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**Abstract**

In this work we report on our experiences with running a Combustion Solver for Engine Simulation on a Bulgaria EGEE Grid site during the study visit at the Institute for Parallel Processing of the Bulgarian Academy of Sciences (IPP-BAS) within the scientific cooperation agreement between CNR and BAS.

## 1 Introduction

The design of modern engines relies on new technologies devoted to enhance fuel conversion efficiency and reduce pollutant emissions, in order to match the stringent limits on $NO_x$, $CO_x$ and soot formation imposed by the Governments. The impact on computational modeling is the need to accurately describe highly complex, different physical-chemical phenomena occurring in each engine cycle, and perform over a wide range of engine operating conditions. Typical mathematical models for the description of the overall problem involve different submodels, including turbulence, spray and combustion models with different characteristic time scales. The solution of the overall model usually relies on an operator splitting technique, where the different physical phenomena are decoupled, and the different submodels are separately solved on a 3d computational grid.

In recent years much attention has been addressed to the combustion submodels, by introducing detailed chemical reaction mechanisms, where the number of the chemical species and the reactions to be considered reach also several hundreds. The main computational kernel in this framework is the solution of stiff systems of non-linear ODEs for which implicit methods have to be employed. Therefore, the numerical solution of chemistry has become one of the most computationally demanding parts in simulations, thus leading to the need of efficient combustion solvers [4, 5, 6, 7]. In [8, 9] we have proposed a new approach for solving the above systems based on a combination of two different implicit solvers: VODE [2] and SDIRK4 [3], in order to balance the accuracy and efficiency requirements in realistic simulations. This approach is based on the information that some species, such as ketones and OH radical intermediate species with low density and short characteristic time scales, are crucial in the so-called *cold combustion phase*, therefore stiff stability and accuracy of the Backward Differentiation Formulas (BDF) implemented in VODE are the

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method of choice. On the other hand, in the so-called *hot combustion phase*, ketone can be rapidly damped while other low-density species such as OH radical remains crucial. In this phase, accuracy remains important but highly oscillating components can be observed, for which L-stability properties of the Singly Diagonally Implicit Runge-Kutta (SDIRK) method implemented in the SDIRK4 package appears more effective for having reliable solution and saving computing time. See section "Combustion Model for Diesel Engines" of [8, 9] for the mathematical description of the combustion model and section "ODE Solvers and Multi-solver Approach" of [8, 9] for a description of the main features of the ODE solvers used, both in terms of employed formulas and in terms of stability properties.
Within the context of a time-splitting technique, where combustion is decoupled by fluid flow, the chemical reactions do not introduce any coupling among grid cells representing the combustion chamber, therefore combustion models show an intrinsic parallelism to be exploited. The software is written in Fortran 77. The parallel software component for combustion modeling is based on the CHEMKIN-II [4] package for managing detailed chemistry and it is interfaced with the sequential KIVA3V-II code [1] for the simulation of the entire engine cycle. In order to reduce the impact of local stiffness and adaptive solution strategies on a possible computational load imbalance, the parallel software component supports a data distribution where systems of ODEs related to contiguous cells are assigned to different processors. To this aim, grid cells are reordered according to a permutation of indices, deduced by a pseudo-random sequence, and the ODE systems per each grid cell are distributed among the available processes, following the new order of the grid cells.

## 2 Using the EGEE Production Grid

We ran some tests of the solver on the Bulgarian EGEE Grid site BG04-ACAD located at the IPP-BAS (Institute for Parallel Processing of the Bulgarian Academy of Sciences) using the Grid environment provided by the EGEE project middleware. In order to be able to access this resource a X.509 Grid certificate was necessary along with the membership to one of the Virtual Organization supported. We applied for membership to the SEEGRID VO. We have used the Resource Broker at the IPP-BAS and our own User Interface node located at Institute for High Performance Computing and Networking of the CNR. To run jobs on that site with such a certiticate a VOMS proxy certificate has to be acquired by issuing

```
voms-proxy-init -valid 24:00 -voms seegrid
```

which generates a temporary proxy certificate valid for 24 hours. The MPI implementation installed on the cluster BG04-ACAD was MPICH-GM 1.2.7 and we have installed our software under the shared file system directory

```
/opt/exp_software/seegrid/engine-grid-0.1
```

