Fast and correct computation A comprehensive test concept to proof the new FDS-SCARC technique

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Abstract

Because CFD programs, like FDS, generally consist of a large number of different components representing the variety of participating numerical algorithms and chemical / physical processes, it is close to impossible to verify such codes in its entirety, for example with comparisons of fire tests. Instead, a careful verification and validation under consideration of mathematical conditions and used numerical schemes is imperative, even for single components as well as groups of components with increasing complexity. In particular, error cancelations between single program components can only be detected by such component-level tests. The article presents the structure of such a comprehensive test concept and the needs of more mathematical and numerically orientated test procedures that are much more suited for a reliable evaluation than only a simple visual comparison of the numerical results of experimental fire tests.

1. Introduction

In [5, 6] we explained a major lack of the current program package FDS concerning the geometric decomposition of the computed domain into smaller subdomains or meshes. We presented a new generalized domain decomposition strategy for the efficient parallel solution of the FDS-pressure equation that guarantees the necessary accuracy. In this second part, we describe a comprehensive test methodology and first tests to proof the correctness of this new strategy.

Given the positive experience with certification processes for tools and components for civil engineering, it seems appropriate to develop analogous quality assessment procedures for fire safety-related CFD programs as described in [11]. In fact, in analogy with fire tests for structural elements, the comparison of CFD-based simulation data with measurements from fire experiments has become one standard approach for testing the applicability of such codes.

However, on the basis of such global comparisons it is not possible to decide whether a CFD code produces good results because it is really correct, or simply because of internal error cancellation. Unfortunately, the required details of the flow fields are often plainly inaccessible due to a lack of appropriate measurement techniques, e.g., in the presence of intense smoke. Thus, quality assessments of CFD codes for fire safety should not rely exclusively on comparisons with experimental results.

This conclusion is further supported by the fact that only a limited range of flow regimes can be reproduced in the laboratory. As a consequence, even if a CFD code has positively passed scrutinizing tests based on comparisons with a large experimental data base, there is no guarantee whatsoever that it will work equally well in flow regimes which the experiments have not covered. For example, it is an open issue whether fire events in very large open-space buildings can be downscaled to laboratory sizes while maintaining all the rules of similarity.

Another disadvantage for a detailed proof of data computed by CFD programs is the fact, that data from fire experiments always consider net effects of all physical processes of a fire. Therefore, cancelation of errors inside the computational results may remain undetected.

Especially the simulation of fire and smoke spreading requires the modeling of complicated and partially not really understood physical and chemical processes. For this reason, the developers of such programs use empirical models as well as many approximations to limit the

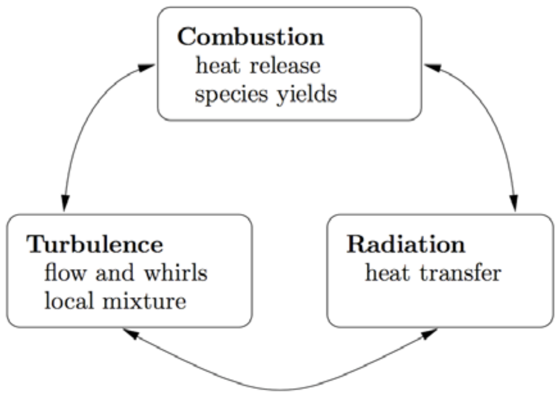

Figure 1: Process interaction

computational costs in an appropriate range. Even more, there is a strong non-linear coupling between these processes, for example between turbulence, combustion, and radiation. And last but not least it is possible, that because of the limited range of experimental facilities errors outside these range can not be detected.

In summary, comparisons with fire experimental data are necessary and useful. However, if adopted as the only means of testing they are insufficient to document the performance of CFD programs. Therefore, a more comprehensive testing strategy is indispensable.

1.1. Component-level and isolated process tests

Verification and validation (V&V) is widely discussed in the CFD community (e.g., [1, 3, 7, 12]). It is beyond the scope of this paper to summarize the discussion regarding different definitions of verification and validation. In contrast, we aim to provide some evidence why other types of tests are necessary to ensure reliable results from CFD programs. Figure 2, from *Schlesinger* [14], illustrates various facets of what we will expand upon in the present text.

