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ROBUST AND SCALABLE SOLVERS IN HPC: RECENT DEVELOPMENTS AND FUTURE CHALLENGES

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ABSTRACT

Multiscale systems, characterized by interactions between different scales in space and time, offer valuable insights into diverse scientific disciplines, including physics, biology, materials science, and engineering. With advances in hardware technologies enabling simulations of larger and more complex systems, the development of robust and scalable numerical methods becomes crucial to fully unlock the potential of modern High-Performance Computing (HPC) architectures. This minisymposium aims to address key topics in this field, including multilevel solvers for partial differential equations, nonlinear optimization, and multi-fidelity techniques. A fundamental, but usually neglected, part of the solution procedure is the choice of the hardware and the representation of infinite dimensional objects such as irrational numbers. Because of this, we also welcome contributions related to hybrid computing, matrix-free solvers and mixed-precision algorithms.

Multilevel solvers and preconditioners: Techniques such as multigrid and domain decomposition methods have emerged as powerful techniques to handle large-scale problems involving high numbers of unknowns. These methods alleviate the computational bottleneck in numerical simulations and improve the efficiency of solving algebraic systems consisting of millions of unknowns.

Nonlinear optimization: Real-world phenomena often exhibit complex behavior, which translates into nonlinearities in their objective function and/or constraints. Nonlinear optimization methods can further leverage the power of multilevel techniques and combine them with nonlinear optimization algorithms and nonlinear preconditioners, providing effective solutions to tackle these challenges. This integration enables more efficient optimization of complex systems.

Multi-fidelity modeling: In many scientific contexts, acquiring high-fidelity data comes at a significant computational cost. To address this trade-off between accuracy and computational resources, multi-fidelity techniques have been developed, such as surrogate modeling, adaptive sampling, and uncertainty quantification.

Hardware choices: Algorithms are ultimately run on a machine, which has a very specific memory distribution (cache, RAM) and bandwidth. Strategies that can leverage different architectures (ARM, CPU, GPU) and represent objects only up to their relevant information (16, 32, and 64 bit floats) can present dramatic speed-ups to the overall computational burden of the solution process. These choices can be distributed among all solver components (preconditioner and solvers), but solid mathematical foundations for these choices are still under active development.

The minisymposium emphasizes the importance of robust and scalable numerical methods, preconditioned solvers, and high-performance algorithms in modern HPC practices.