

Questionnaire:

1) Quality of the project proposal

1a) Originality, scientific importance, prospects of the project and expected benefits of the project for basic research

The applicants intend to establish a large multidisciplinary research team with members from the four scientific fields

- continuum mechanics,
- mathematical analysis,
- numerical analysis, and
- high performance computing (HPC)

and the three institutions

- Charles University (Prague),
- Academy of Sciences of the Czech Republic (Prague), and
- VSB-Technical University of Ostrava.

In total, 39 team members are mentioned in Fig. 1.

The motivation for this joint effort is to bring together researchers from all fields which are the links of the chain from real-world problems in a selected field (here: continuum mechanics) to efficient simulations of these problems on supercomputer systems. Thus, the applicants hope to be able to develop a solid theoretical basis which allows to guarantee accuracy, quality, and reliability of computer simulations while utilizing all available resources efficiently. The investigations are intended to be driven by selected important real-world applications.

Generally, joining the strengths of experienced researchers in these fields appears promising and would be expected to produce new significant contributions to science, because knowledge in all of these fields is the premise for the successful simulation of continuum mechanics problems and today simulation is one of the most important enabling methodologies for research in natural sciences.

One aspect which promises a stimulation of the fields considered even after the lifetime of the project is the multidisciplinary education of young researchers.

The scientific objectives listed in Section 2.1 focus on mathematical modeling of continuum mechanics problems and the development of numerical methods. In this list of objectives, parallel implementation and simulation are mentioned, but not elaborated.

1b) Preparation of the project proposal, aim of the project and proposed deliverables

The proposal mainly emphasizes the qualifications, expertise, and past achievements of the applicants and the team members as indicators for their potential to successfully accomplish the project proposed.

One page of the proposal (Section 2.1) is dedicated to a list of scientific objectives, mainly concerned with modeling and analysis of continuum mechanics problems and the development of corresponding numerical methods.

As intended deliverables the applicants mention scientific publications that will contribute to answers of fundamental questions in the research fields considered, software packages, and the education of a new generation of flexible researchers.

From my point of view, it would have been desirable that the applicants had specified the interactions between the research fields, teams, persons and institutions involved more precisely. To me the list of scientific objectives (Section 2.1) and the research directions (Section 3.2) largely appear as independent topics that could possibly also be investigated in smaller (interdisciplinary) research projects. Only a few research questions are clearly pointed out, where interactions are expected, mainly only between two groups (interactions between locality of finite element basis functions and preconditioning; incorporation of algebraic and modeling errors into a posteriori error analysis; massively parallel simulation of thermal convection; numerical aspects of parallel domain decomposition algorithms). This may be originating from the fact that the research fields involved in the workflow from modeling to simulation (Section 1.1) appear to form an assembly line, i.e., chain rather than a complete graph. Can the applicants explain that the workflow actually is at least a 'closed loop' as stated in Section 2.3.3, i.e., is there any feedback the HPC group can give to the modeling groups so that they can develop new models with improved potential for parallelization?

In my opinion, the role of the HPC group is either understated or its participation in the project is questionable. Among the scientific objectives (Section 2.1), only a single objective can be correlated to this group: the 'implementation of suitable solvers' 'fully exploiting the paradigm of parallel computing'. When the reader reaches Section 3.2.5 ('Large Scale Problems'), it is explained that the HPC group intends to work on several types of domain decomposition techniques. I did, however, not recognize any statements whether these techniques are suitable for all problems considered or if other techniques have to be investigated in addition. More severely, the overall goal of the project is the development of a theoretical basis to guarantee accuracy and reliability of computer simulations, the theoretical background of which is stated to be closely tied to the 'modern mathematical theory of partial differential equations'. I can envision the development of such a common theoretical basis for the different branches of mathematics and theoretical physics. But, since HPC is about parallelization, programming, and parallel performance, it is not clear to me how the work of the HPC group will correspond to this overall goal of the project.

1c) Concept, methodology and timeline

The one-page tentative project schedule (Section 4.2) distinguishes between three parts: a modeling part, the analysis of partial differential equations, and a joint numerical and high performance computing part. Each part contains 2-4 'phases' described by one or two sentences. The time frames of the phases are vaguely specified in terms of years. The expected interactions between groups are also specified vaguely using terms such as 'will provide continuous support'. No precise dependencies are given between phases of different parts, which might mislead to the impression that none of the parts requires definable input in form of scientific results from another part.

In general, the proposal lists many interesting research questions and applications on which the individual team members have been working successfully and on which they intend to continue to work (Section 3.1, 'Expertise overview'). Section 3.2 gives several examples of interesting real-world problems to be studied. However, in my opinion, the proposal does not specify clearly enough (maybe in form of work packages, milestones or similar), which of the 39 team members (or small groups of team members) will work on which topic and what are the deliverable results of these work packages that the persons or small groups will provide to other persons or small groups while the project proceeds.

It is therefore very difficult to evaluate the feasibility of the project within the project duration of 5 years. Moreover, I have no information if the project budget includes salary for additional research personnel. It is also impossible to tell in advance how many students from Master or PhD study programs will contribute to the project.

Junior researchers and students are planned to be educated by providing interdisciplinary topics for master and doctoral theses and by supervising these theses by two advisers from different disciplines. This is a good idea, but it will broaden the view of a student to only one second discipline. Further, the applicants state that the project will have a direct influence on several existing Master and PhD study programs, but they do not give further details. Will there be special multidisciplinary series of courses or summer schools?

The overall quality of the project proposal can be rated as:

Average - B

2) The applicant(s) and his/their publication level

All applicants are excellent and recognized researchers with publications in highly recognized and impacting journals. Also, all applicants have experience in leading small and large projects.

The qualification of the applicant(s), his/their publication level can be rated as:

Excellent - A1

Overall commentary on the project proposal:

a) Strengths of the project proposal:

- consideration of computer simulation -- a tool for natural scientists, which today is as important as real-world experiments
- cooperation between all research fields involved in the workflow from modeling real-world problems to simulating the models on parallel computer systems promises synergistic effects and new scientific results due to a broader view of the participating researchers
- project is to be driven by real-world problems, and practical implementations of parallel simulation software on supercomputers are planned
- selection of the important field of continuum mechanics as the source of real-world problems
- aim at the education of a new generation of multidisciplinary researchers
- applicants and team members are highly experienced researchers

b) Weaknesses of the project proposal:

- presentation of the tasks of and interactions between the individual team members and small groups: Who does what with whom and why, and what are the dependencies between the tasks?
- weak integration of the HPC group into the central concept of developing a theoretical basis
- conception of education of young researchers could be elaborated further

c) General comments: