II.A.11 KIVA-4 Development

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Objectives

- Validate parallelization of KIVA-4 in realistic geometries
- Develop a parallel collocated version of KIVA-4
- Implement advanced combustion models in KIVA-4
- Develop converters to KIVA-4 from established mesh generation software
- Develop remapping capability in KIVA-4
- Reduce spray dependence on grid

Accomplishments

- The parallelization of KIVA-4 was tested in realistic geometries including 4-valve pentroof and 3-valve engine geometries.
- The collocated version of KIVA-4 was parallelized and run in parallel in a vertical valve engine geometry.
- The University of Wisconsin's chemistry and spray submodels were implemented in KIVA-4 and tested in a 2-D sector geometry.
- Reaction Design's chemistry package was interfaced with KIVA-4.
- Mesh converters to KIVA-4 format were developed for the TrueGrid and ICEM software programs.
- Remapping capability was demonstrated in a cylindrical tetrahedral mesh.
- Reduced spray dependence was achieved by using the grid overset method in KIVA-4.

Future Directions

- Continue validation of KIVA-4 in unstructured geometries and in parallel simulations of realistic engine geometries.
- Implement Lawrence Livermore's multi-zone combustion model [1] into KIVA-4.
- Develop the capability to perform turbulent calculations with the large eddy simulation (LES) turbulence model in KIVA-4.

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Introduction

We have focused our efforts on parallelizing realistic geometries, developing a collocated version of KIVA-4, incorporating improved combustion and spray models, building interfaces with mesh generation software packages, developing remapping capability for KIVA-4 and reducing the spray dependence on the grid.

We previously had worked with relatively simple geometries in our parallel version of KIVA-4. In our recent work, we simulated two realistic engine geometries in parallel. These geometries include a 4-valve pentroof geometry and a 3-valve engine which has been studied experimentally by Dick Steeper at Sandia National Laboratory, Livermore.

We also developed a collocated version of KIVA-4 where the velocity is located at the cell-center along with the other field variables (pressure, temperature and density). This version is more appropriate for unstructured meshes that use a large percentage of tetrahedra or prisms. This version also has opened the door to more advanced meshes which include the grid overset technique in which two different meshes can be combined to model engine phenomena.

KIVA-4 inherited the combustion models of KIVA-3V which are Arrhenius type chemistry controlled combustion models. The University of Wisconsin Engine Research Center has had many years of experience with combustion models including mixing controlled models and ignition models which previous versions of KIVA-3V had not incorporated. We implemented the University of Wisconsin's combustion models into KIVA-4 to enhance the code and its applicability.

KIVA traditionally has accommodated large mesh movements with its snapper algorithm, where layers of cells become activated or deactivated during piston or valve movement. We have complemented KIVA's snapper routines with the capability of remapping fields to an entirely different mesh and continuing the engine simulation on the second mesh.

KIVA uses a grid generation program called K3PREP to construct its engine meshes. However, K3PREP can only generate structured meshes while KIVA-4 can accommodate unstructured meshes as well as structured meshes. Mesh generation is a complex field in itself and we felt the best use of time would be spent developing interfaces from existing grid generation software. We have developed interfaces for ICEM (via its CHAD output format). Robert Rainsberger at TrueGrid developed a mesh output format for KIVA-4 with assistance from LANL. We have also run a simple mesh generated with the Cubit mesh generator with KIVA-4.

KIVA uses a set of Lagrangian particles that move through the computational mesh to model the liquid fuel spray. The computational mesh is used to model the gaseous phase. The Lagrangian particles experience a drag during their motion and momentum is transferred from the particles to the grid. The Lagrangian particles also collide and evaporate. Each of these processes is dependent on the resolution of the underlying grid. We have implemented the grid overset method in KIVA-4 which allows one to resolve the region around the spray without resolving the entire engine geometry, thus allowing one to calibrate sprays with a fine resolution.

Approach

We have focused our efforts on continued development of KIVA-4. Our approach is to develop KIVA-4 in areas that are most essential and will have the greatest impact. We believe that KIVA-4 would be adopted more readily and have more applicability if it could be complemented with a grid generator, could perform calculations of realistic geometries in parallel and could access advanced combustion and spray models.

