ScaRC is ready for use in FDS

Alternative solver for the FDS pressure equation

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Agenda

1. Pressure equation
2. FFT solver
3. UGLMAT solver
4. ScaRC solver

FDS pressure Poisson equation

Different discretization types

Pressure equation in FDS

Elliptic partial differential equation of „Poisson“ type

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

Strongly coupled with velocity field,
to be solved at least twice per time step

Source terms of previous time step.
e.g. radiation, combustion pyrolysis, ...

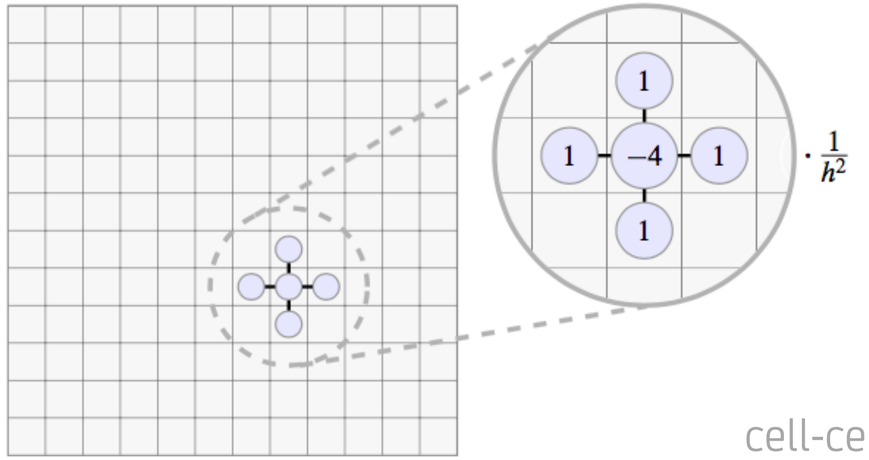
Key feature: Local information is spread immediately over whole domain!

Discretization with finite differences

1

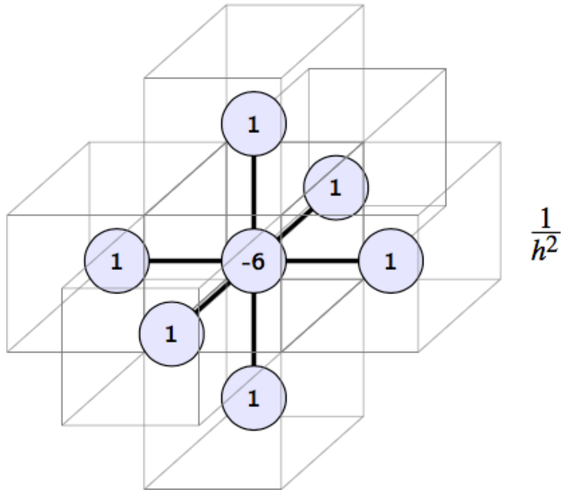
Pressure equation

5-point stencil in 2D



cell-centered

7-point stencil in 3D



Specifies physical relations between grid cells according to elliptic equation

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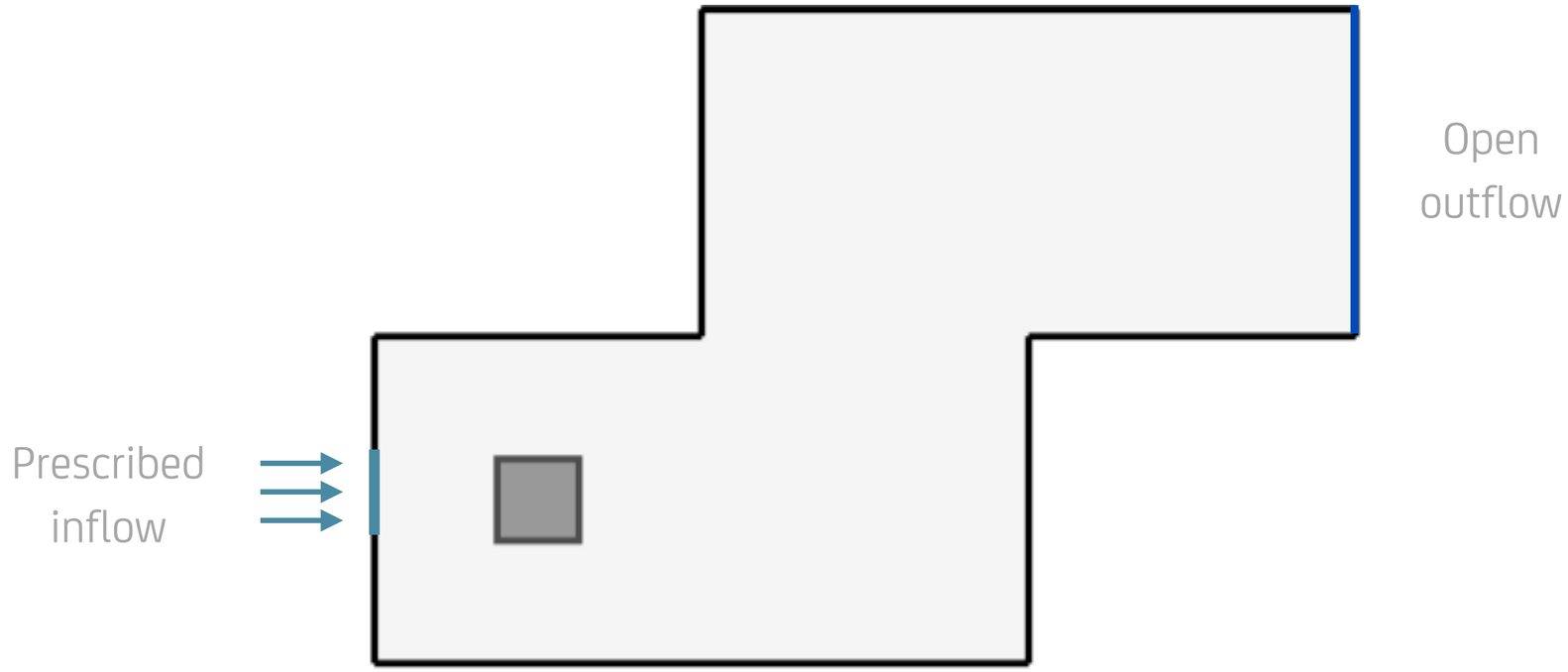
Demo-case ‚2D-pipe with obstruction‘

1

Pressure equation

Simple example to explain the concepts



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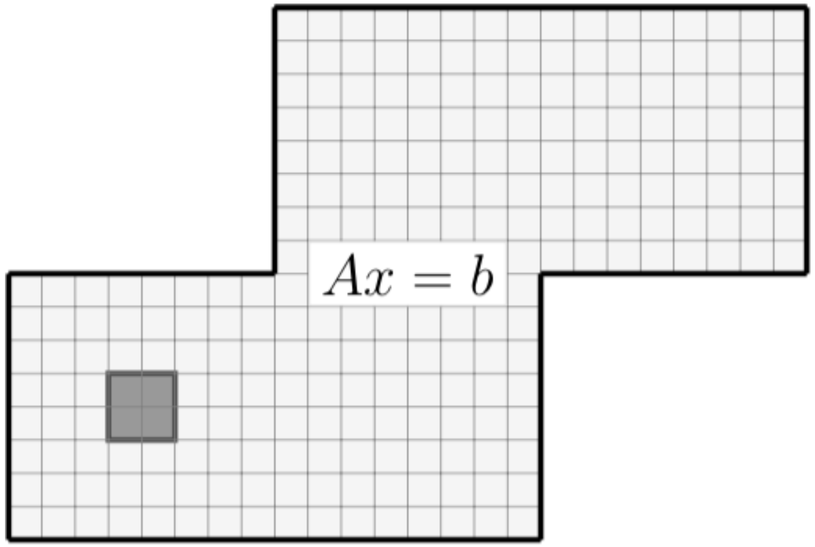
Global versus local discretization

Global discretization

1 global matrix, 1 global right hand side vector



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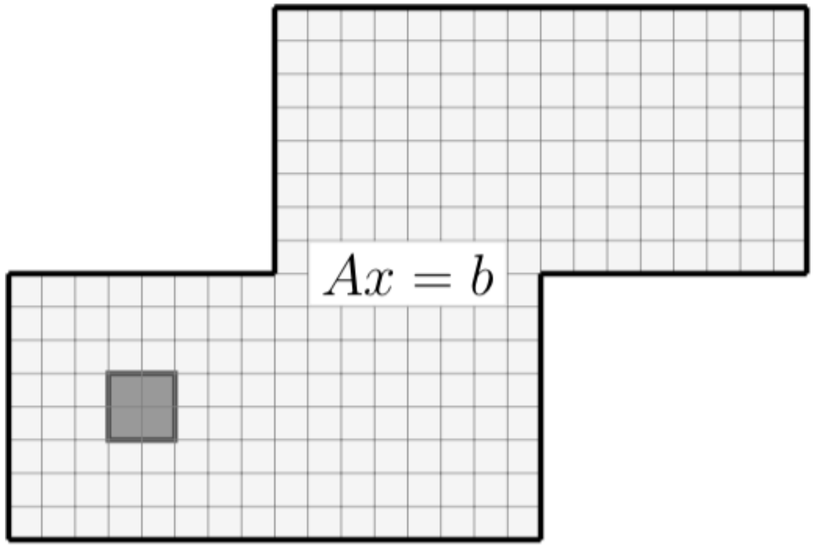
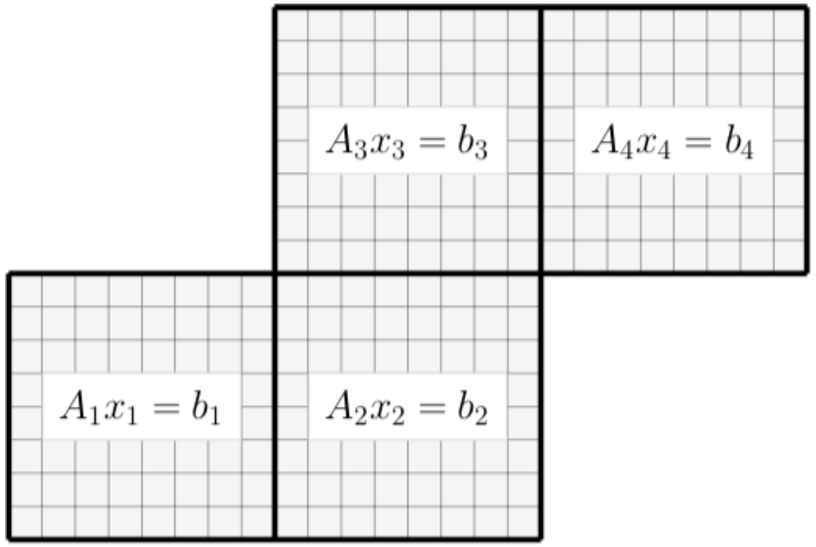


Set of local discretizations

M local matrices, M local right hand side vectors



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Global versus local discretization

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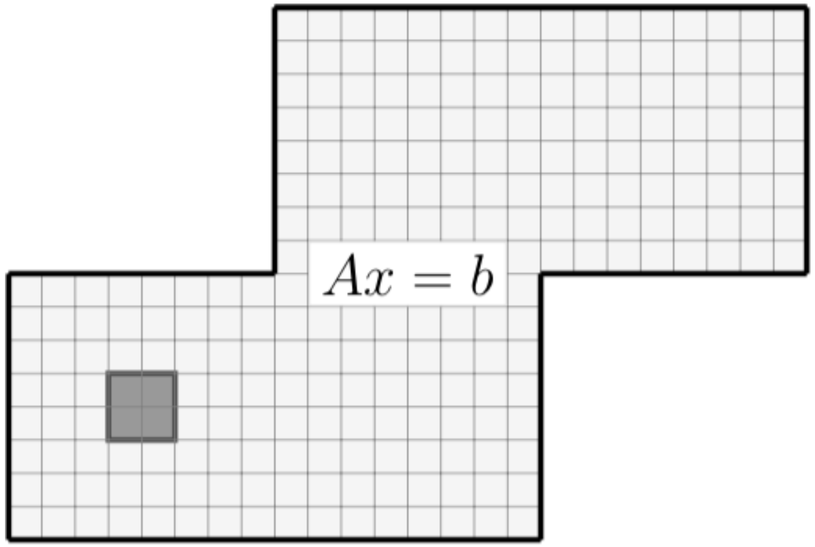
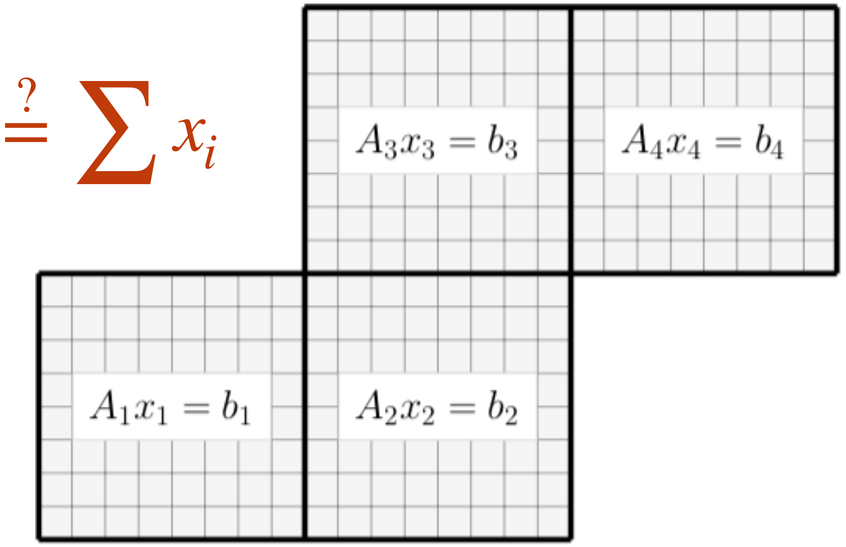


Set of local discretizations

M local matrices, M local right hand side vectors

$$x \stackrel{?}{=} \sum x_i$$



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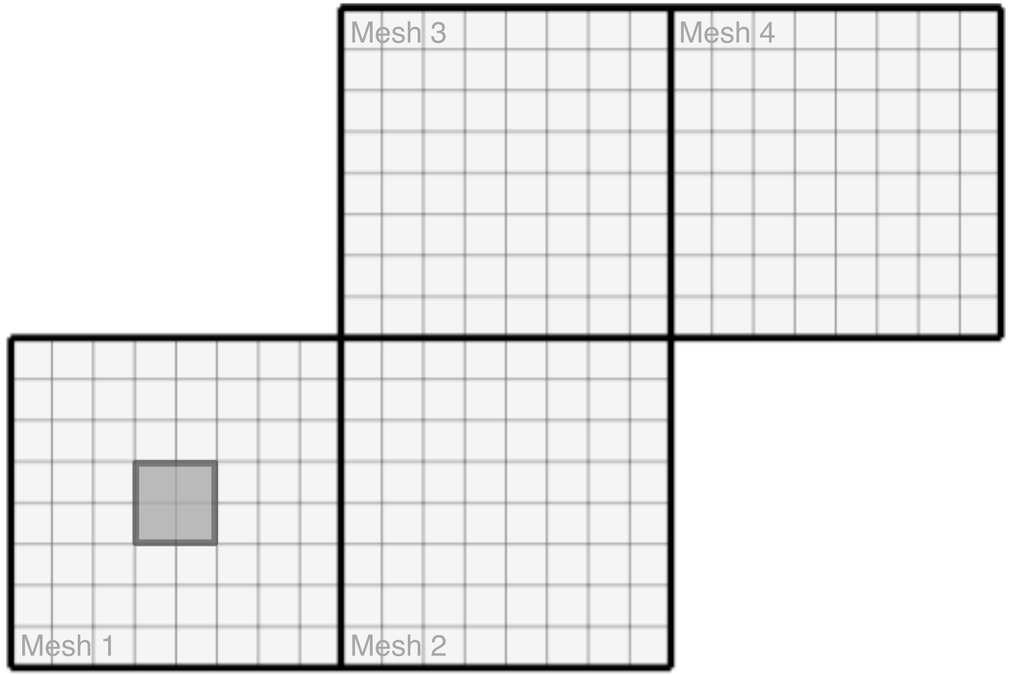
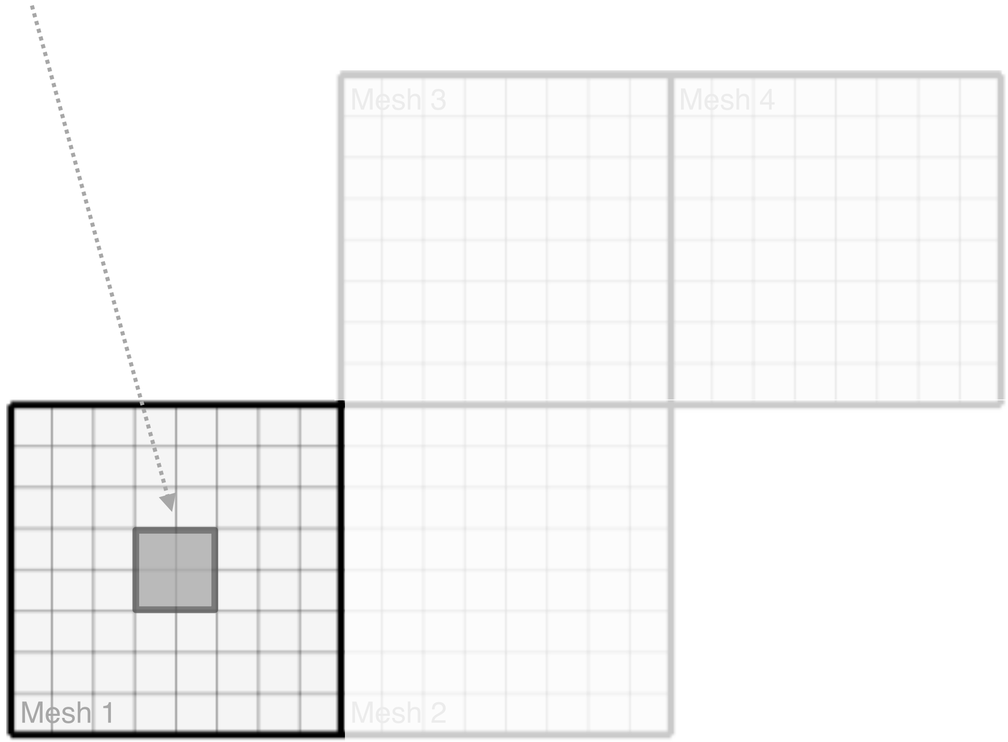
Structured versus unstructured discretization

There are different possibilities to discretize ...



