LA-UR-17-28712
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Title: KIVA-hpFE: Predictive turublent reactive and multiphase flow in engines : Science Supporting Mission of the Laboratory

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Intended for: Report

Issued: 2017-09-26

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

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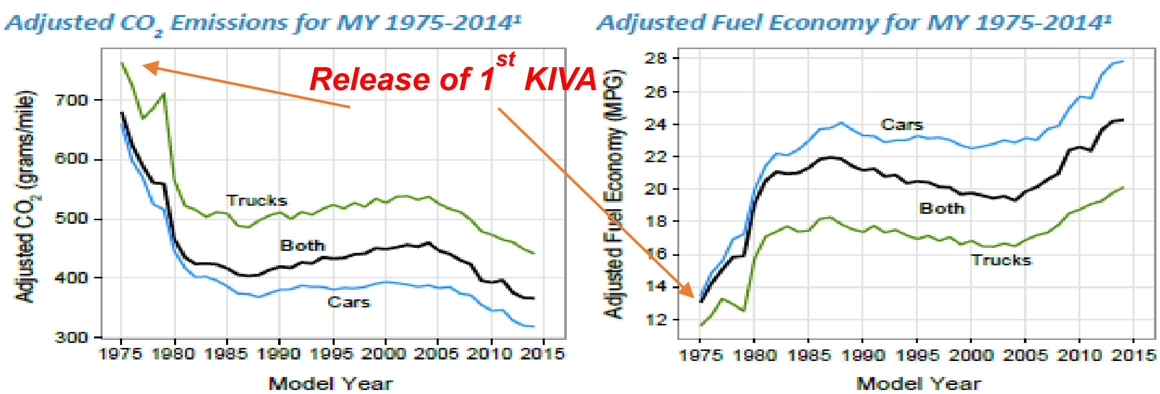
Science Supporting Mission of the Laboratory

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.*

Highly Impactful

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). 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).

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. 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.

KIVA software, a worldwide mainstay in combustion modeling. 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. For example, KIVA software is a highly used modeling tool in engine combustion research at the Universities of Iowa State, Wisconsin, Michigan Technological, and many others throughout the U.S. and the world. Kiva has provided numerical simulation capability to numerous commercial companies and the U.S. government, including FORD Motor Company, Cummins, John Deere, many National Laboratories, and NASA. A simple Google search on "KIVA combustion code" returns over 10,000 hits. A quick library reference search can find over 500 journal papers published using the KIVA software. Various components in the KIVA codes have been applied to diverse engineering problems.

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Currently, Los Alamos National Laboratory licenses KIVA-3V, KIVA-4pmi through a nonexclusive, and nontransferable end user license agreement for a reasonable licensing fee. Soon KIVA-hpFE will be available for engine research by academia and industry. 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 100's of times since January 2012, with researchers and students finding it helpful in determining paths forward and solving reasonably complex reactive flow problems, including engines.

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. 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 modeling of solid mechanics, used in fluid structure interactions problems, solidification, porous media modeling and magneto hydrodynamics.

The 5th generation of KIVA, KIVA-hpFE has the following features to support the ever increasing technological needs of the nation and researchers:

1) 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 [1,2,3,4,5,6].
2) Is 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 [2,3,4,5,6].
3) Uses a newly 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 [7,8,9].

4) Employs 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 [10,11,12,13,14,15].
5) The FEM parallel construction utilizes MPI parallelism FEM's inherently local integration to achieve super linear speed-up [14,15,16,17]
6) Incorporates and implicit viscous solver using only active nodes for speed of solution.
7) Employs ANSYS's ChemKin-Pro for more encompassing reactive chemistry
8) Utilizes a Volume of Fluids (VOF) method for modeling injection spray physics near the nozzle [18,19]
9) Incorporates in-situ preconditioning and LANL developed linear equations solvers [20]
10) Leverages commercial grid generation software for quality of grid and ease of grid generation.

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 super-linear speed-up when running on clusters or high performance computers. Our peers do not include any of the capabilities listed above.

KIVA-hpFE 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 complier. 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 much faster than our previous generation of parallel engine modeling software by a factor of 12x for a comparable engine cycle.

The FEM 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-ω 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.

This FEM projection method can use 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. The interface between liquid and compressible gas is calculated with the conservative VOF system as the flow evolves, allowing for exact determination of the stresses responsible for breaking a stream of liquid into ligaments and droplets.

Supplies the needs of Researchers, Industry and the Nation

The combustion of fuel in an engine involves turbulent flows and many complicating factors which include highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing, turbulence–chemistry interactions, compressibility effects and variable inertia effects. Coupling between these processes occurs over a wide range of time and length scales. Other complications arise when multiple phases are present due to the introduction of dynamically evolving interface boundaries and the complex exchange processes that occur as a consequence.

In the calculation of turbulent flows, the Reynolds time-averaged Navier-Stokes equations (RANS) are widely used and can yield good results for mean velocity and pressure fields when appropriate turbulence models ($e.g. k - \omega$) are employed to represent the averaged effects of turbulence. However, RANS methods are unable to capture detailed flow behaviors and particularly the unsteady turbulent structures. Combustion is notoriously difficult to model at the Reynolds-averaged level, but, the very fine-mesh needed by Direct Numerical Simulations (DNS) as well as the large number of species equations required for a realistic combustion model, currently makes this approach computationally too expensive for engineering use.

