Automatic stabilization of difficult isogeometric analysis simulations with Deep Neural Networks

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1. Introduction

Numerical solutions of Partial Differential Equations with Finite Element Method have multiple applications in science and engineering. Several challenging problems require special stabilization methods to deliver accurate results of the numerical simulations. The advection-dominated diffusion problem is an example of such problems. Unstable numerical methods generate unphysical oscillations, and they make no physical sense. Obtaining accurate and stable numerical simulations is difficult, and the method of stabilization depends on the parameters of the partial differential equations. They require a deep knowledge of an expert in the field of numerical analysis. We propose a method to construct and train an artificial expert in stabilizing numerical simulations based on partial differential equations. We create a neural network-driven artificial intelligence that makes decisions about the method of stabilizing computer simulations. It will automatically stabilize difficult numerical simulations in a linear computational cost by generating the optimal test functions. These test functions can be utilized for building an unconditionally stable system of linear equations. The optimal test functions proposed by artificial intelligence will not depend on the right-hand side, and thus they may be utilized in a large class of PDE-based simulations with different forcing and boundary conditions. We test our method on the model one-dimensional advection-dominated diffusion problem. But the methodology presented here can also be applied in two and three dimensions. It can be extended to challenging computational problems, including Navier-Stokes simulations with high Reynolds number or high contrast Maxwell equations. The artificial neural network's optimal test functions can be used to generate a sparse system of linear equations. This system of equations will have a structure allowing for a fast, accurate, and stable solution of the considered PDE.

2. Automatic stabilization with neural networks

Recently, there is a significant interest in research of possible application of Deep Neural Networks into finite element method simulations [13,14]. Paper [14] is an introduction to Deep Neural Network for computational scientists working already with the simulations. In [15] the authors consider the problem of representing some classes of real-valued univariate functions used in approximation with deep neural networks (deep NN, DNN) based on rectified linear unit (ReLU) activation functions. They show how the so-called ReLU NN calculus rules can be applied to obtain

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the representation of piecewise linear continuous functions. In particular, DNN approximation rates match those achieved by free-knot (h-adaptive) and order-adaptive (hp-adaptive) approximations. In [13] the authors show that it is possible to guide goal-oriented adaptivity for stationary problems using DNN. The finite element method utilizes high-order basis functions, e.g., Lagrange polynomials in the classical finite element method (FEM) [4] or B-spline basis functions in isogeometric analysis (IGA) [1]. There are several challenging problems solved by FEM and IGA, such as analysis of the construction of civil engineering structures, cars or airplanes [6], geophysical applications like identification of oil and gas bearing formations [12], bioengineering simulations like modeling of cancer growth [7], blood flow simulations [11], wind turbine aerodynamics [3] or modeling of propagation of acoustic and electromagnetic waves over the human head [2]. They require special stabilization methods to deliver high accuracy numerical solution.

We plan to train the neural network to find the optimal test functions stabilizing the time-dependent IGA FEM simulations. We also propose a method to solve a Petrov-Galerkin formulation with the optimal test functions in a linear computational cost on tensor product grids. The simulations of difficult, unstable time-dependent problems, like advection-dominated diffusion [8], high-Reynolds number Navier-Stokes equations [9], or high-contrast material Maxwell equations, have several important applications in science and engineering.

There are several stabilization methods, such as Streamline-Petrov Upwind Galerkin method (SUPG) [5], discontinuous Galerkin method (DG) [10], as well as residual minimization (RM) method [8,9]. We will use the Petrov-Galerkin formulation with the optimal test functions. It can be derived directly from the RM method. The RM for a given trial space it uses the larger test space, while for the Petrov-Galerkin formulation, we can compute the optimal test functions living in the subspace of the test space. The number of the optimal test functions is equal to the dimension of the trial space. The Petrov-Galerkin formulation, used for stabilization, enables interfacing with DNN. The DNN can be trained by running several simulations and using the computations of the optimal test functions. The test functions will be parameterized using the B-spline basis. The input to the DNN will be the problem parameters and the trial space. The output from the DNN will be the optimal test functions coefficients. Later, by running the simulations in every time step, using the actual configuration of parameters from the current time step, we can ask the DNN to provide the optimal test functions that will stabilize the computations for a given trial space. Such an efficient, ultra-fast, and automatic way of stabilization of time-dependent simulations is not available nowadays, and it may have a big impact on the computational science community.

3. Applications

We develop a method for ultra-fast solvers using Petrov-Galerkin formulations with optimal test functions for time-dependent problems. These solvers for a given approximation space require determining the optimal test functions that will stabilize the simulations. The solver itself, if properly designed using the alternating-directions algorithms, can deliver a linear computational cost, but the problem of finding the optimal test spaces is computationally hard. We also claim that for transient simulations, where the model parameters change from one time step to another, the test spaces that stabilize the simulations may change from one time step to another.

Thus, we construct and train DNN to find optimal test functions to stabilize Petrov-Galerkin formulations with classical and isogeometric finite element method simulations of time-dependent problems, perform on regular patches of elements. The DNN will approximate the coefficients of linear combinations of B-spline basis functions used to test the Petrov-Galerkin formulation employed within the classical and isogeometric finite element method. Trained on the simulations' parameters, different deep neural networks for different classes of problems, they will deliver in a linear computational cost, the parameters of the optimal test functions that can be used for stabilization of the simulations.

The simulations of difficult, unstable time-dependent problems, like advection-dominated diffusion-reaction, high-Reynolds number Navier-Stokes equations, or high-contrast material Maxwell equations, have several important applications in science and engineering.