Structured versus unstructured discretization

... at cells inside and around a solid obstruction



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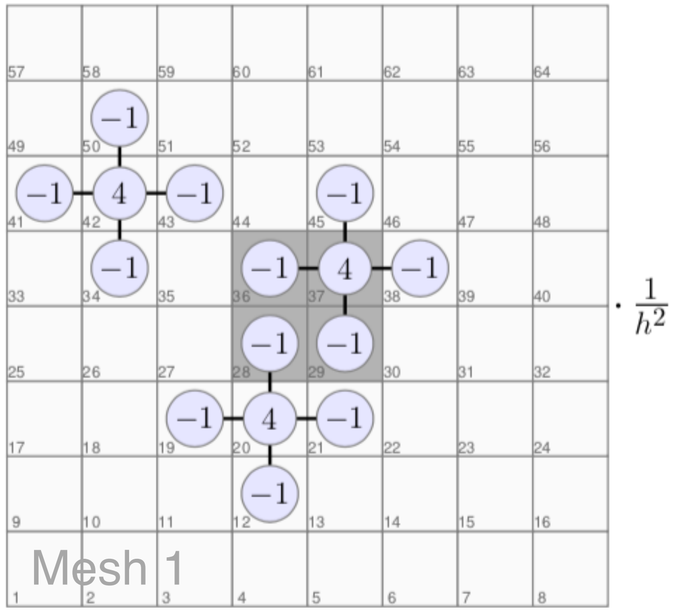
Structured versus unstructured discretizations

Structured

Regular matrix stencils



$\cdot \frac{1}{h^2}$

8x8 cells

Cells inside obstructions are **included**

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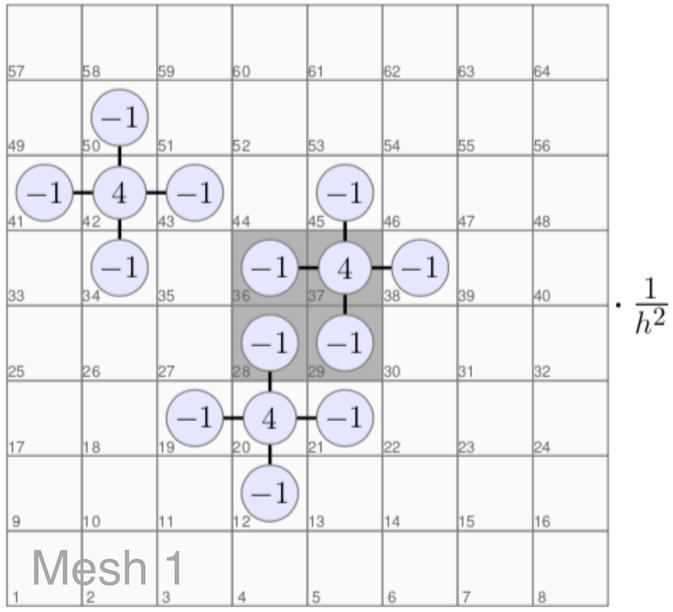
Structured versus unstructured discretizations

Structured

Regular matrix stencils



$\cdot \frac{1}{h^2}$

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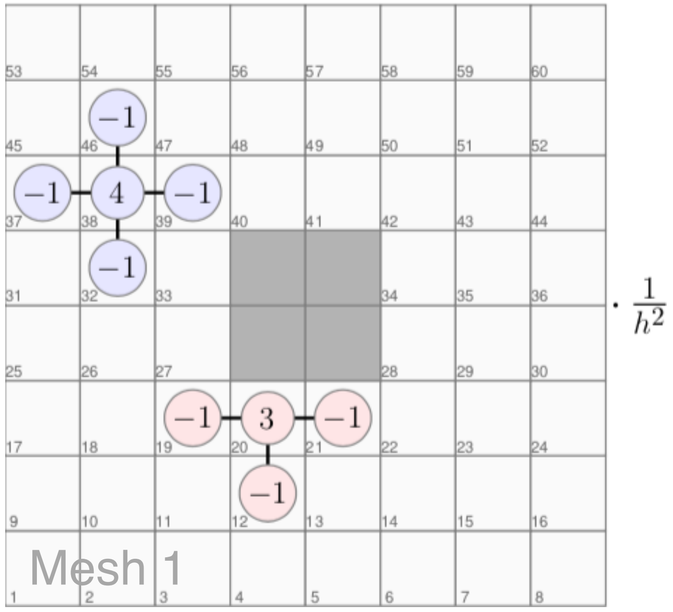
Cells inside obstructions are **included**

Unstructured

Irregular matrix stencils



$\cdot \frac{1}{h^2}$

Cells inside obstructions are **excluded**

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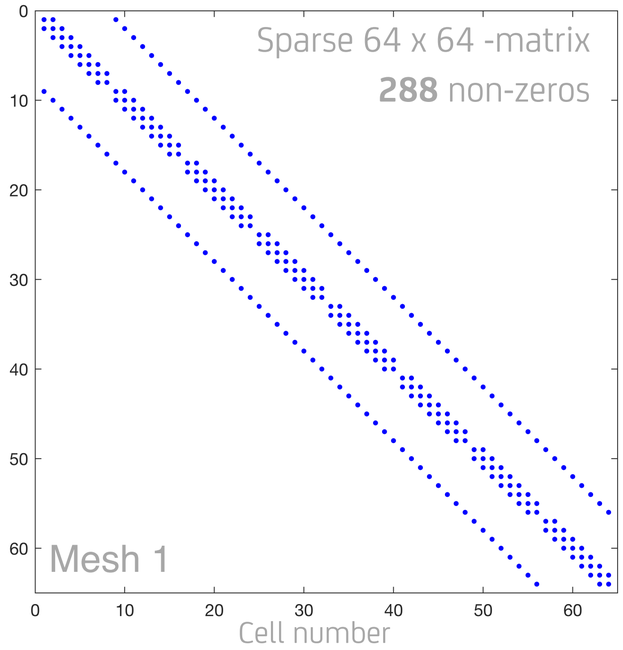
Regular versus irregular Poisson matrix

Structured

Highly regular Poisson matrix A



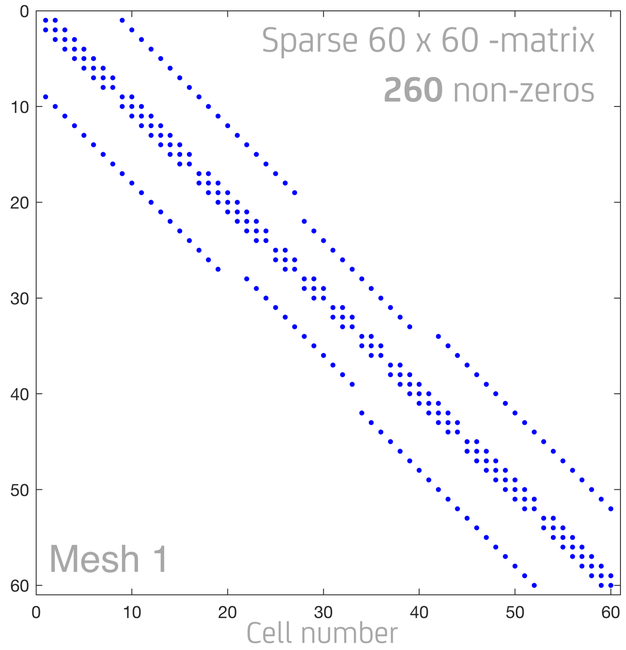
Highly optimized solvers usable (fast!)

8x8 cells

Sparsity patterns

Unstructured

Irregular Poisson matrix A



Need of more robust solvers (slower!)

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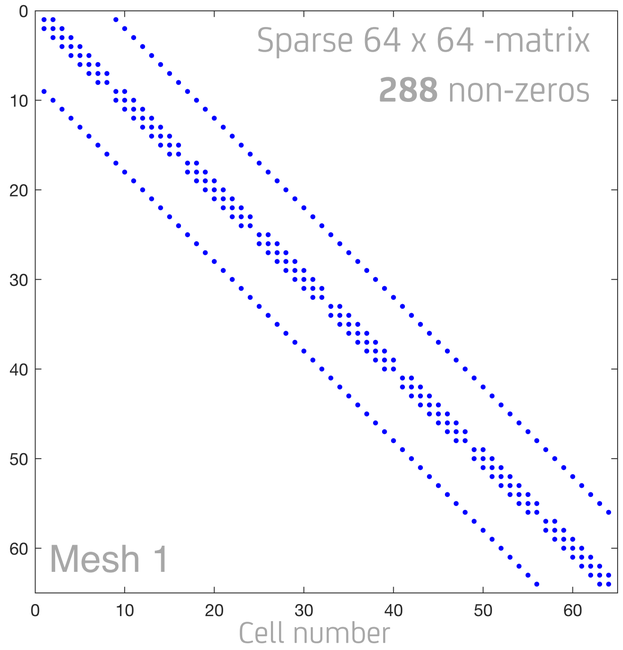
Regular versus irregular Poisson matrix

Structured

Highly regular Poisson matrix A



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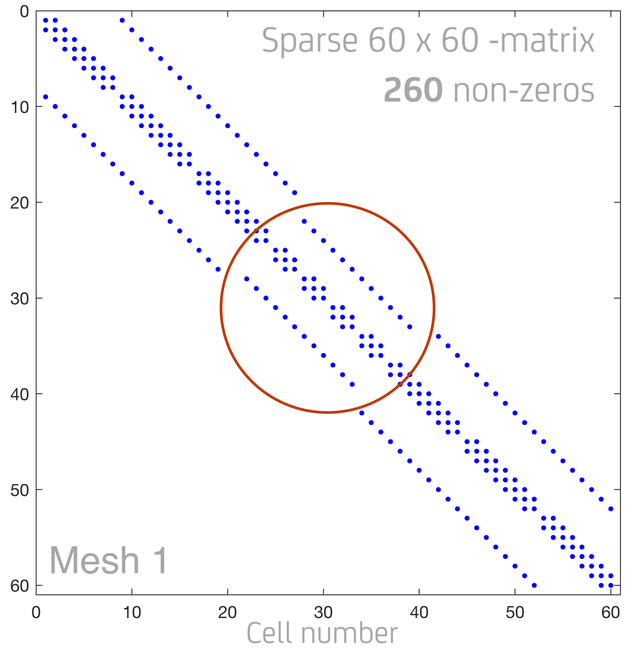

Need of more robust solvers (slower!)

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Current FDS pressure solver

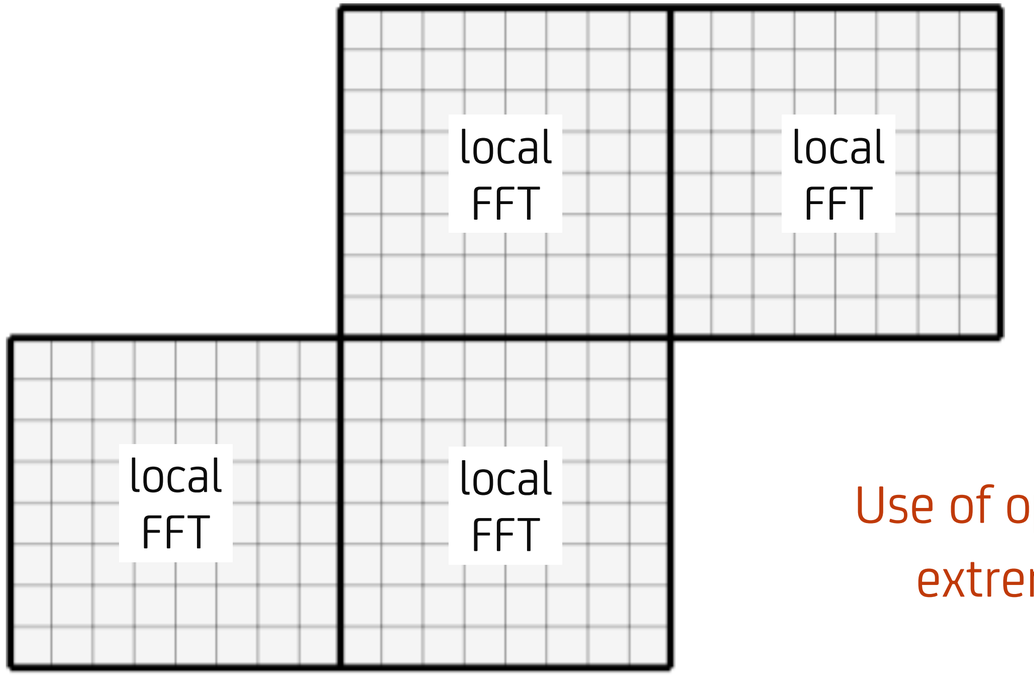
Mesh-wise FFT with pressure iteration

Mesh-wise FFT-solver

2

FFT
solver

Local structured discretizations to solve the local Poisson problems by FFT's



Use of optimized CRAYFISHPAK,
extremely fast and robust

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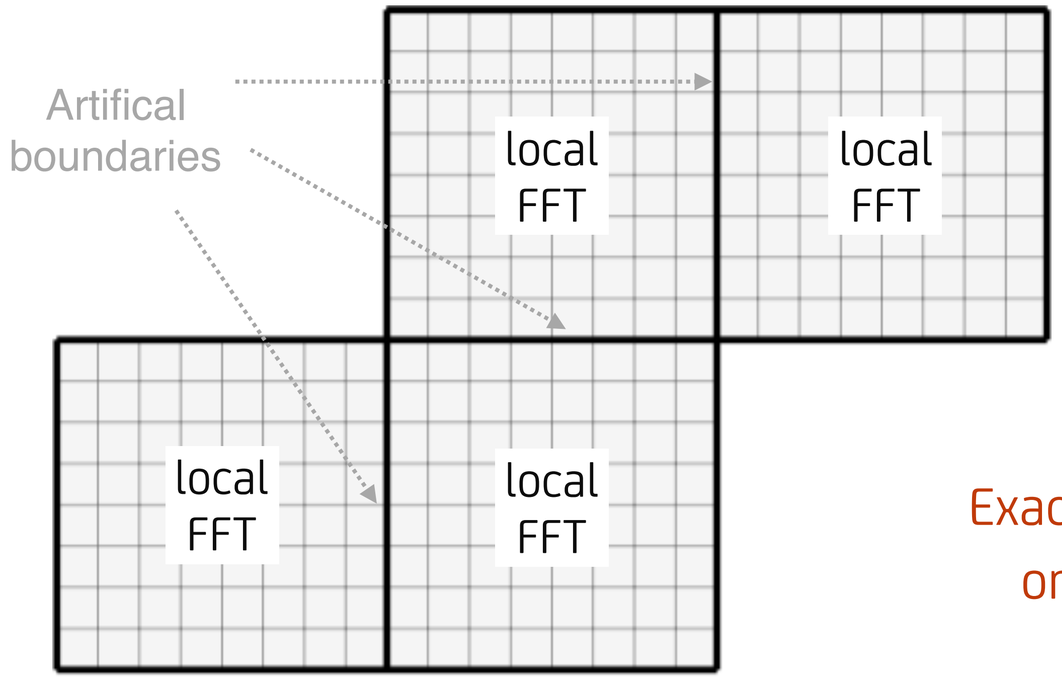
Mesh-wise FFT-solver

2

FFT
solver

Mathematical solvability requires internal boundary conditions for local FFTs ...



