charitable/non-profit status, budgeting and auditing of the institution to be funded. Please include any existing annual report of the applying institution.

## VI. Contact

The Volkswagen Foundation in Hanover will be pleased to provide further information concerning this call.

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## Check-list

### Computer simulation of molecular and cellular bio-systems as well as complex soft matter

Pre-proposals and (renewal) applications written in **English** may be submitted by the specified deadlines. They should be phrased clearly and should provide sufficient information for assessment by the Foundation staff and the scientists involved in peer review. Please submit a signed paper copy of your documents and, additionally, send the corresponding files electronically (preferably as pdf) to the Foundation.

Pre-proposals (deadline: November 2, 2007) should provide the following information:

- cover sheet with short **project title** and name with work address of each **applicant**
- **three to four page project description**  
(1) topic and objectives, (2) short description of the current state of research, the methods employed, and the work plan, (3) added value of the cooperation(s)
- **cost estimation** with projected **duration**  
subdivided in personnel, travel and other recurring costs for each contributing team
- **original signature** of each applicant

As enclosures (and separate files, respectively):

- brief **curriculum vitae** with up to five current, project related publications of each applicant as well as of hitherto known doctoral students or postdoctoral researchers to be employed (one page per person)

Applications are only accepted for project renewals or after positive evaluation of a pre-proposal. Renewal or invited applications (deadlines: November 2, 2007 and August 1, 2008) should provide the following information:

- brief informative **title** of the project
- name and work address (updated where required) of each **applicant**
- **summary** in English and German – approx. 150 words each –
- **ten to twelve page detailed description**  
objectives and justification, own preliminary work and expected results with regard to the international state of the art, complexity of the system, implementation and methods, work plan and schedule, expertise of the research groups involved, and organization of the cooperation
- **cost calculation** with justification of each item as follows:
  - personnel (classification and sum required including social benefits)
  - recurring costs (e.g. travel allowance, supplies, publication charges)
  - non-recurring costs (e. g. small equipment, literature)
- name of the intended **recipient scientific institution(s)**
- **declaration** regarding any submission of this or a related application to another funding institution

- **original signature** of each applicant

As enclosures (and as separate files, respectively):

- **curriculum vitae** and **list of relevant publications** of the last **five years** of all project contributors – three pages maximum per person –
- list of **current or recently completed grants** (title, duration, volume, funding institution, delimitation)
- applicants without secured position during the anticipated project duration only:  
additional **statement** of the head of the institute or the department regarding the feasibility of the project (including computing resources) and the grant administration

Please send your signed pre-proposal / application and the corresponding files to:

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