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Numerical Simulation of Accidental Fires with a Spillage of Oil in Large Buildings

C. Muñoz[a] , D. Vicente[b *]

[a]*BAC Engineering Consultancy Group, Spain*
[b]*Barcelona Supercomputing Center - Centro Nacional de Supercomputación, Spain*

Abstract

BAC's (BAC Engineering Consultancy Group) participation in PRACE programme has made possible to increase its knowledge in the field of fire engineering and the application of advanced computing strategies. These fields may be applied directly to a fire engineering analysis (Performance-Based design) of the steel structure buildings that belong to the International Thermonuclear Experimental Reactor industrial complex in France, which is devoted to research in the field of Nuclear Fusion. In particular, the project could be focused on the building that hosts the cryogenic system of the Tokamak. This building is characterized by its large size. The building hosts a large number of helium and nitrogen compressors, as well as the charcoal filter system, that is necessary for the cryogenic system.

Numerical simulations of the accidental fires that can take place inside of the building have been carried out, some of them as complex as considering the combination of a liquid combustible spillage added to an oil cloud due to the breakage of a high pressure pipe.

1. Introduction

Since 1984, when first Eurocodes [1] were published, the European Union promotes the Performance Based Design. Since then, it is necessary to guarantee the security of building structures against fire action, especially in those buildings where the application of prescriptive laws are often very complicated (in terms of cost, i.e.). The better way to define active and passive protection methods in any building are the risk analysis, according to the people activity, and the analysis of the fires that may occur and its consequences. This analysis often requires the computational simulation of fires, based on computational fluid dynamics software. The software should include flow dynamics, the complex characterization of turbulences, as well as combustion and heat transfer phenomenon. These physical and chemical phenomena require a very high computational capacity.

BAC develops complex computational fluid dynamic simulations in the fields of Fire and Wind engineering, in order to support Building Department to obtain complex structural and architectural designs. Its participation in the SHAPE programme, and the collaboration during the research project with the technical team of the Barcelona Supercomputing Center (BSC), has allowed BAC to carry out a research project to improve the know-how relative to the computational simulation of fires associated to liquid fuels (spillage of oil) in large industrial buildings.

The development of these computational fluid dynamic simulations in the industrial field must be usually carried out with a strict time schedule, coherent with the project and worksite development. For this, it is necessary to use optimized HPC machines to obtain a high parallelization of the models. BAC has a cluster to adapt to the customer's requirements. Thanks to PRACE programme, it has been possible to optimize the parallelization

* Carlos Muñoz, cmunoz<at>bacecg.com ; David Vicente, david.vicente<at>bsc.es

procedure introduced in BAC, identifying the most important weaknesses of its current computing cluster and proposing an optimized and strategic investment to extend its infrastructure to use HPC.

In this way, through BAC's participation in the PRACE programme, and the important collaboration with BSC teams, BAC has improved its knowledge regarding the computational simulation of oil spillages. BAC has also increased its computer simulation capacity, removing different weaknesses of its current infrastructure.

2. Simulations

To improve the know-how relative to the computational simulation of fires associated to liquid fuels and to optimize parallelization tasks in BAC's cluster, different simulations have been carried out.

2.1. Software

The software used in this project is Fire Dynamics Simulator (FDS) [2]. FDS is a computational fluid dynamics model of fire-driven fluid flow. It solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. It is open source software developed by the National Institute of Standards and Technology (NIST).

FDS aims at solving practical fire problems in fire protection engineering, while at the same time providing a tool to study fundamental fire dynamics and combustion. It has the following features [3], [4]:

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- **Hydrodynamic Model**

  FDS solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. The core algorithm is an explicit predictor-corrector scheme, second order accurate in space and time. Turbulence is treated by means of Large Eddy Simulation. It is possible to perform a Direct Numerical Simulation if the underlying numerical mesh is fine enough. LES is the default mode of operation.

- **Combustion Model**

  For most applications, FDS uses a single step, mixing-controlled chemical reaction which uses three lumped species (a species representing a group of species). These are air, fuel, and products. By default the last two are explicitly computed. Options are available to include multiple reactions and reactions that are not necessarily mixing-controlled.

