VERTEX-CFD: A multiphysics platform for fusion applications

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Summary:

The demand for high-performance computational fluid dynamics and multiphysics software packages has grown in recent years as a response to effort in complex engineering and research applications. Although the widespread deployment of high-performance computing (HPC) resources has enabled larger, more complex simulations to be conducted, few commercial or open-source software packages are available that (1) scale performantly on central processing unit (CPU) and graphical processing unit (GPU) computing architectures and (2) represent the multitude of physical processes relevant to these applications. The VERTEX-CFD software is developed to address this technical gap, with a special emphasis on high-fidelity multiphysics modeling of coupled turbulent fluid flow, heat transfer, and magnetohydrodynamics (MHD) for applications in fusion and fission energy and in other spaces. The VERTEX-CFD package was developed to solve the governing equations of these problems using a high-order continuous Galerkin finite element framework and fully implicit monolithic solvers. Special attention is being paid during the development process to verify and to validate the solver and to ensure performance portability across both CPU and GPU computing platforms. A comprehensive verification and validation (V&V) suite and unit tests were designed to assess the accuracy and convergence behavior of the VERTEX-CFD software for problems taken from the published literature.

Statement of need

Fusion energy development draws from a wide range of disciplines to describe design and to develop a functioning system. One challenging engineering task is to develop the fusion core component known as a "blanket." Because this component surrounds the burning plasma and must absorb almost all of the power from nuclear reactions, it must breed fuel, provide nuclear shielding, and provide energy deposition. Molten salt (MS) is a primary choice for cooling the blanket. A "salt blanket" in fusion energy is a layer of molten salt surrounding the fusion plasma. The molten salt acts as both a coolant and a material for neutron absorption, both of which are essential in fusion reactions. The salt blanket absorbs the high-energy neutrons produced by fusion, reducing the wear on reactor components, and converting some of the energy into heat for electricity generation. Molten salts have low electrical and thermal conductivity and experience lesser electromagnetic forces, but they are still turbulent. Heat transfer degradation in an MS flow caused by the reduction of turbulence by a magnetic field is a possible limitation of the MS blanket (R. M. Sergey Smolentsev & Abdou, 2005).

Two approaches are commonly adopted to predict MS flows exposed to a magnetic field: high-fidelity simulation (large-eddy simulation (LES) or direct numerical simulation (DNS)), and Reynolds-averaged Navier-Stokes (RANS) turbulence models. LESs can resolve turbulences at temporal and spatial scales at the expense of large HPC resources. Blanket design with LES is not possible because of current HPC limitations. Design optimization often requires multiple simulation runs to investigate performance under various conditions. The main technique that reduces the computational requirements of the analysis is the RANS turbulence model. This approach filters out the instantaneous velocity component, and the influence of the turbulence is modeled solely by the closure models. Turbulence modeling is a complex problem, and many turbulence models are available as described in the literature (Chen et al., 2022; Menter, 1992), albeit with many limitations (Castro et al., 2003). Furthermore, these models are not readily applicable to the MHD flows and would require modifications (M. A. Sergey Smolentsev Reza Miraghaie & Kunugi, 2002) because MHD effects introduce additional terms in the turbulence balance equations.

VERTEX-CFD is a new open-source package designed to address the modeling of MHD flows in complex geometries. It provides a robust multi-physics solver that can generate high-fidelity simulations by scaling on HPC platforms. VERTEX-CFD package also integrates artificial intelligence and machine learning (AI&ML) tools. These capabilities will provide the needed resources to extend the applicability of turbulence models to MHD flows, and perform design analysis.

Current capabilities and development workflow

Dependencies and deployment

The VERTEX-CFD package is an open-source code that is hosted on the Oak Ridge National Laboratory (ORNL) GitHub account https://github.com/ORNL/VERTEX-CFD. VERTEX-CFD is built on the Trilinos package (Trilinos Project Team, n.d.) that provides a suite of tools for code development on HPC platforms. It has been deployed on a wide variety of HPC platforms, ranging from small clusters to exascale computers including Summit (OLCF, 2024), Frontier (OLCF, 2024), and Perlmutter (NERSC, 2025).

