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A PARALLEL ALGORITHM FOR PSEUDO-ARCLENGTH CONTINUATION

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Over the past 25 year, a number of tools from numerical dynamical systems analysis have been adapted to the study of fluid dynamics. Often these tools, whether they aim to compute periodic or quasi-periodic solutions, homoclinic or heteroclinic connections or invariant manifolds, are cast in the form of a continuation problem.

In this approach, the targeted special flows are realized as solutions to a set of nonlinear equations, underdetermined by a single constraint, which comprises the discretized Navier-Stokes equation as one component. Assuming we have a good approximation to one solution to start from, we can then reconstruct a family of solutions by a prediction-correction method. In the prediction step, we extrapolate from previously computed solutions, and in the correction step an iterative algorithm such as Newton-Raphson is used to refine this prediction. The result is a set of approximate solutions that spans a range of a physical parameter, such as the Reynolds number, or an artificial parameter used to foliate a manifold.

The essential step in adapting such continuation methods to the study of fluid dynamics is usually the elimination of all large matrices, such as the Jacobian matrix that plays a central role in Newton-Raphson iteration. Even for moderately complicated, three-dimensional fluid flow on a small domain, the number of equations to be solved simultaneously can be in the tens of thousands, and the computation and decomposition of system-sized matrices is prohibitively slow. Since the evaluation and time-stepping of the underlying discretized Navier-Stokes equation is usually done in a near optimal way, as the result of decades of intense effort by fluid physicists and numerical analysts, little progress can be expected from re-examining that component of the problem.

Sánchez *et al.* [1] instead addressed the issue by introducing linear solvers based on Krylov subspace iteration to the corrector step. Sometimes in combination with some form of preconditioning, such solvers bring down the computational cost by several orders of magnitude, thereby bringing into the realm a possibility computations that were previously unimaginable. The use of Krylov subspace methods in conjunction with continuation is now standard enough to be simply called Newton-Krylov continuation.

Using this nearly optimal combination of matrix-free linear solving and efficient simulation codes, researchers in fluid dynamics have computed a variety of special flows in channels and pipes that help answer open questions on the transition from laminar to turbulent flow [2]. The answers are far form complete, though, as the results obtained so far are usually far removed from laboratory measurements. In order to bring the computational work closer to observations, and enable direct comparison, larger domains and more complicated flows (as measured, for instance, by Reynolds or Reyleigh numbers) need to be tackled. The main

impediment to such computations is still the time it takes to perform the inner iteration, over Krylov subspace vectors, which, in turn, requires running the underlying fluid simulation code.

In this presentation, we will show how to optimize the continuation algorithm itself. Standard pseudo-arclength continuation is inherently serial, as each sequence of corrector steps must converge completely before a new trial solution is seeded. Moreover, if a corrector sequence fails to converge, a new prediction is made with a smaller step size, and computing time is lost. We employ two stategies to minimize the lost time: we seed new trial solutions from a corrector sequence that has not yet converged, and use multiple step sizes for each prediction. Since all corrector sequences are independent, they are run in parallel. Thus, if a sequence fails, CPU time is lost, but with high likelyhood another sequence, running in parallel, has converged .

For two test cases, one concerning travelling waves in a 1+1D nonlinear partial differential equation and one concerning periodic solutions in weak, isotropic turbulence, we show that the wall time can be reduced by a factor of two using as few as three CPUs. When using up to fourty CPUs, a reduction by a factor of three is possible.

We have released a software package, PAMPAC, that implements the parallel continuation algorithm [3]. The user needs to specify two functions, one for the computation of the residual of the system of nonlinear equations, and one for taking a single corrector step. These functions can be based on any fluid dyamics simulation code.

We will explain the algorithm in detail, using visualization in the form of coloured trees, and demonstrate the use of PAMPAC.

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