LA-UR-17-20058

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Title: HPC Institutional Computing Project: W15_lesreactiveflow KIVA-hpFE
Development: A Robust and Accurate Engine Modeling Software

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Intended for: Report

Issued: 2017-01-05

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HPC Institutional Computing Project: *W15_lesreactiveflow* KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software

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Budget: \$700,000 to \$850,000/year

Introduction to LANL's 5th generation Engine Simulation Software

KIVA-hpFE is a high performance computer software for solving the physics of multi-species and multiphase turbulent reactive flow in complex geometries having immersed moving parts. The code is written in Fortran 90/95 and can be used on any computer platform with any popular compiler. The code is in two versions, a serial version and a parallel version utilizing MPICH2 type Message Passing Interface (MPI or Intel MPI) for solving distributed domains. The parallel version is at least 30x faster than the serial version and much faster than our previous generation of parallel engine modeling software, by many factors.

The 5th generation algorithm construction is a Galerkin type Finite Element Method (FEM) solving conservative momentum, species, and energy transport equations along with two-equation turbulent model $k-\omega$ Reynolds Averaged Navier-Stokes (RANS) model and a Vreman type dynamic Large Eddy Simulation (LES) method. The LES method is capable modeling transitional flow from laminar to fully turbulent; therefore, this LES method does not require special hybrid or blending to walls. The FEM projection method also uses a Petrov-Galerkin (P-G) stabilization along with pressure stabilization. We employ hierarchical basis sets, constructed on the fly with enrichment in areas associated with relatively larger error as determined by error estimation methods. In addition, when not using the hp-adaptive module, the code employs Lagrangian basis or shape functions. The shape functions are constructed for hexahedral, prismatic and tetrahedral elements.

Our work supplies the needs of Researchers, Industry and the Nation

Fuel economy is heavily dependent upon engine efficiency, which in turn depends to a large degree on how fuel is burned within the cylinders of the engine. Higher in-cylinder pressures and temperature lead to increased fuel economy, but they also create more difficulty in controlling the combustion process. Poorly controlled and incomplete combustion can cause higher levels of emissions and lower engine efficiencies.

One of the goals of U.S. and foreign automakers and engine manufacturers is to optimize combustion engines with the objective of reducing fuel usage, retaining or increasing power, and reducing undesirable emissions. In order to optimize combustion processes, engine designers have traditionally undertaken manual engine modifications, conducted testing, and analyzed the results. This iterative process is painstaking slow, costly, and does not lend itself to identifying the optimal engine design specifications.

In response to these problems, Los Alamos National Laboratory (LANL) scientists have developed KIVA, an advanced computational fluid dynamics (CFD) modeling code that accurately simulates the in-cylinder processes of engines. KIVA, a transient, three-dimensional, multiphase, and multicomponent code for the analysis of

chemically reacting flows with sprays has been under development at LANL for many years, producing now the 5th generation software KIVA-hpFE.

KIVA's functionality extends from low speeds to supersonic flows for both laminar and turbulent regimes. Transport and chemical reactions for an arbitrary number of species and their chemical reactions is provided. A stochastic particle method is used to calculate evaporating liquid sprays, including the effects of droplet collisions, agglomeration, and aerodynamic droplet breakup.

KIVA is Highly Impactful

The KIVA family of software has a long history of success. These codes have been instrumental in understanding combustion processes, provided assistance in engine development, and better engine design, particularly internal combustion engines. KIVA software, a worldwide mainstay in combustion modeling, has provided modeling for new engine designs, e.g., a 2007 Cummins diesel engine which was fully designed from computational methods that included the integral use of KIVA. KIVA continues to be a basis for commercial software development, commercial engine development, and a research tool for an uncountable number of professors, students and other researchers. KIVA is a family of Fortran-based Computational Fluid Dynamics (CFD) software that predicts complex multi-species multi-phase turbulent fuel and airflows. KIVA models all engine combustion processes with models for spray, soot formation, spark ignition, and reactive chemistry (including pollutant-formation processes).

Los Alamos National Laboratory and its collaborators are facilitating engine modeling by improving accuracy and robustness of the modeling, and improving the robustness of software. We also continue to improve the physical modeling methods. We are developing and implementing new mathematical algorithms, those that represent the physics within an engine. We provide software that others may use directly or that they may alter with various models e.g., sophisticated chemical kinetics, different turbulent closure methods or other fuel injection and spray systems.