Exact values not known,
only approximately

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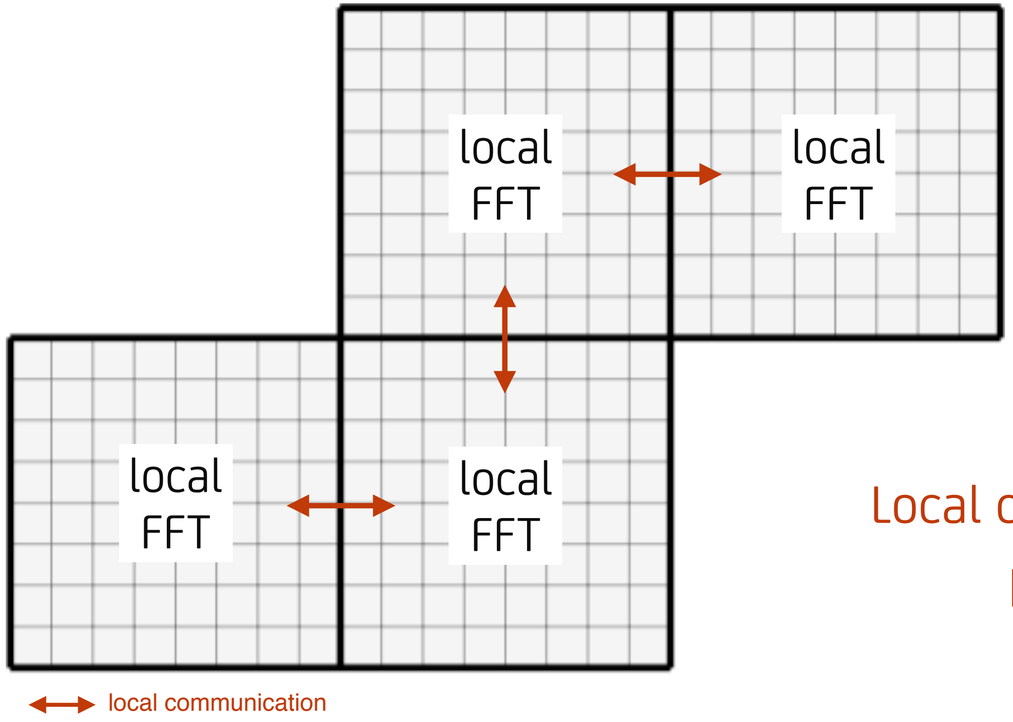
Mesh-wise FFT-solver

2

FFT
solver

... average of neighboring cells from previous time step is used



Local communication required
per FDS time step

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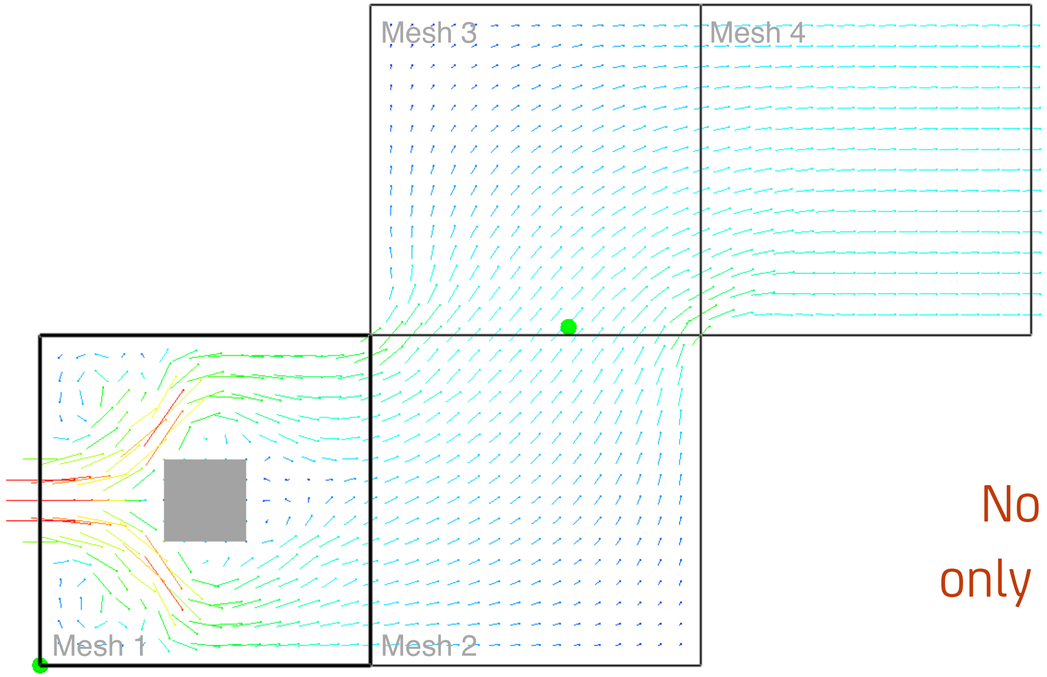
Accuracy along mesh interfaces?

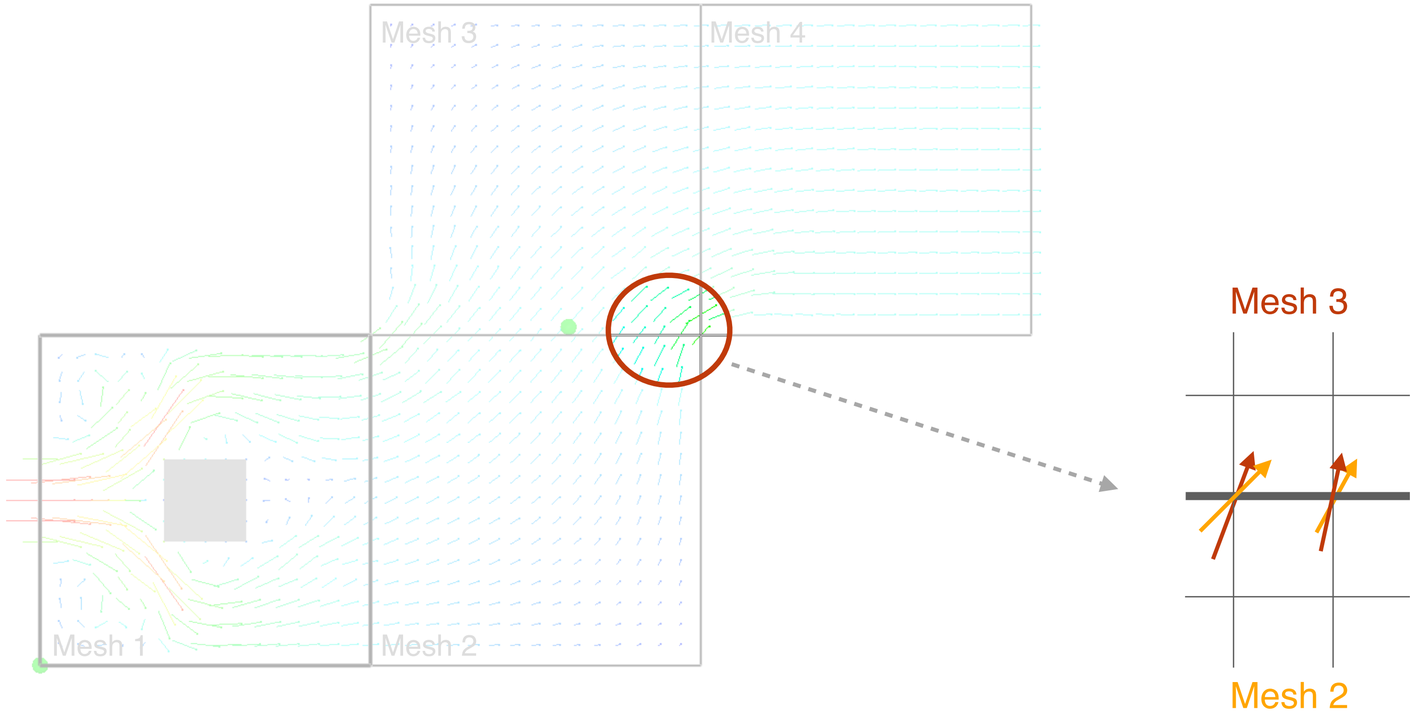
Question: How accurate is the velocity field at mesh interfaces?



No global discretization,
only collection of local ones

Accuracy along mesh interfaces?

Local velocity components may be different along mesh interfaces



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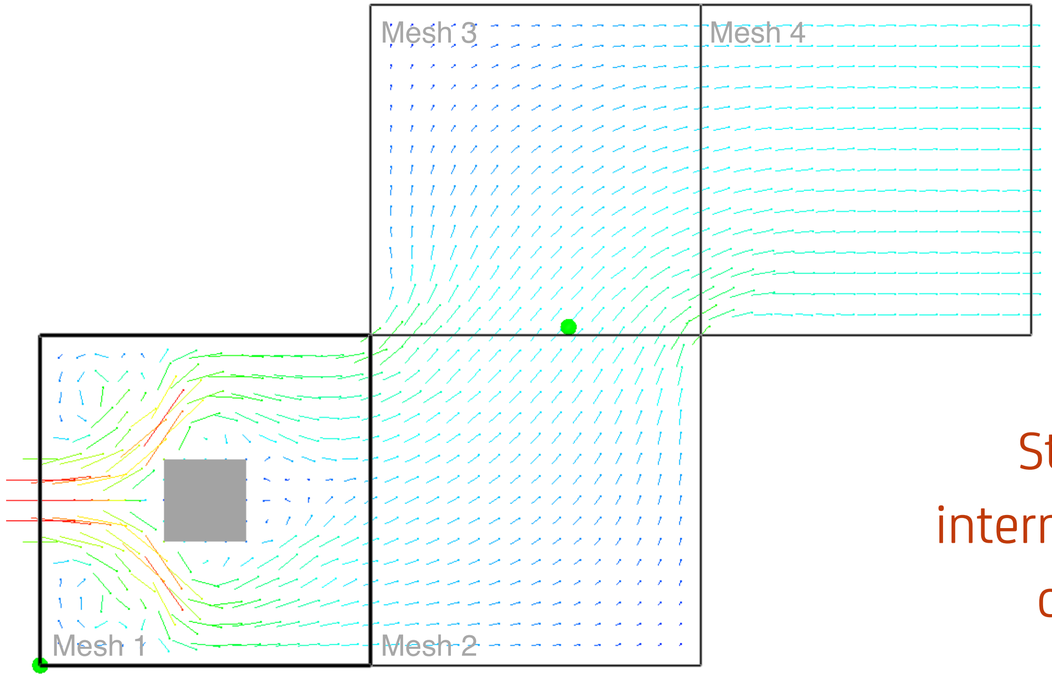
Accuracy along internal obstructions?

2

FFT
solver

Question: How accurate is the velocity field along inner obstructions?



Structured grids only,
internal boundary conditions
cannot be specified

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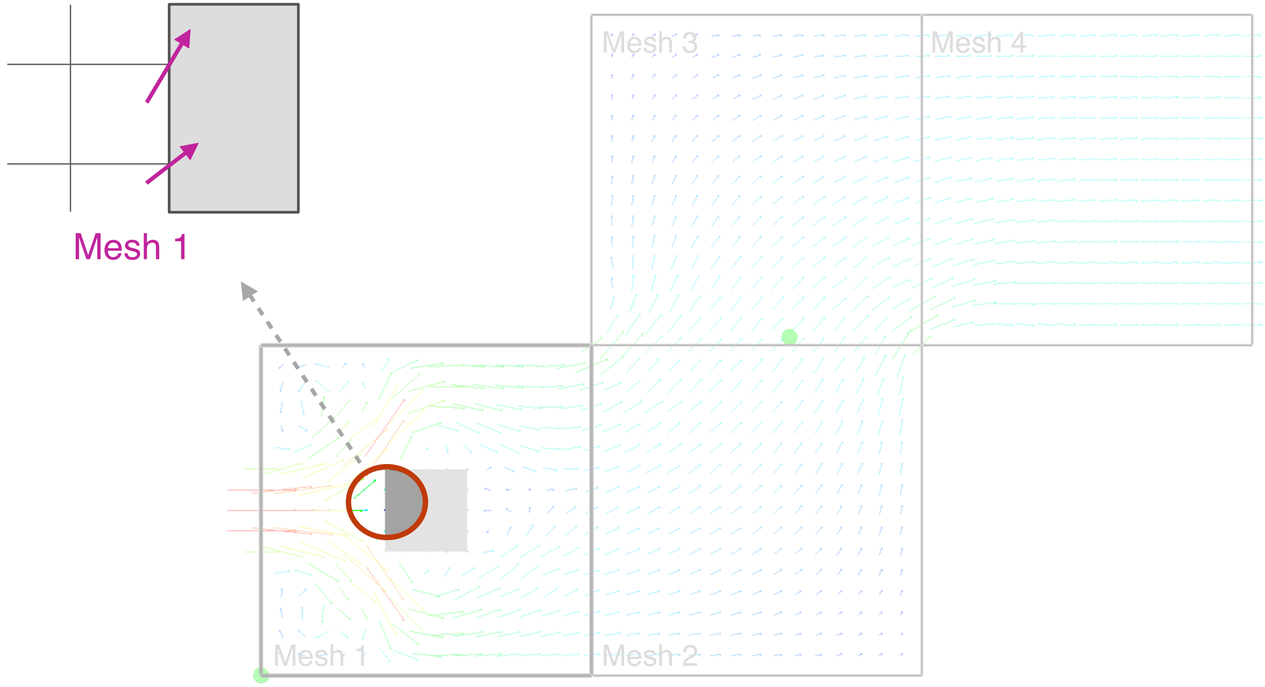
Accuracy along internal obstructions?

2

FFT
solver

Velocity components may penetrate into the inner obstructions



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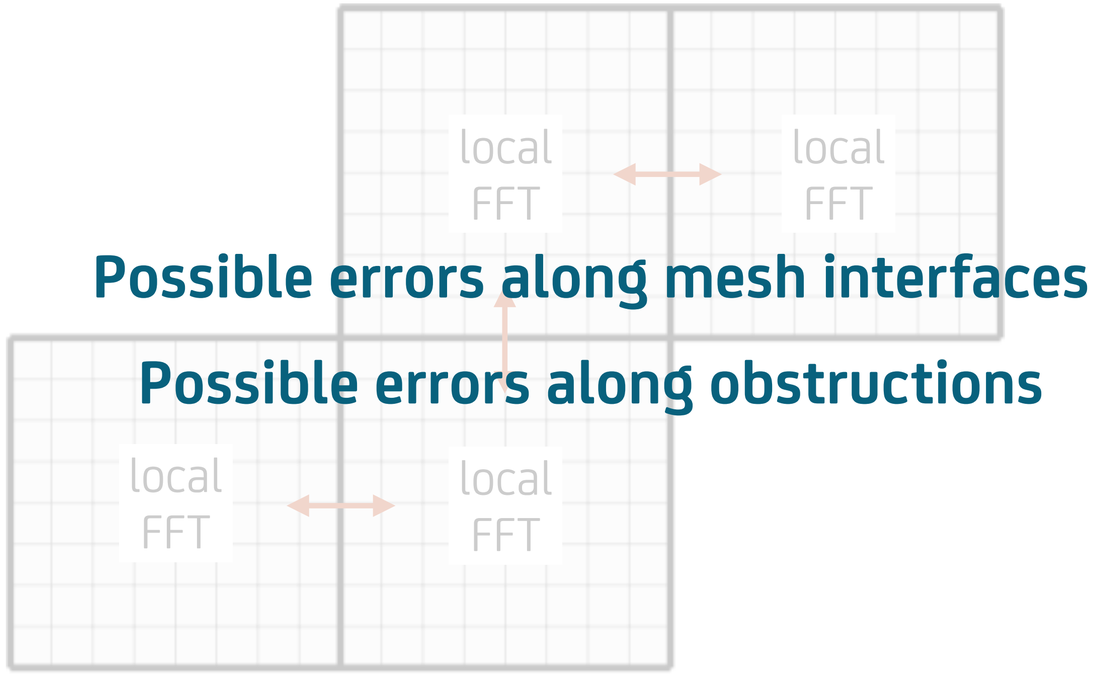
Mesh-wise FFT-solver

2

FFT
solver



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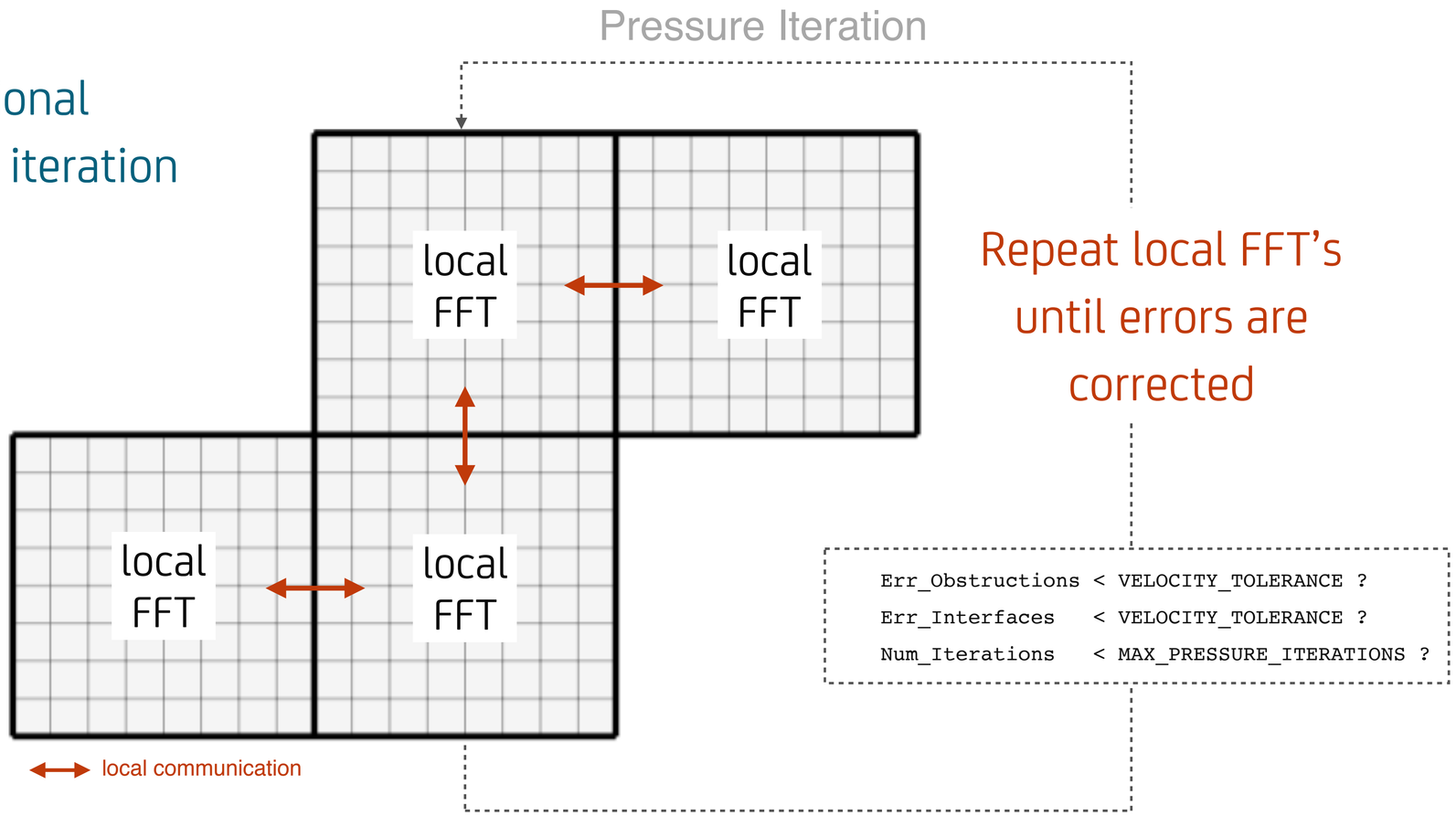
Mesh-wise FFT-solver with pressure iteration