- **Radiation Transport**

  Radiative heat transfer is included in the model via the solution of the radiation transport equation for a gray gas, and in some limited cases using a wide band model. The equation is solved using a technique similar to finite volume methods for convective transport, thus the name given to it is the Finite Volume Method. Using approximately 100 discrete angles, the finite volume solver requires about 20% of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer. The absorption coefficients of the gas-soot mixtures are computed using the RadCal narrow-band model. Liquid droplets can absorb and scatter thermal radiation. This is important in cases involving mist sprinklers, but also plays a role in all sprinkler cases. The absorption and scattering coefficients are based on Mie theory.

- **Geometry**

  FDS approximates the governing equations on a rectilinear mesh. Rectangular obstructions are forced to conform to the underlying mesh.

FDS is parallelized with a hybrid strategy. The combination of MPI and OpenMP approaches enables a two-level parallelization: at first the computational domain is decomposed into meshes for distributed memory, and then, within each mesh the multi-threading approach on some selected code regions is applied for shared memory [5].

2.2. Cases configuration

The project included the analysis of six different simulations. Initially, the typical fire that was intended to be characterized in the project would have a duration between 1200-1500 seconds, depending on the combustible amount. However, based on the fire characteristics that BAC is analysing, we consider that is not necessary to understand the behaviour of the spillage of oil and to obtain the mesh optimization to develop all the fire duration. It is for this reason that the time simulation developed is close to 50 seconds in all cases. It is important to highlight that the fire has a steady behaviour already from the 10 seconds. The growth of an oil spillage is very fast.

The project has consisted in the following phases:

1. Installation: The software Fire Dynamics Simulator has been handed over to the PRACE partner and installed on the target system
2. Verification and validation: Verification and validation of the FDS software with example test cases and benchmarks. The purpose of this testing process has been to ensure that the software installation is successful and that any corruption of the software executable or libraries has occurred.
3. Simulation and analysis of the results: BAC has carried out six fire simulations, including an oil spillage in the centre of a large domain (360,000 m^3). This domain represents a standard benchmark of a large industrial building. The time of simulation is close to 50 seconds (in the highest Rate of Heat Release (RHR) period).

A domain of 100m x 60m x 60m has been designed, with 23 million of finite volume cells. A localized fire of 100m^2 is simulated in the centre of the domain, with a Rate of Heat Release (RHR) of 50MW. The fire is fully developed after the first 10 seconds of simulation. The finite volume cells have a uniform edge size of 250mm.

The cases tested have been the following:

- 64 cores: 360,000 elements/core
- 256 cores: 90,000 elements/core
- 1,024 cores: 22,460 elements/core
- 2,048 cores: 11,230 elements/core

The scalability of the models proposed to analyse the simulation of spillage of oil and fuel is evaluated. The results variability obtained depending on the mesh segmentation has also been analysed.

3. Results

The code scales properly up to 256 MPI processes and using up to 2 OpenMP (OMP) threads per core. The results for 1024 and 2048 cores were better than 256 but the speedup was less than 60% of the ideal, so we consider the best number of processes to execute the simulation is around 256 and 512 cores depending on the size of the input (Table 2).

The use of up to 2 threads was decided following the numbers obtained with the execution with 1, 2 and 4 threads of an example with mesh of 23M elements executed with 64 MPI processes (Table 1).

Number of cores used	Number of MPI processes	Number of OMP Threads x process	Wall clock time (s)	Measured speedup	Lineal speedup
64	64	1	820	x1	x1
128	64	2	580	x1.41	x2
256	64	4	473	x1.73	x4

Table 1: Scalability analysis developed in BSC machine

The scalability curve when the number of processors varies for a fixed total problem size is shown in Figure 1.