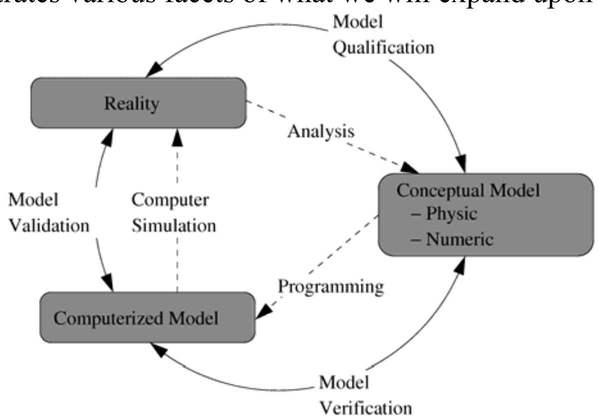

Figure 2: The issue of verification and validation [14]

1. **Model Qualification:** is the process of determining whether an adopted conceptual model accurately represents the real world as far as its intended uses are concerned. To do so, the conceptual model should include descriptions of all physical system components and processes that are of interest for the intended use. Conceptual models for CFD consist of the equations of fluid dynamics extended by auxiliary model equations, e.g., for turbulence and chemical reactions, and of initial and boundary conditions, [12].
2. **Model Verification:** is the process of determining whether a computerized model accurately represents the developer's conceptual model and its solutions [1]. The fundamental goal of verification is the identification and quantification of errors in the computational model and its solution. In verification activities, the accuracy of a computational solution is primarily measured relative to two types of references: analytical solutions and highly accurate numerical solutions [12].
3. **Model Validation:** is the process of determining the degree to which the computerized model is an accurate representation of the real world from the perspective of the in-

tended utilization [1]. The strategy of validation is to assess how accurately computational results match with experimental data, with quantified error and uncertainty estimates for both [12].

Because computerized models, namely the CFD programs, generally consist of very large numbers of different components representing the variety of participating system components and processes, it is close to impossible to verify a CFD program in its entirety. Instead, careful verification and validation of single components as well as groups of components of increasing complexity are imperative. In particular, error cancelations between a program's components can only be detected by such component-level tests. To illustrate the scope of the issue, here is a sample of the components of a CFD program that will require individual assessment:

- **Physical submodels:** turbulence, radiation, boundary conditions …
- **Numerical algorithms:** flux functions, time integrators, linear algebra solvers…
- **Data handling components:** data structures, parallelization, load balancing …
- **Grid handling components:** discretization techniques, domain decomposition, grid refinement …

All these components interact in various ways, so that component-level tests must process the components themselves as well as the interactions between them.
Although all steps are important, in the present paper we focus on the verification issues to test the implementation of the new scheme FDS-SCARC in comparison to the current scheme. Even more, we give a rough introduction of some useful strategies to proof the quality of numerical schemes that are much more suited for a reliable evaluation than only a simple optical comparison of the numerical results.

2. Test of numerical qualities

2.1. Consistency, convergence and stability

As demonstrated in the previous paper of this series [5], numerical discretization schemes have a crucial influence on a CFD code's quality. It is beyond the scope of the present paper to provide more than a rough overview of the related theory for convergence investigations, but some basics are necessary to understand the main ideas behind.
The current von-Neumann computer operates with a finite precision representation of real numbers called floating-point numbers. It can form only a finite number of such floating-point values and can store only a finite number of them in its memory space. Therefore, it cannot handle continuum problems described by differential equations such as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \tag{1}$$

directly. Instead, the continuum equations are approximated by discrete analogues through a "discretization scheme". A common way to derive discrete approximations, e.g., for the partial derivatives in (1), uses Taylor series expansions. The Taylor expansion for $\varphi(x_{i+1})$ of a function $\varphi(x)$ around $x=x_i$ reads as

$$\varphi_{i+1} = \varphi_i + \left(\frac{\partial \varphi}{\partial x}\right)_i \cdot \Delta x + \left(\frac{\partial^2 \varphi}{\partial x^2}\right)_i \cdot \frac{\Delta x^2}{2!} + \left(\frac{\partial^3 \varphi}{\partial x^3}\right)_i \cdot \frac{\Delta x^3}{3!} + \cdots \tag{2}$$

A change in the sequence of terms leads to an approximation for the gradient of φ at point *i*

$$\left(\frac{\partial\varphi}{\partial x}\right)_i \approx \frac{\varphi_{i+1}-\varphi_i}{\Delta x} \underbrace{-\left(\frac{\partial^2\varphi}{\partial x^2}\right)_i\cdot\frac{\Delta x}{2!}-\left(\frac{\partial^3\varphi}{\partial x^3}\right)_i\cdot\frac{\Delta x^2}{3!}-\dots}_{\text{truncation error } \mathcal{O}(\Delta x)} \tag{3}$$

For the approximation of the gradient of φ only a finite number of terms in (3) can be considered. The rest is necessarily neglected and remains as a "truncation error". This type of discretization is widely used in CFD programs and a range of concepts of numerical analysis exists for characterizing the accuracy and correctness of the resulting numerical approximation schemes.

