

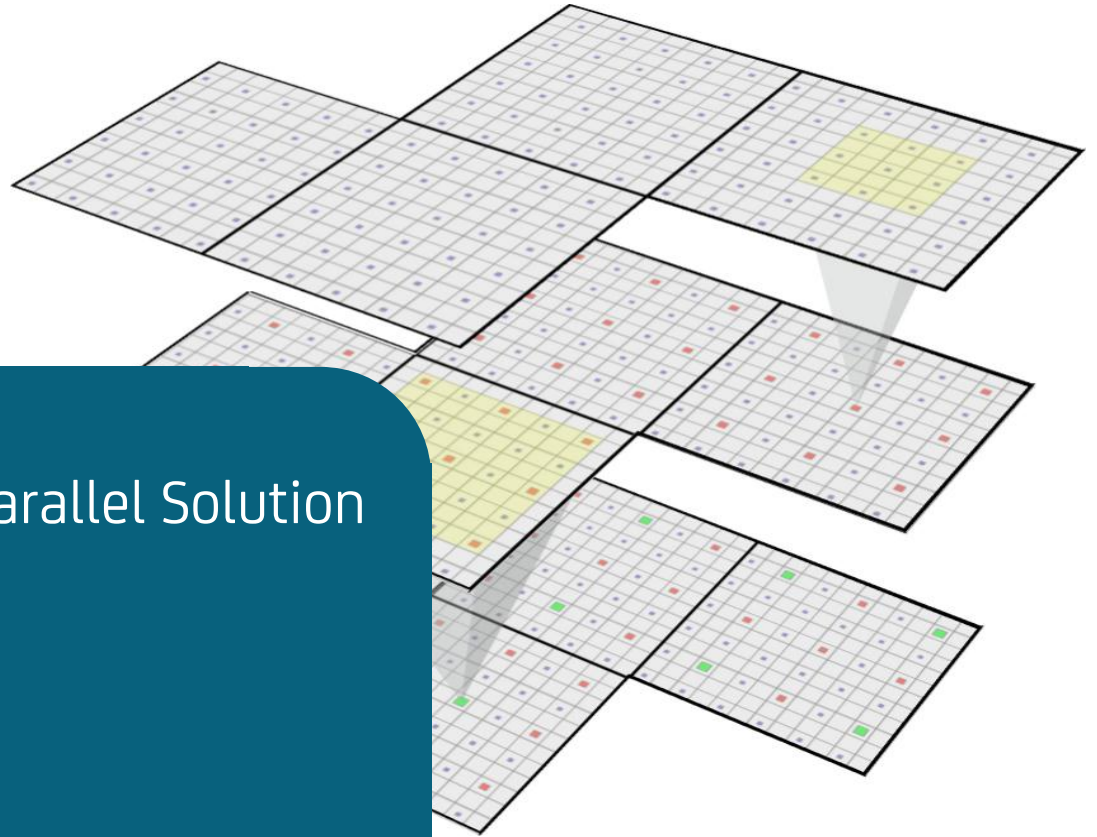
# Numerical Insights into the Parallel Solution of the FDS Pressure Equation

## Scalability and Accuracy

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# Content

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Characteristics of  
the FDS pressure  
equation

2

Different  
parallel FDS  
pressure solvers

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# Characteristics of the FDS pressure equation

# Mathematical properties

➤ Elliptic partial differential equation of Poisson type

$$\nabla^2 \mathcal{H} = -\frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} - \nabla \cdot \mathbf{F}$$

Source terms from previous time step (momentum flux terms)

- Important component in complete solution process
- Solved at least twice in every time step
- Strongly linked with the computation of the other required quantities

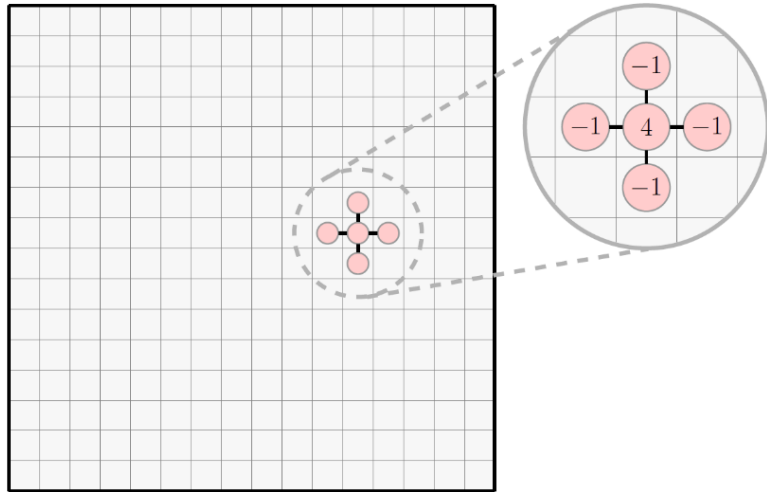
➤ Pressure solution strongly influences the quality of the whole simulation