LES is rapidly becoming more widely used to study combustion. Extensions of subgrid-scale models to variable-density flows are straightforward. True compressibility effects of the weak subgrid-scale motions are likely to be negligible. This assumption is valid because the growth in the compressible shear layer is not related to dissipation, but rather to production and pressure-strain. Production is determined by the large scales and initiates the turbulent energy cascade, while dissipation mainly happens at the small scales. It could indicate that the large-scale turbulence is considerably altered by compressibility while the small eddies are more incompressible, see Vreman [21] for further explanation

LES uses filtered equations in time and space and the method requires a finer grid than RANS, but the grid scale is not as fine as needed in DNS. The use of h-adaptation (Carrington et al. [6]) refines the mesh where the local relative error is large (measured by a percentage of the average total error in the domain). This refinement process assists LES modeling by producing a solution with a specified error on the domain utilizing a minimal number of elements, thereby reducing the computational time, i.e., minimizes the computer time of solution for a given error in the solution (Carrington, et. al [2,3,4,5]). In addition, this h-adaptive method is especially helpful to capture shocks and other flow features that might not be resolvable with the grid resolution used at the start of a simulation. Results of LES applications to flows that include shock-induced boundary-layer separation are also discussed.

Filtration of the conservation equations over finite mesh sizes gives rise to physical scales that are smaller than the mesh size and cannot be resolved by LES methods, subsequently requiring the use of subgrid correlations, which model those subgrid scales. Since the filtered grid scale in general needs to contain perhaps 80% of the turbulent kinetic energy, the non-resolved small scales are more isotropic than large scales (Kolmogorov [22], Smyth and Moum [23], some of the effects can be reasonably accounted for by means of a subgrid-scale (SGS) model.

Modeling of the subgrid correlations is performed on the assumption that SGS can be obtained based on the information of large or resolved scales. One of the early approaches is due to Smagorinsky [24] who developed a subgrid model, called by its acronym SM and which is still widely used. In the Smagorinsky SGS model, the eddy viscosity ν_t is modeled as $\nu_t = (C_s\Delta)^2\sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$, where C_s is the eddy viscosity coefficient and is assumed to be a constant, Δ is the grid size and $\bar{S}_{ij}$ is the strain rate tensor. There are two key reasons for the success of the Smagorinsky model. First, it yields sufficient diffusion and dissipation to stabilize the numerical computations (Pope [25] and Deardorff [26]); second, low order statistics of the larger eddies are usually insensitive to the subgrid scale motions (Meneveau [27] and Ghosal and Rogers [28]). The subgrid-scale stresses vanishing in laminar flow and at a solid boundary, and having the correct asymptotic behavior in the near-wall region of a turbulent boundary layer, allows one to conclude that Cs should vary in time (Germano [29]). However, most investigators choose to keep Cs constant throughout the flow or make modifications to the SGS model, (Smagorinsky [24]), Piomelli et al. [30], Moin and Kim [31], Yakhot et al. [32], Vreman [33]).

Vreman [33] proposed a different invariant coefficient model, here termed VM, which appears to have many advantages over SM. The Vreman model not only guarantees vanishing SGS dissipation for various laminar shear flows, but also eliminates the need to use a wall-damping function in boundary layer flows (Vreman [33] and Lau et. al. [34]). This makes the method is especially suitable for LES simulations of wall-bounded shear flows. VM has also been more successful than SM in modeling highly anisotropic transitional flows and appears well suited for complex flows containing laminar, transitional and turbulent flows (Vreman [33] and Kemenov et al. [35]).

Unlike most turbulence models, this VM-LES model does not involve any explicit filtering, averaging, or clipping procedure to stabilize the numerical procedure, enabling it to be used in simulations of reacting flows with complex geometries.

Turbulent Flow with Multi-Species

The Favre-filtered continuity and momentum which govern the evolution of large-scale eddies are expressed as

$$\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\left(\bar{\rho}\tilde{u}_i\right)}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial\left(\bar{\rho}\tilde{u}_i\right)}{\partial t}+\frac{\partial\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right)}{\partial x_j}=\frac{\partial\tilde{t}_{ji}}{\partial x_j}-\frac{\partial\bar{p}}{\partial x_i}+\frac{\partial\tau_{ji}}{\partial x_j}+\bar{f}_{drop}+\bar{\rho}\sum_{k=1}^{NumSpecies}\tilde{\mathrm{Y}}_k f_{k,j} \tag{2}$$

where the body forces related to droplet or particulate a shown for completeness of model equations in the code, although not invoked in this paper. The stress tensor, $\tilde{t}_{ij}$ is evaluated using the Stoke's hypothesis as

$$\tilde{t}_{ij}=\mu\left(\frac{\partial\tilde{u}_i}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_i}\right)-\frac{2}{3}\mu\frac{\partial\tilde{u}_k}{\partial x_k}\delta_{ij} \tag{3}$$