Results

We present the results of parallel computations in a 4-valve engine shown in Figure 1. Table 1 shows the speed-up achieved with varying amounts of processors. One can see that four processors are being used effectively. Beyond four processors, the speed-up diminishes. The parallel performance tends to plateau for two reasons. First, the grid is relatively small using 38,392 cells. For comparison, we have achieved a speed-up of 10.21 in a cylinder with 430,000 cells with 14 processors in KIVA-4. Second, the mesh partitioning could be improved considering the fact that cells become deactivated when the piston moves up. Partitioning refers to how the mesh is subdivided among processors (or equivalently the way the computational load is divided among processors). We have implemented a means of repartitioning a mesh during the course of a simulation, thus providing a means of improving the parallel performance with larger amounts of processors. Figure 2 shows the 3-valve engine run in parallel. We were able to achieve a speed-up of 1.71 with 2 processors and 2.62 with 4 processors. In the 3-valve engine parallel computation, entire ports become deactivated during the course of the simulation which makes an effective single partitioning even more difficult.

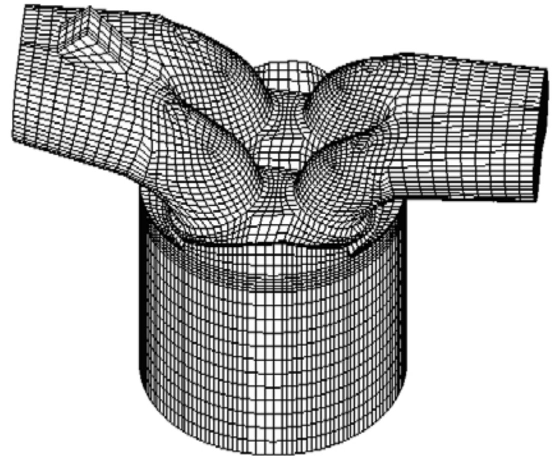

FIGURE 1. 4-Valve Pentroof Geometry Simulated in Parallel with KIVA-4

TABLE 1. Parallel Speed-Up with 4-Valve Engine

Number of Processors	Time (hours)	Speed-up
1	9.6	1.0
2	5.24	1.83
4	3.0	3.2
8	2.76	3.48
16	2.36	4.1

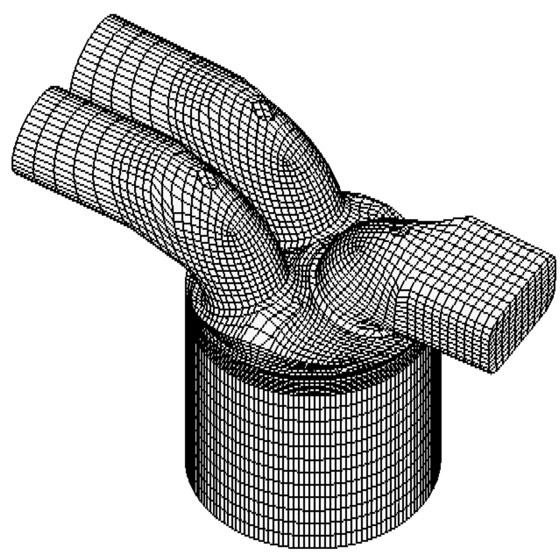

FIGURE 2. 3-Valve Geometry Run in Parallel with KIVA-4

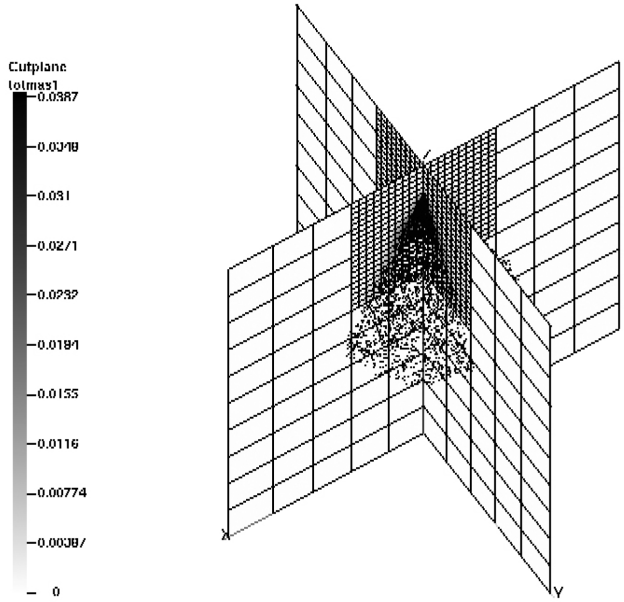

FIGURE 3. Use of Grid Overset Method to Resolve Spray

Our repartitioning algorithm should prove effective in improving the 3-valve parallel efficiency.