1

Characteristics of the FDS pressure equation

# Finite Difference Discretization

## ➤ Single-Mesh Case



1 linear system of equations:

$$Ax = b$$

**Discretization stencil** (cell-centered):

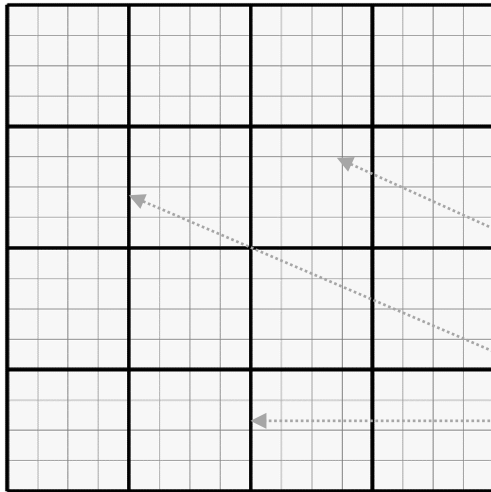
Specifies the physical relationships between grid cells

# 1

Characteristics of the FDS pressure equation

# Finite Difference Discretization

## ➤ Multi-Mesh Case



M linear systems of equations:

$$A_i x_i = b_i$$

Multiple meshes, assigned to different processors of a parallel computer

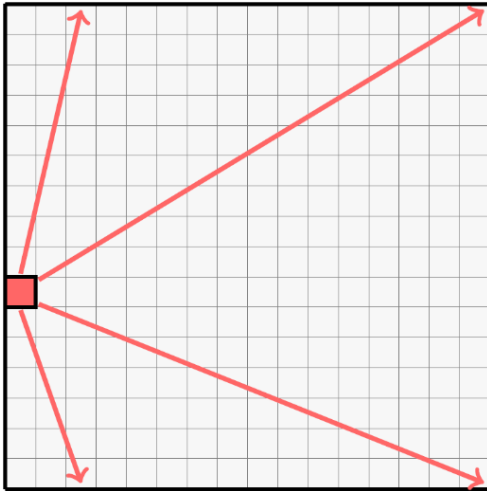
New artificial interior boundaries:  
Data exchange for coupling needed

# 1

Characteristics of  
the FDS pressure  
equation

# Properties in the Single-Mesh case

➤ High velocity for the propagation of information



Local information spreads immediately across whole domain

Local data have impact to entire solution

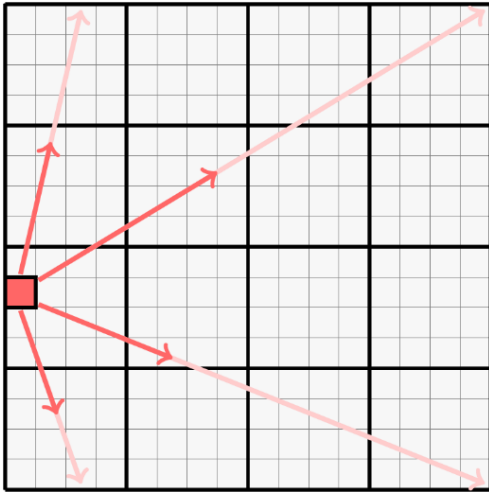
Very strong global coupling

1

Characteristics of the FDS pressure equation

# Properties in the Multi-Mesh case

## ➤ Requirements to the Multi-Mesh pressure solver



Fast spread of data must be reproduced best possible

Fragmentation of physical connectivity must be avoided

Approximation quality of Single-Mesh solver should be preserved

1

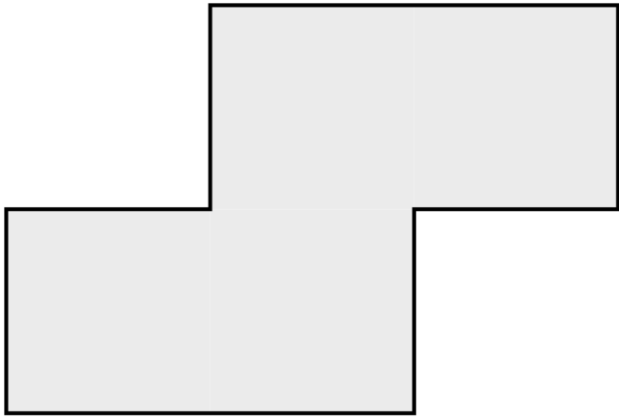
Characteristics of the FDS pressure equation



