hp3D: A Scalable MPI/OpenMP hp-Adaptive Finite Element Software Library for Complex Multiphysics Applications

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Summary

The hp3D finite element (FE) library is a tool for computational modeling of engineering applications. The library provides a framework for discretization of three-dimensional[1] multiphysics problems described by systems of partial differential equations. hp3D can be compiled in real or complex mode to accommodate the need for real- or complex-valued physics variables, respectively. The library is written entirely in Fortran; user applications interfacing with the library are also written in Fortran. The hp3D software can be installed and runs efficiently on various CPU-based compute architectures, from laptops and single workstations to state-of-the-art supercomputers.

Statement of need

hp3D combines a list of unique features and algorithms setting it apart from other publicly available finite element libraries. The software supports hybrid meshes combining elements of "all shapes:" hexahedra, tetrahedra, prisms, and pyramids. The internal Geometric Modeling Package (GMP) provides support for *exact geometry* elements and *isoparametric* elements. Exact geometry elements directly use the parametrizations provided by GMP resulting in computations with no geometry error; isoparametric elements approximate the geometry maps with polynomials spanning the element space of shape functions. hp3D's shape functions package provides compatible discretization of energy spaces forming the $H^1 - H(\text{curl}) - H(\text{div}) - L^2$ exact sequence (Demkowicz, 2023; Fuentes et al., 2015). Additionally, the hp3D FE code sets itself apart from other advanced FE libraries (e.g., MFEM (Anderson et al., 2021) or deal.II (Bangerth et al., 2007)) by supporting *hp-adaptive* solutions with *anisotropic refinements* in both element size h and polynomial order p. Such hp-adaptive methods are the most efficient way to converge to difficult solutions, e.g., resolving solutions with boundary layers, adapting toward geometric singularities, etc. (Chakraborty et al., 2023). hp3D features a number of unique algorithms, including *constrained approximation* routines for assembling elements with hanging nodes (Demkowicz et al., 1989; Oden et al., 1989; Rachowicz et al., 1989), and *projection-based interpolation* for computation of nodal constraints (Demkowicz, 2008). Besides discretization with the standard Bubnov-Galerkin FE method, the hp3D library also supports discretization with the discontinuous Petrov-Galerkin (DPG) method (Demkowicz & Gopalakrishnan, 2017). The hp3D software leverages hybrid MPI/OpenMP parallelism to run efficiently on large-scale computing facilities (Badger et al., 2023; Henneking, 2021).

[1]The hp2D FE library for two-dimensional problems is conceptually equivalent to hp3D but has not yet been released publicly.

Dependencies

hp3D interfaces with several well-established third-party libraries: for mesh partitioning (ParMETIS (Karypis & Kumar, 1998), PT-Scotch (Chevalier & Pellegrini, 2008)), for dynamic load balancing (Zoltan (Devine et al., 2002)), for linear solvers (MUMPS (Amestoy et al., 2001), PETSc (Balay et al., 2023)), and for I/O (pHDF5 (The HDF Group, 1997)). We note that all of these dependencies can be directly installed via PETSc. Additionally, the geometry mesh and the solution can be exported to VTK and visualized with ParaView (Ahrens et al., 2005).

Examples of applications

Some examples of 3D applications that have been implemented in hp3D include modeling of acoustic wave propagation in the human head (Gatto, 2012), modeling of electromagnetic waves with thermal effects in the human head (Kim, 2013), electromagnetic and acoustic scattering and high-frequency beams (Petrides, 2019; Petrides & Demkowicz, 2021), modeling of insulators in high-energy density electric motors (thermo-viscoelasticity) (Fuentes et al., 2017), and modeling of optical amplifiers (nonlinear Maxwell equations coupled with the heat equation) (Henneking et al., 2022, 2021; Nagaraj et al., 2019).

Further reading

Instructions on installing and using the code are available in the hp3D user manual (Henneking & Demkowicz, 2022). hp3D's underlying algorithms are described in various published articles and books. Many parts of the current version of the hp3D software are based on the algorithms described in the two-volume hp book series (Demkowicz, 2006; Demkowicz et al., 2007) on the former 2D and 3D versions of the code (which were not published as open-source libraries). A third hp book volume detailing the additions and modifications of the newest version, including its MPI/OpenMP parallel algorithms, will be published soon (Henneking, Demkowicz, et al., 2024). The orientation-embedded shape functions package is described in Fuentes et al. (2015). Details on the FE methodology and conforming discretization of exact-sequence elements are given in Demkowicz (2023).

