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Title: KIVA-hpFE: Predictive turbulent reactive and multiphase flow in engines - An Overview

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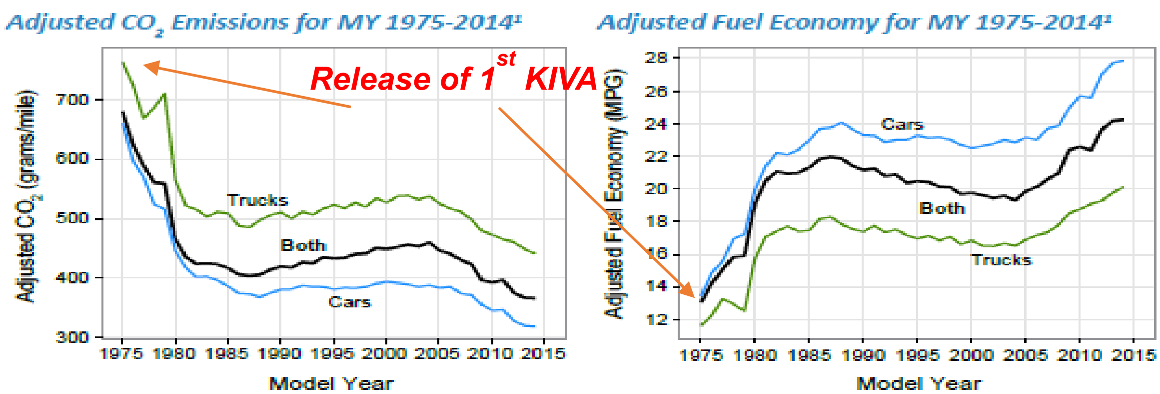
An Overview

Connection to the Goals and Mission of the Laboratory

Research and development of KIVA-hpFE for turbulent reactive and multiphase flow particularly as related to engine modeling program has relevance to National energy security and climate change. Climate change is a source problem, and energy national security is consumption of petroleum products problem. Accurately predicting engine processes leads to, lower greenhouse gas (GHG) emission, where engines in the transportation sector currently account for 26% of the U.S. GHG emissions. Less dependence on petroleum products leads to greater energy security. By Environmental Protection Agency standards, some vehicles are now reaching 42 to the 50 mpg mark. These are conventional gasoline engines. Continued investment and research into new technical innovations, the potential exists to save more than 4 million barrels of oil per day or approximately $200 to $400 million per day. This would be a significant decrease in emission and use of petroleum and a very large economic stimulus too! It is estimated with further advancements in combustion, the current emissions can be reduced up to 40%.

Enabling better understanding of fuel injection and fuel-air mixing, thermodynamic combustion losses, and combustion/emission formation processes enhances our ability to help solve both problems. To provide adequate capability for accurately simulating these processes, minimize time and labor for development of engine technology, are the goals of our KIVA development program.



[1] *Adjusted CO_2 and fuel economy values reflect real world estimates and are not comparable to automaker standards compliance levels. Adjusted CO_2 values are, on average, about 25% higher than the unadjusted laboratory CO_2 values that form the starting point for GHG standards compliance, and adjusted fuel economy values are about 20% lower, on average, than unadjusted fuel economy values.*

Research Breadth and Impact

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 manufactures 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. The older codes use an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite-volume technique. The codes use an implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving manner.

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 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). Employing KIVA software helps to optimize internal combustion engine processes, including diesel engines, for higher efficiency and lower emissions. KIVA engine modeling routines such as spray and core CFD Arbitrary Lagrangian-Eulerian (ALE) algorithms are now ubiquitous in the industry of engine code simulators. In addition, many engineers and researchers have made modifications to or enhanced our routines to address specific problems in engine designs. Using Los Alamos National Laboratory's KIVA code, Cummins reduced development time and cost by 10%–15% in developing its high-efficiency ISB 6.7-L diesel engine that was able to meet emission standards. At the same time, the company realized a more robust design and improved fuel economy while meeting all environmental and customer constraints. This engine was the first to go from CAD and CFD to production without the use of prototyping.

This software is ever evolving and continues building from its origins. The KIVA development software team is constantly employing and inventing the newest algorithms, numerical methods, and models in response to industry, national and world 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.