# Different parallel FDS pressure solvers

# Presentation of two different approaches

➤ Explanation of both strategies for pipe-shaped geometry in 2D



Allows for a simple graphical visualization of the underlying concepts

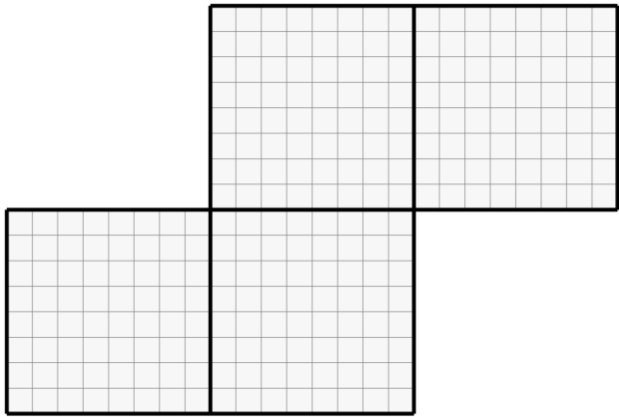
2

Different parallel FDS pressure solvers

# Presentation of two different approaches

➤ Explanation of both strategies for pipe-shaped geometry in 2D

2  
Different parallel  
FDS pressure  
solvers



Subdivision in 4 submeshes

# Current official approach: Multi-Mesh FFT



## Fast Fourier Transformation:

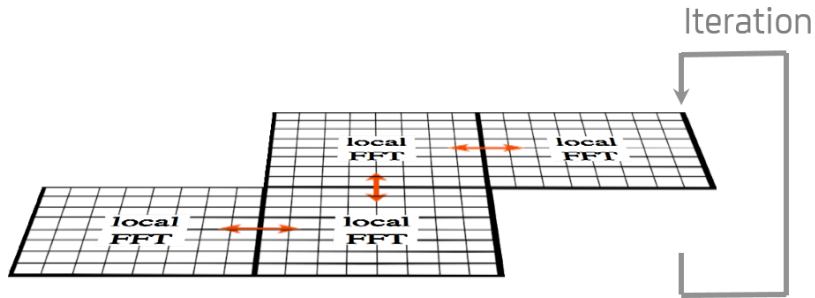
- Locally working method
- Embedded in an iterative averaging process along internal boundaries (and solid obstructions)
- Doesn't solve the same system of equations as a corresponding Single-Mesh solver would do (if available)

2

Different parallel  
FDS pressure  
solvers

# Current official approach: Multi-Mesh FFT

➤ Local FFT-methods plus averaging process



**Local FFT-methods on subgrids:**

Data exchange only between direct neighbors (computationally cheap)

**Surrounding iteration:**

Responsible for the consistency along internal boundaries

➤ High local efficiency, but only slow global data flow

2

Different parallel FDS pressure solvers

# Current official approach: Multi-Mesh FFT

2

Different parallel  
FDS pressure  
solvers

## ➤ Stopping criterion:

Difference of velocity components at internal mesh boundaries < tol !!

```
&PRES VELOCITY_TOLERANCE=0.01, MAX_PRESSURE_ITERATIONS=100
```

Default: (characteristic mesh size)/10

Default: 10

## ➤ Optimal choice of the tolerance for a given case: tol = ?

- tolerance too coarse: insufficient accuracy
- tolerance too fine: computational time too high

# Alternative approach: ScaRC



## Scalable Recursive Clustering:

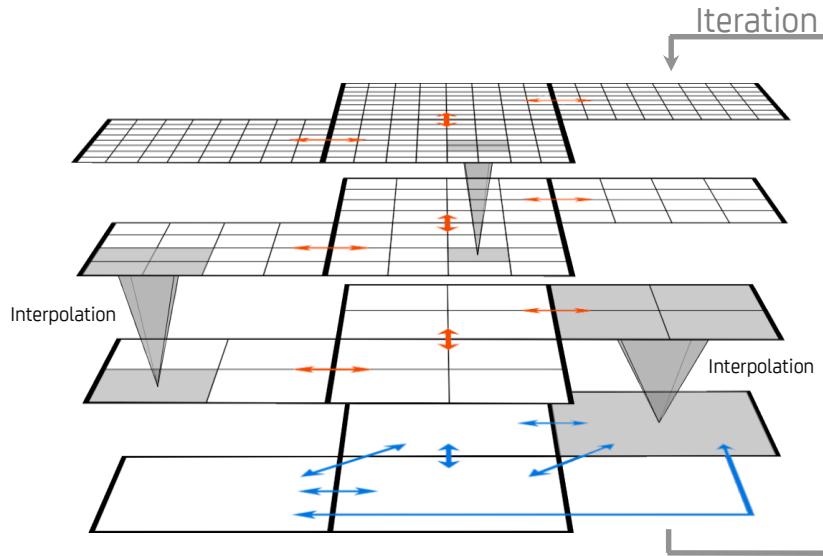
- Globally working method
- Combines domain decomposition techniques with multigrid methods
- Solves the same system of equations as a corresponding Single-Mesh solver would do (if available)

2

Different parallel  
FDS pressure  
solvers

# Alternative approach: ScaRC

## ➤ Geometric multigrid variant:



Sequence of grid levels with different resolutions:

Data exchange only between direct neighbors  
(computationally cheap)

Averaging process on coarse grid:

Data exchange between all meshes  
(computationally expensive)

➤ Each level covers a different range of the global information (strong coupling)

