

National Science Foundation 4201 Wilson Boulevard Arlington, Virginia 22230

Long Time Behavior (LTB) of Numerical Methods in Large Scale Scientific Computing

Dear Colleague:

The Computational Mathematics Program of the Division of Mathematical Sciences at the National Science Foundation has a long history of supporting basic research on numerical methods and algorithm design in large-scale computation for problems in science and engineering. This letter is to inform the mathematics community that the program has a focused topic area in Fiscal Year 2007 that addresses long-time behavior (LTB) of numerical methods in large scale scientific computing. This area of emphasis should not discourage the community from submitting proposals in the usual wide variety of computation-related fields, but should be viewed as a special topic of interest.

The number of degrees of freedom, in particular the number of time steps, for solving partial differential equations grows as computational resources grow. Errors or numerical artifacts that may be insignificant when the number of time steps to solution is relatively small can dominate a calculation as this number reaches the tens or hundreds of thousands. Such non-physical artifacts can come in a variety of forms, from the accumulation of numerical truncation error, round-off error, uncertainty in physical parameter values, model uncertainty, etc. Theoretical error estimates containing constants that grow exponentially with time are not adequate to address these effects. Further, as computational platforms grow in size with increasing numbers of CPUs, the advent of commodity multi-core processors, and the increasing heterogeneity of computing environments, increasing care must be paid to designing algorithms that are conducive to such architectures. The trend in computational hardware is to have tens or hundreds of thousands of processors with limited memory associated with each processor and nodes that contain clusters of processors. It is critical that proposed numerical approaches take into account various latencies and load balancing issues that will certainly be encountered on such architectures. Such large calculations produce very large data sets. Algorithms for the efficient analysis and visualization of very large data sets on such modern architectures in order to uncover hidden correlations and structures are also of interest. Above all, the physical correctness of the calculation is the most important issue. Arriving at a physically relevant answer requires careful attention to the above issues as well as others.

The Division of Mathematical Sciences (DMS) of the Directorate for Mathematical and Physical Sciences (MPS) of the National Science Foundation (NSF) recognizes the needs and opportunities posed by this recent surge in interest in long-time and large-scale computing. Unsolicited research proposals to DMS addressing cross-cutting topics in one or more aspects of large-scale scientific computing are considered a focused topic area by the Computational Mathematics Program. We invite novel and creative numerical approaches that address solving real physical problems in such environments.

Proposals addressing this focused topic area should include the label "LTB:" at the beginning of the proposal title. The target date for submitting such proposals to the Computational Mathematics Program is December 7, 2006, see the NSF web site, http://www.nsf.gov/div/index.jsp?div=DMS. Prior to submitting a proposal, PI's are strongly encouraged to contact the Computational Mathematics Program.

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Sincerely, Peter March Division Director Division of Mathematical Sciences