This software is ever evolving and continues building from its origins, now in a 5th generation code. The software team is constantly employing and inventing the newest algorithms, numerical methods, and models in response to industry needs. Each version has added significant elements to the previous licensed version; with the current progression changing the entire numerical method to the state-of-the-art for CFD modeling, known as **KIVA-hpFE** with a newly invented, accurate and robust local-ALE system for immersed moving parts. This new code is a finite element based method that employs parallelism for rapid solution to complex and highly resolved engine physics.

5th Generation KIVA-hpFE and HPC

This FEM projection method is designed for all flow regimes from laminar incompressible to fully turbulent compressible flow and high Mach flows. Higher-order polynomial approximation for model dependent physical variables (p-adaptive) for greater accuracy and grid enrichment (locally higher grid resolution – h-adaptive) is available to supply exponential convergence of spatial error. The hp-adaptive FEM is at a minimum of: 2nd order in space and 3rd order on advection terms everywhere in the solution and is higher order when and where required as prescribed by the adaptive procedures. The time-dependent scheme is a semi-implicit projection method that employs and backward Euler time stepping with an implicit solve for the viscous terms. Other time integration schemes are available for use in the simulation as well, such as Crank-Nicholson method or can also employ a Taylor-Galerkin/Characteristic method by pulling in different modules not distributed with the code.

The moving immersed parts are represented with an overset surface grid. A new type of ALE, a local-ALE scheme, provides for second-order accuracy as the part's surface move through the fluid's hexahedral grid. A number of commercial packages provides for initial grid generation, where the parts themselves are not represented in the complex geometry. The moving parts are derived from CAD surfaces and overlay the fluid dynamics grid. This makes for easy grid generation on complex geometries.

The system includes the KIVA multi-component spray model. The spray model is Lagrangian Particle method, for atomized droplets. A Volume of Fluids (VOF) module is available for multiphase flow simulation and can be used to model the initial spray break-up.

Reactive chemistry can be performed within the code and utilizes a fuel library of 30 types. In addition, the software also links to high-fidelity reactive chemistry models found in *ChemKin-Pro* by ANSYS for comprehensive reaction analysis. The software accommodates add-on models in addition through a module and templates, all called from the upper level of the code. The model also includes a 3-soot transport model.

The software is designed to solve many types of reactive flow problems, from burners to internal combustion engines and turbines. In addition, the formulation allows for direct integration of solid bodies (conjugate heat transfer), as in heat transfer through housings, parts, cylinders. It can also easily be extended to stress modeling of solids, used in fluid structure interactions problems, solidification, porous media modeling and magneto hydrodynamics.

FY 2016 Publications/Presentations

- 1) Waters J., Carrington, D. B., Pepper, D.W. (2016), "An Adaptive Finite Element Method with Dynamic LES for Turbulent Reactive Flows," Journal of Computational Thermal Sciences, Begell House Inc., vol. 8, no. 1, pp. 57-71
- 2) V. D. Hatamipour, David B. Carrington, Juan C. Heinrich (to appear), "Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh," Progress in Computational Fluid Dynamics, An International Journal
- 3) Carrington. D. B., Mazumder, M., Heinrich, J.C., (to appear), "Three-Dimensional Local ALE-FEM Method for Fluid Flow in Domains Containing Moving Boundaries/Objects Interfaces", Progress in Computational Fluid Dynamics, An International Journal.
- 4) Waters, J ; Carrington, D. B., (2016), "A parallel Large Eddy Simulation in a finite element projection method for all flow regimes," Numerical Heat Transfer Part A-Applications, vol.70 (2), pp.117-131
- 5) J. Waters, D.B. Carrington (2016), "Modeling Turbulent Reactive Flow in Internal Combustion Engines with an LES in a semi-implicit/explicit Finite Element Projection Method," *Procs. of the ASME 2016 Internal Combustion Engine Fall Tech. Conf.*, ICEF2016, Oct. 9-12, 2016, Greenville, SC, USA
- 6) J. Waters, D.B. Carrington, D.W. Pepper (2015), "Application of a dynamic LES model with an H-adaptive FEM for fluid and thermal processes," *Procs. of 1st Thermal and Fluid Engineering Summer Conference - TFESC*, 2015-08-09/2015-08-12, N.Y., N. Y., United States
- 7) J. Waters, D.B. Carrington, D.W. Pepper (2015), "Parallel Large Eddy Simulation for Turbulent Reactive Flow Modeling," *Procs. of the Int. Conf. Computational & Experimental Engr. & Sci.* (ICCES'15), Reno, NV.
- 8) J. Waters, D.B. Carrington, D.W. Pepper (2015), "An Adaptive Finite Element Technique with Dynamic LES for Incompressible and Compressible Flows," *Procs. of the 15th Computational Heat Transfer Conference, CHT-15*, Piscataway, New Jersey