In response to industry and researcher's needs, we implemented (or are implementing) the following methods to enhance the accuracy, robustness and ease of use of the code for turbulent reactive multiphase flow in engines:

1) Developed a fractional step FEM method for all flow regimes, all flow speeds, from laminar to turbulent. The method is extremely flexible by design, allowing for ease of incorporation of other methods, such as those listed below. By virtue of this base, the following listed methods and models function well [1, 2].
2) Implemented an hp-adaptive method, allowing for higher order and higher resolution when and where it is needed. Higher order polynomial approximation for model dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution – *h*-adaptive) provide for a high-order of accuracy and robust solutions in the next generation of KIVA, KIVA-hpFE, particularly on complex domains [1,2].
3) Invented a local-ALE method that is accurate and robust for moving parts. This method employs overset grids for actuated and immersed moving part, eliminating the need to retain any grid history, and hence eliminates the possibility of grid entanglement [3,4,5].
4) Implemented a dynamic LES method that doesn't require wall function or wall damping, spans the transitional flow and therefore produces both laminar, turbulent or transitional flow, flow types all found within the engine at various times [6,7,8,9].
5) MPI parallelism for superlinear speed-up [10,11]
6) Implicit viscous solver using only active nodes for speed of solution.
7) Implemented a Plasma spark model for more accuracy in the spark ignition process
8) Implementing ChemKin III for more encompassing reactive chemistry
9) Volume of fluids method for modeling injection spray physics very near the nozzle
10) Implemented in-situ preconditioning and LANL developed linear equations solvers
11) Grid generation, quality of grid and ease of grid generation

Comparison with Peers

Currently, Los Alamos National Laboratory licenses KIVA-3V, KIVA-4, and KIVA-4pmi source code through a nonexclusive, nontransferable end user license agreement for a reasonable licensing fee. A demo version is also available and can be accessed online. The demo version has been downloaded more than 600 times since January 2012.

The methods and algorithms for CFD modeling with moving boundaries and the use of ALE developed at LANL, along with the spray modeling methods and algorithms are now ubiquitous in others' codes, for example the spray modeling, the ALE and the moving parts methods. Our newest methods currently being developed in KIVA-hpFE are more accurate, more robust, and easier to use that earlier versions of KIVA. In addition, the system is faster than our older versions, along with having superlinear speed-up when running on clusters or high performance computers. Our peers do not include any of the capabilities listed above.

These peers include Convergent, LLC and ANSYS' Fluent along with Star-CD. Convergent code although easy to use, hasn't demonstrated reliable results. ANSYS's has asked if we'd like them to include our new KIVA-hpFE into their suite of solver tools -- saying a good deal about our effort.

Status of the Capabilities

The current progression of code development is 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.

1) The fractional step (predictor-corrector) FEM method for all flow regimes, all flow speeds, from laminar to turbulent has been developed and well tested with RANS and LES turbulent, sprays, some combustion, and engine type simulations. The method is extremely flexible by design, allowing for ease of incorporation of other methods, such as those listed below. By virtue of this base, the following listed methods and models function well [1,2].
2) The hp-adaptive method allowing for higher order and higher resolution when and where it is needed, is completed for 2-D quads and 3-D hexahedral methods and incorporates, that is, wraps around the all flow solver predictor-correction fractional step method. Work continues on the hp-adaptive module to function with moving parts. Currently, the algorithm should be capable of handling moving parts with flat surfaces. Memory utilization is being optimized at this time via coding structure changes [1,2].
3) The local-ALE method for moving parts has been implemented and tested in both 2-D and 3-D and is implemented in the all flow solver predictor-correction fractional step method for any surface type on the immersed part. This method creates new elements as needed, including tetrahedral and prism types. We continue to test this method, and are finding some issues to overcome still, all of which have been solved for moving parts with flat surfaces [3,4,5].
4) The dynamic LES method is shown to span the transitional flow, produces both laminar, turbulent and transitional flow, and is implemented in the predictor-corrector FEM flow solver. In fact, the LES is quite good and appears to produce a RANS two-equation type solution of courser grids, perhaps negating the need for assumptions that are involved in the two-equation turbulence closure [6,7,8].
5) MPI parallelism is providing superlinear speed-up functioning or tested on many platforms [9,10].
6) Implicit viscous solver using only active nodes for speed of solution is implemented and saves a great deal of computational cost.
7) The plasma kernel spark model for more accurately providing simulated spark ignition functions as desired and has been tested on few cases.
8) Implementation of ChemKin III for more encompassing reaction chemistry is in progress.
9) Volume of fluids method for modeling injection spray physics very near the nozzle has been implemented an is being tested. The first portion of the effort neglects stresses surface that cause the liquid portion of the flow to break-up into ligaments.
10) LANL developed linear equations solvers (PCG package) and oure in-situ preconditioning is implemented and functioning well.
11) Grid generation, quality of grid and ease of grid generation continues with an informal collaboration from GridPro.
12) A Request for Information (RFI) to commercialize KIVA and support industry and researchers' needs closed at the end of the April. LANL received 3 responses to commercialize RFI for the KIVA suite of software. Two of the three have been identified as great candidates to work with and the Feynman Center for Innovation is now doing further diligence with each to determine the most appropriate path forward. Both candidates maybe provided KIVA codes in a nonexclusive manner.