The energy equations which govern the evolution of large-scale eddies are expressed as

$$\begin{aligned}\frac{\partial\tilde{E}}{\partial t}=&-\frac{\partial}{\partial x_i}\left(\tilde{E}\tilde{u}_i+p\tilde{u}_i\right)+\frac{\partial}{\partial x_i}\kappa\frac{\partial\tilde{T}}{\partial x_i}-\frac{\partial\left(C_p q_i\right)}{\partial x_i}+\frac{\partial}{\partial x_i}\left(t_{ij}+\tau_{ij}\right)\\&+\frac{\partial}{\partial x_i}\left(\bar{\rho}\sum_{j=1}^{NumSpecies}\bar{H}_K\left(D_K+\frac{\mu_{sgs}}{Sc_t}\right)\frac{\partial\tilde{\mathrm{Y}}_K}{\partial x_i}\right)\\&+\bar{\rho}\sum_{j=1}^{NumSpecies}\tilde{\mathrm{Y}}_j f_j\left(x_i\right)\bullet\tilde{u}_i-\sum_{k=1}^{NumSpecies}H_{o,k}w_k\end{aligned} \tag{4}$$

Material properties are determined by an mass weight aggregation process returning the gas properties gas when multi-components are in the gas, for example if the gas is air and made of only oxygen and nitrogen.

The turbulent species equation has the same form as the thermal energy transport equation given by

$$\frac{\partial\bar{\rho}\tilde{\mathrm{Y}}_j}{\partial t}=-\frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\tilde{\mathrm{Y}}_j\right)+\frac{\partial}{\partial x_i}\bar{\rho}\left[\left(D_{j,N}+\frac{\mu_{sgs}}{Sc_t}\right)\frac{\partial\tilde{\mathrm{Y}}_j}{x_i}\right]+\bar{\rho}\tilde{\mathrm{Y}}_j f_j\left(x_i\right)+\dot{w}^j_{chem}+\dot{w}^j_{spray} \tag{5}$$

In Eqs. (1)–(5), $\bar{\rho}$ is the filtered density, $\tilde{T}$ is the filtered temperature, $\tilde{u}_i$ is the filtered velocity vector, $\tilde{E}$ is the filtered energy, $\tilde{\mathrm{Y}}$ is the filtered species, Pr is the molecular Prandtl number, μ is the dynamic viscosity, and C_p is the specific heat capacity at constant pressure, Sc_t is the turbulent Schmidt number. The SGS stress tensor τ_{ij} and SGS heat flux vector q_i in Eqs. (6) and (8) are defined respectively as

$$\tau_{ij}-\frac{1}{3}\tau_{kk}\delta_{ij}=-2\mu_{sgs}\left(\tilde{S}_{ij}-\frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) \tag{6}$$

$$q_j=-\frac{\mu_{sgs}}{Pr_{sgs}}\frac{\partial\tilde{T}}{\partial x_j} \tag{7}$$

where μ_{sgs} is the turbulent eddy viscosity, Pr_{sgs} is the SGS Prandtl number, and

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) \tag{8}$$

is the strain rate tensor.

LES Vreman SGS model with dynamic coefficient

Although the Vreman SGS model with fixed coefficient produces better results than the ad hoc modification of the Smagorinsky coefficient in transitional and turbulent flows, Germano et al. [29] concluded that it is impossible to find a single, universal constant for different flows. In addition, none of any fixed coefficient SGS models can account for the energy transfer from unresolved to resolved scales (backscatter), which may also occur intermittently while on average, energy is transferred from the large to the small scales (forward scatter) (Piomelli et al. [30]). The development of the dynamic subgrid-scale Smagorinsky model (DSGS) reflects significant progress in the subgrid-scale modeling of non-equilibrium flows. The DSGS model can be used to calculate the eddy viscosity coefficient by sampling the smallest resolved scale, rather than by setting a priori parameters. The second filter is larger than the grid filter with the grid filter equal to the resolved scale. The idea is to minimize the difference between this larger test filter and grid filter. The dynamic SGS stress model uses this minimization process to model the local subgrid eddy viscosity and forming the proper coefficient. This is performed by sampling the smallest resolved scales and using this information to create the model for the subgrid scales, providing closure to the turbulence.

The DSGS is obtained by two filtering processes: in the first process, the grid filter Δ is applied, where the filtered expressions are given by (1)-(5), with the SGS Reynolds stress included. In the second process, a test filter $\hat{\Delta} = 2\Delta$ is added to the grid filtered equations (1)-(5), leading to the subtest-scale stress tensor T_{ij} and subtest-scale heat flux vector Q_j :

$$T_{ij} - \frac{1}{3}T_{kk}\delta_{ij} = -2\mu_{sgs}\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) \tag{9}$$

And

$$Q_j = -\frac{\mu_{sgs}}{Pr_{sgs}}\frac{\partial \tilde{T}}{\partial x_j} \tag{10}$$