The source code for hp3D has been archived to Zenodo (Henneking, Petrides, et al., 2024).

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References

Ahrens, J., Geveci, B., & Law, C. (2005). Paraview: An end-user tool for large data visualization. In *The visualization handbook*. Elsevier. https://doi.org/10.1016/b978-012387582-2/50038-1

Amestoy, P. R., Duff, I. S., L'Excellent, J. Y., & Koster, J. (2001). A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM Journal on Matrix Analysis and Applications*, *23*(1), 15–41. https://doi.org/10.1137/s0895479899358194

Anderson, R., Andrej, J., Barker, A., Bramwell, J., Camier, J.-S., Cerveny, J., Dobrev, V., Dudouit, Y., Fisher, A., Kolev, T., & others. (2021). MFEM: A modular finite element methods library. *Computers & Mathematics with Applications*, *81*, 42–74. https://doi.org/10.1016/j.camwa.2020.06.009

Badger, J., Henneking, S., Petrides, S., & Demkowicz, L. (2023). Scalable DPG multigrid solver for Helmholtz problems: A study on convergence. *Computers & Mathematics with Applications*, *148*, 81–92. https://doi.org/10.1016/j.camwa.2023.07.006

Balay, S., Abhyankar, S., Adams, M. F., Benson, S., Brown, J., Brune, P., Buschelman, K., Constantinescu, E., Dalcin, L., Dener, A., Eijkhout, V., Faibussowitsch, J., Gropp, W. D., Hapla, V., Isaac, T., Jolivet, P., Karpeev, D., Kaushik, D., Knepley, M. G., … Zhang, J. (2023). *PETSc/TAO users manual* (ANL-21/39 - Revision 3.20). Argonne National Laboratory. https://doi.org/10.2172/2205494

Bangerth, W., Hartmann, R., & Kanschat, G. (2007). Deal.II–general-purpose object-oriented finite element library. *ACM Transactions on Mathematical Software*, *33*(4), 24–es. https://doi.org/10.1145/1268776.1268779

Chakraborty, A., Henneking, S., & Demkowicz, L. (2023). An anisotropic hp-adaptation framework for ultraweak discontinuous Petrov–Galerkin formulations. *arXiv Preprint arXiv:2309.00726*. https://doi.org/10.48550/arXiv.2309.00726

Chevalier, C., & Pellegrini, F. (2008). PT-Scotch: A tool for efficient parallel graph ordering. *Parallel Computing*, *34*(6-8), 318–331. https://doi.org/10.1016/j.parco.2007.12.001

Demkowicz, L. (2006). *Computing with hp Finite Elements. I. One and Two Dimensional Elliptic and Maxwell Problems*. Chapman & Hall/CRC Press, Taylor; Francis. https://doi.org/10.1201/9781420011685

Demkowicz, L. (2008). Polynomial exact sequences and projection-based interpolation with application to Maxwell equations. In *Mixed finite elements, compatibility conditions, and applications* (pp. 101–158). Springer. https://doi.org/10.1007/978-3-540-78319-0_3

Demkowicz, L. (2023). *Mathematical theory of finite elements*. Society for Industrial; Applied Mathematics. https://doi.org/10.1137/1.9781611977738

Demkowicz, L., & Gopalakrishnan, J. (2017). Discontinuous Petrov–Galerkin (DPG) method. *Encyclopedia of Computational Mechanics Second Edition*, 1–15. https://doi.org/10.1002/9781119176817.ecm2105

Demkowicz, L., Kurtz, J., Pardo, D., Paszyński, M., Rachowicz, W., & Zdunek, A. (2007). *Computing with hp Finite Elements. II. Frontiers: Three Dimensional Elliptic and Maxwell Problems with Applications*. Chapman & Hall/CRC. https://doi.org/10.1201/9781420011692

Demkowicz, L., Oden, J. T., & Rachowicz, W. (1989). Toward a universal hp adaptive finite element strategy. Part 1: Constrained approximation and data structure. *Computer Methods in Applied Mechanics and Engineering*, *77*, 79–112. https://doi.org/10.1016/0045-7825(89)90129-1

