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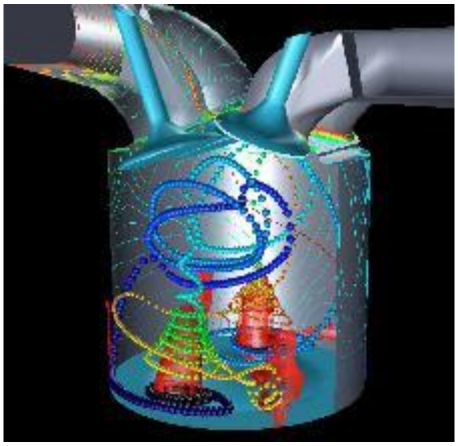
Los Alamos National Security, LLC Request for Information on how industry may partner with the Laboratory on KIVA software.

Los Alamos National Security, LLC (LANS) is the manager and operator of the Los Alamos National Laboratory (LANL) for the U.S. Department of Energy (DOE) National Nuclear Security Administration (NNSA) under contract DE-AC52-06NA25396. LANS is a mission-centric Federally Funded Research and Development Center focused on solving the most critical national security challenges through science and engineering for both government and private customers. LANL has advanced expertise in development of computational fluid dynamics software for predicting complex fuel and air flows as well as ignition, combustion, and pollutant-formation processes in engines, as well as other applications.



KIVA SOFTWARE AND FINITE ELEMENT ENHANCEMENTS

KIVA is a family of Fortran-based computational fluid dynamics software developed by LANL. The software predicts complex fuel and air flows as well as ignition, combustion, and pollutant-formation processes in engines. The KIVA models have been used to understand combustion chemistry processes, such as auto-ignition of fuels, and to optimize diesel engines for high efficiency and low emissions.

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 temperatures 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.

In order to optimize combustion processes, engine designers have traditionally undertaken manual engine modifications, conducted testing, and analyzed the results. This iterative process is painstakingly slow, costly, and does not lend itself to identifying the optimal engine design specifications. In response to these problems, LANL scientists developed KIVA, an advanced computational fluid dynamics (CFD) modeling code that accurately simulates the in-cylinder processes of engines.

The KIVA suite of software in general is a transient, three-dimensional, multiphase, multi-component code for the analysis of chemically reacting turbulent flows with sprays and has been under development at LANL for decades. The older codes (KIVA-3v, KIVA-4 and KIVA4-mpi) use an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite volume method. These codes use either an explicit or implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving manner and solved in the Lagrangian system. Also, the convection calculations can be subcycled in the desired regions to avoid restricting the time step due to Courant conditions. KIVA's functionality extends from low speeds to supersonic flows for both laminar and turbulent regimes. A stochastic particle method is used to calculate evaporating liquid sprays, including the effects of droplet collisions, agglomeration, and aerodynamic breakups.

The newest code, KIVA-hpFE is an Eulerian methodology employing and local-ALE technique for moving immersed parts. In addition, the moving parts system allows for fast grid generation by commercial grid generators, such as ICEM, MeshTool, Cubit, TrueGrid or GridPro. The grid generating software is required to produce hexahedral meshes without concern for gridding around the moving parts; the local-ALE algorithm allows the immersed parts to move through the hexahedral grid quickly. As the parts move new elements are created as needed. Because the way the local-ALE method works, there can be no mesh tangling -- the method is robust. The KIVA-hpFE is capable of handling transition flows, from laminar to turbulent using the dynamic LES model. Transport for an arbitrary number of species and their chemical reactions is provided.

The modularity of the code facilitates easy modifications for solving a variety of hydrodynamics problems involving chemical reactions. The versatility and range of features have made KIVA programs attractive to a variety of non-engine applications; these range from convection towers to modeling silicon dioxide condensation in high pressure oxidation chambers. Other applications have included the analysis of flows in automotive catalytic converters, power plant smokestack cleaning, pyrolytic treatment of biomass, design of fire suppression systems, Pulsed Detonation Engines (PDEs), stationary burners, aerosol dispersion, design of heating and ventilation, spray deposition and cooling. With somewhat more development the KIVA-hpFE code is capable of modeling non-Newtonian flows, solidification, 3-D printing for manufacturing, free surface flows, mesoscale atmospheric flow, indoor air transport, magneto-hydrodynamics aerospace fluid dynamics, multiphase flow, fluid-structural interaction problems, and general CFD problems with heat transfer, and wildfire modeling. The code has found a widespread application in the automotive industry. The code is extensible to many engineering applications.