Here we define $\mu_{sgs} = \bar{\rho} C_{DVMG} \Pi^t$ and $Pr_{sgs} = Pr_{DVMG}$, and $\hat{\tilde{S}}_{ij} = \frac{1}{2}(\frac{\partial \hat{\tilde{u}}_i}{\partial x_j} + \frac{\partial \hat{\tilde{u}}_j}{\partial x_i})$ is the test filtered strain rate tensor. Using the Germano [29] identity and the least-squares error minimization technique of Lilly [36], the coefficients C_{DVMG} and Pr_{DVMG} are obtained (see Lau et al. [34]) as

$$C_{DVMG} = \frac{L_{ij}M_{ijV}}{M_{ij}M_{ijV}} \tag{11}$$

and

$$Pr_{DVMG} = \frac{\langle M_j^\theta M_j^\theta \rangle_V}{\langle L_j^\theta M_j^\theta \rangle_V} \tag{12}$$

respectively, where

$$M_{ij} = -2\left(\bar{\rho}\Pi^t \tilde{S}_{ij} - \bar{\rho}\Pi^g \tilde{S}_{ij}\right) \tag{13}$$

$$M_j^\theta = -C_{DVMG}\left(\bar{\rho}\Pi^t \frac{\partial \tilde{T}}{\partial x_j} - \bar{\rho}\Pi^g \frac{\partial \tilde{T}}{\partial x_j}\right) \tag{14}$$

$$\Pi^t = \sqrt{\frac{B_\beta^t}{\hat{\alpha}_{ij}\hat{\alpha}_{ij}}} \tag{15}$$

$$B_\beta^t = \beta_{11}^t\beta_{22}^t - \beta_{12}^t\beta_{12}^t + \beta_{11}^t\beta_{33}^t - \beta_{13}^t\beta_{13}^t + \beta_{22}^t\beta_{33}^t - \beta_{23}^t\beta_{23}^t \tag{16}$$

$$\beta_{ij}^t = \sum_{m=1}^{3} \hat{\Delta}_m^2 \hat{\alpha}_{mi}\hat{\alpha}_{mj} \tag{17}$$

$$\hat{\alpha}_{ij} = \frac{\partial \tilde{u}_j}{\partial x_i} \tag{18}$$

$$L_{ij} = \bar{\rho}\tilde{u}_i\tilde{u}_j - \frac{1}{\bar{\rho}}\bar{\rho}\tilde{u}_i\,\bar{\rho}\tilde{u}_j \tag{19}$$

$$L_j^\theta = \bar{\rho}\tilde{u}_j\tilde{T} - \frac{1}{\bar{\rho}}\bar{\rho}\tilde{u}_j\,\bar{\rho}\tilde{T} \tag{20}$$

where $\langle \quad \rangle_V$ is volume integral over the entire domain to mitigate the effect of locally (highly) oscillating eddy viscosity fields. The DSGS coefficient remains the same throughout the entire domain and only varies in time.