Remedy:
Use additional
corrective iteration



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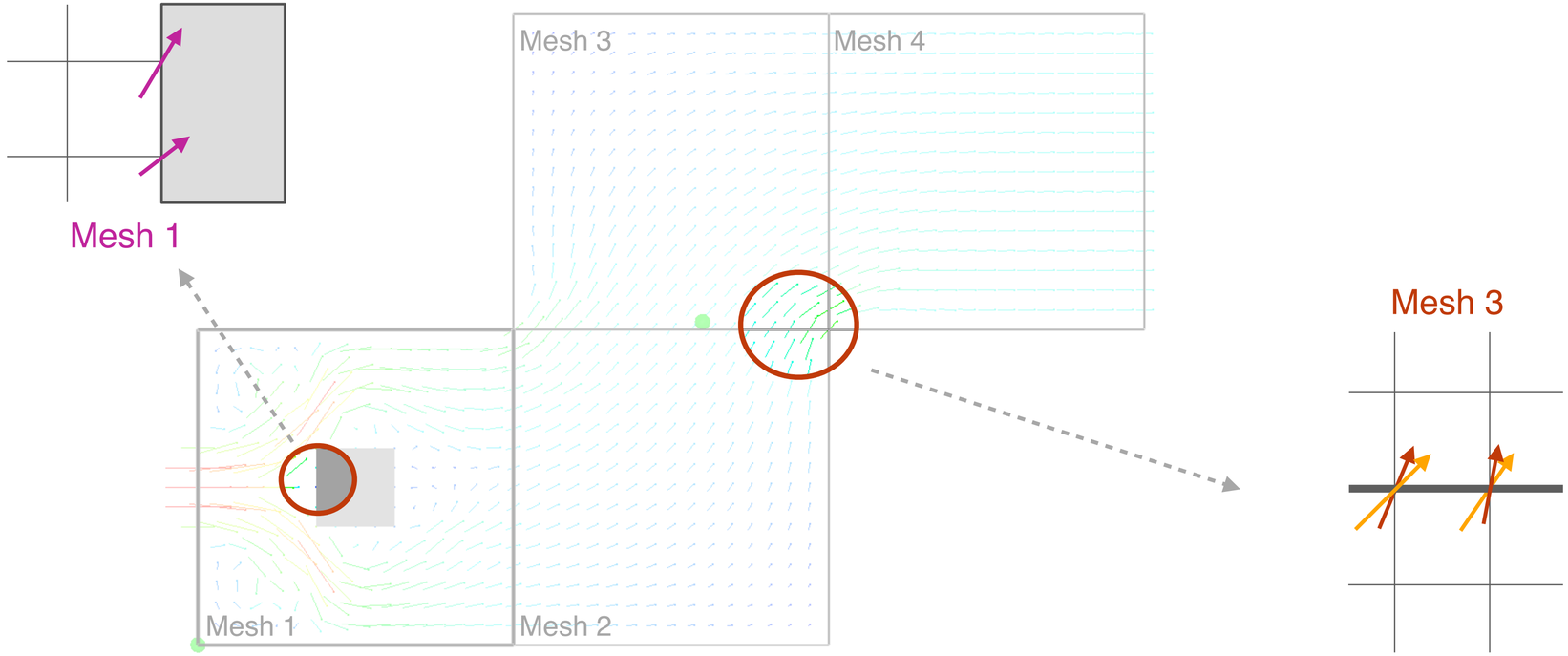
Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

Start iteration: Initial velocity errors



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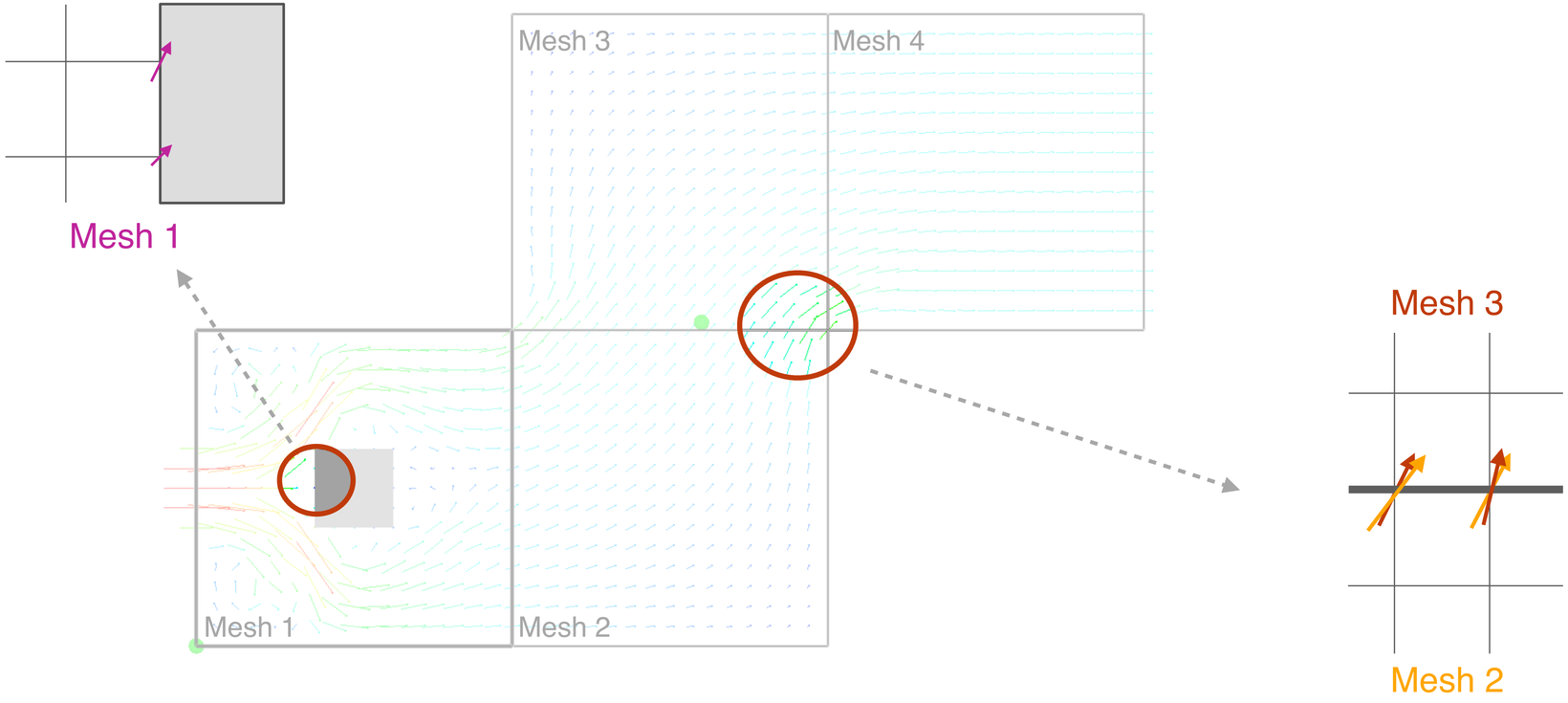
Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

Intermediate iteration: Velocity errors are reduced more and more



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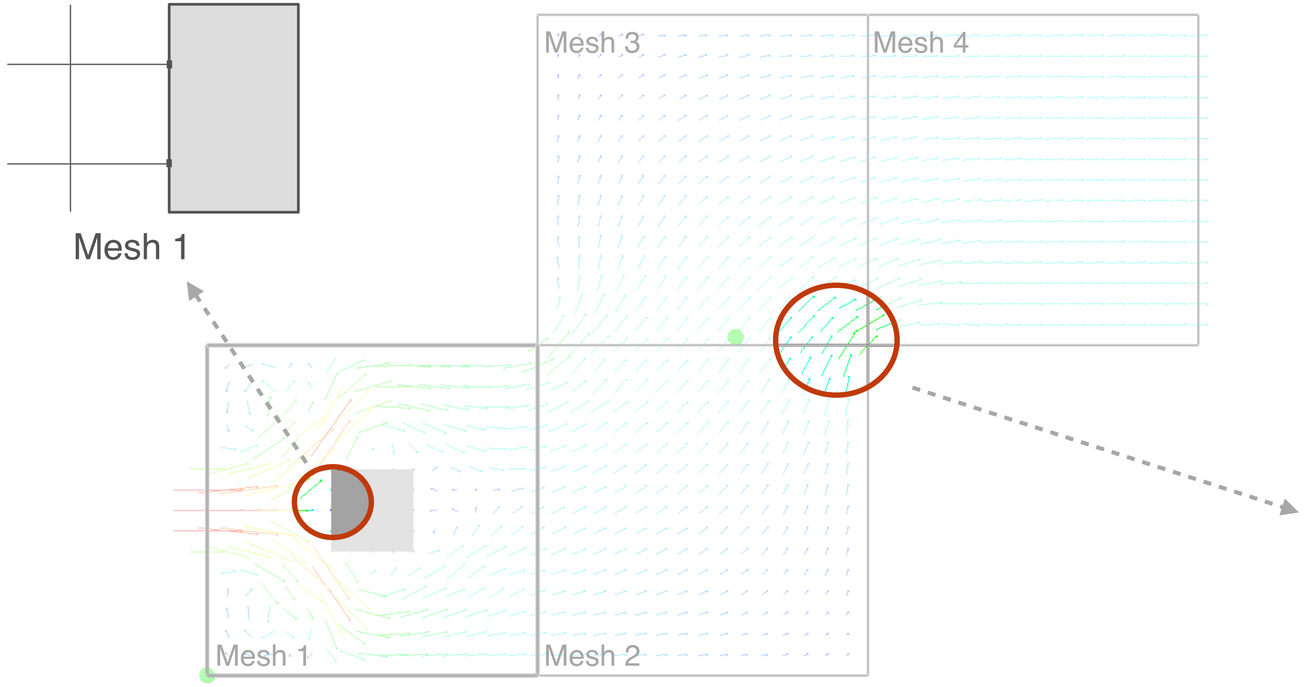
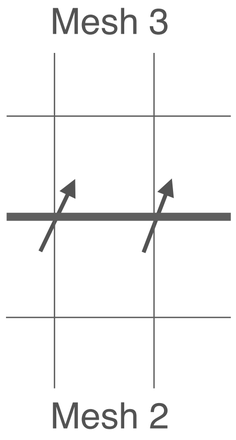
Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

End of iteration: Velocity errors are below specified tolerance





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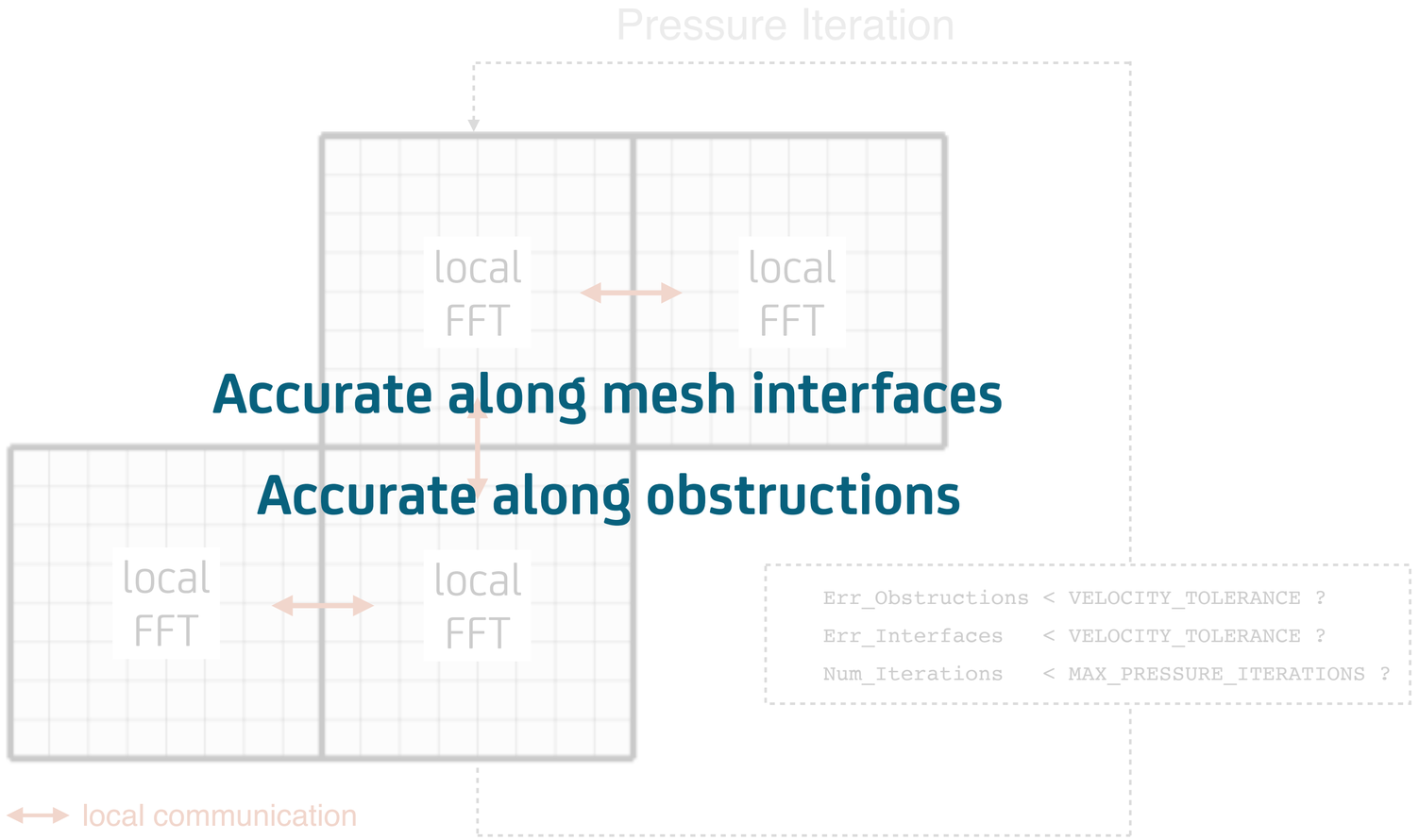
Mesh-wise FFT-solver with pressure iteration

2

FFT
solver



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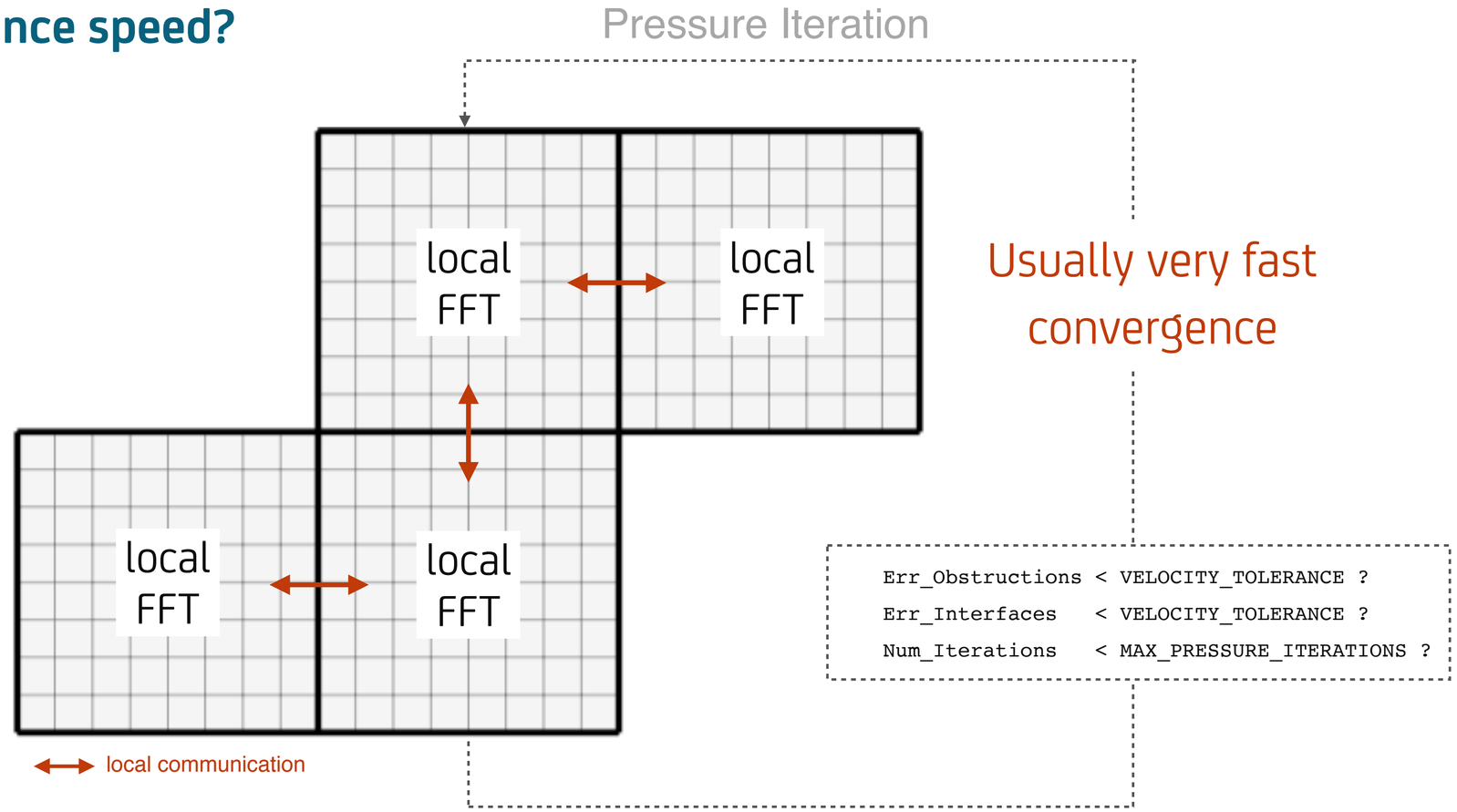
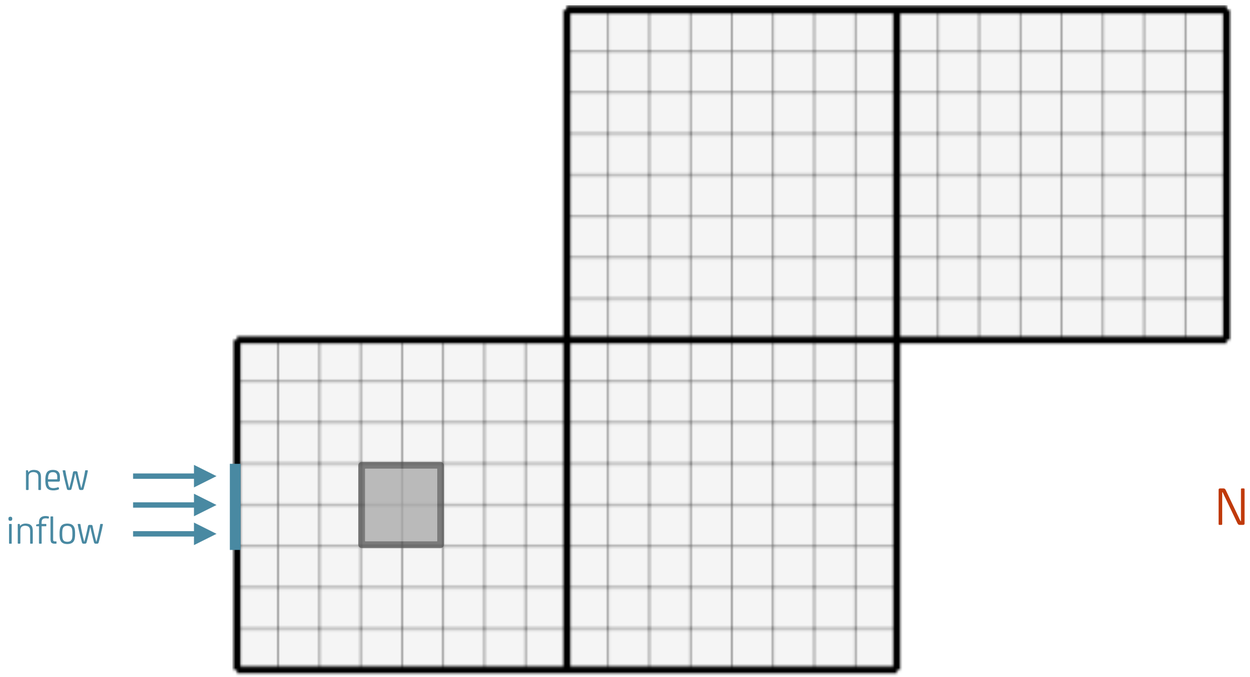
Mesh-wise FFT-solver with pressure iteration

