Contemporary approaches for the high-fidelity simulation of large-scale physical systems

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Linear Operator Learning Using GreenONets and a Multi-Level Neural Network Approach

In collaboration with Ziad Aldirany (Polytechnique Montréal), Régis Cottereau (Aix-Marseille Université), and Serge Prudhomme (Polytechnique Montréal).

The solution of boundary-value problems using deep learning approaches, such as physics-informed neural networks [Raissi et al., JCP, 2019] or deep operator networks [Lu et al., NMI, 2021], has been extensively investigated in recent years. However, achieving high accuracy in the approximations obtained from these methods often remains a significant challenge. A multi-level neural network approach was proposed in [Aldirany et al., CMAME, 2024] that allows one to iteratively reduce the errors, sometimes within machine precision, when approximating a solution using PINNs. In this work, we extend the multi-level approach to approximate linear operators using Green operator networks (GreenONets) as described in [Aldirany et al., CMA, 2024]. Starting with an initial approximation of the operator, we correct the solution by considering a different Green operator network involving higher frequencies. The method enables one to iteratively reduce the high-frequency component of the residuals. Numerical examples will be presented to demonstrate the efficiency of the proposed multi-level approach.

YVES BOURGAULT, Université d'Ottawa

Linearly-Implicit Backward Difference Formulas for Navier-Stokes Equations

We propose a linearly-implicit method (called LBDFT) to solve the incompressible Navier-Stokes equations. Linearly-implicit methods have an algorithmic complexity that lies between fully-implicit and semi-implicit time-stepping schemes. In LBDFT, the nonlinear advection in the Navier-Stokes equations is split into three linear terms using a Taylor series expansion. One term is taken explicitly and the other two are updated with the linear diffusion term at each time step. Linearly-implicit methods were also proposed in [Garcia-Archilla & Novo, IMA J Num Analysis, 2022][Wang et als, CAM, 2023], in this case based on extrapolation formulae as for semi-implicit methods. These methods are then compared with various fully-implicit and semi-implicit time-stepping methods in terms of accuracy, stability, computing time and ability to compute various flows. We first use two standard test cases to assess the methods. We observed that linearly-implicit methods are more CPU efficient compared to fully-implicit BDF, both at second- and third-order of accuracy. Our third test case explores the ability of the methods to compute steady flows at high Reynolds numbers. LBDFT was able to compute steady cavity flows for Reynolds up to 500,000. Our last test case explores unsteady flows at large Reynolds numbers. It was observed that the linearly-implicit methods allow significantly larger critical time step (40-50 times larger) compared to the semi-implicit methods, the latters needing a stabilization term to maintain their stability. This article is co-authored with Kak Choon Loy, Faculty of Computer Science and Mathematics, Universiti Malaysia Terengganu, Malaysia.

DIANE GUIGNARD, University of Ottawa

SALAH IBDELOUCH, Polytechnique Montréal

PHILIPPE-ANDRÉ LUNEAU, Université Laval

Accelerating Nonexpansive Iterative Schemes with On-the-fly Reduced Order Modeling

Whether for solving nonlinear equations, optimization problems, or autonomous dynamical systems, fixed-point-type iterations are widely used in numerical sciences. However, when the goal is to iteratively solve a problem that depends on the solution of a partial differential equation, a large linear system typically needs to be solved at each iteration. On-the-fly reduced-order modeling enables the construction of a low-dimensional, self-correcting approximation of the solution to this system during the iterative process. When the process itself is nonexpansive, theoretical guarantees regarding convergence can be established. Numerical examples will illustrate that, in some cases, this methodology can lead to speedups compared to a classical fixed-point scheme.

CONOR MCCOID, McMaster University
Symmetrized cells in adaptive optimized Schwarz

Adaptive optimized Schwarz methods update transmission conditions at each iteration to achieve superlinear convergence. For multiple subdomains, this can be done by considering each subdomain individually, forming symmetrized cells, building transmission conditions for each cell, and then reconstructing a fast global Schwarz method. The process of building transmission conditions for the symmetrized cells has continuous analogues in methods for perfectly matched layers. This talk explores implementation options as well as issues such as crosspoints and scaling.

MATHIEU MULLINS, ETS Montréal

ALEJANDRO ALFONSO RODRIGUEZ, Université Laval
Analyzing Convergence of Schwarz Waveform Relaxation Methods Using Exponential Weighting

The Schwarz Waveform Relaxation (SWR) method represents a class of numerical domain decomposition techniques developed for solving space-time partial differential equations using iterative procedures. The approach begins by dividing the physical spatial domain into several overlapping or non-overlapping subdomains. For each subdomain, the corresponding time-dependent problem is solved independently and in parallel over the entire time interval. After solving, information at the subdomain interfaces is exchanged across the entire time window. This process is repeated iteratively, with updated interface values, until the global solution converges. Analyzing and predicting their convergence behavior can be challenging. In many cases, the convergence estimates require evaluating inverse Laplace transforms of complicated expressions. Unfortunately, for some types of interface conditions, there are no known explicit formulas for these inverse transforms. To overcome this obstacle, we will show how exponential weighting techniques can be used to derive superlinear convergence estimates without computing the inverse Laplace transform explicitly. These techniques simplify the analysis while still capturing the essential features of the SWR iteration. It will be used to analyze the convergence of SWR with the Dirichlet and Robin transmission conditions.

DAVE SUJAL, University of Calgary

VINCENT THIBEAULT, Université Laval/Dynamica