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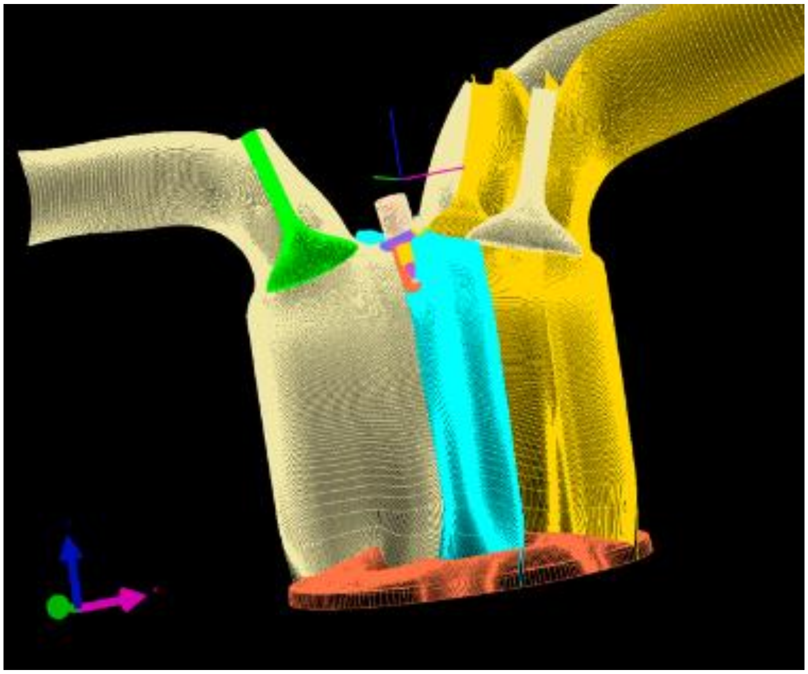
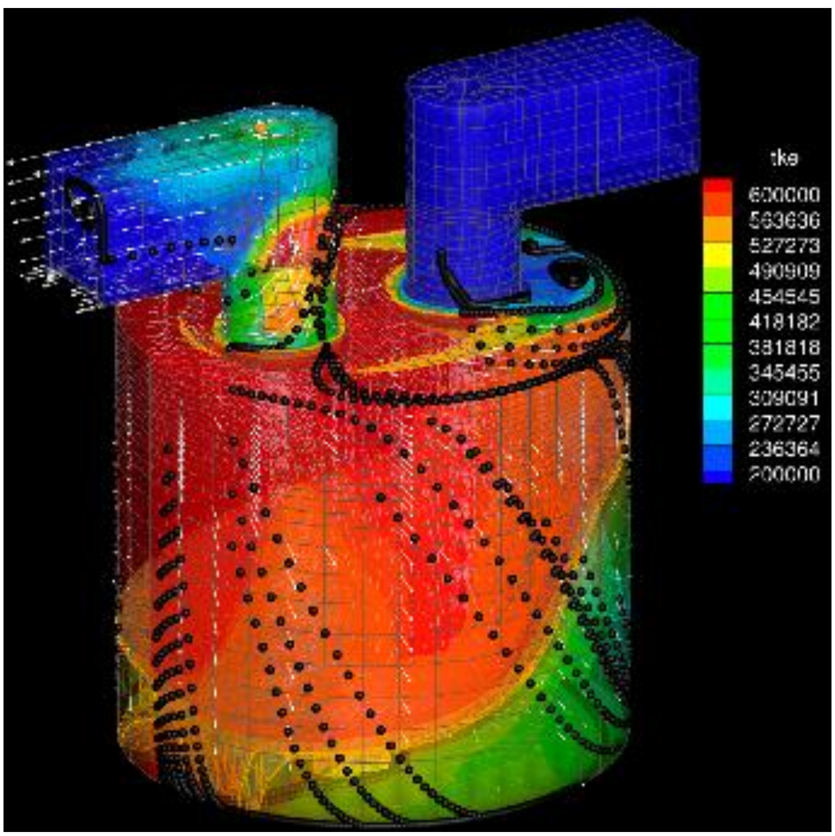
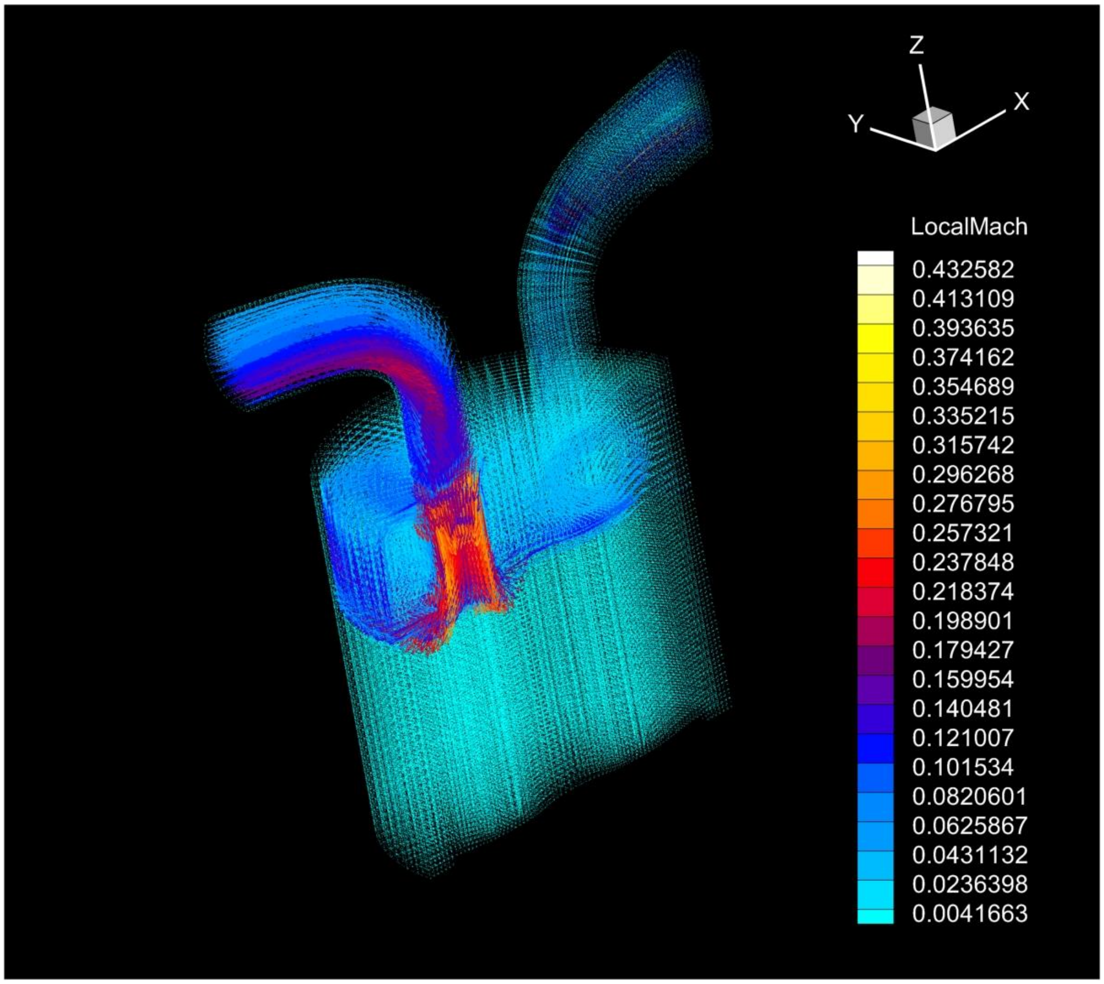