Convergence speed?



Mapping of the global flow of information?

Question: How quickly does new local information spread?



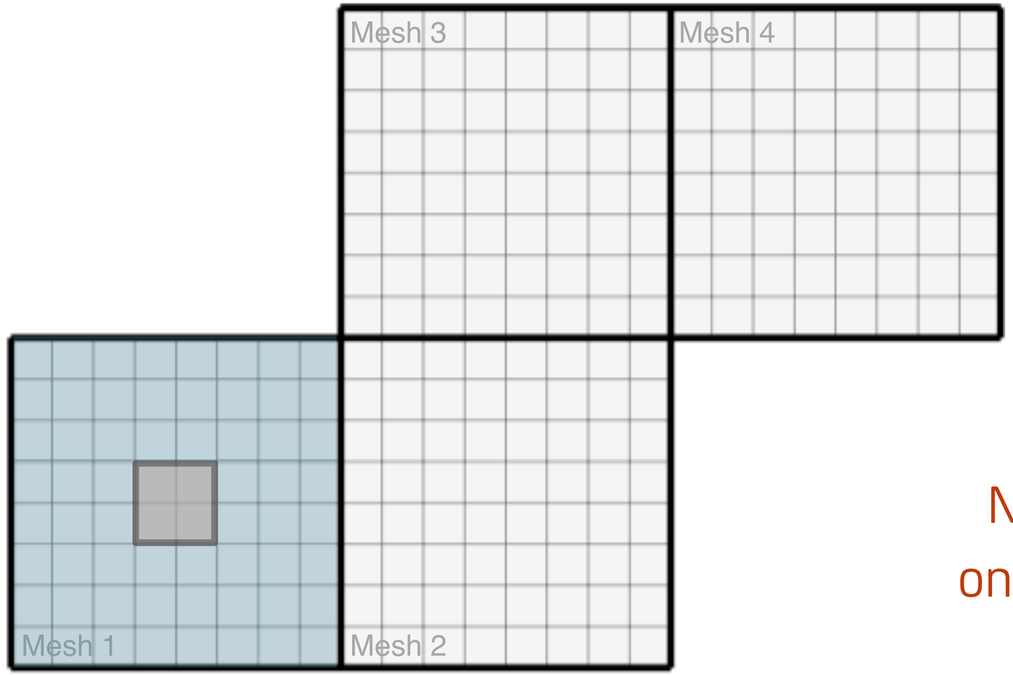
No global discretization,
only local solutions

Mapping of the global flow of information?

2

FFT
solver

1. Cycle: Information reaches Mesh 1



No global data transfer,
only local communication

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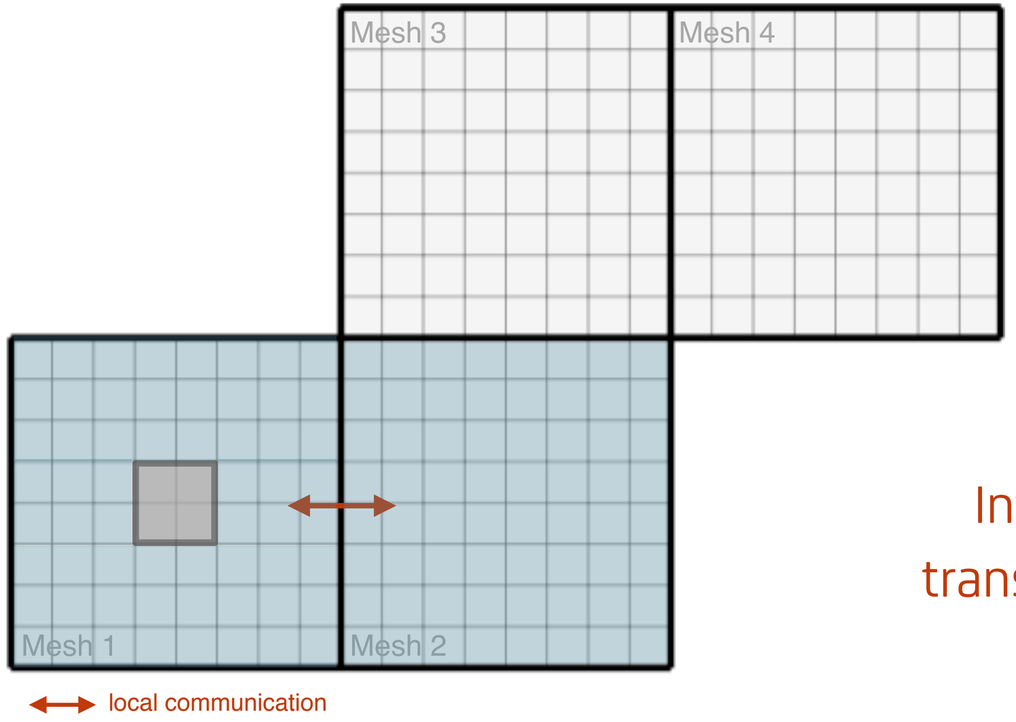
Mapping of the global flow of information?

2

FFT
solver

2. Cycle: Information reaches Mesh 2



Information can only be
transferred mesh-by-mesh ...

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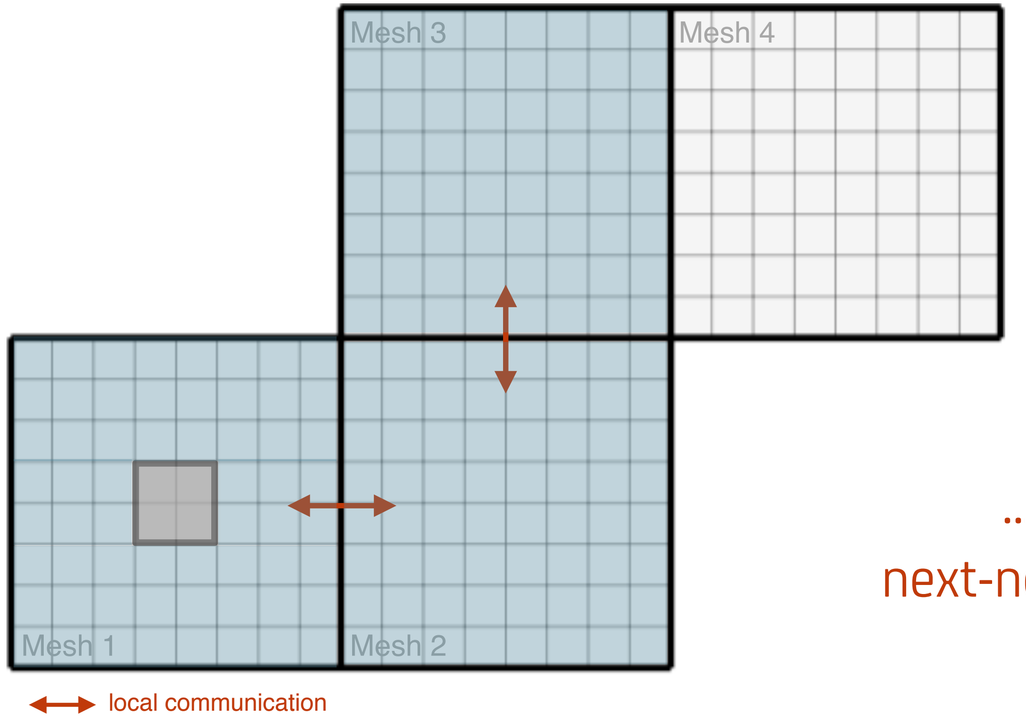
Mapping of the global flow of information?

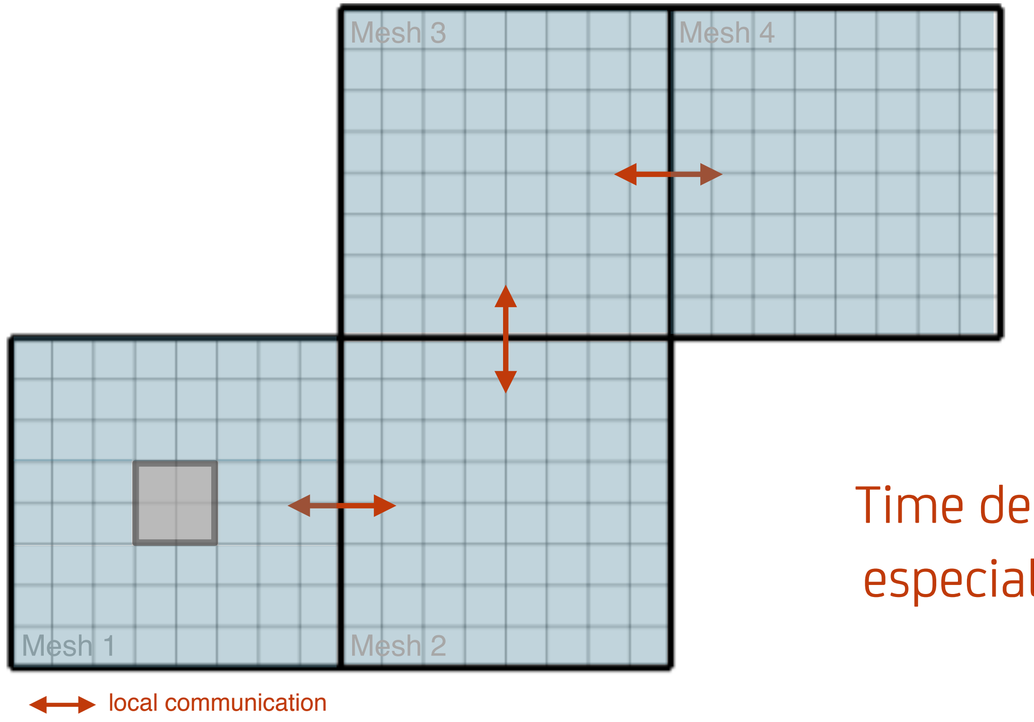
3. Cycle: Information reaches Mesh 3



... successively using
next-neighbor communications

Mapping of the global flow of information?

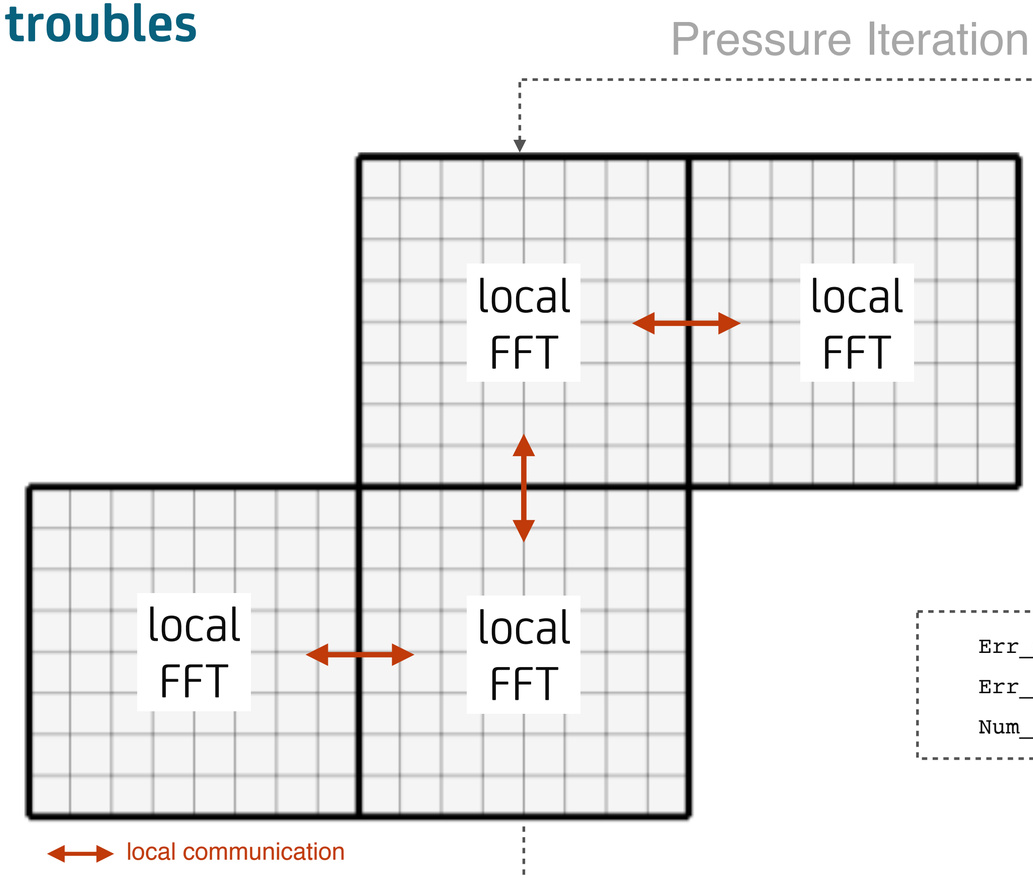
4. Cycle: Information finally reaches Mesh 4



Time delay compared to 1-mesh,
especially for large mesh counts

Mesh-wise FFT-solver with pressure iteration

Possible troubles



For large mesh counts or very transient cases slow convergence and large overhead

```
Err_Obstructions < VELOCITY_TOLERANCE ?
Err_Interfaces   < VELOCITY_TOLERANCE ?
Num_Iterations   < MAX_PRESSURE_ITERATIONS ?
```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UGLMAT solver

Optimized parallel LU-decomposition

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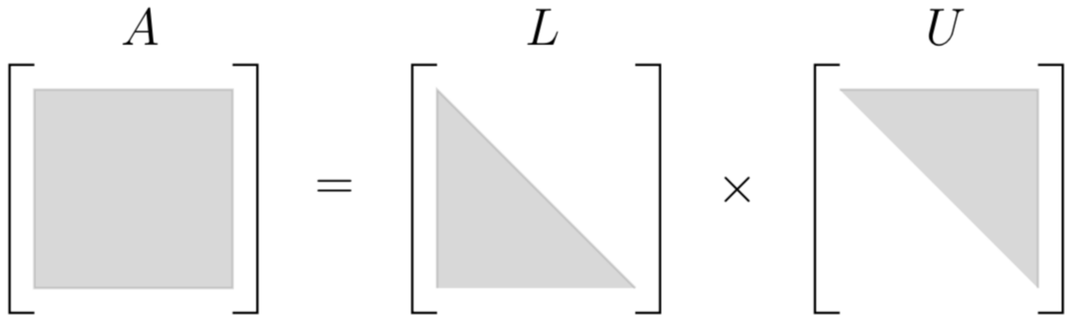
Alternative pressure solver UGLMAT

3

UGLMAT
solver

- **Global unstructured discretization** of whole domain
- Decomposition of global Poisson matrix A in lower and upper triangular matrices L and U



Parallel
LU-decomposition

- Usage of optimized LU - solver from Intel Math Kernel Library (MKL)

Alternative pressure solver UGLMAT

3

UGLMAT
solver

- **Global unstructured** discretization of whole domain
- Decomposition of global Poisson matrix A in lower and upper triangular matrices L and U

Accurate along mesh interfaces

Accurate along obstructions

Parallel
LU-decomposition

- Usage of optimized LU - solver from Intel Math Kernel Library (MKL)

