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Title: UNSTRUCTURED KIVA

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Los Alamos
NATIONAL LABORATORY

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ABSTRACT

Los Alamos National Laboratory has developed an efficient unstructured version of KIVA-3V, which will be called KIVA-4. KIVA-4 like its predecessor KIVA-3V solves the three-dimensional compressible Navier-Stokes equations in complex geometries with moving boundaries (e.g. pistons and valves). KIVA-4 also inherits the spray and combustion capabilities of KIVA-3V in that it models vaporizing fuel droplets and combusting fuel vapor. KIVA-4 improves the capabilities of KIVA-3V by allowing computations to be performed on unstructured grids, which are generally better and more easily generated grids. KIVA-4 also can use multiple fuel species in vaporizing fuel particles, in contrast to KIVA-3V, which only can use one fuel species. Most importantly, KIVA-4 is no more than 10% slower than KIVA-3V.

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Unstructured KIVA

D. J. Torres and P.J. O'Rourke

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Abstract

Los Alamos National Laboratory has developed an efficient unstructured version of KIVA-3V, which will be called KIVA-4. KIVA-4 like its predecessor KIVA-3V solves the three-dimensional compressible Navier-Stokes equations in complex geometries with moving boundaries (e.g. pistons and valves). KIVA-4 also inherits the spray and combustion capabilities of KIVA-3V in that it models vaporizing fuel droplets and combusting fuel vapor. KIVA-4 improves the capabilities of KIVA-3V by allowing computations to be performed on unstructured grids which are generally better and more easily generated grids. KIVA-4 also can use multiple fuel species in vaporizing fuel particles, in constrast to KIVA-3V, which only can use one fuel species. Most importantly, KIVA-4 is no more than 10% slower than KIVA-3V.

1 Introduction

In the past, Los Alamos has generated parallel unstructured codes to replace KIVA-3V. These codes included CHAD (Computational Hydrodynamics for Advanced Design) and KIVA-AC (AC stands for Arbitrary-Connectivity). These codes scale well in parallel (the computational speed with multiple processors is equal to the computational speed with one processor times the number of processors). CHAD in particular was designed to be significantly more accurate than KIVA-3V. However the single processor speed of KIVA-AC and CHAD are about 10 and 20 times slower respectively than KIVA-3V for a simple 3D compression test. The single processor speed of KIVA-AC and CHAD has prevented them from being adopted by industry. Consequently, Los Alamos has made an effort in the last year to develop an unstructured code that is comparable to KIVA-3V in efficiency.

Los Alamos National Laboratory has developed an efficient unstructured version of KIVA-3V, which will be called KIVA-4. KIVA-4 like its predecessor KIVA-3V solves the three-dimensional compressible Navier-Stokes equations in complex geometries with moving boundaries (e.g. pistons and valves). KIVA-4 also inherits the spray and combustion capabilities of KIVA-3V in that it models vaporizing fuel droplets and combusting fuel vapor. KIVA-4 improves the capabilities of KIVA-3V by allowing computations to be performed on unstructured grids which are generally better and more easily generated grids. KIVA-4 also can use multiple fuel species in vaporizing fuel particles, in constrast to KIVA-3V, which only can use one fuel species. Most importantly, KIVA-4 is no more than 10% slower than KIVA-3V.

2 Indexing changes

KIVA-3V uses an indexing convention where the left-front-bottom node index of a cell is the same as the cell index. KIVA-3V also assumes for example that the left face of a cell is the right face of the neighboring cell. These conventions have been eliminated in KIVA-4. KIVA-4 like KIVA-3V assumes cells are logical hexahedra. However, in KIVA-4 edges and/or faces can degenerate into points which allows for the use of prisms, tetrahedra, and pyramids.