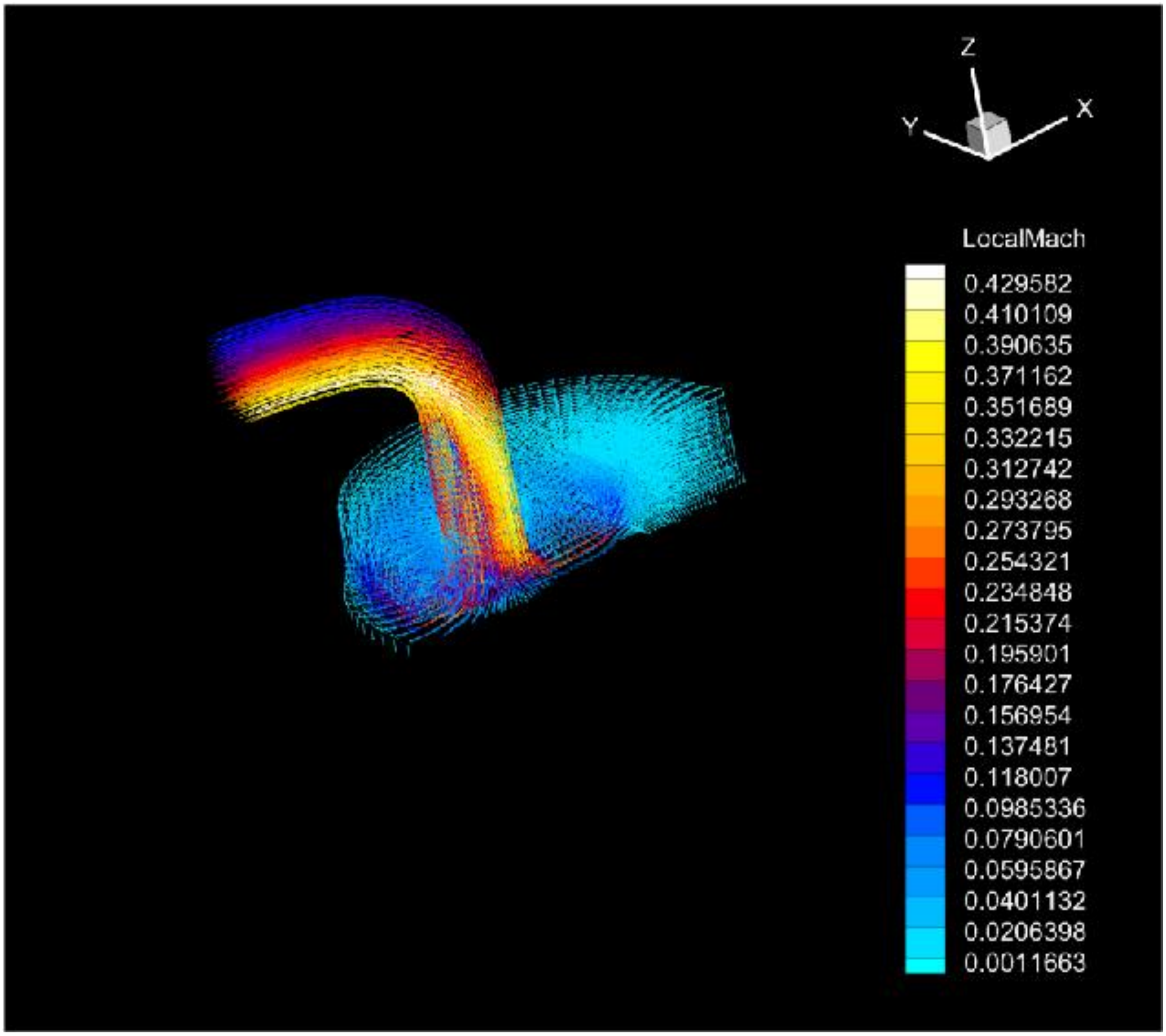
Direct Injection Spark Ignition (DISI) 4-valve engine grid, made of approximately 10 million hexahedral cells using GridPro commercial grid generation software.