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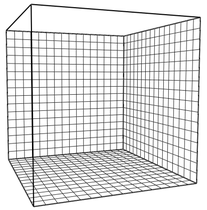
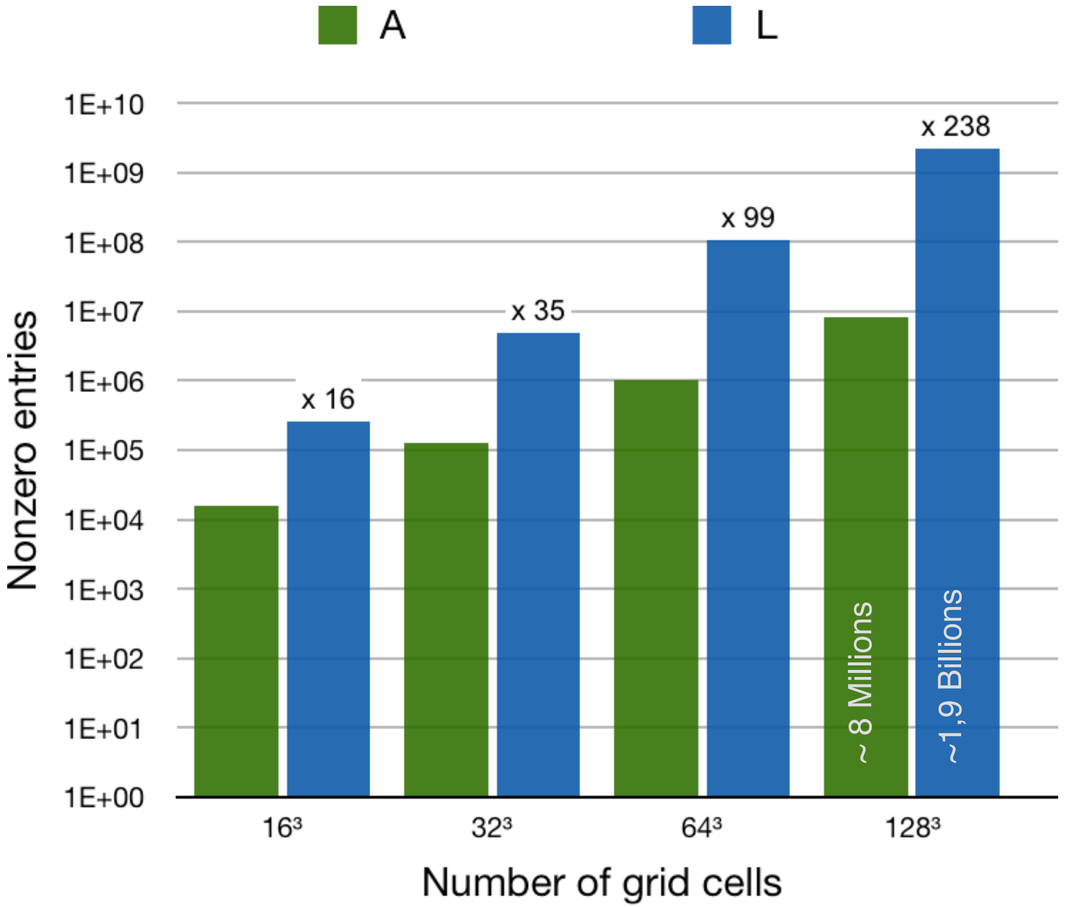


UGLMAT - Memory needs for 3D-cube



L has much more non-zero entries than A due to ‚fill-in'

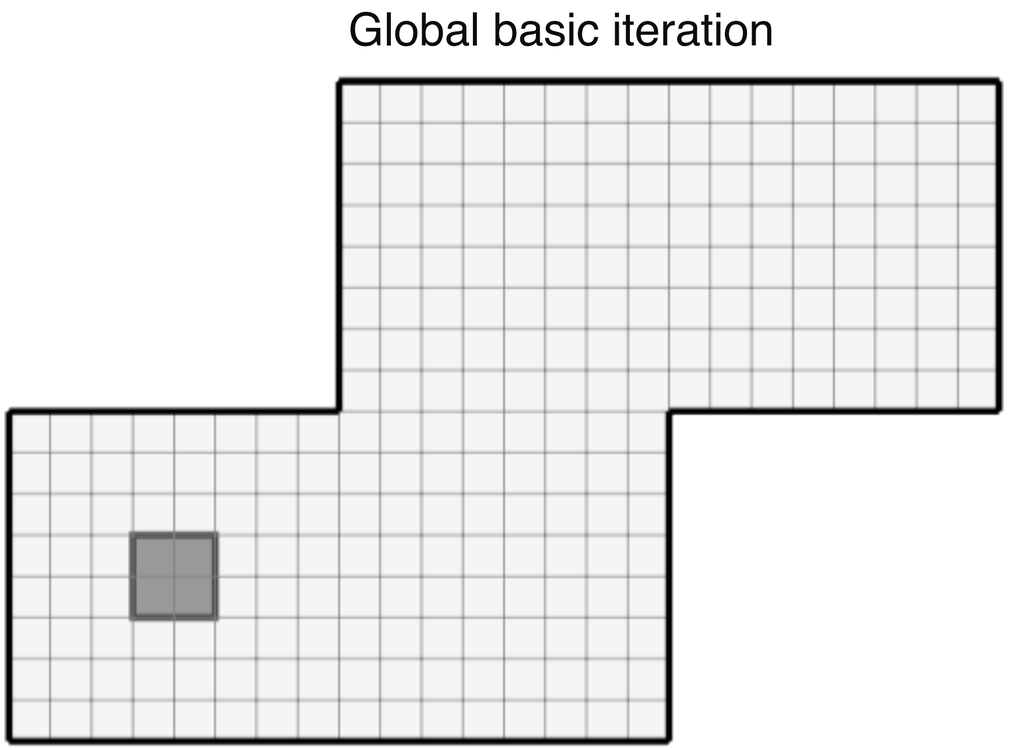
Huge memory requirements if grid is refined

ScaRC

Scalable Recursive Clustering

hhpberlin

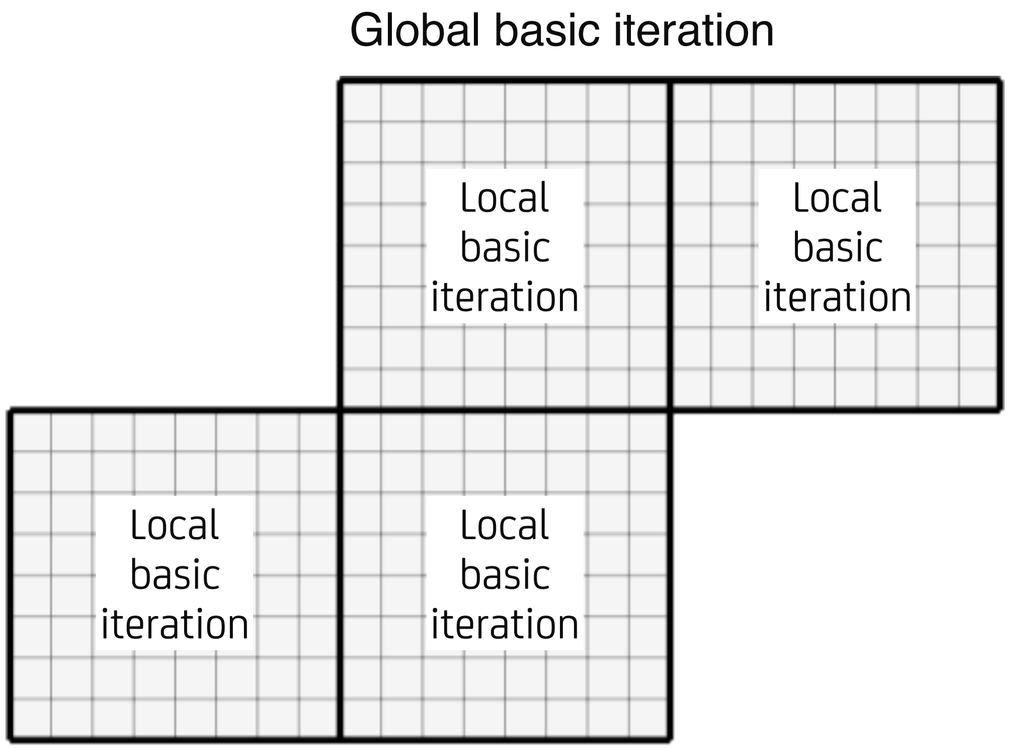
ScaRC Core: Overall global iterative method



Global structured discretization

Data-parallel iterative method for global Poisson matrix

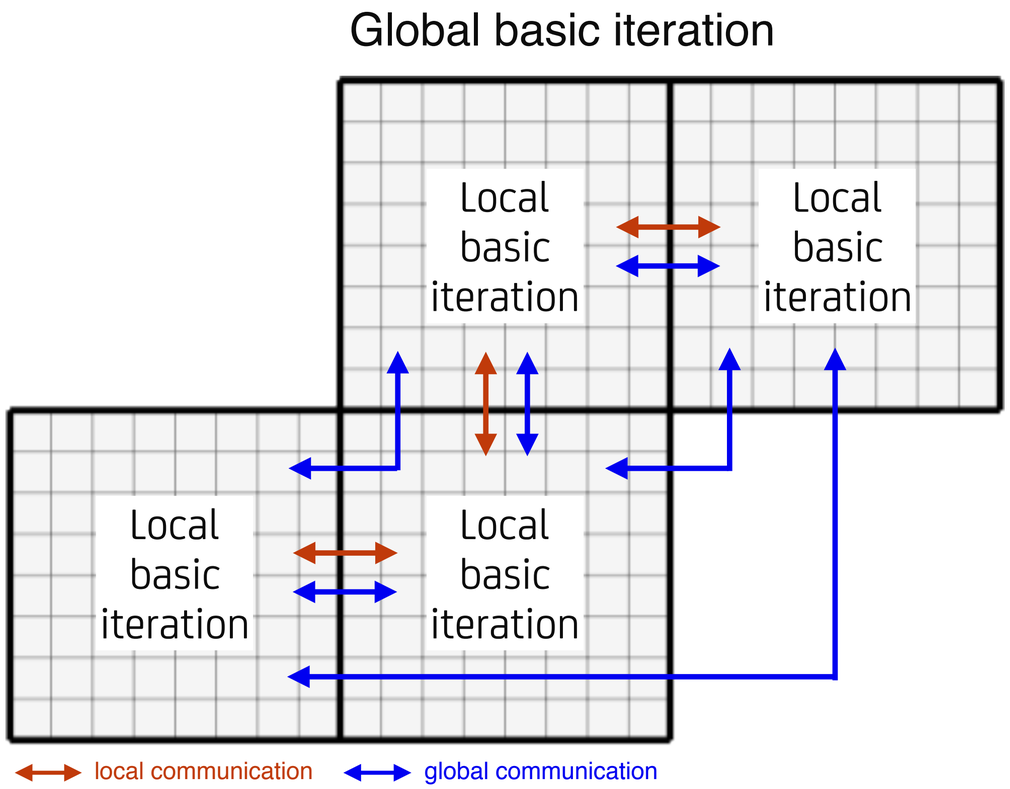
ScaRC Core: Additional local iterative methods



Not used as
stand-alone solvers

only as corrections
to global solution

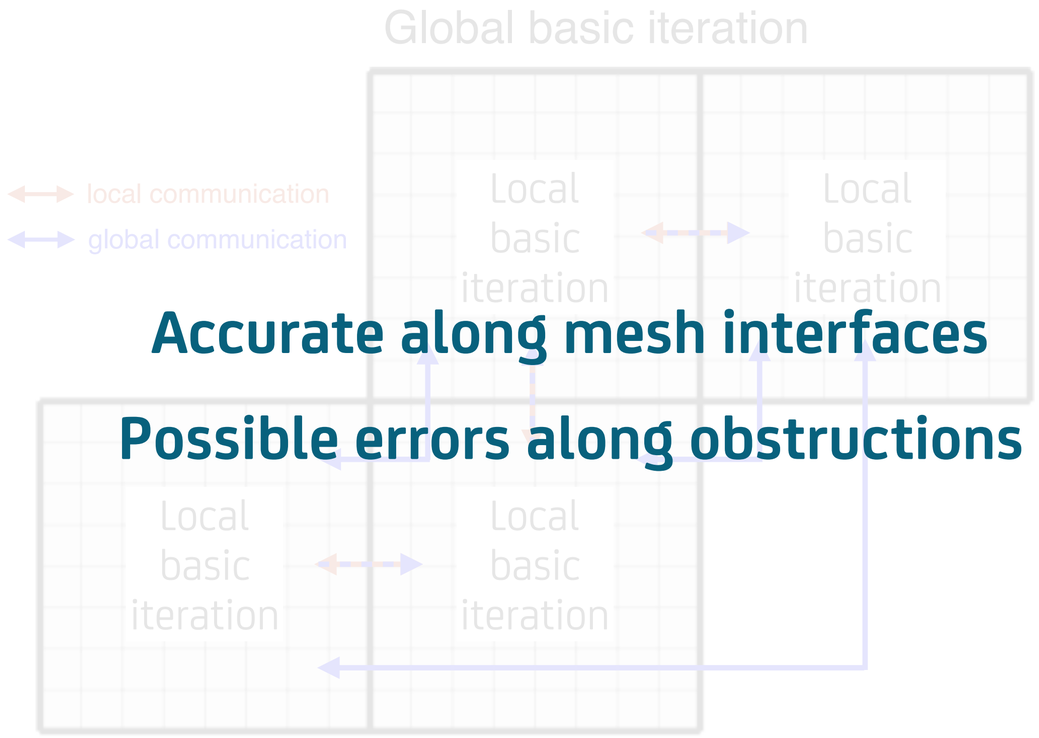
ScaRC Core: Local and global communication



Local solvers offer
fine grid accuracy

Basic information transfer
is provided globally

ScaRC Core: Structured basic version



Accurate along mesh interfaces

Possible errors along obstructions

Multiple variations of different techniques

Use of different discretization techniques

- Pressure iteration for structured case → Fix errors at obstructions
- Global unstructured discretization → No errors at obstructions

Use of different global solvers

- Conjugated Gradient method (CG) → Exploit basic robustness
- Geometric Multigrid method (MG) → Improve global coupling

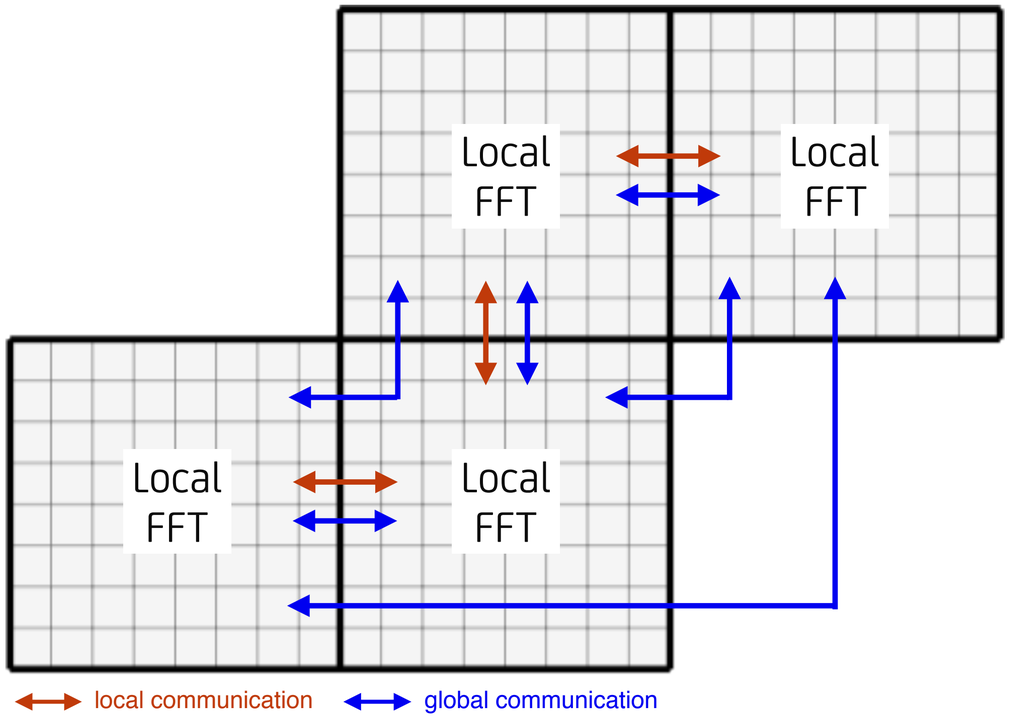
Use of different local solvers

- Optimized FFT (CRAYFISHPAK) → Speed up local solutions in structured case
- Optimized LU (Intel MKL) → Speed up local solutions in unstructured case