- **Order of consistency:** The quality of the numerical solution will depend on the order of the scheme, described by the truncation error. The "order of a discretization" is determined by the power of the discretization parameter (here Δx) that appears in the first neglected term of the Taylor expansion. Therefore, the discretization in (3) is of first order (Δx). For modern CFD programs, second order discretization is state of the art.

- **Convergence:** With convergence tests, the correctness of a numerical scheme can probed empirically. As the grid size Δx vanishes, the truncation error should vanish as well, and at a rate determined by the order of the scheme,

$$\lim_{\Delta x \to 0}\left(\frac{\partial\varphi}{\partial x}-\frac{\Delta\varphi}{\Delta x}\right)=0. \tag{4}$$

  Convergence studies involving calculations of the same problem on grids with varying mesh sizes are necessary to check this basic aspect. Only a series of convergence tests on well-selected non-trivial test problems can establish with reasonable certainty that a code correctly implements the discretization schemes that it has been built upon. Unless a code has passed such tests, one cannot expect that it produces reliable results for realistic application problems. Therefore, authorities should insist on a detailed documentation of convergence tests, before accepting data derived from numerical simulations.

- **Stability:** There will be a large number of input data x defined by the user, for many of which only coarse estimates will be available. Essentially, a numerical scheme $F(x)$ for evaluating a function $f(x)$ is called stable if small input errors result in controlled, small changes in the computed output, i.e., $|F(x+\delta x)-F(x)|\to 0$ as $\delta x\to 0$. In the graphical illustration the stability of the numerical scheme means, that the ratio between the hatched area of the input deviation and the hatched area of the total deviation of the numerical result must be limited.

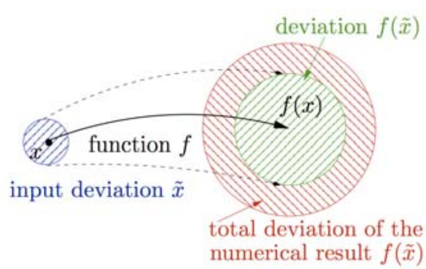

Figure 3: Stability and error propagation

All these requirements are known for a long time. Already in 1902, the French mathematician Hadamard identified consistency, convergence, and stability as necessary conditions for a useful mathematical model. Additionally, the efficiency of the code is another very important quality criterion, because the computational results must be available in a reasonable time. Ultimately, the base of all is the correctness of the underlying numerics.

2.2. Practical relevance

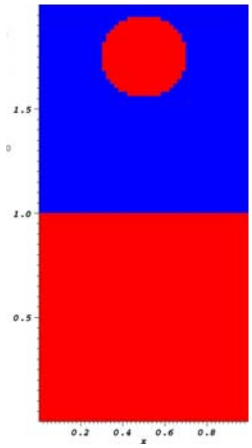

Figure 4: Falling droplet

Besides of the mathematical and numerical argumentation, there is even a physical relevance. Often practitioners argued, that as long as important input data can only be roughly estimated, digits after the decimal point could be neglected.
In the context of numeric schemes this argumentation fails. Even the small terms of the Taylor series (3) represent physical properties. This should be demonstrated by a simple numerical experiment, the falling droplet.
Let us assume that we drop a droplet into a fluid surface, as shown in figure 4. Now we simulate the falling droplet. For this purpose, we use a CFD program, which can switch between first and second order accuracy according to neglecting the second term (1st order) or third term (2nd order) in the approximation of the gradient (5).
Now we compare the density and velocity field after the impact of the droplet into the fluid surface at the same time. Whereas in the right picture (2nd order) a compact wave roll to the right, the left picture (1st order) looks more like a small fluid hill with a flow along a line to the right upper edge of the picture.

