Effect of grid resolution on combustion simulations of large scale experiments

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One major concern with numerical simulations of combustion processes is the accuracy of the solution. In one and two dimensional calculations it is usually possible to perform calculations with sufficiently fine grids. The convergence of the solution can then be shown by comparison to an even finer grid with higher resolution. This approach becomes difficult for transient three dimensional calculations as the number of grid cells increases with the third power and the computational effort with the fourth power of the inverse of the cell size. For large scale applications with complex geometries the cell size is typically limited by the available computational resources and not by the requirements of the physical model. Therefore it is generally not possible to demonstrate a fully converged solution by comparison to an over resolved reference calculation.

In order to study the effect of grid size on the solution, the only option is to use simulations with coarser grids than the resolution we can effort. Since we know that these grids are to coarse to give a fully converged solution, we must expect differences between the solutions on different grids. However, these differences should provide insight into the behavior of the solution on different grids and should, hopefully, allow to judge the quality of the best possible (that is affordable) solution.

At Forschungszentrum Karlsruhe we are interested in hydrogen distribution and combustion problems in large scale facilities with complex geometries. The background of our work is the study of severe accidents in nuclear power plants, where in a certain class of accidents large amounts of hydrogen (several hundred kg) are released from the reactor pressure vessel into the containment building ($\approx 100000\ m^3$). The phenomena involved are studied experimentally and by numerical simulations. The different stages of such an accident scenario are dominated by different physical effects which proceed on different time and length scales. To cover the whole sequence of events several specialized fluid dynamics codes have been developed. The distribution phase is covered by GASFLOW [1], fast turbulent combustion processes are described by COM3D [2] and detonations by DET3D [3]. Although these codes have been developed for safety studies of nuclear fission plants, they also have been proven useful in fusion reactor applications and in studies concerning facilities in a developing hydrogen economy.

In the present work we will focus on turbulent combustion applications. The above mentioned code COM3D solves the Navier-Stokes equations together with a k-ϵ turbulence model and an Eddy-Breakup combustion model on an equidistant structured grid. While these models have their limitations, they are still widely used in production environments, since many more advanced models are computationally too demanding.

On order to allow for local grid refinement, the code was included into a parallel framework for adaptive mesh refinement. This framework is based on the work of Marsha Berger and coworkers [4, 5] and uses the solver and physical models from COM3D. The new code was named COMPA (COM Parallel Adaptive) in order to honor its ancestor [6]. Together with the new AMR framework pre and post processing tools were developed to support the more complex data structures needed with refined grid geometries. The preprocessing tools allow the automatic generation of structured grids from CAD files of the problem geometry. While this might not seem too important, it turned out, that a major obstacle to grid sensitivity studies in complex geometries was the work involved in setting up the required computational grids.

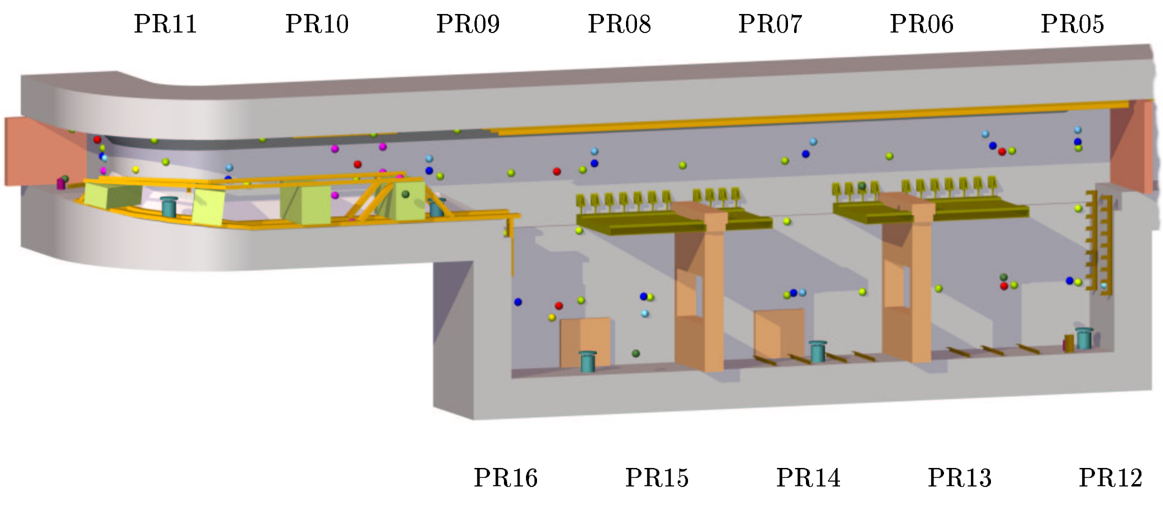

Figure 1: Schematic view of test facility with approximate positions of pressure probes