The job submit command we used is

```
edg-job-submit --config seegrid_ui_var.conf --config-vo seegrid_ui.conf \
-r ce02.grid.acad.bg:2119/jobmanager-pbs-seegrid mpi.jdl
```

which specifies the resource and the queue we wanted to use. An example of the job description file *mpi.jdl* is shown in Figure 1.

This job description file specifies the type of a MPI job using 40 nodes for its execution. It also defines the files which have to be staged in. In our case the job execution script *launch_kiva_40.sh* and the input files *itape*5 and *itape*5.*IM*. The corresponding job execution script is shown in Figure 2

```
JobType="MPICH";
NodeNumber = 40;
Executable="launch_kiva_40_1.sh";
StdOutput="report_out.txt";
StdError="report_err.txt";
InputSandbox={"launch_kiva_40.sh","ITAPE5/itape5","ITAPE5/itape5.IM"};
OutputSandbox={"report_out.txt","report_err.txt","thermo.dat","otape12"};
RetryCount = 0;
```

Figure 1: Example of a Job description file.

```
#!/bin/bash
#PBS -l nodes=80:ppn=1
export PATH=/opt/mpich-mx/bin:$PATH:/opt/globus/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/opt/mx/lib
export MPIRUN_DEVICE=ch_mx
export MX_RCACHE=1
cat $PBS_NODEFILE |uniq |head -n 40 > /opt/exp_software/seegrid/engine-grid-0.1/bin/machinefile
SANDBOX_DIR=‘pwd‘
mv $SANDBOX_DIR/itape5 /opt/exp_software/seegrid/engine-grid-0.1/bin/itape5
mv $SANDBOX_DIR/itape5.IM /opt/exp_software/seegrid/engine-grid-0.1/bin/itape5.IM
cd /opt/exp_software/seegrid/engine-grid-0.1/bin/
/opt/mpich-mx/bin/mpirun --mx-copy-env -np 40 -machinefile $PBS_NODEFILE ./kiva_stat_misto_v2
mv /opt/exp_software/seegrid/engine-grid-0.1/bin/otape12 $SANDBOX_DIR
mv /opt/exp_software/seegrid/engine-grid-0.1/bin/thermo.dat $SANDBOX_DIR
```

Figure 2: Example of a Job execution script.

# 3 Numerical experiments and Performance Results

In this Section we show results concerning engine simulations performed on a prototype, single cylinder Diesel engine, having characteristics similar to the 16 valves EURO IV Fiat 1.9 JTD Multijet. Main engine parameters are reported in Table 1.

| | |
|---|---|
| Bore[mm] | 82.0 |
| Stroke[mm] | 90 |
| Compression ratio | 16.5 : 1 |
| Engine speed | 1500 rpm |
| Displacement[$cm^3$] | 475 |
| Valves per cylinder | 4 |
| Injection system | $2^n d$ gen. Common Rail |
| Electro-injector | microsac, 7 holes, $\phi = 140mm$ |
| | $440mm^3/30sec/100bar$ |

Table 1: Multijet 16V Engine Characteristics

Three different operating conditions have been considered, corresponding to different values of Exhaust Gas Recir-

culation (EGR), rail pressure, and injection timing, which characterized three different test cases (*Case 1–3*) for our simulation software.

Our typical computational grid was a 3d cylindrical sector representing a sector of the engine cylinder and the piston bowl. It was formed by about 3000 cells, numbered in counter-clockwise fashion on each horizontal layer, from bottom-up. Note that, the structure of the active computational grid changes within each simulation of the entire engine cycle in order to follow the piston movement into the cylinder. The limit positions of the piston, that is the lowest point from which it can leave and the highest point it can reach, are expressed with respect to the so-called Crank angle values and they correspond to $-180^o$ and $0^o$. During the typical interval of the Crank angles ($[-20^o$, $40^o]$) in which main combustion phenomena happen, the total number of active cells is about 1000.

