An Unstructured Parallel Solver for Multi-phase and Reactive Flows in Internal Combustion Engines

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Keywords: CFD in Engines, Combustion

Since years IFP applies CFD for understanding and developing internal combustion engines (see for example [1,2]). The finite volume solver KMB [3], a home-developed version of KIVA-II [4], is fully designed for vectorial super computers. The hexaedrical structured multi-blocks approach of this solver is well adapted to these machines but induces a high computing cost due to their expensive price and also drives to very strong constrains on 3D grids especially during grid motion during valves and piston displacement. Then, few years ago, IFP began to develop a new solver, called KIFP [5], designed for less expensive parallel super-scalar machines (SMP machines) in a new hexaedrical unstructured formalism. Figure 1 illustrates the step done in term of possible grid design. Now free set of conformable hexaedra can be used for discretizing the complex 3D engine's geometries. In order to minimize the development cost and time, the OPEN-MP paradigm was chosen for parallelization. This paradigm allows us to work only on the most CPU time consuming routines and ensures the code portability on workstations and PCs.

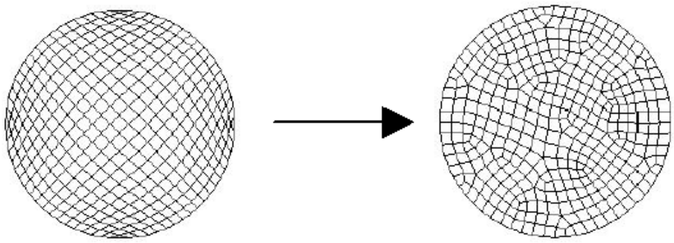

Fig. 1. Old and new grid capabilities; 2D cut-plane in a cylindrical combustion chamber.

KIFP solves the full Reynolds Averaged Navier-Stokes equations for multi-species with sprays and turbulent combustion using the well known time-splitting decomposition. First of all source terms are explicitly solved. For gasoline or Diesel DI (Direct Injection) engines, spray is initiated and the localization of all lagrangian particles is done in the 3D eulerian grid using a very efficient algorithm. Then evaporation and breakup are computed. So far, spray source terms are not too much CPU expensive and their computation is done sequentially. For gasoline turbulent combustion, Extented Coherent Flame Model terms are computed including air/fuel ratio fluctuations in the chamber (ECFM model [6,7]). A phenomenological correlation is used to take into account convection at spark plug for ignition [7]. Due to their CPU cost, some of them are parallelized like chemical kinetic for pollutant formation (CO and NO). A local speed-up of 2.5 for 4 processors is achieved.

Follows the diffusion terms. Species, energy and k-ε turbulent diffusion terms are all implicitly solved by a generic diffusion routine. The conjugate residual method with the SOR algorithm is used to inverse matrices and parallelization is there very efficient. The SIMPLE method [8] is applied for solving in a coupled way the pressure-velocity system. All gradient

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terms used for pressure and Reynolds stress tensor are parallelly computed. Also preconditioning efficiently the pressure matrix [9] drastically reduces the simulation time. The speed-up in this part of the code reaches 3 with 4 processors.

Finally, after the coupling between the lagrangian liquid particles and the gaseous eulerian volume, the convection terms are explicitly sub-cycled. The second order upwind scheme for scalars and momentum convection, a combination of Super-bee and Van Leer limiters [10], is parallelized. Here again a local speed-up of 3 with 4 processors is achieved.

Globally, all parallel sections, more than 50% of the code, give a very good and scalable speed-up around 3 over 4 processors for production cases. Parametric studies drive us to run several time the code at the same time with several parametric variations on large set of processors and not to run case by case on the total set. This allows us to keep the speed-up of 3 over each set of 4 processors. Furthermore, being tomorrow as fast as we are today with the vectorial computer seems to be achievable soon with faster super scalar computers and also nicer unstructured grids allowing higher time step. Figure 2 gives the performances obtained on several modern platforms including sequential time and speed-up for an injection case without combustion (checking the spray performances) and a combustion case without injection (checking the combustion performances). Depending on the machine sequential time may be very interesting and a global speed-up of 3.4 can be reached for the total run.

