Variational Formulations in the Non-Isothermal Thermo-Chemo-Mechanics of Nonlinear Materials: Co-Design of Theoretical Model Development and Parallel Solvers — New Aspects in Funding Phase 2

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In this project, complex material behavior is modeled, in which interacting thermo-chemo-mechanical processes play a dominant role. Such problems arise in a variety of engineering fields. Our approach centers on the co-design of modeling, based on variational principles, and numerical solution methods for the arising discretized nonlinear and linearized problems, that employ state-of-the-art parallel iterative solvers from domain decomposition. The co-design is of particular importance in multi-field scenarios, since many more possible combinations of variational settings, finite element formulations and solver types and configurations are conceivable. Moreover, for complex thermo-chemo-mechanical problems, solutions may only become obtainable, if efficient and parallel solvers, carefully adapted for the particular variational model formulation, are available. During the first phase, a common software environment was defined and implemented as a cross-sectional activity between the groups. It is composed of the open source finite element library deal.II (with user-defined material models and element formulations), p4est (for the decomposition), and the Fast and Robust Overlapping Schwarz (FROSch) solver framework. FROSch has been under active development in this project. It is part of the ShyLU-FROSch-package in the open source Trilinos software library. Based on this implementation it was possible to investigate the numerical and parallel scalability of monolithic FROSch solvers for problems with strong, nonlinear coupling between mechanics and diffusion. Moreover, three-level FROSch solvers have been investigated, which will be needed in the second phase to achieve parallel scalability for the challenging problems under investigation. For the second funding phase, solution strategies for minimization principle-based formulations of chemo-mechanics shall be accompanied by saddle point formulations and developed in a closed loop with adapted FROSch solvers. Moreover, a major emphasis is placed on phasefield (diffuse interface) problems on the modeling side. In particular, we are interested in simulating dissipative, non-equilibrium processes, in which multiple chemical components may react and diffuse across the boundaries of multiple phases. Here, the governing equations appear as coupled sets of Allen-Cahn, Cahn-Hilliard and Fickian diffusion equations. Again, we will study the advantages and disadvantages of different formulations regarding physical interpretability of boundary conditions, required ansatz functions, as well as robustness and scalability of the iterative solvers by means of representative numerical examples. Other aspects on the theoretical side include the formulation of variationally-consistent homogenization schemes and their extension to non-isothermal chemo-mechanical processes. On the solver side we will develop monolithic three-level approaches as well as monolithic nonlinear approaches tailored to the problems.