3 Timing comparison

Figure 1 shows the mesh used to compare the efficiency of KIVA-3V and KIVA-4. The darkened vertical port is a pressure inflow boundary held at 2 bars. A fuel rich iso-octane mixture flows in from this pressure inflow boundary. The opposite vertical port is a pressure outflow boundary held at 1 bar. In a 1000 cycle run, KIVA-4 required 201 seconds and KIVA-3V required 183 seconds.

Figure 2 shows the time spent in the 8 most computational demanding subroutines for both KIVA-3V and KIVA-4. KIVA-4 spends a larger amount of time in the momentum fluxing, velocity solver, and mass fraction solver than does KIVA-3V.

Figure 3 shows an unstructured mesh used to model a single cylinder engine with vertical valves and spray with KIVA-4.

4 Limitations

Since KIVA-4 like KIVA-3V places the velocities at the nodes and all other variables (pressure,density,temperature,ect.) at cell centers, it is not advisable to use a grid with a large percentage of degenerate cells, without suffering a loss in numerical accuracy.

KIVA-4 also presently requires a vertical layering of cells be employed in order for the valve and piston snappers to work properly. Specifically cells at one level in the cylinder must be logically equivalent to cells at another level in the cylinder. We hope to relax this limitation in the near future.

While multicomponent vaporization is properly accounted for in KIVA-4, the combustion routines still can only handle one reacting fuel species.

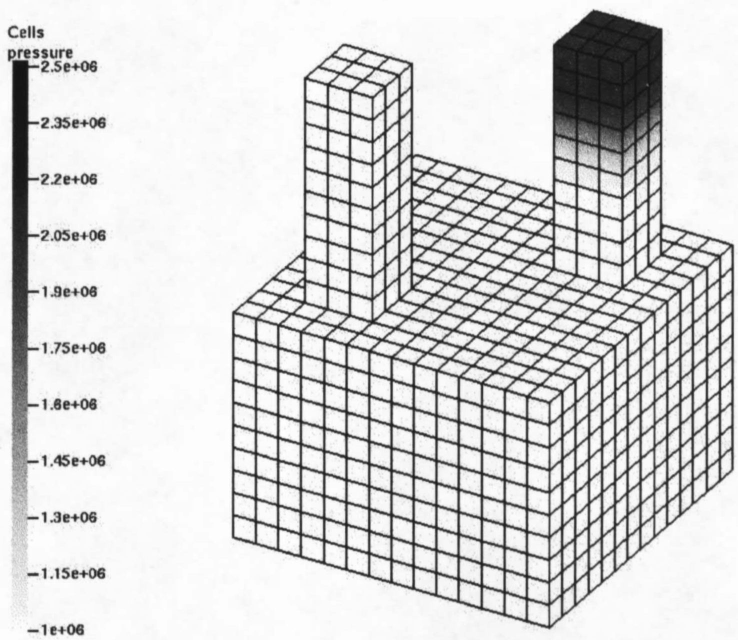

Figure 1: Mesh used for timing comparison of KIVA-3V and KIVA-4.