Devine, K., Boman, E., Heaphy, R., Hendrickson, B., & Vaughan, C. (2002). Zoltan data management services for parallel dynamic applications. *Computing in Science and Engineering*, *4*(2), 90–97. https://doi.org/10.1109/5992.988653

Fuentes, F., Demkowicz, L., & Wilder, A. (2017). Using a DPG method to validate DMA experimental calibration of viscoelastic materials. *Computers & Mathematics with Applications*, *325*, 748–765. https://doi.org/10.1016/j.cma.2017.07.012

Fuentes, F., Keith, B., Demkowicz, L., & Nagaraj, S. (2015). Orientation embedded high order shape functions for the exact sequence elements of all shapes. *Computers & Mathematics with Applications*, *70*(4), 353–458. https://doi.org/10.1016/j.camwa.2015.04.027

Gatto, P. (2012). *Modeling bone conduction of sound in the human head using hp-finite elements* [PhD thesis, The University of Texas at Austin]. https://hdl.handle.net/2152/19517

Henneking, S. (2021). *A scalable hp-adaptive finite element software with applications in fiber optics* [PhD thesis, The University of Texas at Austin]. https://doi.org/10.26153/tsw/13716

Henneking, S., & Demkowicz, L. (2022). hp3D User Manual. *arXiv Preprint arXiv:2207.12211*. https://doi.org/10.48550/arXiv.2207.12211

Henneking, S., Demkowicz, L., Petrides, S., Fuentes, F., Keith, B., & Gatto, P. (2024). *Computing with hp Finite Elements. III. Parallel hp3D Code*. In preparation.

Henneking, S., Grosek, J., & Demkowicz, L. (2022). Parallel simulations of high-power optical fiber amplifiers. *Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2020+1*, 349–360. https://doi.org/10.1007/978-3-031-20432-6_22

Henneking, S., Grosek, J., & Demkowicz, L. (2021). Model and computational advancements to full vectorial Maxwell model for studying fiber amplifiers. *Computers & Mathematics with Applications*, *85*, 30–41. https://doi.org/10.1016/j.camwa.2021.01.006

Henneking, S., Petrides, S., Fuentes, F., Badger, J., & Demkowicz, L. (2024). *hp3D: A scalable MPI/OpenMP hp-adaptive finite element software library for complex multiphysics applications (v1.0)*. https://doi.org/10.5281/zenodo.10763375

Karypis, G., & Kumar, V. (1998). A fast and high quality multilevel scheme for partitioning irregular graphs. *SIAM Journal on Scientific Computing*, *20*(1), 359–392. https://doi.org/10.1137/s1064827595287997

Kim, K. (2013). *Finite element modeling of electromagnetic radiation and induced heat transfer in the human body* [PhD thesis, The University of Texas at Austin]. https://hdl.handle.net/2152/21292

Nagaraj, S., Grosek, J., Petrides, S., Demkowicz, L., & Mora, J. D. (2019). A 3D DPG Maxwell approach to nonlinear Raman gain in fiber laser amplifiers. *Journal of Computational Physics*, *2*, 100002. https://doi.org/10.1016/j.jcpx.2019.100002

Oden, J. T., Demkowicz, L., Rachowicz, R., & Westermann, T. A. (1989). Toward a universal hp adaptive finite element strategy. Part 2: A posteriori error estimation. *Computer Methods in Applied Mechanics and Engineering*, *77*, 113–180. https://doi.org/10.1016/0045-7825(89)90130-8

Petrides, S. (2019). *Adaptive multilevel solvers for the discontinuous Petrov–Galerkin method with an emphasis on high-frequency wave propagation problems* [PhD thesis, The University of Texas at Austin]. https://doi.org/10.26153/tsw/2153

Petrides, S., & Demkowicz, L. (2021). An adaptive multigrid solver for DPG methods with applications in linear acoustics and electromagnetics. *Computers & Mathematics with Applications*, *87*, 12–26. https://doi.org/10.1016/j.camwa.2021.01.017

Rachowicz, W., Oden, J. T., & Demkowicz, L. (1989). Toward a universal hp adaptive finite element strategy. Part 3: Design of hp meshes. *Computer Methods in Applied Mechanics and Engineering*, *77*, 181–212. https://doi.org/10.1016/0045-7825(89)90131-X

The HDF Group. (1997). *Hierarchical data format version 5*. http://www.hdfgroup.org/HDF5