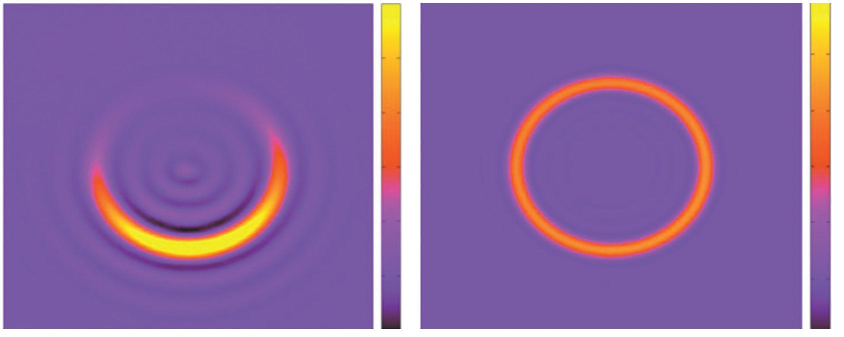

Figure 1. Stabilization of advection-diffusion simulations.

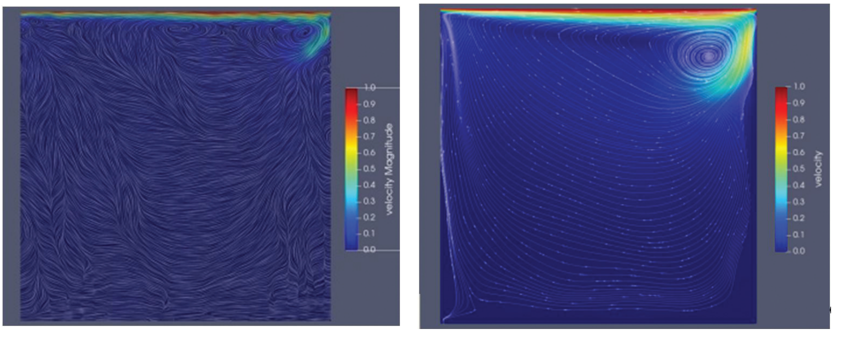

Figure 2. Stabilization of Navier-Stokes simulations.

References

1. Cottrell J.A., Hughes T.J.R., Bazilevs Y.: *Isogeometric analysis: toward integration of CAD and FEA*. John Wiley & Sons, 2009.
2. Demkowicz L., Gatto P., Kurtz J., Paszyński M., Rachowicz W., Bleszynski E., Bleszynski E.: *Hamilton M., Champlin C., Pardo D., Modeling of bone conduction of sound in the human head using hp finite elements i. code design and verification*. Computer Methods in Applied Mechanics and Engineering, 21-22, 2011, 1757–1773.
3. Hsu M.-C., Akkerman I., Bazilevs, Y.: *High-performance computing of wind turbine aerodynamics using isogeometric analysis*. Computers & Fluids, 49, 2011, 93–100.
4. Hughes T.J.R., Belytschko T.: *The finite element method: Linear static and dynamic finite element analysis*. Computer-Aided Civil and Infrastructure Engineering, 4, 1989, 245–246.
5. Hughes T.J.R., Franca L., Mallet M.: *A new finite element formulation for computational fluid dynamics: Vi. convergence analysis of the generalized supg formulation for linear time-dependent multidimensional advective-diffusive systems*. Computer Methods in Applied Mechanics and Engineering, 63, 1987, 97–112.
6. Hughes T.J.R., Cottrell J.A., Bazilevs Z.: *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*. Computer methods in applied mechanics and engineering, 194, 2005, 4135–4195.

7. Łoś M., Kłusek A., Hassaan M.A., Pingali K., Dzwinel W., Paszyński M.: *Parallel fast isogeometric l2 projection solver with galois system for 3d tumor growth simulations*. Computer Methods in Applied Mechanics and Engineering, 343, 2019, 1–22.
8. Łoś M., Munoz-Matute J., Muga I., Paszyński M.: *Isogeometric residual minimization method (igrm) with direction splitting for non-stationary advection–diffusion problems*. Computers & Mathematics with Applications, 79, 2019, 213–229.
9. Łoś M, Munoz-Matute J., Muga I., Paszyński M.: *Isogeometric residual minimization for time-dependent stokes and navier-stokes problems*. Computers & Mathematics with Applications, 95, 2021, 200–214.
10. Pietro D., Ern A.: *Mathematical Aspects of Discontinuous Galerkin Methods*. Springer, 2011.
11. Taylor C.A., Hughes T.J.R., Zarins C.K.: *Finite element modeling of blood flow in arteries*. Computer Methods in Applied Mechanics and Engineering, 158, 1998, 151–196.
12. Pardo D., Torres-Verdin C., Nam M.J., Paszyński M., Calo V.M.: *Fourier series expansion in a non-orthogonal system of coordinates for the simulation of 3d alternating current borehole resistivity measurements*. Computer Methods in Applied Mechanics and Engineering, 45–48, 2008, 3836–3849.
13. Brevis I., Muga I., van der Zee K.: *Data-driven finite elements methods: Machine learning acceleration of goal-oriented computations*. arXiv:2003.04485, 2020, 1-24.
14. Higham C.F.: *Deep learning: An introduction for applied mathematicians*. SIAM Review, 61, 2019, 860– 891.
15. Opschoor J.A.A., Petersen P.C., Schwab C.: *Deep relu networks and high-order finite element methods*. Analysis and Applications, 18, 2020, 715–770.

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