Publication list:

1. "An *hp*-adaptive Predictor-Corrector Split Projection Method for Turbulent Compressible Flow," *Proceedings of the 15th International Heat Transfer Conference, IHTC-15,* Kyoto, Japan, August 10-15, 2014. David Carrington, Xiuling Wang, Darrell Pepper
2. "A predictor-corrector split projection method for turbulent reactive flow," Journal of Computational Thermal Sciences, Begell House Inc., vol 5, no. 4, pp.333-352, 2014, David B. Carrington, Xiuling Wang, Darrell Pepper
3. "Three-Dimensional Local ALE-FEM Method for Fluid Flow in Domains Containing Moving Boundaries/Objects Interfaces ," Progress in Computational Fluid Dynamics, an Int. Jour (submitted) David Carrington, Monayem Mazumder, Juan Heinrich
4. "A local ALE for flow calculations in physical domains containing moving interfaces," Progress in Computational Fluid Dynamics, an Int. Jour. vol 14, no, 3, pp. 139-150, 2014 David B. Carrington, Dominic Munoz, Juan Heinrich
5. "Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh," Progress in Computational Fluid Dynamics, an Int. Jour, (submitted) V. D. Hatamipour, David B. Carrington, Juan C. Heinrich
6. "An Adaptive Finite Element Technique with Dynamic LES for Incompressible and Compressible Flows," Journal of Computational Thermal Sciences, Begell House Inc. Waters J., Carrington, D.B., Pepper, D.W. (to appear)
7. "An Adaptive Finite Element Technique with Dynamic LES for Incompressible and Compressible Flows," *Proceedings of the 15th Computational Heat Transfer Conference, CHT-15, Piscataway, New Jersey*, May 25-29, 2015. Jiajia Waters, David B. Carrington, Darrell Pepper
8. "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, J.Waters, D.B. Carrington, D.W. Pepper (2015)
9. "Modeling Turbulent Reactive Flow in Internal Combustion Engines with an LES in a semi-implicit/explicit Finite Element Projection Method," *Proceedings of the ASME 2016 Internal Combustion Fall Technical Conference*, ICEF2016, Oct 9-12, 2016, Greenville, SC, USA, Waters, J, Carrington, D.B.
10. "A Parallel Large Eddy Simulation in a Finite Element Projection Method for all Flow Regimes," Numerical Heat Transfer, Part A: Applications. (to appear) Waters,Jiajia and Carrington,David, (2016)
11. "Parallel Large Eddy Simulation for Turbulent Reactive Flow Modeling," *Procs. of the Int. Conf. Computational & Experimental Engr. & Sci***.** (ICCES'15), Reno, NV., J.Waters, D.B. Carrington, D.W. Pepper (2015)
12. "Sensitivity analysis of the grad-div stabilization parameter in finite element simulations of incompressible flow," Journal of Numerical Mathematics, (to appear) M. Neda, F. Pahlevani, L. Rebholz & J. Waters
13. "Time relaxation algorithm for flow ensembles, Numerical Methods for Partial Differential Equations, 1098-2426, 2015, T. Aziz, M. Neda & J. Waters
14. "Fluid Models and Parameter Sensitivities: Computations and Applications," International Journal of Novel Ideas: Mathematics, (submitted) Sept. 2015, L. Davis, M. Neda , F. Pahlevani , & J. Waters
15. "A Local Meshless Method for Approximating 3D Wind Fields," Journal of Applied Meteorology and Climatology, 2015, D.W. Pepper & J. Waters,
16. "Global Versus Localized RBF Meshless Methods for Solving Incompressible Fluid Flow with Heat Transfer," Numerical Heat Transfer, Part B: Fundamentals, Vol. 68, Issue. 3, 2015, J. Waters & D. W. Pepper
17. "A meshless method for modeling convective heat transfer" , Journal of Heat Transfer, ASME Journals, vol 135, no. 1, 2013 Darrell Pepper, Xiuling Wang, David B. Carrington