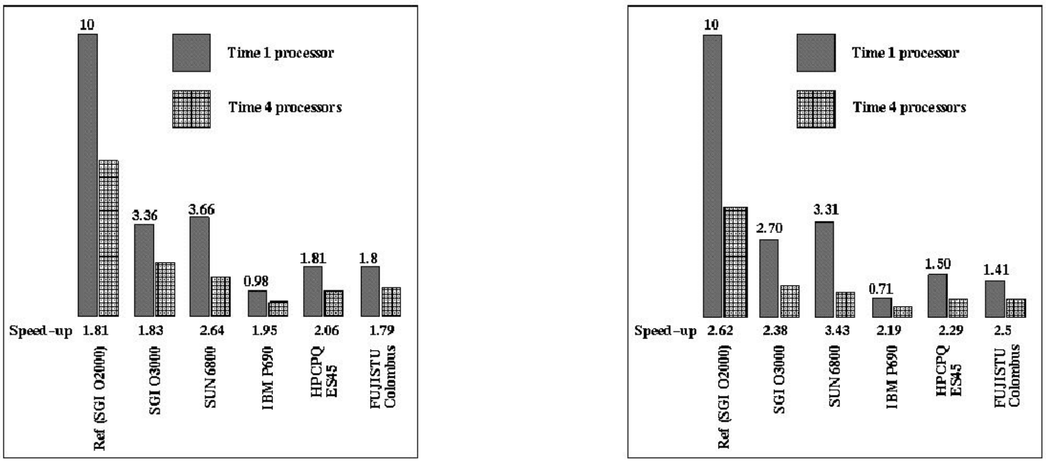

Fig. 2. Normalized performances for an injection case (left) and a combustion case (right).

A gasoline direct injection engine is shown as an example for application runs [7]. The engine is meshed from the CATIA CAD definition. Figure 3 shows the actual engine principle and the actual piston shape with a hemispheric bowl. The half-chamber unstructured grid is shown on figure 4. O and C-shape in all directions of the grid are widely used.

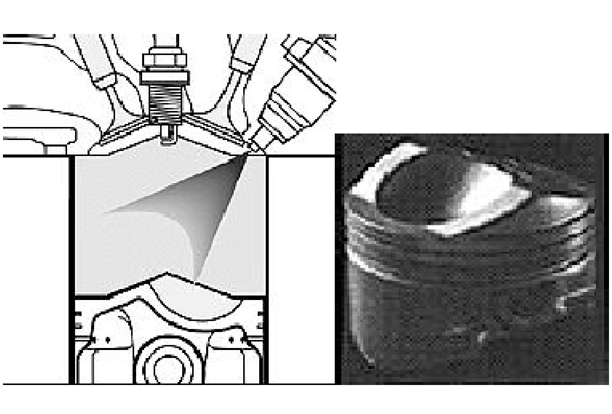

Fig. 3. GDI engine principle and Piston shape.

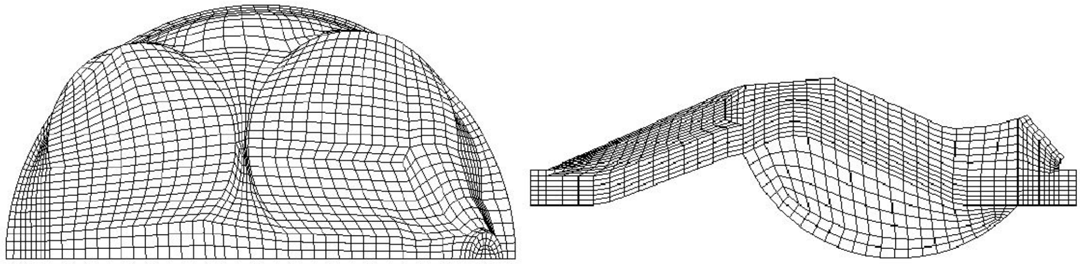

Fig. 4. GDI engine grid; Half cylinder is meshed (top and front views).

For parametrical study, two stratified experimental points are computed. Table 1 gives their characteristics. Computations are initiated at intake valve closing time, 149 crank angle degrees (cad) before top dead center (BTDC), by a tumble motion inside the cylinder.