ScaRC-CG: Default for structured grids

Pressure Iteration

Global data-parallel Conjugate Gradient method

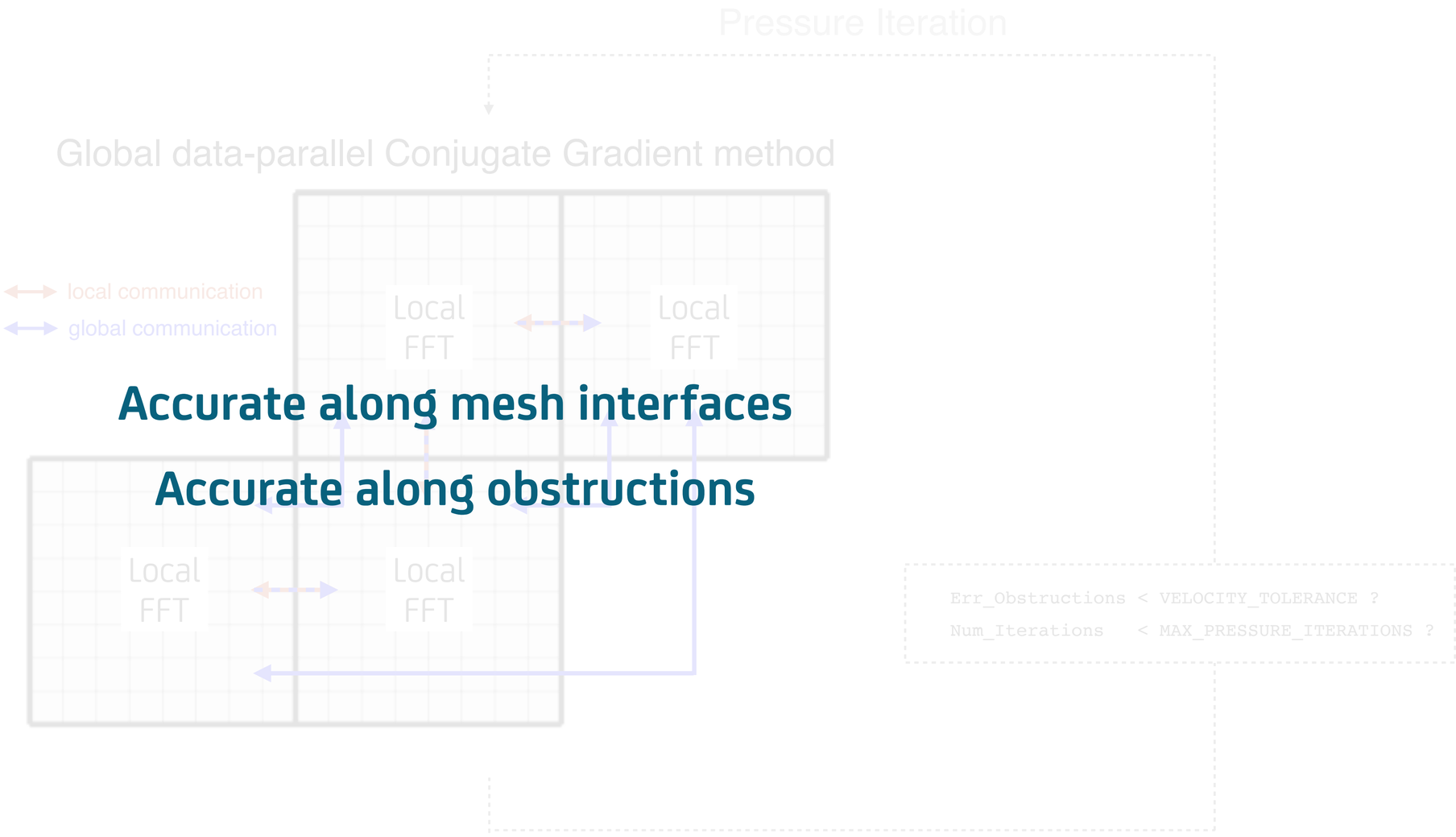


Optimize globally (CG)
Optimize locally (FFT)

Pressure iteration for
inner obstructions

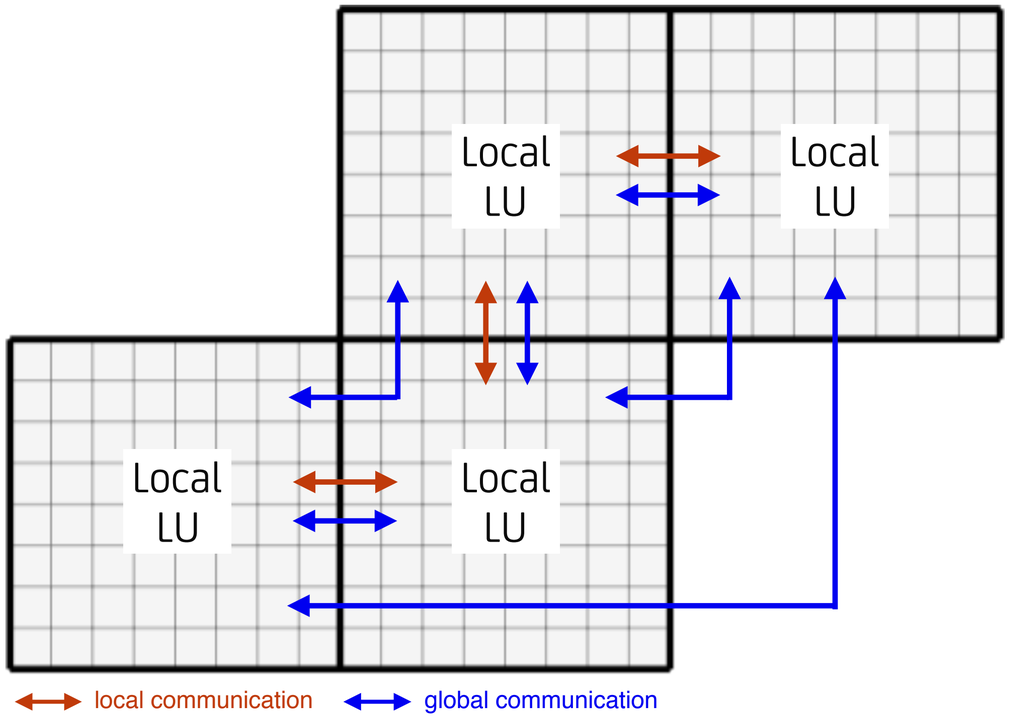
```
Err_Obstructions < VELOCITY_TOLERANCE ?
Num_Iterations   < MAX_PRESSURE_ITERATIONS ?
```

ScaRC-CG: Default for structured grids



UScaRC-CG: Default for unstructured grids

Global data-parallel Conjugate Gradient method



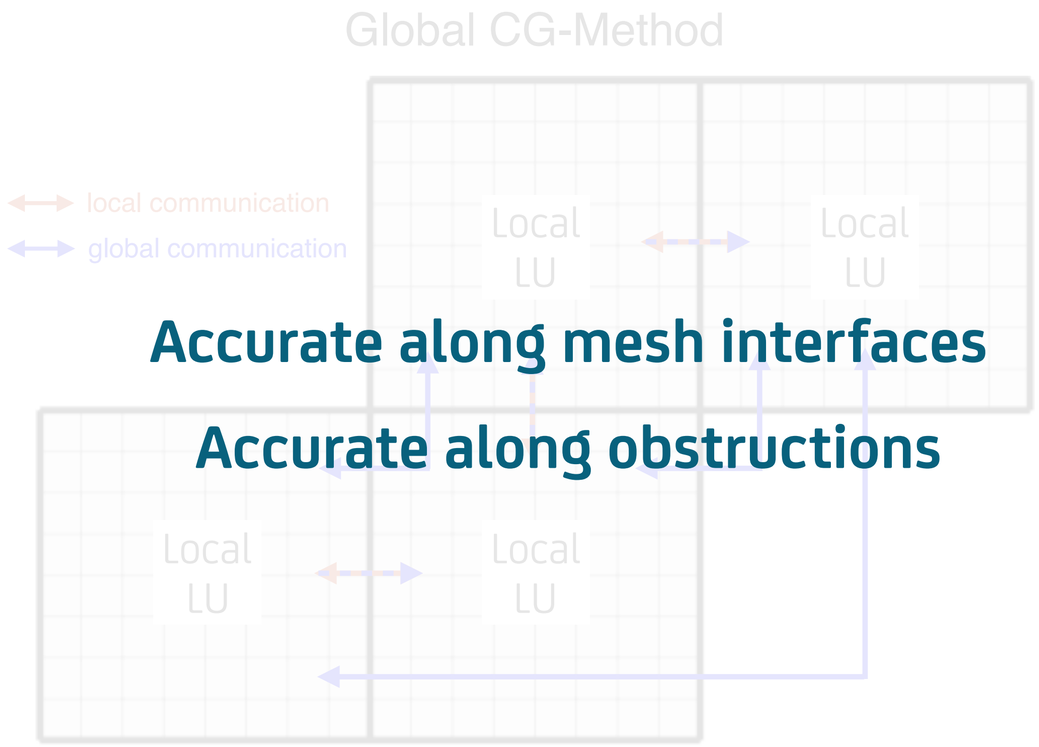
Optimize globally (CG)
Optimize locally (LU)

No need for
pressure iteration

UScaRC-CG: Default for unstructured grids

4

ScaRC
solver



Accurate along mesh interfaces

Accurate along obstructions

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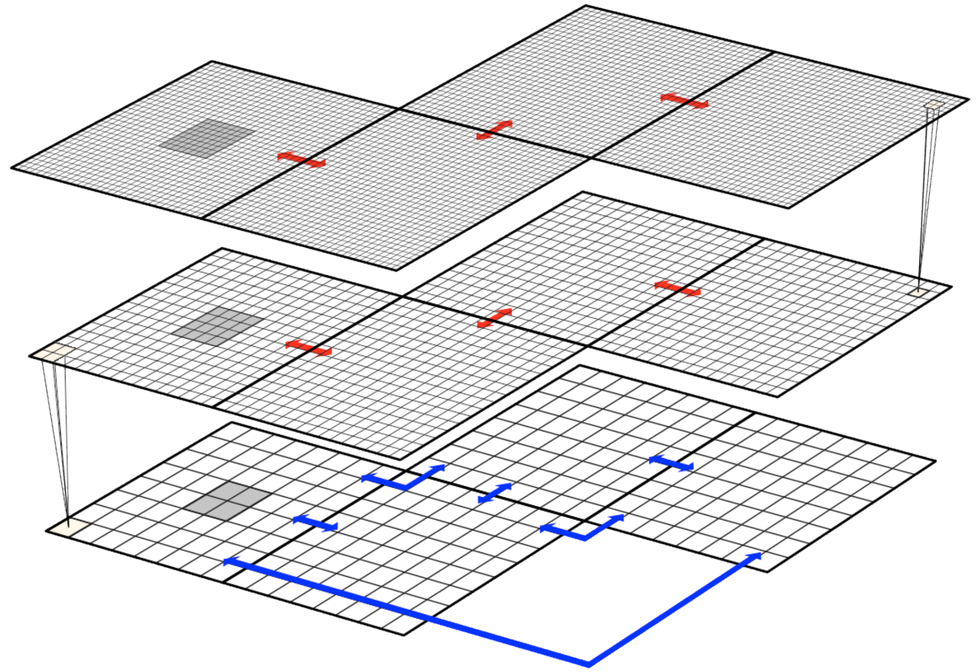
ScaRC-MG: Alternative for structured grids

Pressure Iteration

Global data-parallel Multigrid method



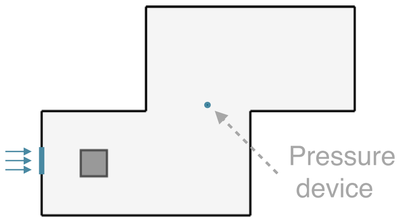
local communication global communication

Improve global coupling (MG)

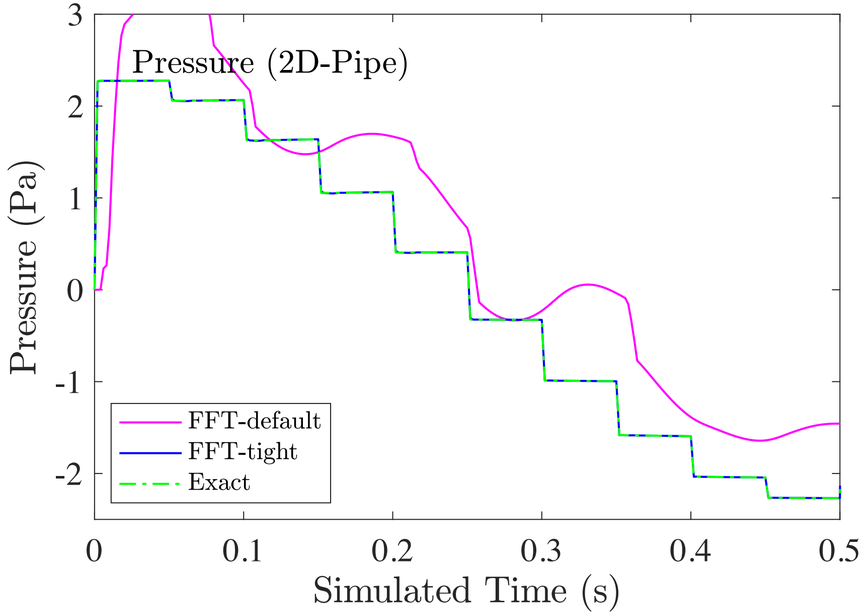
Pressure iteration for inner obstructions

```
Err_Obstructions < VELOCITY_TOLERANCE ?
Num_Iterations   < MAX_PRESSURE_ITERATIONS ?
```

Pressure trace for 2D-pipe

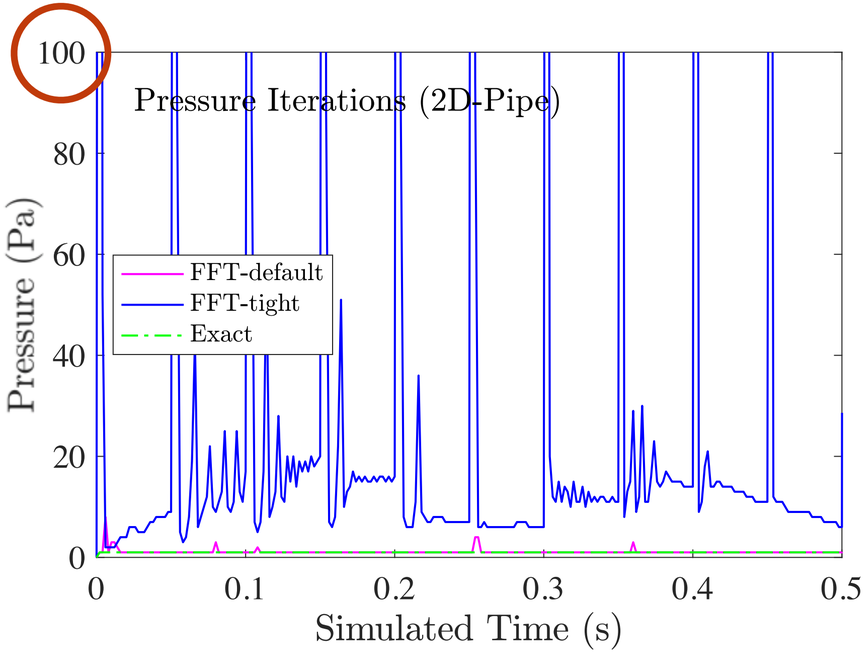


FFT default and tight (tol=10^{-5} m/s)

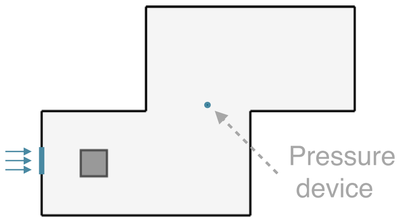


Only accurate for tight pressure iteration

Number of required pressure iterations

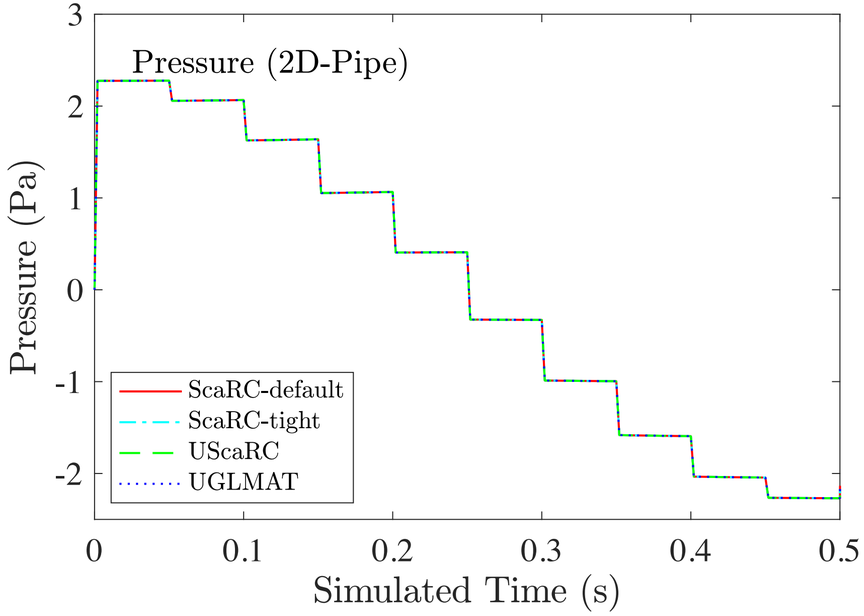


Increased number of pressure iterations (Ø 28)