2

Different parallel  
FDS pressure  
solvers



# Alternative approach: ScaRC

2

Different parallel  
FDS pressure  
solvers

## ➤ Geometric Multigrid (GMG):

- Uses only the geometric information included in the problem/grid
- Works efficiently for problem classes with certain regularity properties

## ➤ Algebraic Multigrid (AMG):

- Uses only algebraic information included in the system of equations
- Works efficiently for more general and irregular problem classes

**Common requirements:** Interpolation between levels / Suitable stopping criterion

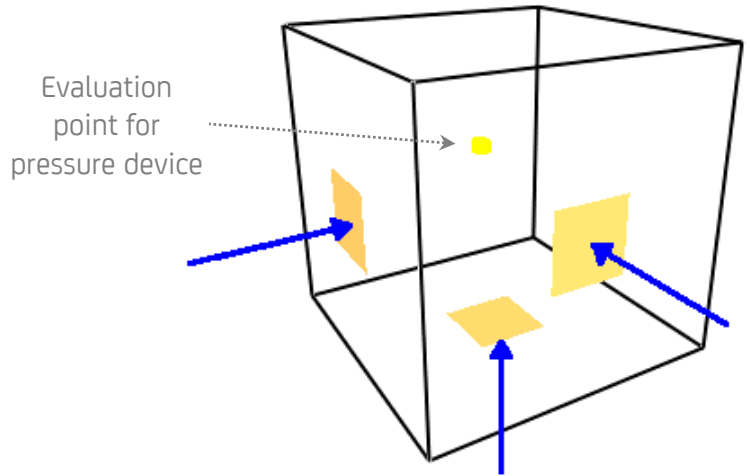
# Numerical accuracy and scalability tests

# Scarc3D: Frequently changing global behavior

3

Numerical accuracy and scalability tests

➤ ScaRC verification case for a cube-shaped domain in 3D



Grid resolution  $128^3$

Different inflows from three sides

Global situations changes in small time intervals of 0.05 s

Great challenge for different solvers

➤ Can Multi-Mesh FFT and ScaRC reproduce the global data flow?

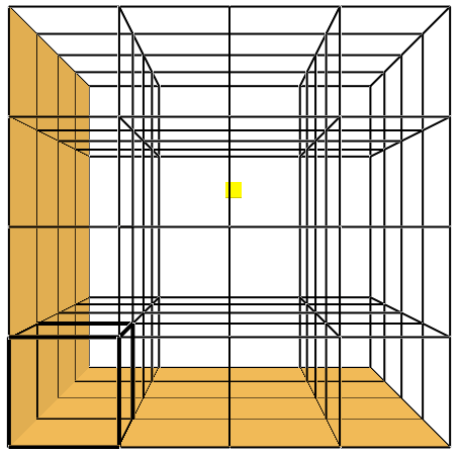
# Scarc3D: Frequently changing global behavior

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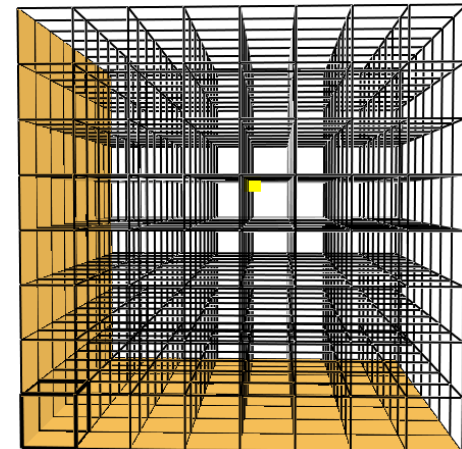
➤ High level of fragmentation by subdivision

Numerical accuracy and scalability tests

64 Meshes (4x4x4)



512 Meshes (8x8x8)



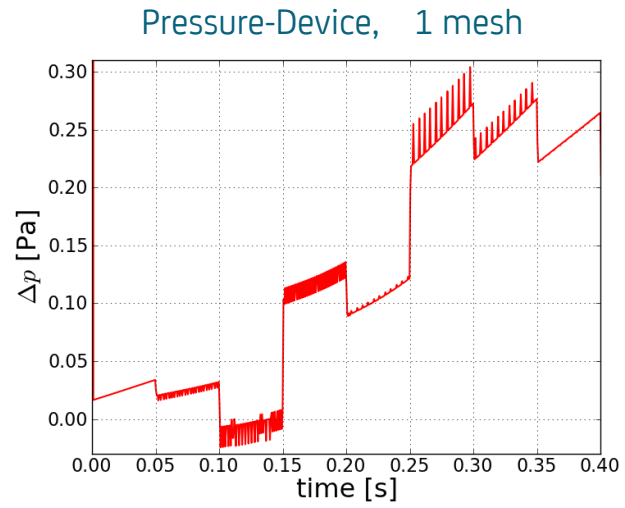
➤ Compare pressure devices: “Multi-Mesh FFT & ScaRC versus Single-Mesh FFT”