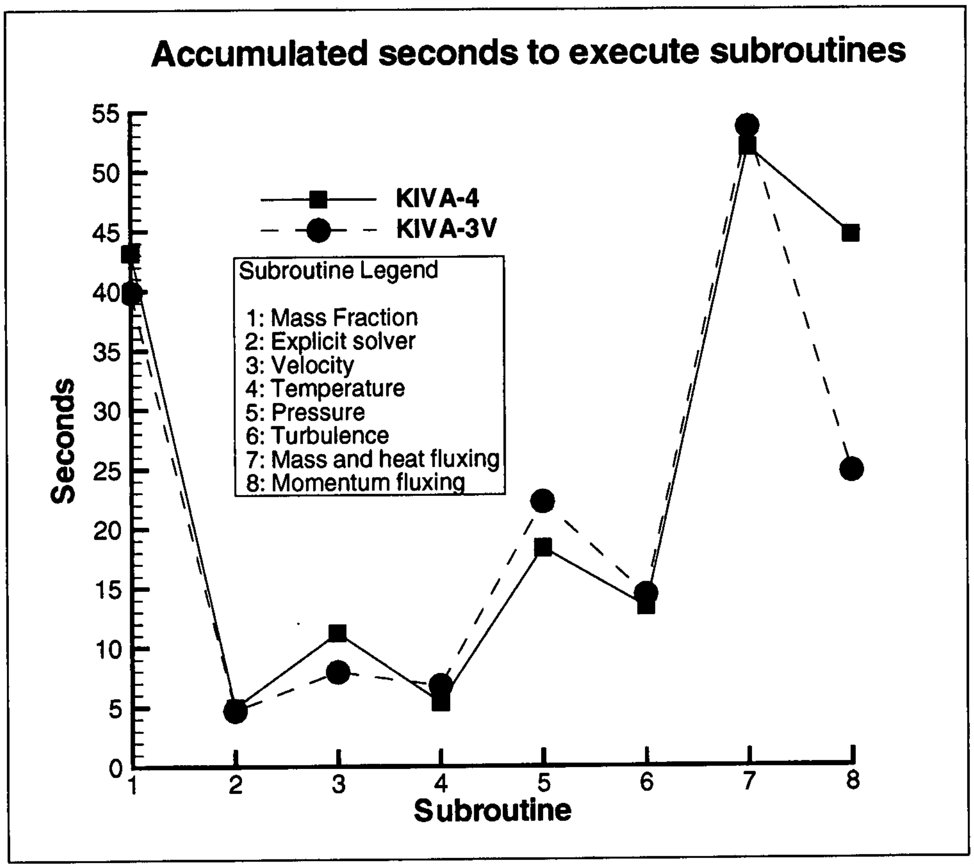

Figure 2: Timing profile comparison of KIVA-3V and KIVA-4.

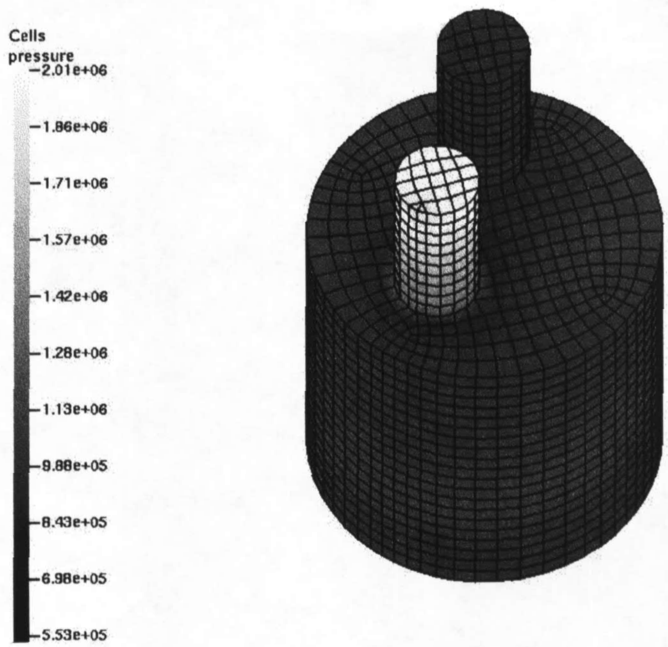

Figure 3: Unstructured grid with valves used for computations with KIVA-4.

We also hope to make the modifications to allow multiple combusting fuel species.

5 Future Plans

A manual describing the features of KIVA-4 and changes to KIVA-3V will be compiled. Since KIVA-4 will be an open source code, the manual should provide an important resource for users who wish to modify the code.

A meshing strategy which uses the meshing capabilities of a software package (GridPro or ICEM) to generate a KIVA-4 compatible mesh will be explored.

Future plans also include parallelizing KIVA-4 possibly with MPI (Message-Passing-Interface). MPI will avoid the considerable parallel overhead penalty inherent in using PGSLIB which is the parallel library used by KIVA-AC and versions of CHAD.