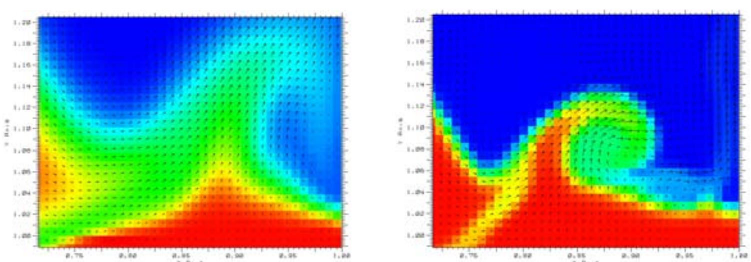

Figure 5: Comparison of a first and second order solution

The reason is, that the approximation of a curvature, necessary to form waves, needs the second derivation. Nevertheless, this curvature term is neglected in the first order approximation.

$$\left(\frac{\partial\varphi}{\partial x}\right)_i \approx \underbrace{\underbrace{\frac{\varphi_{i+1}-\varphi_i}{\Delta x}}_{\text{1st order approximation}} - \left(\frac{\partial^2\varphi}{\partial x^2}\right)_i \cdot \frac{\Delta x}{2!}}_{\text{2nd order approximation}} - \left(\frac{\partial^3\varphi}{\partial x^3}\right)_i \cdot \frac{\Delta x^2}{3!} - \dots \tag{5}$$

2.3. Usefulness for code testing

From a physical point of view the solution of the underlying set of equations must be independent of the underlying domain decomposition. Simplified: the solution of a single- and multi-mesh-calculation should be the same. But what does that explicitly mean? Domain decomposition methods to solve boundary value problems always lead to more or less additional numerical errors and increase the inaccuracy of a numerical scheme. Nevertheless, the numerical error of a domain decomposition method or parallelization strategy must be limited by the numerical error defined by the order of the underlying numerical scheme. In case of FDS the scheme should be of second order accuracy in time and space (see [8]). Therefore convergence tests provide an appropriate quality criteria.

3. Concept and Strategy

One important feature of the program package FDS is the possibility to decompose the computed domain geometrically into smaller subdomains or meshes. This technique is a prerequisite for parallel computing and a time efficient numerical computation of practical problems. But, the usage of multi-meshes in serial as well as parallel simulations in FDS may cause inaccuracies or instabilities, as demonstrated by different authors e.g. [2, 4, 5, 6, 9, 13].

These errors result from deficiencies in the domain decomposition strategy in conjunction with the FFT-solver used to solve the pressure equation in FDS (see [5, 6]). These deficiencies suggest to develop completely new strategies for the solution of the pressure equation. Subsequently, a new parallelization concept, the generalized domain decomposition/multigrid method SCARC is presented [5].

In this part we describe a comprehensive test strategy to proof the correctness of this new strategy. Following the idea of component-level tests and the described V&V rules, the test strategy focuses at the hydrodynamic solver and the domain decomposition method first. Nevertheless the concept is expandable.

3.1. Classification

There will be different sources for reference data, which can be used for V&V work. The presented concept differs between:

- A **Analytical tests**
  The results of these analytical tests are known because of mathematically or numerically based considerations. One example is the presented pipe test.
- SE **Semi-experimental tests**
  Semi-experimental tests used a closely restricted number of physical or chemical processes. For example we focus only on heat conduction.
- N **Numerical tests**
  Numerical tests are comparisons with results from more detailed or higher qualified programs. See the example in the pipe test subsection.
- E **Experimental tests**
  These are small- or full-scale fire tests as well as complex buoyancy-driven fluid flow experiments.

To realize the component-level strategy the classification differentiates between the physical and chemical processes and more numerical criteria like order, convergence, and symmetry. Additionally the implementation of boundary conditions plays an important role for error-detection. At the current state, we subsume these criteria under the term structure test (DD: domain decomposition, OC: order and convergence, PA: parallelization, BC: boundary condition, SY: symmetry). At the end a comprehensive test table is presented. Inside this table the classification of each test is described.

Test	Type	Physical. components							
		Gasdynamic	Gravitation	Viscosity	Radiation	Turbulence	Combustion	...	Structure test
Pipe	A	✓							DD,OC
Hydrostatic	A	✓	✓						BC
Orifice	SE	✓		✓		✓			BC,OC
...									