# Scarc3D: Frequently changing global behavior

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➤ Stepwise/oscillating evolution of pressure device

Numerical accuracy and scalability tests



➤ Pressure device of corresponding Single-Mesh FFT case is taken as reference

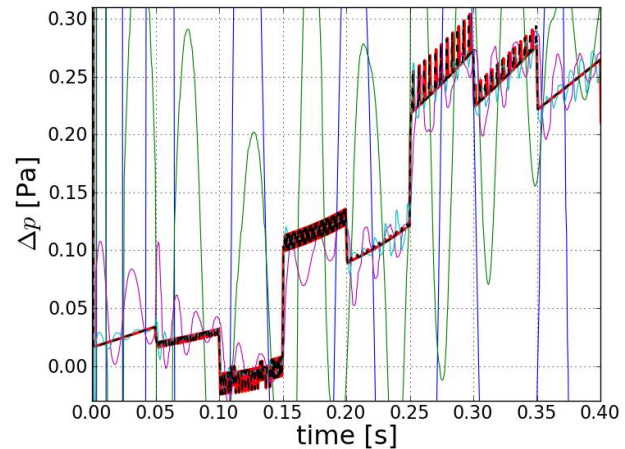
# Scarc3D: Frequently changing global behavior

3

➤ Stepwise/oscillating evolution of pressure device

Numerical accuracy and scalability tests

Pressure-Device, 64 meshes



Comparison of:

- Single-Mesh FFT
- Multi-Mesh FFT with tol = default,  $10^{-2}$ ,  $10^{-3}$ ,  $10^{-4}$
- ScaRC

—	1 mesh, FFT (default)
—	64 meshes, FFT (default)
—	64 meshes, FFT (tol=0.01)
—	64 meshes, FFT (tol=0.001)
—	64 meshes, FFT (tol=0.0001)
- -	64 meshes, ScaRC

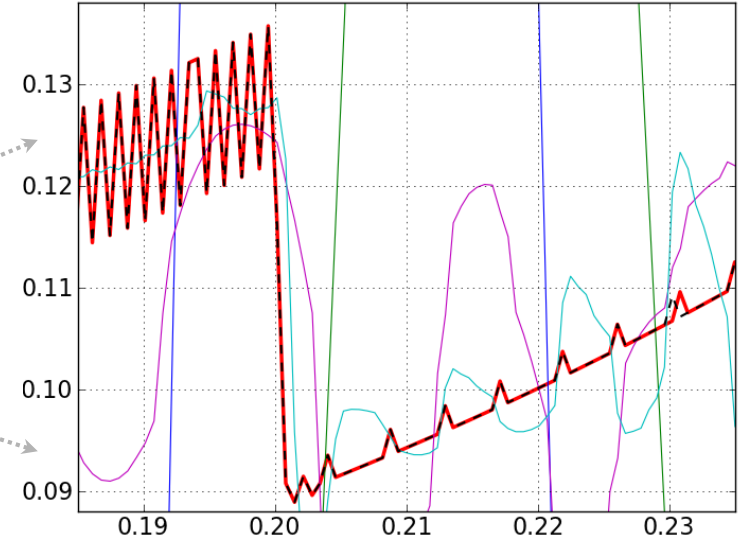
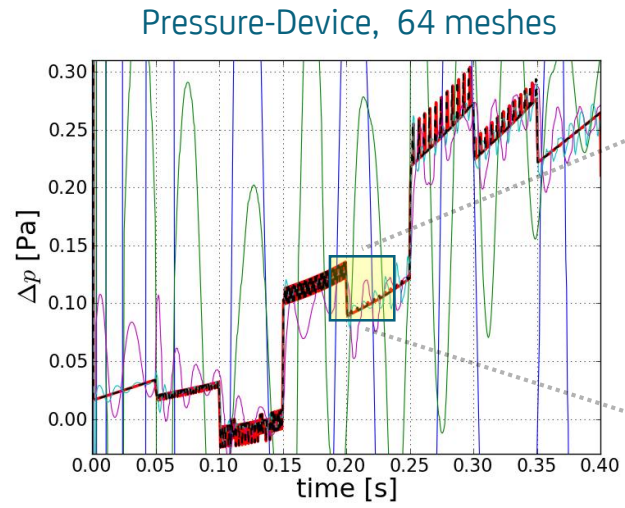
➤ Acceptable consistency only for Multi-Mesh FFT( $10^{-4}$ ), full consistency for ScaRC

# Scarc3D: Frequently changing global behavior

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Numerical accuracy and scalability tests



- 1 mesh, FFT (default)
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➤ Acceptable consistency only for Multi-Mesh FFT( $10^{-4}$ ), full consistency for ScaRC