The most recent developments to the software suite (KIVA-hpFE) have included algorithm construction that is a Galerkin type Finite Element Method (FEM) solving conservative momentum, species, and energy transport equations along with two-equation turbulent model k-ω; Reynolds Averaged Naiver-Stokes (RANS) model and a dynamic Large Eddy Simulation (LES) method. The LES method does not require the law-of-the-wall and is capable modeling transitional flow from laminar to fully turbulent. The FEM projection method also uses a Petrov-Galerkin (P-G) stabilization along with pressure stabilization. The LANL team employs hierarchical basis sets, constructed on the fly with enrichment in areas associated with relatively larger error as determined by the Zienkiewicz-Zhu stress-error estimation method among other error 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. 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 or 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.

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. Initial grid generation is provided for by a number of commercial packages, where the parts themselves are not represented in the complex geometry, but are derived from CAD surfaces. This makes for easy grid generation on complex geometries.

The suite of software includes a multi-component spray model and reactive chemistry with 32 fuels in the library. KIVA utilize ChemKin III with additional interfacing for comprehensive reaction mechanisms. The software can utilize sophisticated commercial chemical reaction solvers and 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.

LICENSING AND PARTNERSHIP OPPORTUNITY

LANS is seeking partners to license and distribute the software to users as well as to further collaborate in development of the software as needed based on the technical expertise at LANL.
LANS has identified several areas for potential partnership:

- Supply pre- and post-processing capabilities;
- Reactive chemistry technical expertise and support;
- Technical support for engineering simulations and their setup including combustion and engine problem setup;
- Training with pre- and post-processing along with CFD/combustion solver setup; and
- Assistance with documentation in the form of a manual (through the example suite on test cases and web-based examples).

Please note that the foregoing list is non-exhaustive, and LANS is open to collaboration in any suitable field that supports the Laboratory’s primary mission deliverables. To that end, LANS is opening this formal Request for Information to industry, academia, and the not-for-profit research sectors to gauge the level of interest and potential for a strong collaboration in advancing KIVA. This offering is made without prejudice to any form of agreement, collaborative arrangement, alliance, number of entities, or partnering mechanism. Those companies interested in pursuing this opportunity should direct a Letter of Interest, as well as any comments or questions, to the undersigned on or before ________________.

Below you will find a listing of certain partner attributes that LANS prefers. Please properly mark any information that is considered proprietary or business-sensitive. LANS will supply a Non-Disclosure Agreement to any entity or person that requires it.

LANS INTELLECTUAL PROPERTY
International copyright on KIVA software

Please note that the U.S. Government retains a worldwide, royalty-free, non-exclusive right to practice any LANS-owned patents and/or copyrighted software. Accordingly, any and all partners will have open access to any LANS intellectual property in performance of a Government contract.

PREFERRED PARTNER ATTRIBUTES

The following is a list of the preferred partner attributes:

- Demonstrated knowledge of product marketing, sales, and worldwide software distribution;
- Ability to set up and maintain software licensing and security mechanisms (or equivalent) for appropriate protection of source and executable versions of the code(s);
- Software marketing and packaging expertise to perform the following:
  - Make a beta version of the software available for testing;
  - Make an educational version of the software available at no/low cost for graduate research students to promote the adoption of KIVA;
- Ability to provide or acquire support for maintenance and further development of the KIVA software suite;
- Expertise to continue development of the software suite to enhance its functionality around the technical areas listed in the "Licensing and Partnership Opportunity" section
- Partners possessing knowledge and expertise in:
  - Grid generation
  - Post processing
  - CFD and combustion modeling
  - Fortran90
- Expertise in solution of linear equation systems with good solution methods or ability to use equation solver system used by LANL (PCG and Lapack); and
- Expertise in parallel solution processes, MPICH2, Intel-MPI.

The foregoing are negotiable preferences; LANS welcomes all Letters of Interest from any suitable party.

WHAT WE ARE REQUESTING

Please submit a written response on how your organization envisions utilizing this technology in partnership with Los Alamos. This may include a business or product plan, a business model, or just information regarding your company with contact information. We look forward to reviewing your ideas on how together we can bring the KIVA software portfolio to the private sector. If you have questions please contact Kathleen McDonald by email Kathleen_m@lanl.gov or (505) 667-5844. Please submit responses by email to Kathleen_m@lanl.gov by _____________. You will be contacted in a timely manner upon receipt of this information.