Table 1: V&V test table

4. Pipe test example of V&V test table

To demonstrate the possibilities of a numerically orientated test strategy we present the pipe test, an analytical test case. The left side of a channel with a constant density flow is impinged with the accelerated velocity $u(t)=\sin(C\ t)$. The right side of the channel is open. To test the accuracy of the domain decomposition method, we subdivide the computational domain in n=1 up to $M=10$ subdomains as demonstrated in figure 6.

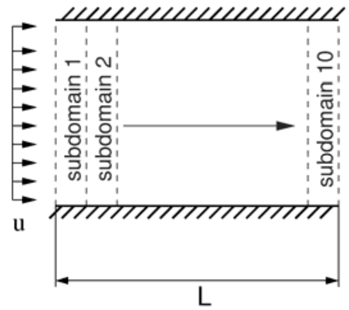

Figure 6: Multi-mesh pipe test

The gradient of the pressure drop between the left and right side of the channel can be analytically determined from the momentum equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} \quad +(\mathbf{u}\cdot\ \nabla)\mathbf{u}\right)+\ \nabla p \quad = \mathcal{S}_{\rho\mathbf{u}}.$$

This is true, because the flow velocity is spatially homogeneous therefore the advection term of the momentum equation vanishes. Furthermore, the source term $S_{\rho u}$ in this example is zero. This leads to equation

$$\rho\frac{\partial \mathbf{u}}{\partial t} = -\ \nabla p \approx -\frac{\Delta p}{\Delta x}$$

With Δx=L and $u(t)$=$u_0\sin(2\pi t)$ the mean pressure drop between in- and outflow is

$$\Delta\tilde{p} = -\rho u_0 2\pi \cos(2\pi t)L. \tag{6}$$

4.1. Test of the hydrodynamic solver

Starting with $M=1$ we investigate the solution of a one-mesh computation with $u_0=1\ m/s$, $\rho=1.188\ kg/m^3$, and L=1.0 m. As shown in figure 7 the computed results of FDS-FFT and FDS-ScaRC reproduce the analytical solution of (6) well. However, there are oscillations at the minima and maxima of the graph.

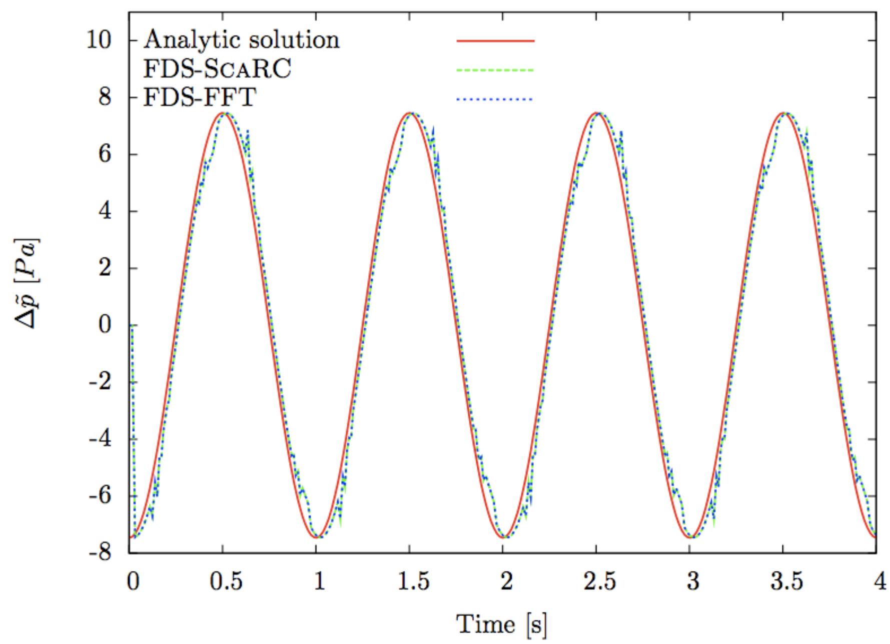

Figure 7: Pipe test, Results of a one-mesh computation

To verify, that these oscillations are not an inevitable consequence of the underlying zero-Mach scheme, we compare the result with the research code *MOLOCH*, see figure 8. This code is based on a comparable zero-Mach scheme of second order accuracy [10]. The research code matches the analytical solution very well and no oscillations are observable. This indicates that the oscillations are a result of deficiencies in the implementation of the scheme or the open boundary concept in FDS. The reasons are still unknown. Following the component-level strategy the hydrodynamic solver and the open boundary function must be decoupled for further investigations.