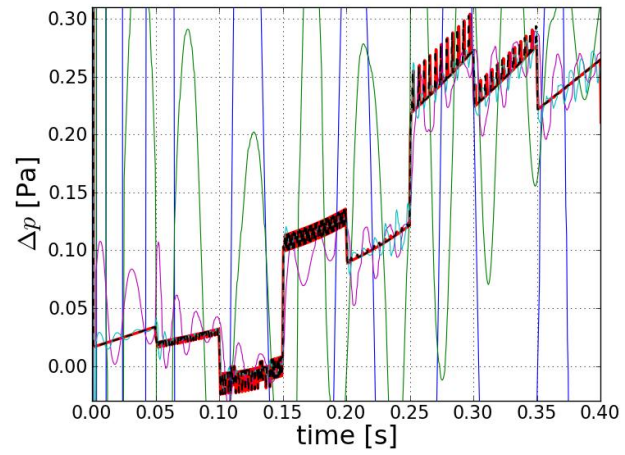
# Scarc3D: Frequently changing global behavior

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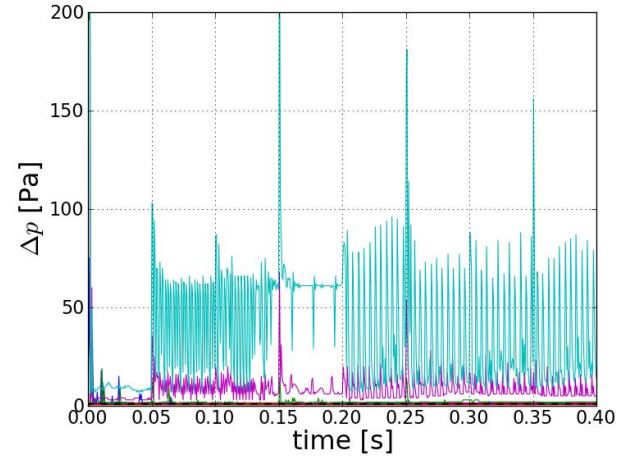
➤ Multi-Mesh FFT: Drastic increase of iteration numbers

Numerical accuracy and scalability tests

Pressure-Device, 64 meshes



Number of iterations, Multi-Mesh FFT



- 1 mesh, FFT (default)
- 64 meshes, FFT (default)
- 64 meshes, FFT (tol=0.01)
- 64 meshes, FFT (tol=0.001)
- 64 meshes, FFT (tol=0.0001)
- 64 meshes, ScaRC

➤ Big rise of computational overhead to achieve a sufficient accuracy



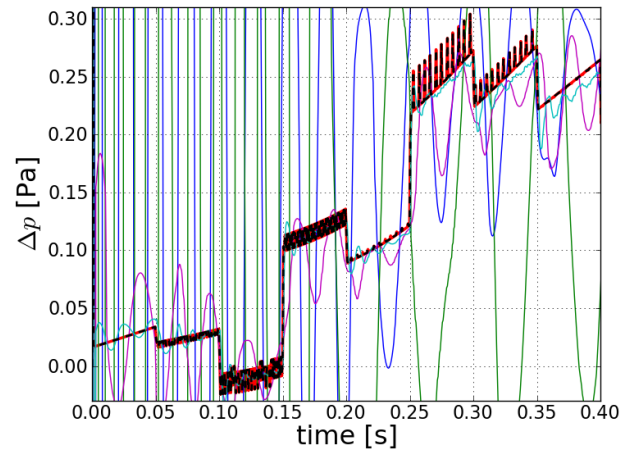
# Scarc3D: Frequently changing global behavior

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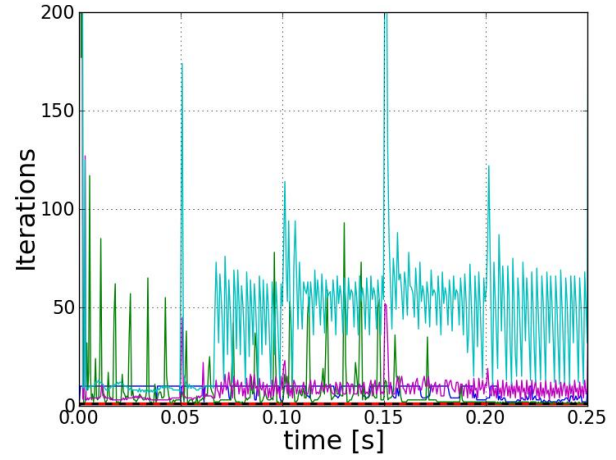
➤ Similar comparisons for the 512-mesh case

Numerical accuracy and scalability tests

Pressure-Device, 512 meshes



Number of iterations, Multi-Mesh FFT



- 1 mesh, FFT (default)
- 512 meshes, FFT (default)
- 512 meshes, FFT (tol=0.01)
- 512 meshes, FFT (tol=0.001)
- 512 meshes, FFT (tol=0.0001)
- - 512 meshes, ScaRC