Governing equations and discretization methods

The VERTEX-CFD software is still under active development and currently implements a set of partial differential equations (PDEs) discretized with a finite element method (FEM) and high-order temporal integrators: entropically damped artificial compressibility (EDAC) Navier-Stokes equations (Clausen, 2013), temperature equation, and induction-less MHD equations. Coupling between the different physics is ensured by source terms, including the buoyancy force f^B and the Lorentz force f^L. A conservative form of the set of PDEs is implemented in VERTEX-CFD, as shown in Equation 1, and it solves for pressure P, temperature T, velocity $\mathbf{u}$, and electric potential φ. Density ρ, heat capacity C_p, electrical conductivity σ, thermal conductivity k, and thermal expansion β are fluid properties and are all assumed to be constant. The external magnetic field, the reference temperature for buoyancy force, and the volumetric heat source are denoted by $\mathbf{B^0}$, T_0, and $q^{'''}$, respectively.

$$\begin{cases} \partial_t P + \nabla \cdot (P\mathbf{u}) = \frac{1}{M^2}\nabla \cdot \left(\frac{C_p \mu}{\gamma k}\nabla P\right) \\ \partial_t \rho \mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla P + \rho\nu\Delta\mathbf{u} + f^L - f^B \\ f^B = \rho \mathbf{g}\beta(T - T_0) \\ f^L = \mathbf{J}\times\mathbf{B^0} = \sigma\left(-\nabla\varphi\times\mathbf{B^0} + (\mathbf{B}\cdot\mathbf{u})\cdot\mathbf{B^0} - ||\mathbf{B^0}||^2\mathbf{u}\right) \\ \rho C_p\left(\partial_t T + \mathbf{u}\cdot\nabla T\right) = \nabla\cdot(k\nabla T) + q^{'''} \\ \nabla\cdot(\sigma\nabla\varphi) = \nabla\cdot[\sigma\mathbf{u}\times\mathbf{B^0}] \end{cases} \tag{1}$$

The set of equations presented above can be augmented with RANS turbulence models and the wall-adapting local eddy (WALE) viscosity model (Nicoud & Ducros, 1999) to simulate turbulent flows. Solvers, FEMs, and other relevant tools are provided by the Trilinos package (Trilinos Project Team, n.d.). The VERTEX-CFD software is designed to scale and to be compatible with various CPU and GPU architectures on HPC platforms by leveraging Kokkos (Trott et al., 2022) programming language. VERTEX-CFD software has demonstrated second-order temporal and spatial accuracy (Delchini et al., 2024).

Development workflow: testing, validation and verification

The long-term objectives of the VERTEX-CFD project are to facilitate the addition of new physical models by relying on a plug-and-play architecture and to guarantee the correctness of the implemented model over time. New physics and equations are easily added to the global tree and allow for quick deployment of new physical models on HPC platforms.

Such approach can only be made possible by setting clear requirements and review processes for all developers contributing to the project code: any changes and additions to the source code are reviewed and tested before being merged. VERTEX-CFD software is tested daily on a continuous integration (CI) workflow hosted on the ORNL network. Each new physics is implemented in closure models with unit tests that are run on CPU and GPU nodes.

Physical models and coupling between equations were verified and validated against benchmark problems taken from the published literature: isothermal flows (Clausen, 2013; Lane & Loehrke, 1980; Taylor & Green, 1937), heated flows (Kuehn & Goldstein, 1976; Tritton, 1959), transient and steady-state cases, turbulent cases (NASA Langley Research Center, 2024; Nicoud & Ducros, 1999), and MHD flows (Smolentsev et al., 2015).

Conclusions and current development activities

VERTEX-CFD is an open-source CFD solver that relies on a finite element discretization method to solve for the incompressible Navier-Stokes equations coupled to a temperature equation and MHD equation. RANS turbulence models and LES models are also available. The code relies on the Trilinos package and offers a wide range of temporal integrators, solvers, and preconditioners to run on CPU- and GPU-enabled platforms. VERTEX-CFD software was verified and validated for steady and unsteady incompressible flows with benchmark cases taken from the published literature: natural convection, viscous heating, laminar flow over a circle, and turbulent channels. VERTEX-CFD software has also been demonstrated to scale on CPU (Perlmutter) and GPU (Perlmutter and Summit) architectures.

Development tasks are currently focusing on the following three main activities:

- Implementation of a conjugate heat transfer model.
- Coupling with TensorFlowLite (Abadi et al., 2015) for AI&ML applications.
- Implementation of wall function for RANS models to enable high-Reynolds turbulence models.
- Optimization of the source code for Frontier supercomputer (OLCF, 2024).

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