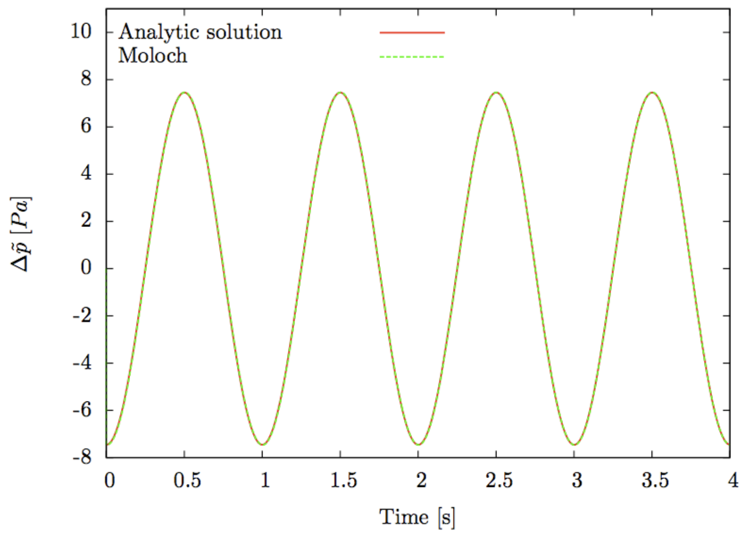

Figure 8: Pipe test, Comparison with research code

4.2.Test of the domain decomposition

To compare the pressure drop of the analytic solution with the numerical results in conjunction with the domain decomposition method, the domain is split up to *M*=10 subdomains and computed in a serial run. As shown in figure 9 the computed results become erroneous if the computational domain is divided into single subdomains. Although this case is a simple parallel flow with constant density, FDS-FFT is not able to compute the correct results in this case.

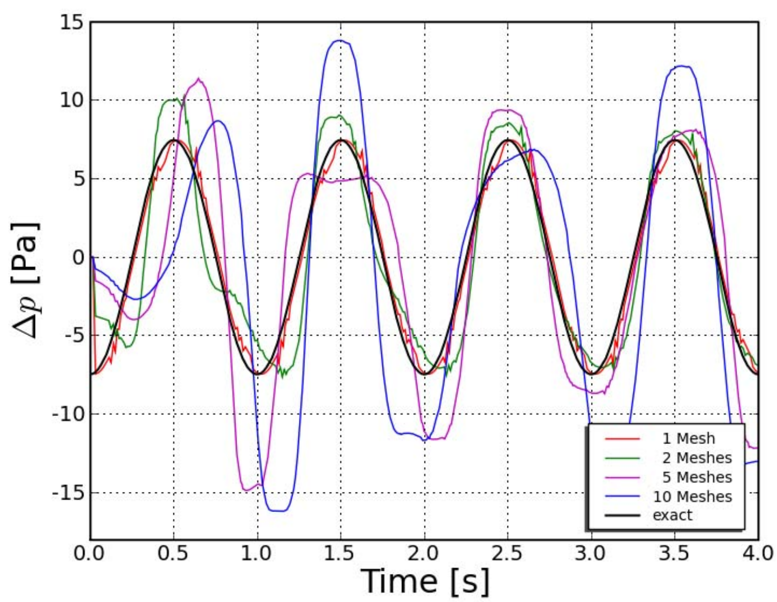

Figure 9: Pipe test, Mean pressure drop for FDS-FFT

Taking the differences between the analytic solution (6) and the results for the different M-mesh computations gives unacceptable errors up to 14 Pa, as illustrated in figure 10.