➤ The more meshes, the bigger the differences

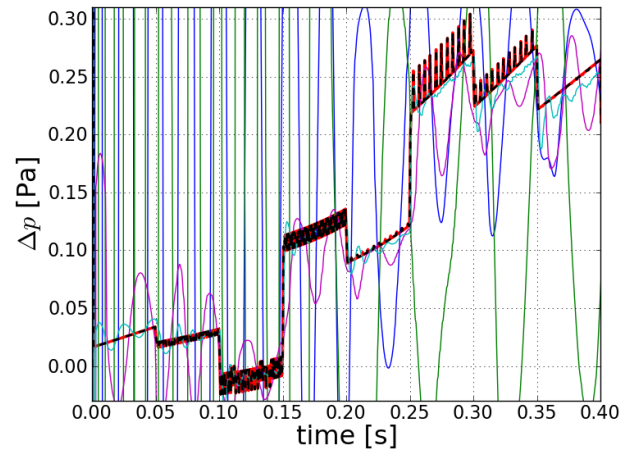
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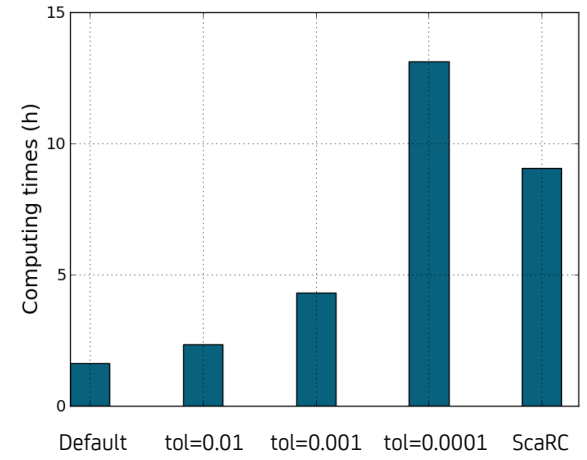
➤ Very different computing times

Numerical accuracy and scalability tests

Pressure-Device, 512 meshes



Computing times, 512 meshes



- 1 mesh, FFT (default)
- 512 meshes, FFT (default)
- 512 meshes, FFT (tol=0.01)
- 512 meshes, FFT (tol=0.001)
- 512 meshes, FFT (tol=0.0001)
- 512 meshes, ScaRC

➤ Fair comparison only for Multi-Mesh FFT( $10^{-4}$ ) and ScaRC

# Shunn3: Multi-Mesh convergence study

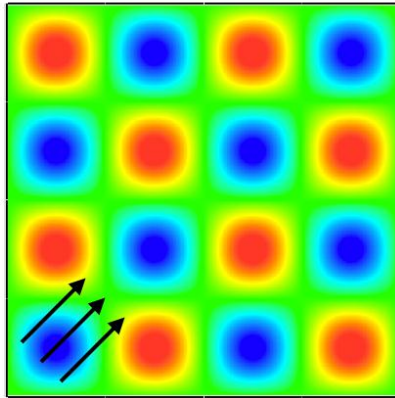
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Numerical  
accuracy and  
scalability tests

➤ From Verification Guide: „Variable Density Manufactured Solution“

1 Mesh

Smokeview 6.0.1 - Jun 20 2012



Slice  
rho  
kg/m3



mesh: 1

Frame: 0  
Time: 0.0

Constant velocity field:  $U = W = 0.5$

$CFL = 0.5$

$N = \{ 32, 64, 128, 256, 512 \}$

Analytical solutions for different  
quantities are known

➤ 2. order convergence of FDS time-stepping algorithm for Single-Mesh case

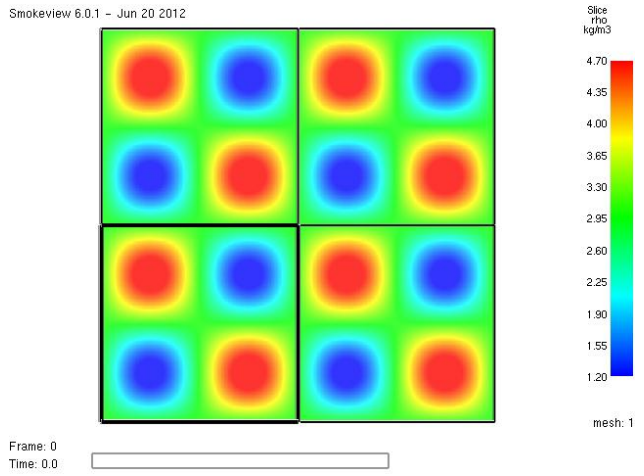
# Shunn3: Multi-Mesh convergence study

3

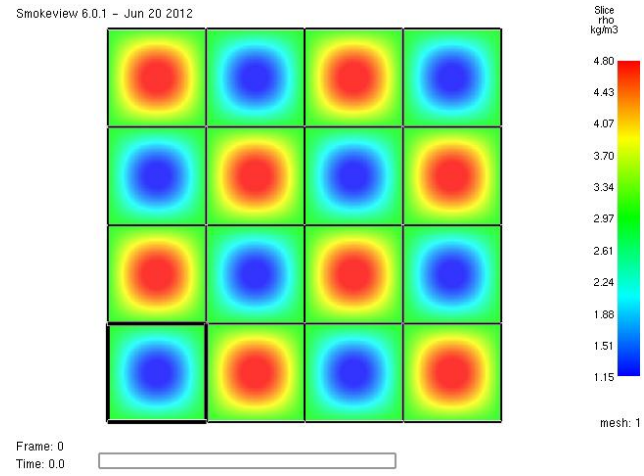
➤ Analyze convergence behavior for different subdivisions with ScaRC

Numerical accuracy and scalability tests

4 Meshes



16 Meshes



➤ Can ScaRC preserve the 2. order convergence of the Single-Mesh case?

