

# A micro-macro parareal algorithm for slow-fast systems with applications to molecular dynamics

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We introduce a micro-macro parareal algorithm for the time-parallel integration of multiscale-in-time systems. The algorithm first computes a cheap, but inaccurate, solution using a coarse propagator (simulating an approximate slow macroscopic model), which is iteratively corrected using a fine-scale propagator (accurately simulating the full microscopic dynamics). This correction is done in parallel over many subintervals, thereby reducing the wall-clock time needed to obtain the solution, compared to the integration of the full microscopic model. We provide a numerical analysis of the algorithm for a prototypical example of a micro-macro model, namely singularly perturbed ordinary differential equations. We show that the computed solution converges to the full microscopic solution (when the parareal iterations proceed) only if special care is taken during the coupling of the microscopic and macroscopic levels of description. The convergence rate depends on the modeling error of the approximate macroscopic model. We illustrate these results with numerical experiments, including a non-trivial model inspired by molecular dynamics.