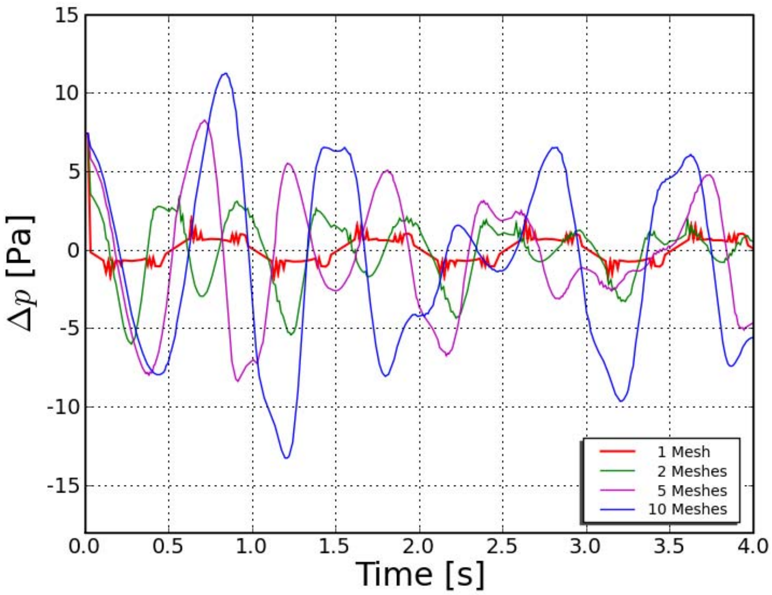

Figure 10: Pipe test, Error of mean pressure drop for FDS-FFT

In comparison with these insufficient FDS-FFT results, the new FDS-SCARC technique demonstrates the advantage of a numerical scheme following the mathematical characteristics of the underlying set of equations.

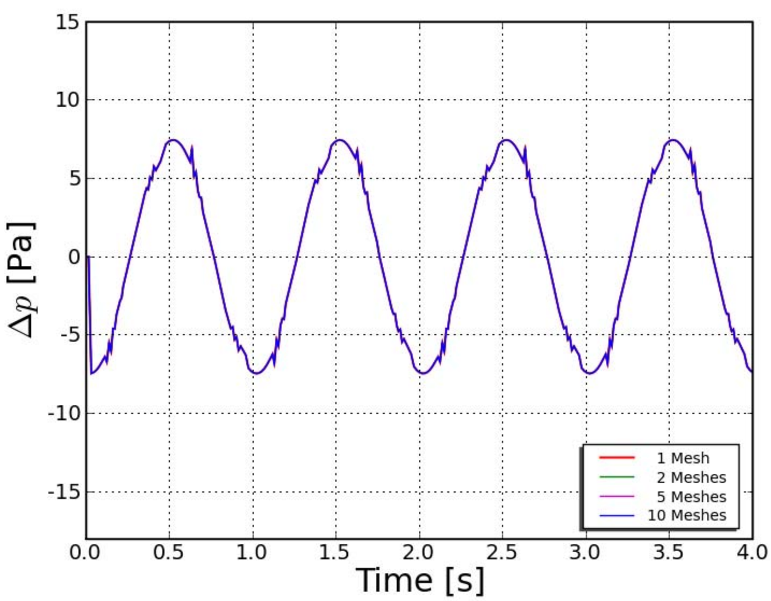

Figure 11: Pipe test, Mean pressure drop for FDS-SCARC

Obviously, FDS-SCARC produces much better results than FDS-FFT. As described before, the solution of FDS-SCARC is independent with respect to the number of subdomains *M*, whereas FDS-FFT leads to unacceptable large errors. A convergence analysis supports these results. In the multi-mesh case, FDS-FFT does no longer possess second order accuracy. The reasons are described in [6]. It should be noted, that the ScaRC technique cannot produce better results than the 1-mesh FFT version because it only replaces the FFT pressure solver, but not the surrounding parts of the code. Therefore the same oscillations occur at the minima and maxima as for the 1-mesh computation. The underlying reasons will be analyzed in the near future.

5. Summary and Outlook

In the present article, we have explained why the widely used comparison with fire experimental data are necessary and useful, but that they are insufficient to properly prove CFD programs.

The demonstrated results underline the necessity of a more comprehensive testing strategy, which has to include investigations of numerical qualities (convergence, stability, and order), and component-level tests. Our pipe test example shows the advantages of analytical and numerical component-level tests.

Until today, the Fire Dynamics Simulator is based on the FFT-solver scheme with all the risk involved. The exclusive focus on computational costs, the motivation to use the FFT-scheme, affects the correctness of the underlying numerical scheme.

The consequences of the detected problems in case of multi-mesh computations in the large area of fire safety applications cannot be estimated by us. However, authorities and fire safety engineers would be advised to be aware of the current multi-mesh problems. Maybe some critical projects must be reviewed.

In close collaboration with Susanne Kilian, hhpberlin, we enhanced this comprehensive testing strategy in conjunction with the development of the FDS-SCARC technique. Correct computations are not inconsistent with fast computations. Nevertheless, fast and faulty computations are questionable.

Acknowledgement:

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