# Shunn3: Multi-Mesh convergence study

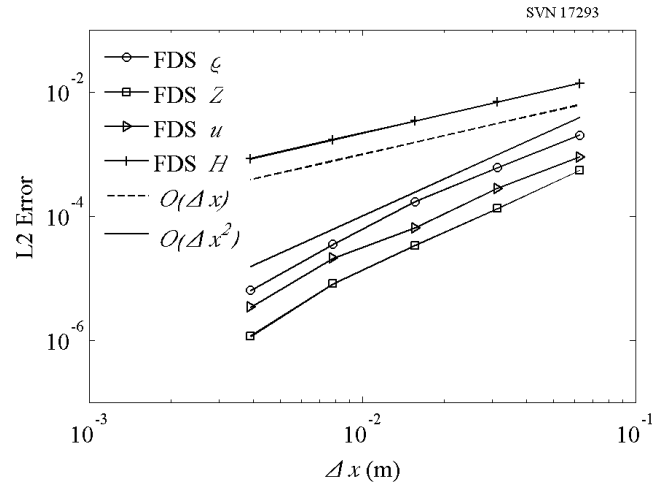
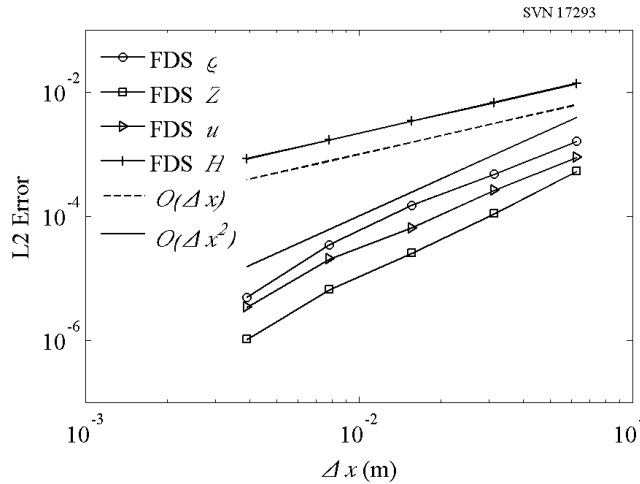
3

➤ L2-errors for mixture fraction, density, velocity and pressure

Numerical accuracy and scalability tests

4 Meshes

16 Meshes



➤ ScaRC is able to keep the 2. order convergence for both subdivisions

# Conclusions

# Conclusions for Multi-Mesh FFT



## Advantages:

- Local FFT-solvers on the single submeshes are extremely fast and robust (high local efficiency)



## Disadvantages:

- Slow/delayed computation of global effects (scalability questionable)
- Optimal stopping tolerance only hardly to predict (parameter choice difficult)
- Possibly many pressure iterations necessary (slow convergence)
- Usually differences to corresponding Single-Mesh case (no full consistency)

4

Conclusions

# Conclusions for ScaRC

4

Conclusions

## ➤ Advantages:

- Better accordance to Single-Mesh case (**good consistency**)
- Higher approximation accuracy than Multi-Mesh FFT (**good accuracy**)
- Better reproduction of global dependencies even for high number of submeshes (**good scalability**)

## ➤ Disadvantages:

- Method parameters must be chosen carefully (**parameter choice difficult**)
- Computing times mostly higher than for Multi-Mesh FFT (**higher computational costs**)



# Outlook

# Outlook

- Further optimizations:
- Improving the algebraic multigrid variant (AMG)
  - Including concepts to use meshwise different grid resolutions
  - Improving the run-time behavior

5

Outlook

# Outlook



## Further optimizations:

- Improving the algebraic multigrid variant (AMG)
- Including concepts to use meshwise different grid resolutions
- Improving the run-time behavior



## Further verification tests:

Analyzing separated physical phenomena, possibly with analytical solution

5

Outlook

# Outlook



## Further optimizations:

- Improving the algebraic multigrid variant (AMG)
- Including concepts to use meshwise different grid resolutions
- Improving the run-time behavior



## Further verification tests:

Analyzing separated physical phenomena, possibly with analytical solution



## Further application tests:

Checking the applicability of ScaRC on realistic, complex geometries

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Outlook

Thank you very much for your attention!

Questions ?



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