Number of cores used	Number of Nodes (16 cores per node)	Number of MPI processes	Number of OMP Threads x process	Wall clock time (s)	Measured speedup	Lineal speedup
64	4	64	1	33,970	x1	x1
256	16	256	1	10,528	x3.2	x4
1024	64	1024	1	3,197	x7.7	x16
2048	128	1024	2	2,689	x11.2	x32

Table 2: Scalability analysis developed in BSC machine

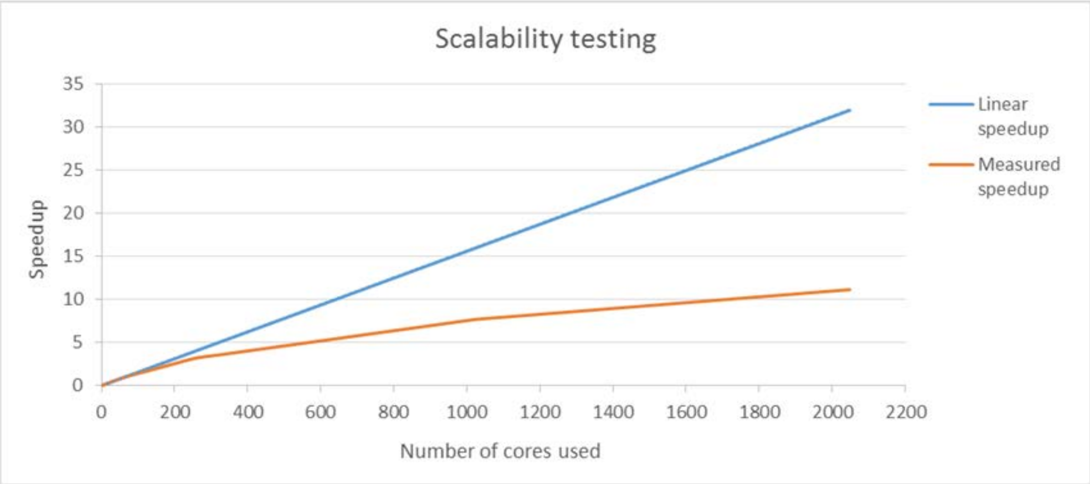

Figure 1: Scalability curve.

The influence of the partitioning of the model in different meshing parts in which to solve the Navier-Stokes equations has been analysed. Not only the time of the simulation has been analysed, but also in the numerical results obtained, depending whether the combustion area is involved in a mesh contact surface or whether the contact surfaces are located in an inert zone of the global computational domain (Figure 2).

The example of a combustion process of 50MW in the centre of the computational domain is showed in Figure 3. It is important to highlight that in this case the flame zone is directly affected by two connection surfaces of domains passing through the combustion zone by the centre of the mesh vertically, one in each main direction of the mesh, both orthogonal between them.

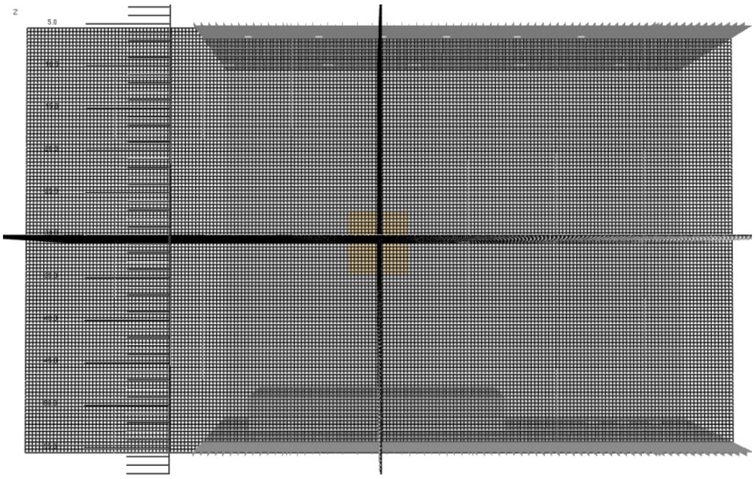

Figure 2: Mesh domain.

There are analyses and papers developed by different researchers [8] that highlight the possible divergence of results obtained in the initial versions of the FDS software due to the mathematical methods of resolution of the pressure Poisson equation. In the resolution of the domain in a single mesh (single processor) the solution for the Poisson equation is very precise, but in multiple meshes there may be a delay in the communication of the information through the general domain, since the Poisson equation is solved in each mesh individually, without taking into account the general domain.