As part of the validation procedure of COMPA numerical simulations of combustion experiments in a large scale combustion facility (see Figure 1 and [7]) were performed for different grids. The experiments were performed to provide a database for blind benchmark tests of different combustion codes. While the original COM3D code took part in the blind benchmark exercise, the COMPA code was not ready in time. Therefore all simulation results in the present paper are from post test calculations. For the configuration shown four experiments have been performed with different ignition locations and with different hydrogen concentrations (10 % and 11.5 % hydrogen in air). These concentrations are at the transition from fast to slow combustion modes.

With the usage of the preprocessing tools we have two possibilities to create grids with different cell sizes. The first option is to use the same geometry for all grid resolutions. With decreasing cell size the number of cells increases, but the level of geometrical detail, that is included in the computational grids, does not change, e.g. a coarse cell is split into finer cells, but no additional obstacles are introduced in the finer cells. The other option is to increase the level of detail with decreasing cell size. Thus more and more small features of the problem geometry are included in the computational grid. A coarse cell is in this case split into cells containing gas and cells containing obstacles.

Numerical simulations were performed with four different cell sizes as indicated in Table 1. In these grids the level of geometrical details increases with decreasing cell size. In the coarsest grid only the major obstacles can be modeled. The next grid with dx=0.3m already includes the venting tubes at the bottom of the canyon. At dx=0.1m the connecting structures between obstacles appear, and with the finest grids the steel structures at the walls are partially included. The simulations were performed using a standard k-ϵ model and a standard eddy-breakup model. For each grid the model parameter in the combustion model was chosen to give good agreement with the experimental data.

Table 1: Main parameters of computational grids

	cell size	**grid size**	**gas/total**	**hardware**
G0500	dx = 0.5m	60 x 17 x 17	2364/ 17340	Linux workstation, 2 workers
G0300	dx = 0.3m	97 x 25 x 25	10699/ 60625	Linux workstation, 2 workers
G0100	dx = 0.1m	281 x 67 x 70	282127/ 1317890	Linux cluster, 9 workers
G0050	dx = 0.05m	567 x 126 x 133	2286940/2923160	Cray T3E, 31 workers

The results indicate that a reasonable description of the combustion processes is possible even with the coarsest grid. With decreasing cell size more and more details become visible, but the general appearance of the pressure histories does not change. It seems that the finest grid does not offer any further advantage in the frame of the physical models used. However, the different simulations require different values for the parameter in the combustion model with values ranging from 10 to 13.

A second set of simulations with different cell sizes and identical geometries is currently under way. Results of these simulations will be presented also. This second set of computations will help to decide whether the observed variation in the combustion model constant is due to the grid resolution or to the level of detail with which the geometry is described.

References

[1] J.R. Travis, P. Royl, R. Redlinger, G. Necker, J.W. Spore, K.L. Lam, T.L. Wilson, B.D. Nichols, C. Müller. GASFLOW II: A three dimensional finite volume fluid-dynamics code for calculating the transport, mixing and combustion of flammable gases and aerosols in geometrically complex domains. Report FZKA-5994, LA-13357-M, Forschungszentrum Karlsruhe, 1997.

[2] A. Kotchourko, W. Breitung. Numerische Simulation der turbulenten Verbrennung von vorgemischten Gasen in komplexen 3D-Geometrien. Nachrichten - Forschungszentrum Karlsruhe 32 (2000) 3, pp.243-249.

[3] R. Redlinger, L. Obholz. Numerical simulation of gaseous detonations in the ITER-FEAT Fusion Reactor. Nachrichten - Forschungszentrum Karlsruhe 34 (2002) 4, pp.295-301.

[4] M. Berger. Adaptive Mesh Refinement for Time-Dependent Partial Differential Equations. Ph.D. dissertation, Stanford University, Computer Science Report No. STAN-CS-82-924, 1982.

[5] M. Berger, A. Jameson. Automatic Adaptive Grid Refinement for the Euler Equations. AIAA Journal, volume 23, number 4, pp.561-568, 1985.

[6] U.Bielert. Documentation of program package COMPA. Under development. Hopefully available soon at http://www.iket.fzk.de.

[7] A.Efimenko, A. Bezmelnitsin, A. Denkevits. Data report on large scale test configurations 1 and 2. Integral large scale experiments on hydrogen combustion for severe accident code validation. Deliverable No. 11 of HYCOM project, FIKS-CT1999-00004, December 2001.