2019-2020 Grand Challenge Award Final Report

Awardee: **Leszek Demkowicz, Professor**
Aerospace Engineering & Engineering Mechanics

Research Award Title: **Development of A Scalable MPI *hp*-Adaptive Finite Element Software Library for Complex Multiphysics Applications**

Research Summary

A scalable parallel version of hp3D—a finite element (FE) software for analysis and discretization of complex three-dimensional multiphysics applications has been developed. The software supports hybrid MPI/OpenMP parallelism for large-scale computation on modern manycore architectures. The focus of the effort lies on the development and optimization of the parallel software infrastructure underlying all distributed computation. While the code supports standard Galerkin methods, special emphasis is given to systems arising from discretization with the discontinuous Petrov–Galerkin (DPG) method. The method guarantees discrete stability by employing locally optimal test functions, and it has a built-in error indicator which we exploit to guide mesh adaptivity. In addition to interfacing with thirdparty packages for various tasks, we have developed our own tools including a parallel nested dissection solver suitable for scalable FE computation of waveguide geometries. For weak-scaling results with up to 24 576 CPU cores and numerical simulations with more than one billion degrees of freedom see [3].

The new software capabilities enable solution of challenging wave propagation problems with important applications in acoustics, elastodynamics, and electromagnetics. These applications are difficult to solve in the high-frequency regime because the FE discretization suffers from significant numerical pollution errors that increase with the wavenumber. It is critical to control these errors to obtain a stable and accurate method. We studied [4] the pollution effect for waveguide problems with more than 8 000 wavelengths in the context of robust DPG FE discretizations for the time-harmonic Maxwell equations. We also discussed adaptive refinement strategies for multi-mode fiber waveguides where the propagating transverse modes must be resolved sufficiently. Our study shows the applicability of the DPG error indicator to this class of problems.

As promised, an extensive documentation is underway. A book documenting the code [5] is under preparation and should be finished in year 2021.

Presentations made

The following presentations acknowledged the award.

- S. Henneking, "A Numerical Study of the Pollution Error and DPG Adaptivity for Long Waveguide Simulations", FE Rodeo, Baylor University, Waco, Feb. 28-29, 2020.
- L. Demkowicz, "Short course on the DPG Method." Aachen University, July 16, 2020 (remote).

The work will also be presented by S. Henneking during the oncoming CSE conference (remote) in March 2021.

Papers published

The development of the parallel MPI/openMP hp3D code has been the subject of the dissertation of Stefan Henneking [3]. Papers [2, 4, 6] describe projects in which we have used the parallel MPI/openMP hp3D code or have done a substantial new development in the code. The serial version of the code was used in papers [9, 1] and dissertations of Socratis Petrides [8], and Jaime Mora-Paz [7].

Awards or recognition received

We managed to secure a small grant from Sandia National Labs: "A Scalable MPI/OpenMP hp-Adaptive Finite Element Software Library for Complex DoD Multiphysics Applications", 04/01/2019 - 9/30/2019, $50,000. In October 2020, we submitted to NSF the proposal on: *Elements:Software. A Scalable Open-Source hp-Adaptive FE Software for Complex Multiphysics Applications* (pending).

References

1. C. Bacuta, L. Demkowicz, J. Mora Paz, and Ch. Xenophontos. Analysis of non-conforming DPG methods on polyhedral meshes using fractional Sobolev norms. *Comp. and Math. Appl.*, 2020. Special Issue on Minimum Residual Methods, in print, see also Oden Institute Report 2020/3.

2. J. Badger, S. Henneking, and L. Demkowicz. Fast integration of DPG matrices based on tensorization (Part II: Prismatic elements). *Finite Elements in Analysis & Design*, 172:103385, 2020. In print, see also Oden Institute Report 2019/15.

3. S. Henneking. *A Scalable hp-Adaptive Finite Element Software with Applications in Fiber Optics.* PhD thesis, The University of Texas at Austin, Austin, TX 78712, March 2021. Computational Science, Engineering and Mathematics (CSEM) program.

4. S.Henneking and L.Demkowicz. A numerical study of the pollution error and DPG adaptivity for long waveguide simulations. *Comp. and Math. Appl.*, 2020. In print, see also Oden Institute Report 2019/20.

5. S. Henneking and L. Demkowicz. *Computing with hp Finite Elements III. Parallel hp Code.* 2021. i preparation, 40 pages and growing.

6. S. Henneking, J. Grosek, and L. Demkowicz. Model and computational advancements to full vectorial Maxwell model for studying fiber amplifiers. *Comp. and Math. Appl.*, 85:30–41, 2021.

7. J. Mora-Paz. *PolyDPG: A discontinuous Petrov-Galerkin methodology for polytopal meshes with applications to elasticity.* PhD thesis, The University of Texas at Austin, Austin, TX 78712, November 2020. Computational Science, Engineering and Mathematics (CSEM) program.

8. S. Petrides. *Adaptive multilevel solvers for the discontinuous Petrov-Galerkin method with an emphasis on high- frequency wave propagation.* PhD thesis, The University of Texas at Austin, Austin, TX 78712, March 2019. Computational Science, Engineering and Mathematics (CSEM) program.

9. S. Petrides and L. Demkowicz. An adaptive multigrid solver for DPG methods with applications in linear acoustics and electromagnetics. *Comp. and Math. Appl.*, 2021.