We carried out our tests using 1, 4, 8, 16, 32 and 40 CPUs of the BG04-ACAD cluster. The nodes of the cluster are equipped with Dual 2.4 GHz AMD Opteron processors and 4 GByte of main memory and are interconnected by a Myrinet network.

The total execution times obtained for a complete engine cycle for the different number of CPUs used are reported in Table 2.

| | Case 1 | Case 2 | Case 3 |
|---|---|---|---|
| 1 procs | 11935 | 13769 | 11023 |
| 4 procs | 6530 | 7424 | 6496 |
| 8 procs | 3748 | 4137 | 3354 |
| 16 procs | 2349 | 2564 | 2048 |
| 32 procs | 1682 | 1755 | 1390 |
| 40 procs | 1510 | 1530 | 1254 |

Table 2: Total execution times (in seconds) of the simulations.

The corresponding speedups are shown in Table 3.

| | Case 1 | Case 2 | Case 3 |
|---|---|---|---|
| 4 procs | 1.83 | 1.85 | 1.70 |
| 8 procs | 3.18 | 3.33 | 3.29 |
| 16 procs | 5.08 | 5.37 | 5.38 |
| 32 procs | 7.09 | 7.85 | 7.93 |
| 40 procs | 7.90 | 9.00 | 8.79 |

Table 3: Speedups.

One can see that the parallel efficiency decreases relatively fast with the number of processors. This effect is due to the overhead of the sequential part of the code that becomes more significant as the number of the processors increases.

In Figure 3 the in-cylinder pressure graph for the three available test cases is shown.

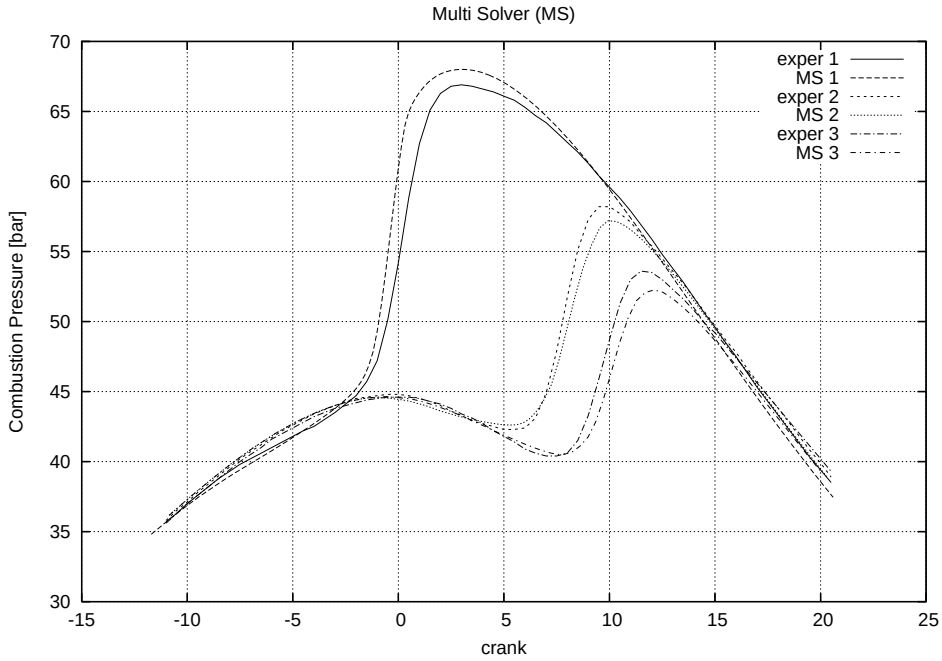


Figure 3: Combustion pressure for the three available test cases: experimental pressure values are compared to predicted ones testing results reliability.

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