Interesting alternatives have been developed, such as the FDS-ScaRC resolution method [7]. Compared to the FDS-FFT method [3], FDS-ScaRC features a greater stability and quality in the results obtained regardless of the number of meshes. The FFT-based method may diverge for high number of meshes [8], [9].

This question has important effects on the simulation time of the computational models and on the parallelization capacity. To produce connections between different meshes with a high numerical computational load from the fluid governing equations can imply a delay in parallelization. This delay, which can be seen in the scalability curve, is accentuated when the connection between computing nodes has not a dedicated high performance network like infiniband, increasing the latency periods of the processing.

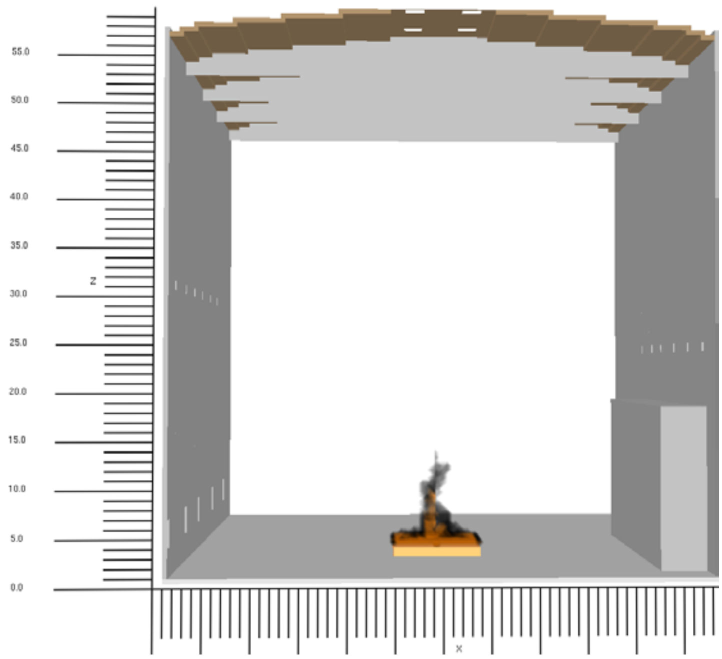

Figure 3: Fire plume in the centre of the domain.

Based on this study, it has been possible to compare BSC and BAC architectures (Table 2), identifying BAC's weaknesses to obtain the maximum performance of its cluster. The latter has the configuration shown in Table 4.

	BAC machine 3-4	**BSC**
PROCESSORS	2 x Intel Xeon E5-2670 8 core	2 x Intel Xeon E5-2670 8 core
O.S.	Windows Server	Linux SuSe Distribution 11 SP3
MPI	mpich2	Intel MPI 5.1.2 for Linux v3.0
OpenMP	Disabled	Enabled
FDS	6.0.0	6.4.0
NODE CONNEXION	Switch 1 Gb	Infiniband Mellanox FDR10
RAM/node	40Gb/node DDR3-1333MHz	32Gb/node DDR3-1600DIMMs
Hard Disk	1 TB 7200 rpm SAS	500Gb 7200rpm SATA II local HDD

Table 3: Architecture differences.

Machine 1	Dell R620 2 Intel Xeon E-5 2640 (12 cores – 24 threads with Hyperthreading) RAM 40Gb DDR3 – 1,333 MHz O.S.: Windows Hard Disk: SAS 7,200rpm; 500Gb
Machine 2	Dell R620 2 Intel Xeon E-5 2640 (12 cores – 24 threads) RAM 40Gb DDR3 – 1,333 MHz O.S.: Windows Hard Disk: SAS 7,200rpm; 500Gb
Machine 3	Dell R620 2 Intel Xeon E-5 2670 (16 cores – 32 threads) RAM 40Gb DDR3 – 1,333 MHz O.S.: Windows Hard Disk: SAS 7,200rpm; 1Tb
Machine 4	Dell R620 2 Intel Xeon E-5 2670 (16 cores – 32 threads) RAM 40Gb DDR3 – 1,333MHz O.S.: Windows Hard Disk: SAS 7,200rpm; 1Tb
Connection between machines	Switch 1 Gb/s

Table 4: BAC's cluster specifications.

