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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., 2020)), 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 et al., 2023). 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).

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