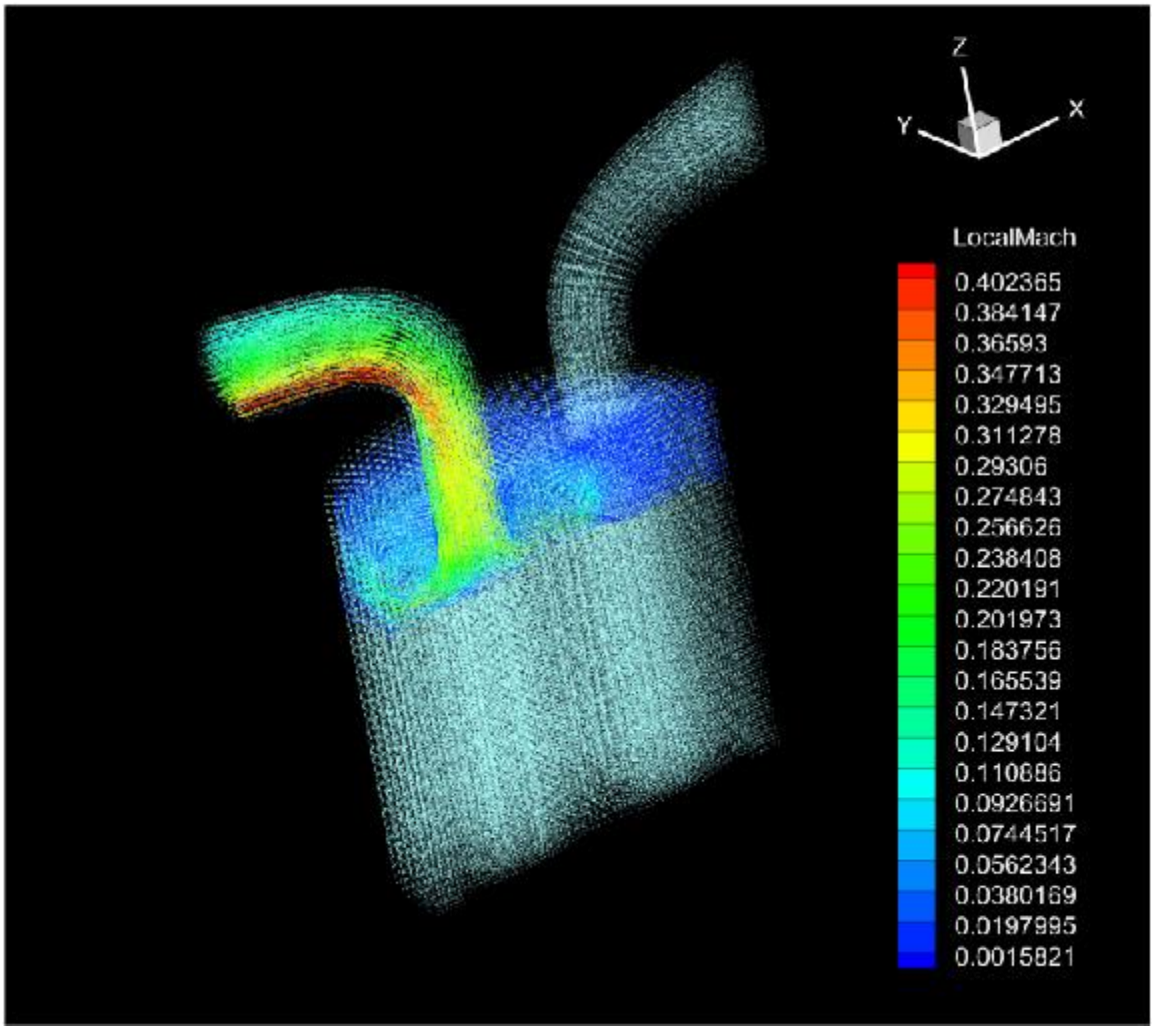
Direct Injection Spark Ignition (DISI) 2-valve test case engine grid using KIVA-4 finite volume method and snapper system for moving parts. Turbulence modeling with the k-ε two-equation closure method.



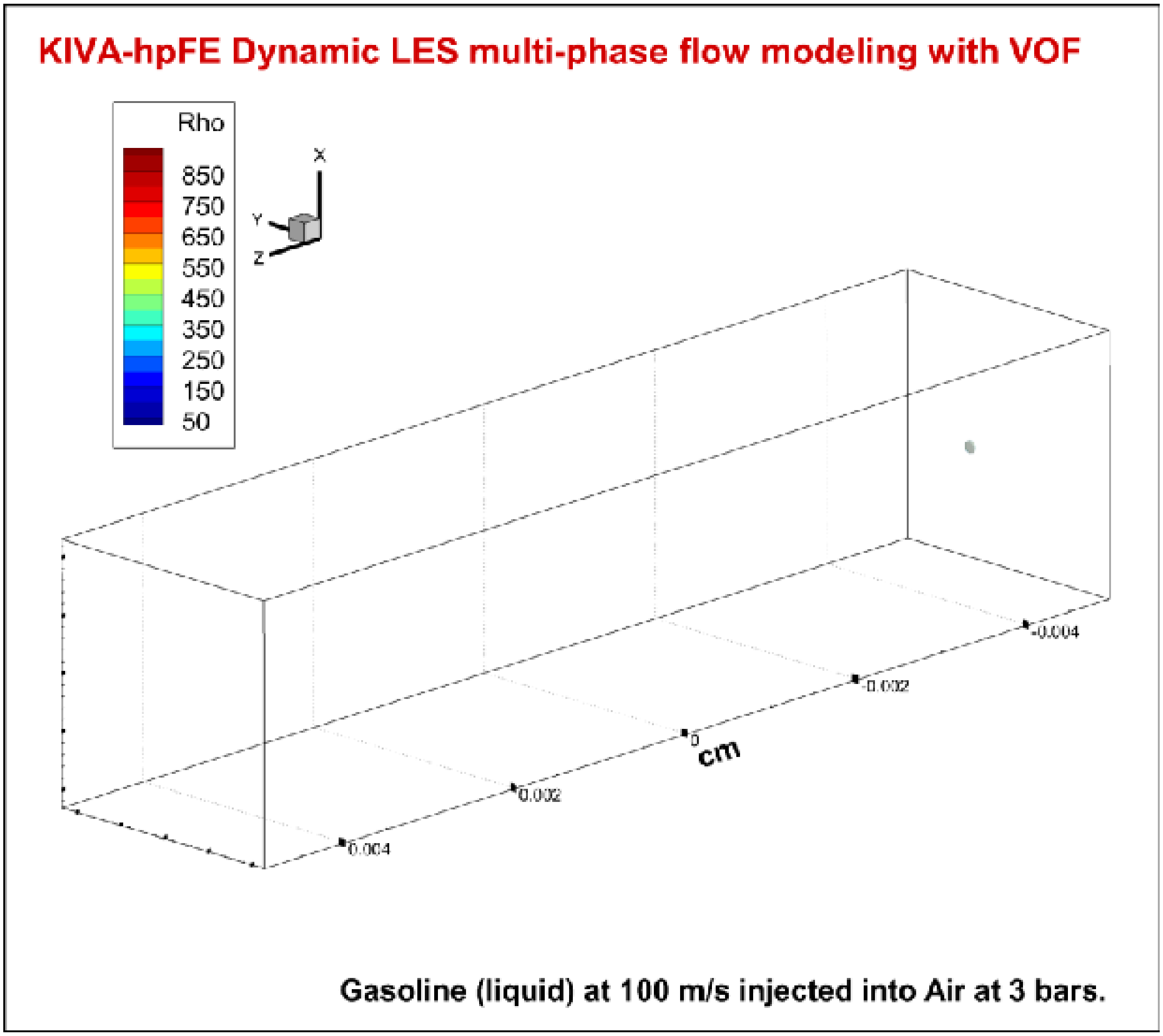
Direct Injection Spark Ignition (DISI) 2-valve test case engine grid – Vreman LES in FEM projection method using Immersed Boundary Method for moving immersed parts (KIVA-hpFE).