It has been detected a phase of high number of MPI communications between nodes that is critical in the parallelization with Fire Dynamics Simulator, especially with a high number of processes in the fire simulation. The simulation of liquid fuels requires the generation of highly refined meshes in the area where the combustion process is produced. This refinement of the mesh implies, in large industrial buildings, the use of a very high number of processes, which imply several nodes. If an interconnection system of 1Gb/s is considered the calculation speed can be seriously affected, compared with an architecture in which there is Infiniband interconnection. In the case of MareNostrum, the technology used is Infiniband FDR10 with up to 40Gb/s. The verification related to the interconnection between nodes has been verified simulating 50 seconds of combustion with a total of 64 meshes.

In BAC architecture different simulations have been developed with 32 processes in a single node, and have been compared with the same number of processes in the BSC-MareNostrum HPC machine (Table 5). These simulations have determined a speed increase in the BSC of ~28%. However, the increase in the velocity is spectacular when the domain is discretized in 32 processes, using 2 nodes and launching 16 MPI processes in each node. The connection between nodes in this case is highly penalized in BAC architecture case, comparing it with BSC-MareNostrum machine, with a difference in time simulation of more than 13 times.

This analysis allows BAC to obtain important conclusions about the requirements of FDS code in terms of scalability and performance. This analysis will permit the adaptation and improvement of the BAC architecture to run parallel calculations with a high numbers of processes and with a good performance and also to understand the limitations of the code in HPC systems.

The study has also included the decomposition of the domain of analysis in different proportions of sub-domains, according to Table 6, evaluating the best options to simulate the liquid fuels combustion in large closed spaces. The global domain partition has been made to evaluate, based on MareNostrum's (MN) simulation time, the maximum optimization that could be obtained with the company's architecture, and how to improve it by optimizing the investment.

Number of MPI processes	OMP Threads	Simulation time [s] in BAC machine	Simulation time [s] in BSC HPC machine	Ratio BAC over MN times
32	1	3,532 (1 node, 32 procs/node) 37,105 (2 nodes, 16 procs/node)	2,758	1.2 13.45
32	2	N/A	1,984	--
64	1	N/A	1,712	--

Table 5: Analysis comparing MN and BAC simulation times.

Initial Time Step	Simulation time (s)	Elapsed time (s)	Ratio over reference
300	11.26	34916	**1.00**
Final time Step	Simulation time (s)		
2400	41.33		Memory requirements (Gb)
			9.58

Initial Time Step	Simulation time (s)	Elapsed time (s)	Ratio over reference
300	11.18	51196	1.47
Final time Step	Simulation time (s)		
2400	40.33		Memory requirements (Gb)
			7.5

Initial Time Step	Simulation time (s)	Elapsed time (s)	Ratio over reference
300	11.2	53247	1.53
Final time Step	Simulation time (s)		
2400	40.72		Memory requirements (Gb)
			7.5

Initial Time Step	Simulation time (s)	Elapsed time (s)	Ratio over reference
300	11.25	54455	1.56
Final time Step	Simulation time (s)		
2400	41.15		Memory requirements (Gb)
			7.5

Initial Time Step	Simulation time (s)	Elapsed time (s)	Ratio over reference
300	11.25	46047	1.32
Final time Step	Simulation time (s)		
2400	41.23		Memory requirements (Gb)
			9.08

Domain divisions		
X	Y	Z
8	**8**	**1**
4	4	4
2	8	4
4	8	2
1	8	8

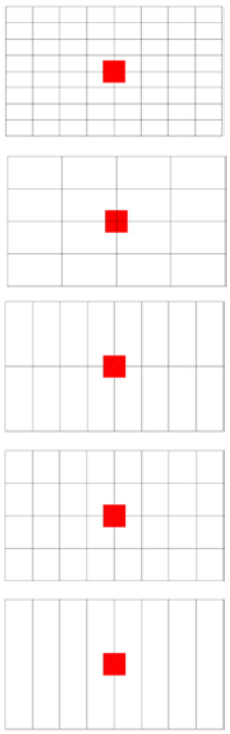

Table 6: Domain division optimization

From the simulation with different partitions of the general domain it can be determined that in the case of the simulation of combustion liquid fuels, maximum efficiency has been achieved by performing the decomposition in two of the three directions of the space in which the Navier-Stokes and pressure Poisson equations must be solved.