Figure 3 shows a computation in a cylinder with the overset grid method where two grids are simultaneously used – one specifically for the spray and another for the engine geometry. Finer resolutions will improve the accuracy of the spray dynamics up to a point. We also hope to incorporate the collision improvements of Abani, et al. (2006) in the future to further decouple the spray dynamics from the underlying grid.

Figure 4 shows a mesh with tetrahedra and prisms that was simulated with KIVA-4. This mesh was created by Valmor de Almeida at Oak Ridge National Laboratory. We expect to use this strategy of using tetrahedra in the bowl and head region and prisms in the squish region for future simulations of engine meshes.

Conclusions

KIVA-4 has simulated realistic geometries in parallel. Advanced combustion models have been tested in KIVA-4. Grid converters have been developed to convert meshes to KIVA-4 format. Restart capability has been developed to remap fields from one mesh to another mesh and continue the KIVA-4 simulation on the second mesh. The grid overset method has been developed in KIVA-4 to reduce the dependence of the spray on the grid.

We would also like to acknowledge the help and suggestions of Qingluan Xue, Yuanhong Li and Song-Charng Kong of Iowa State University, Zheng Xu at Ford Motor Corporation and Valmor de Almeida at Oak Ridge National Laboratory.

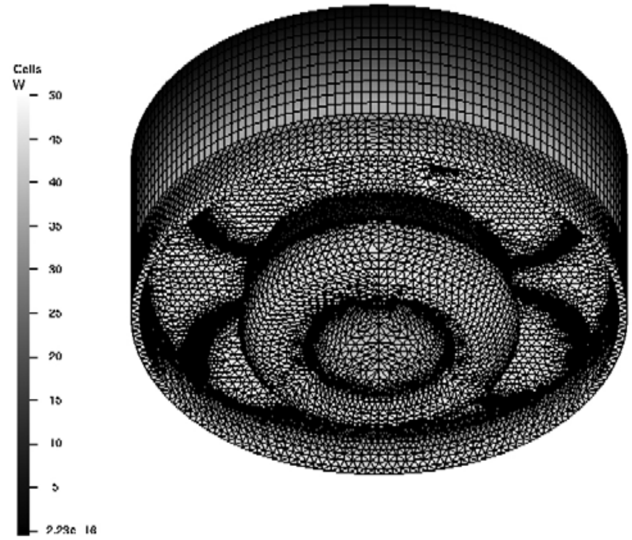

FIGURE 4. Vertical Velocity in Tetrahedral and Prism Mesh

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1. A. Babajimopoulos, D.N. Assanis, D.L. Flowers, S.M. Aceves and R.P. Hessel, A Fully Coupled Computational Fluid Dynamics and Multi-zone Model with Detailed Chemical Kinetics for the Simulation of Premixed Charge Compression Ignition Engines, International Journal of Engine Research, 2005.

2. N. Abani, A. Munnannur and R. Reitz, Reduction of Numerical Parameter Dependencies in Diesel Spray Models, ILASS Americas, 19th Annual Conference of Liquid Atomization and Spray Systems, 2006.

FY 2007 Publications

1. D. J. Torres, Collocated KIVA-4, International Multidimensional Engine Modeling User's Group Meeting Proceedings at SAE Congress, April 2007.

2. Q. Xue, S.C. Kong, D.J. Torres, Z. Xu and J. Yi, DISI Spray Modeling using Local Mesh Refinement, submitted to Society of Automotive Engineers.

3. M. Fife, P. Miles, M. Bergin, R. Reitz and D.J. Torres, The Impact of a Non-Linear Turbulent Stress Relationship on Simulations of Flow and Combustion in an HSDI Diesel Engine, submitted to Society of Automotive Engineers.

FY 2007 Presentations

1. D. J. Torres, "KIVA-4 Development", Advanced Engine Combustion Working Group Meeting, Detroit, October 2007.

2. D. J. Torres, "KIVA Modeling to Support Diesel Combustion Research", DOE National Laboratory Advanced Combustion Engine R&D, Merit Review, Washington, D.C., June 2007.

3. D.J. Torres, "Collocated KIVA-4", International Multidimensional Engine Modeling User's Group Meeting, April 2007.

4. D.J. Torres, "KIVA-4 Development", Advanced Engine Combustion Working Group Meeting, Livermore, February 2007.