

A MICRO/MACRO PARAREAL ALGORITHM FOR MULTISCALE-IN-TIME SYSTEMS

F. Legoll^{1,*}, T. Lelièvre² and G. Samaey³

¹ Laboratoire Navier, École des Ponts ParisTech, Université Paris-Est and MICMAC team-project, INRIA Rocquencourt, FRANCE, legoll@lami.enpc.fr

² CERMICS, École des Ponts ParisTech, Université Paris-Est and MICMAC team-project, INRIA Rocquencourt, FRANCE

³ Scientific Computing, Department of Computer Science, KU Leuven, BELGIUM

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The question of coarse-graining is ubiquitous in materials science. It often amounts to going from a high-dimensional description of a system, with degrees of freedom which possibly evolve on different characteristic times, to a low dimensional description, only retaining the “slow” degrees of freedom. Think e.g. of molecular simulation (where coarse-grained models are written in terms of low-dimensional reaction coordinates) or complex fluids (where coarse-grained models are used to circumvent or simplify the simulation of the evolving microstructure).

We introduce and analyze a micro/macro parareal algorithm for the time-parallel integration of this type of problems [1]. The algorithm first computes a cheap macroscopic solution using a propagator of the coarse-grained model. This solution is iteratively corrected by using a propagator of the fine-scale model, in the parareal algorithm spirit. The iterative procedure converges to the solution of the fine-scale model.

The efficiency of the approach is demonstrated on the basis of numerical analysis arguments and numerical experiments on a simple class of problems.

REFERENCES

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