Based on the vertical main turbulence movement of the air in fire's plume during the combustion process it is considered that the best option is to divided the domain in X and Y directions, and to avoid big data transfer between different meshes in Z-direction. To avoid big data transfer between meshes could increase simulation speedup, especially if network connection is not optimal. Any other option that has included subdivision in the three directions of space, especially the subdivision in Z-global, has generated a higher data transfer between common contact surfaces, which has penalized the simulation time.

4. PRACE cooperation and benefits for the SME

The Partnership for Advanced Computing in Europe (PRACE) has provided the expert support to install the code, adapt their scripts for running the system, helped in their local installation and fixing technical problems in their use of Tier-0 systems and also within their own company cluster. In addition, PRACE provided through a PRACE Preparatory Access Type-B the required computational time needed to perform these initial simulations.

The numerical simulations have allowed the understanding the possible fire situations and their effects on large industrial buildings, for example in one of the most representative international projects and non-pollutant energy icon for the future generations.

The SHAPE programme has enabled BAC Engineering Consultancy Group to carry out the optimization of simulations where it is necessary to consider the interaction between large industrial buildings and the combustion of liquid fuels, such as oil and fuels pools. Under these conditions, the optimization of the calculation processes is the key to develop the characterization of all combustion and turbulence phenomena with the maximum possible accuracy, while ensuring that the HPC architecture allows the simulation with the maximum processing velocity.

The participation in the SHAPE programme has made possible to test the scalability of the code in an HPC environment and to develop the capacities inside the company to use HPC when required.

The high capacity of parallelization and calculation of HPC has allowed the company to use fine spatial meshes and guarantee the correct resolution of the numerical simulation in a suitable time.

Knowing the best meshes configuration for the simulation of oil spillages, BAC has improved its knowledge in relation to this type of simulations in industrial buildings. In addition, the participation in the SHAPE programme has enabled BAC to know the best way to improve its parallel calculation architecture, optimizing the investment to be made in the improvement of those aspects more relevant to increase the velocity of simulation in parallel.

In summary, this project has improved BAC's know-how on high performance computing and has strengthened its position for next challenges.

In addition, the important collaboration of BSC members has enabled BAC to detect weaknesses in the company's cluster architecture, suggesting the most appropriate strategies to improve parallelization and reduce latency times during the simulation of liquid fuels combustion in large industrial buildings. It has been detected that the connection between BAC nodes is one of the weaknesses of its cluster. Taking into account the economic cost of implementing an Infiniband network in an SME, it has been considered that the best strategy to improve BAC's architecture is the connection with a 10Gbits network. However, the possibility of implementing an Infiniband network is also considered, taking into account shorter latency periods that would greatly improve the company's simulation time.

There is also a possible node-to-node Windows communication delay because network-level optimizations are more improved on Linux than on Windows O.S. Currently the company runs its simulations in Windows. However, analysing the results in a Linux O.S., BAC is considering changing to Linux O.S. on its cluster.

5. Conclusions

The SME performed benchmarking and scalability tests of the Fire Dynamics Simulator (FDS) code in BSC's MareNostrum machine up to 2,048 cores and then the results were compared with its in-house cluster. The company verified that its infrastructure is not optimal with respect to node connectivity and system configuration that minimize the scalability of the code. The BSC team supported them to improve parts of the local installation helping to optimize their current infrastructure and detect the bottlenecks to tackle for future clusters and installations.

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Acknowledgements

This work was financially supported by the PRACE project funded in part by the EU's Horizon 2020 research and innovation programme (2014-2020) under grant agreement 653838.