Table 1

	Rpm	Equivalence ratio	Injection Timing (cad BTDC)	Spark Timing (cad BTDC)
Case 1	2000	0.4	74	28
Case 2	2000	0.5	78	28

Figure 5 shows the spray inside the chamber during injection. More than 45000 particles are used for discretizing the injected mass. Equivalence ratio is also shown until flame kernel deposition prediction which occurs around 20cad BTDC. Due to the bowl in piston shape, a rich area of fuel is located near the spark plug facilitating ignition for lean stratified combustion. At last figure 6 gives the predicted in-cylinder pressure predicted by KIFP compared with experiments. It can be seen that, for case 1, the ignition seems under-estimated although the maximum pressure in the chamber, an important characteristic for engines, is retrieved. On the other side, case 2 ignition is well predicted but maximum pressure is then over-estimated. Discussions may be done on ignition [11] and injection models [12]. Computations are done on LINUX PC 2.4GHz with 2 processors in few hours only.

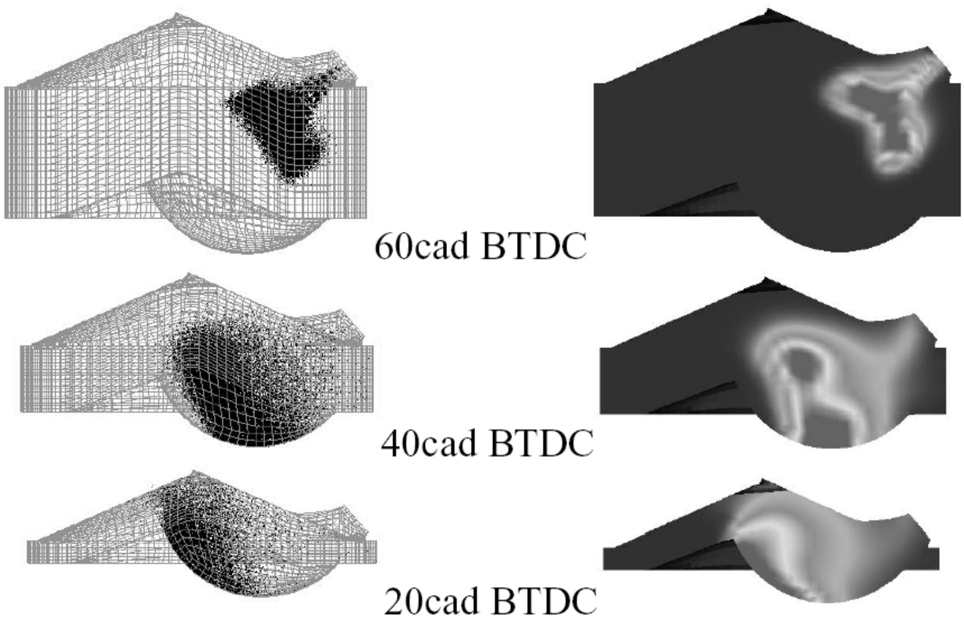

Fig. 5. Spray (left) and equivalence ratio (right) for GDI engine.

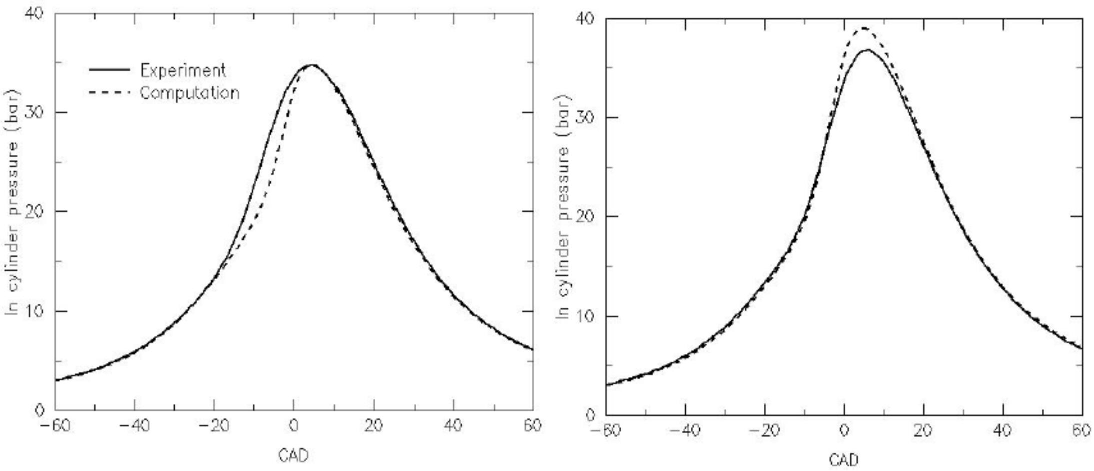

Fig. 6. Predicted cylinder pressure (case 1 left, case 2 right).

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