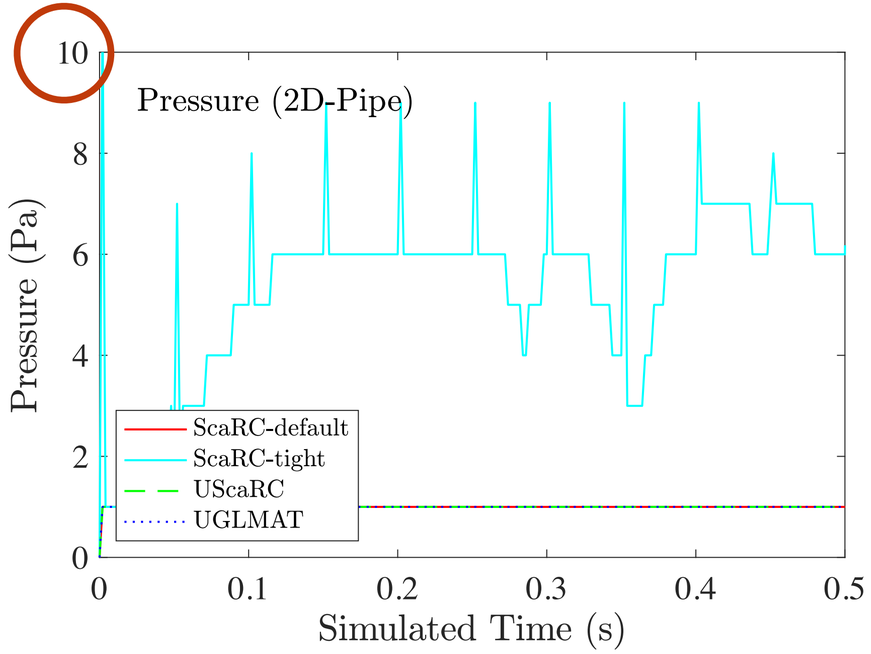
Pressure trace for 2D-pipe

Different variants of ScaRC and UGLMAT



Accurate for all variants

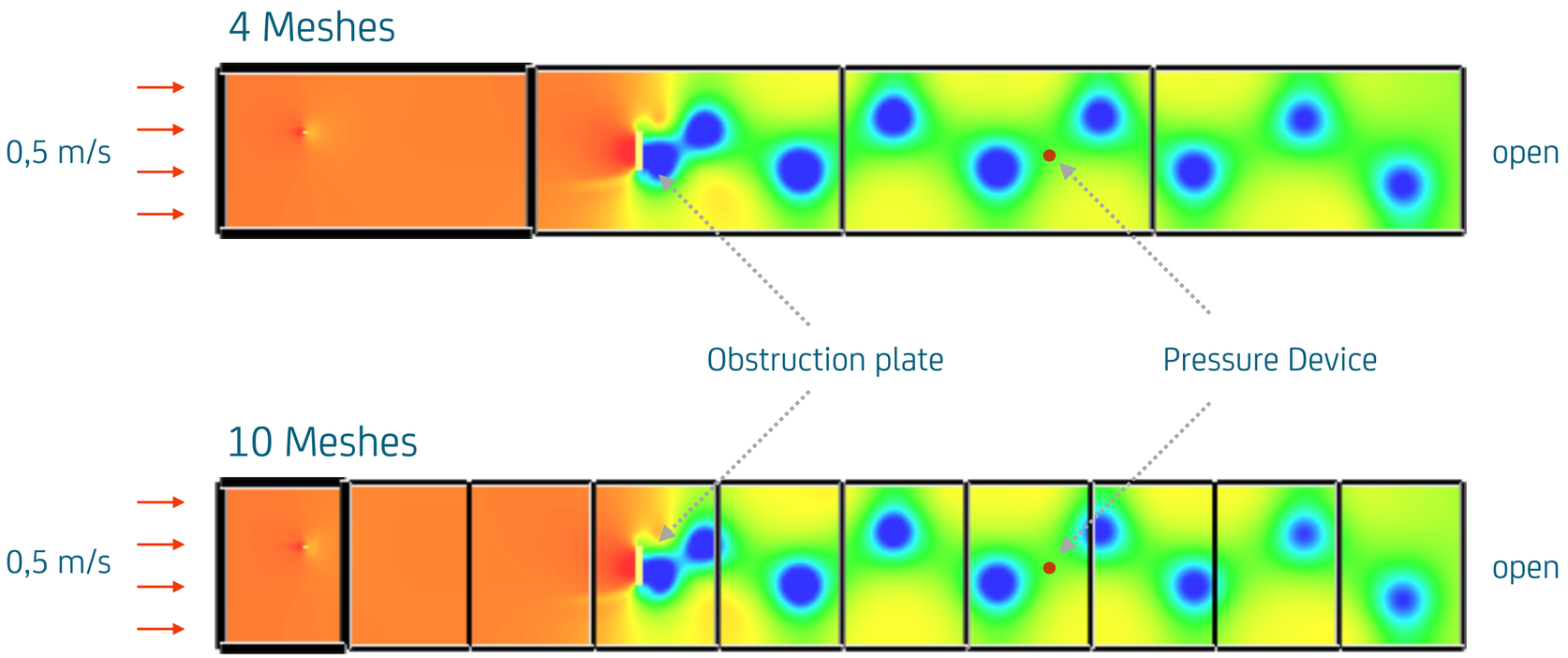
Number of required pressure iterations

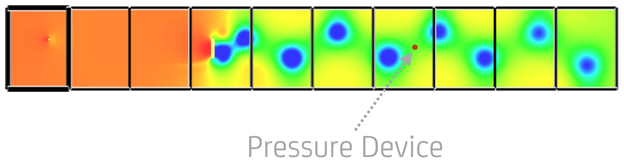


Less pressure iterations: 1 (default), max 9 (tight)

Verification case: Karman vortex street

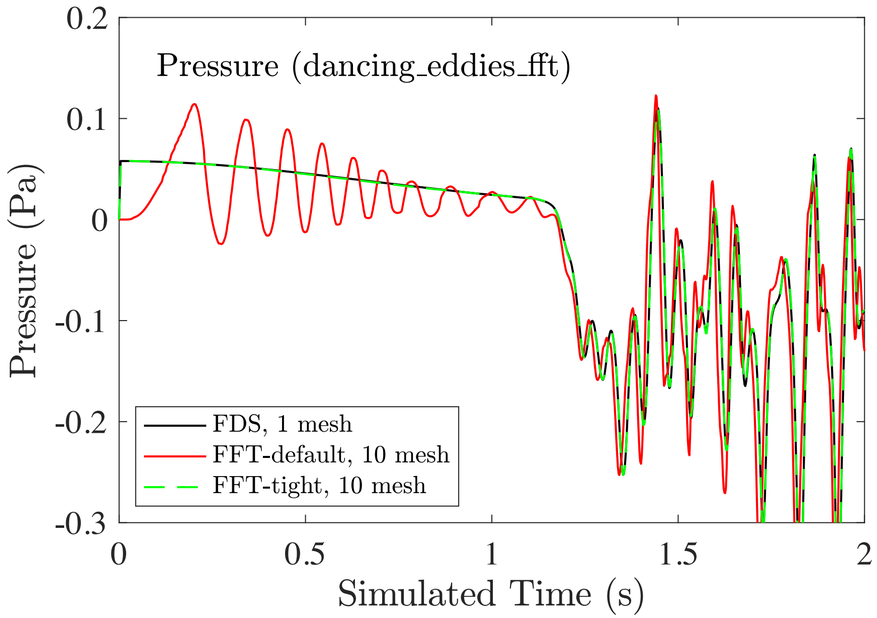
dancing_eddies





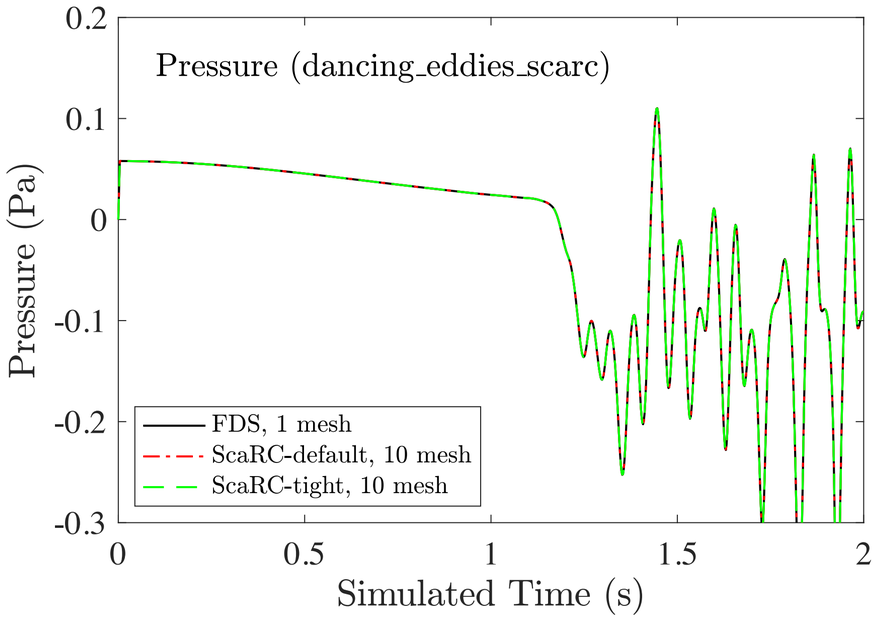
Pressure trace 10-mesh case

FFT default and tight (tol=10^{-5} m/s)



Accurate only for tight tolerance,
but increased number of pressure iterations (Ø 28)

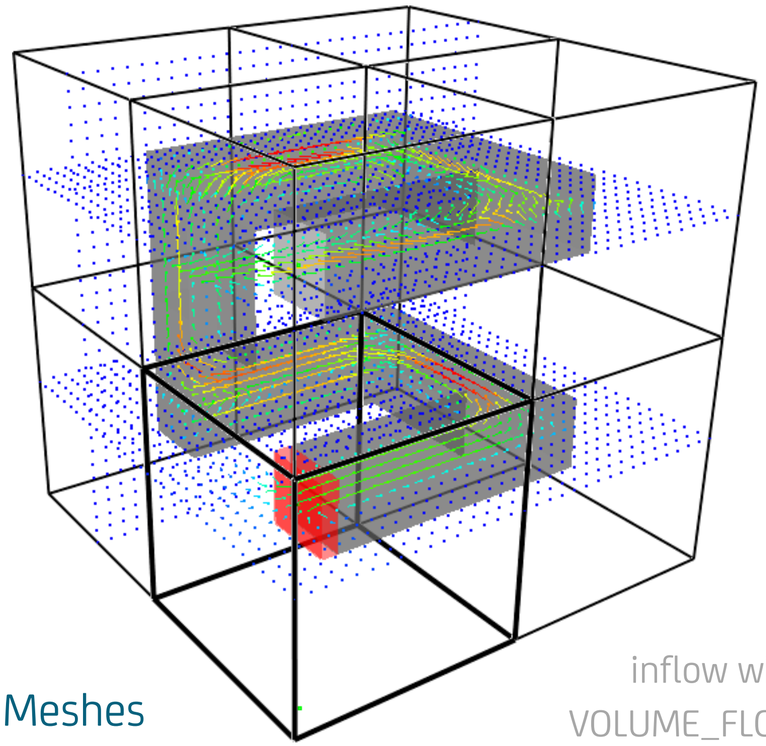
ScaRC default and tight (tol=10^{-5} m/s)



Accurate already for default tolerance,
max 4 pressure iterations for tight tolerance

Verification Case: Flow through a channel

duct_flow



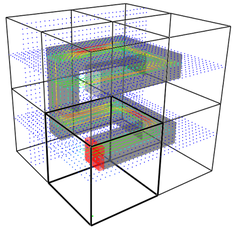
8 Meshes

inflow with
VOLUME_FLOW = 1

Many internal obstructions

which cause frequent

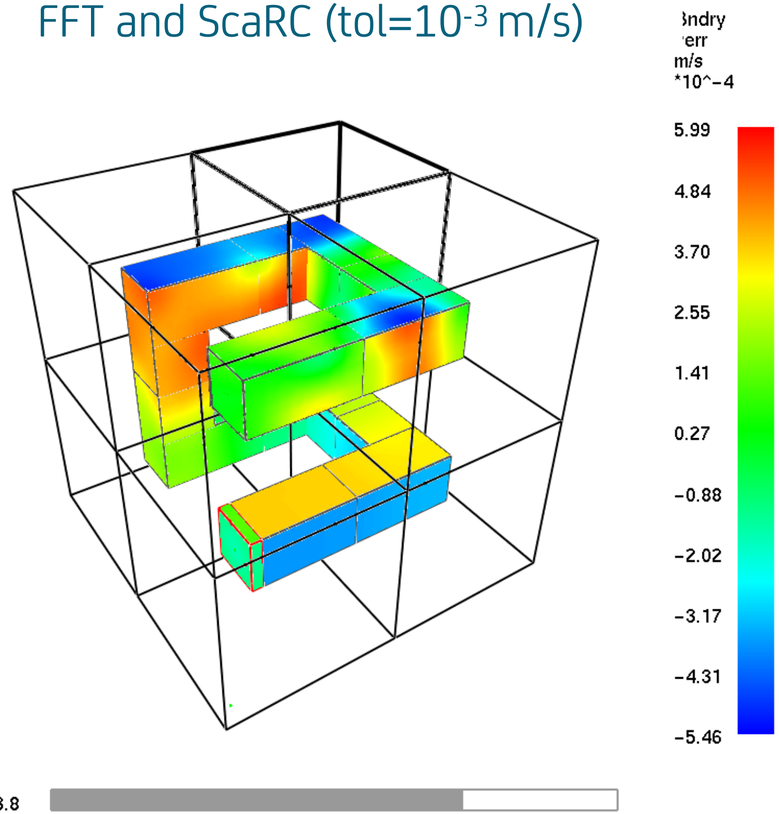
changes of flow direction



Velocity error along channel

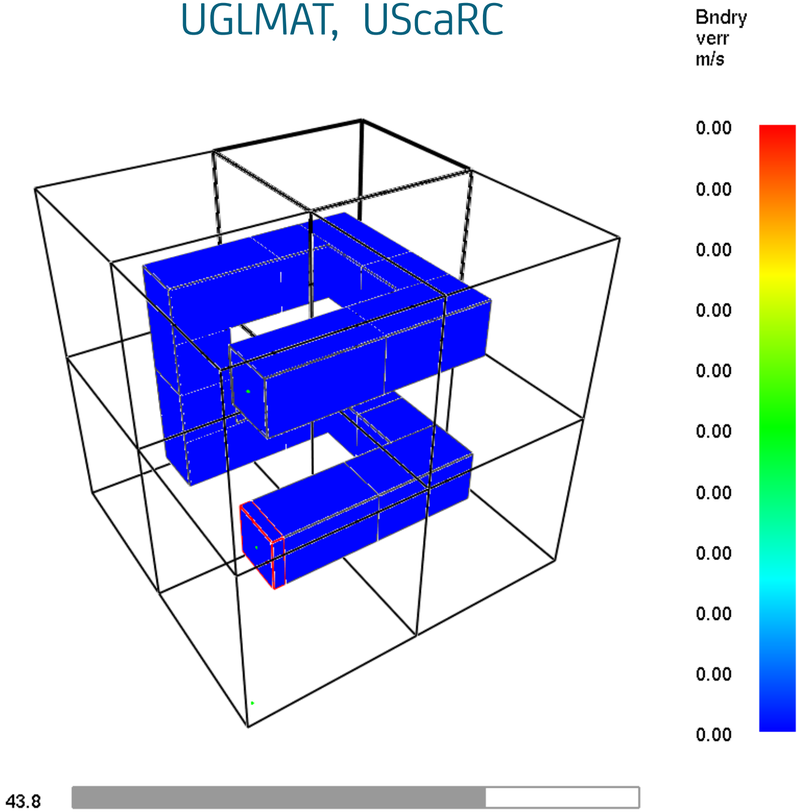
Structured

FFT and ScaRC (tol=10^{-3} m/s)



Unstructured

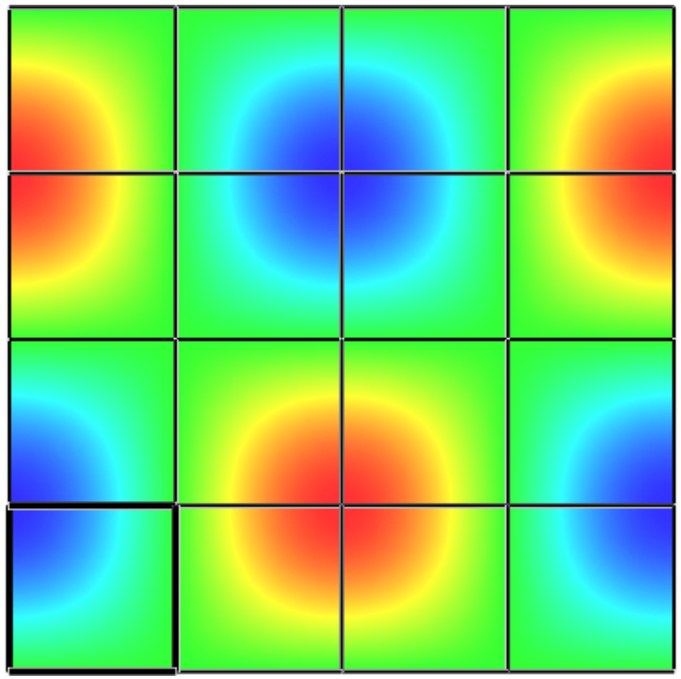
UGLMAT, UScaRC



Verification cases: Periodic boundaries

NS_Analytical_Solution

u - component velocity

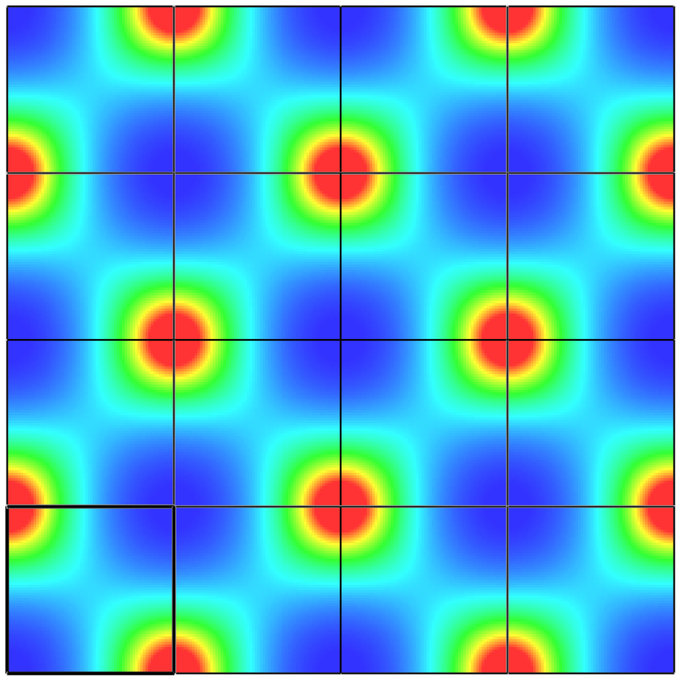


ScaRC
16 meshes

Preserves
periodic
behavior

shunn3

mixture fraction Z



Outlook

Still to do/to improve

- use different refinement levels between meshes (currently same is needed)
- test further global methods (i.e. algebraic multigrid) and local methods (ILU)
- optimise runtime of single components and incorporate OpenMP-directives
- optimise parameter settings for global and local iterations

Verification & Validation

- run all pressure related verification tests
- run selected validation tests

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