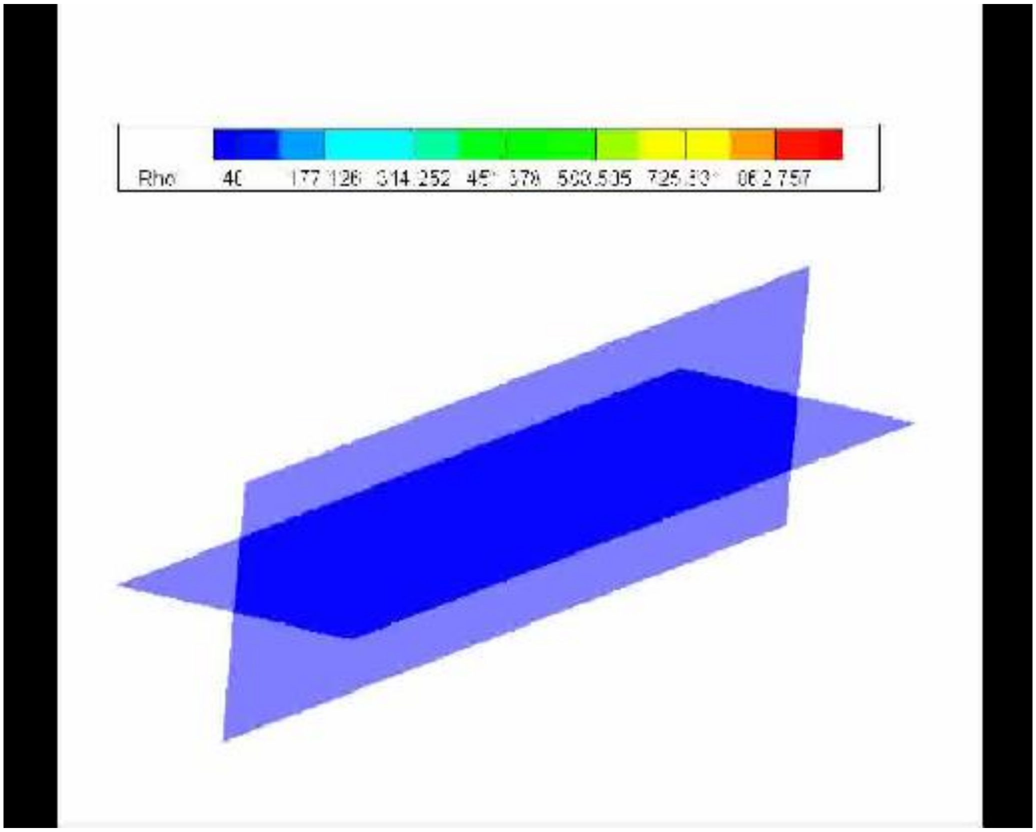
Direct Injection Spark Ignition (DISI) 2-valve test case internal combustion engine simulation
Cut-away showing the highly variable fluid flow field. Flow field is varying in regions of low speed and low turbulence to highly turbulent (Local Mach number in color). Modeled with a Vreman dynamic LES implemented in a stabilized FEM projection scheme using an immersed boundary method for actuated parts.



Direct Injection Spark Ignition (DISI) 2-valve test case internal combustion engine simulation
Cut-away showing the highly variable fluid flow field and mesh. Flow field is varying in regions of low speed and low turbulence to highly turbulent (Local Mach number in color). Modeled with a Vreman dynamic LES implemented in a stabilized FEM projection scheme using an immersed boundary method for actuated parts.



Liquid Jet break-up to ligaments and droplets. Modeled with conservative Volume of Fluid method in a stabilized Finite Element Method to create a predictive simulation of fuel injection for internal combustion engines. Liquid gasoline being injected into a chamber at 3 bars.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