

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

1

Elliptic partial differential equation of „Poisson“ type

Pressure
equation

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

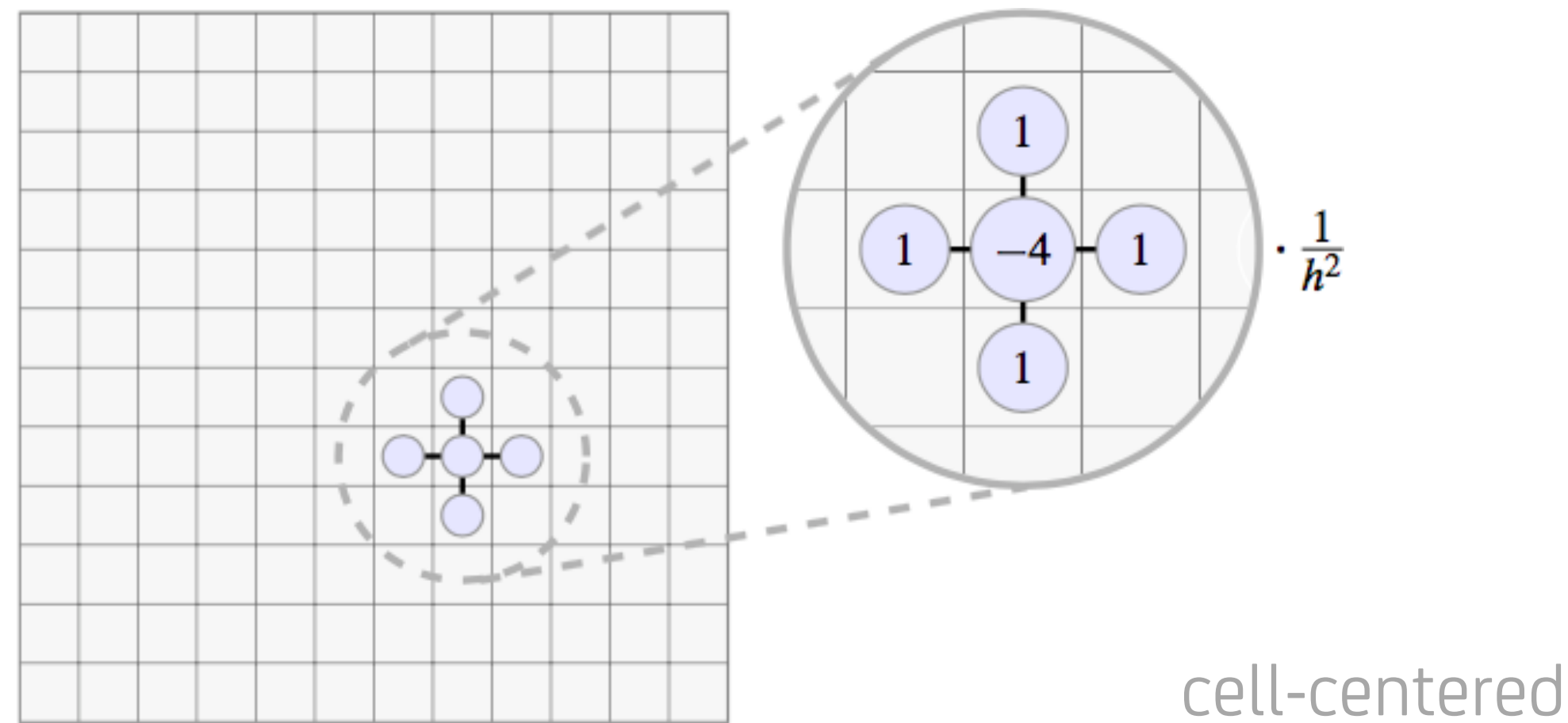
Strongly coupled with velocity field,
to be solved at least twice per time step

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

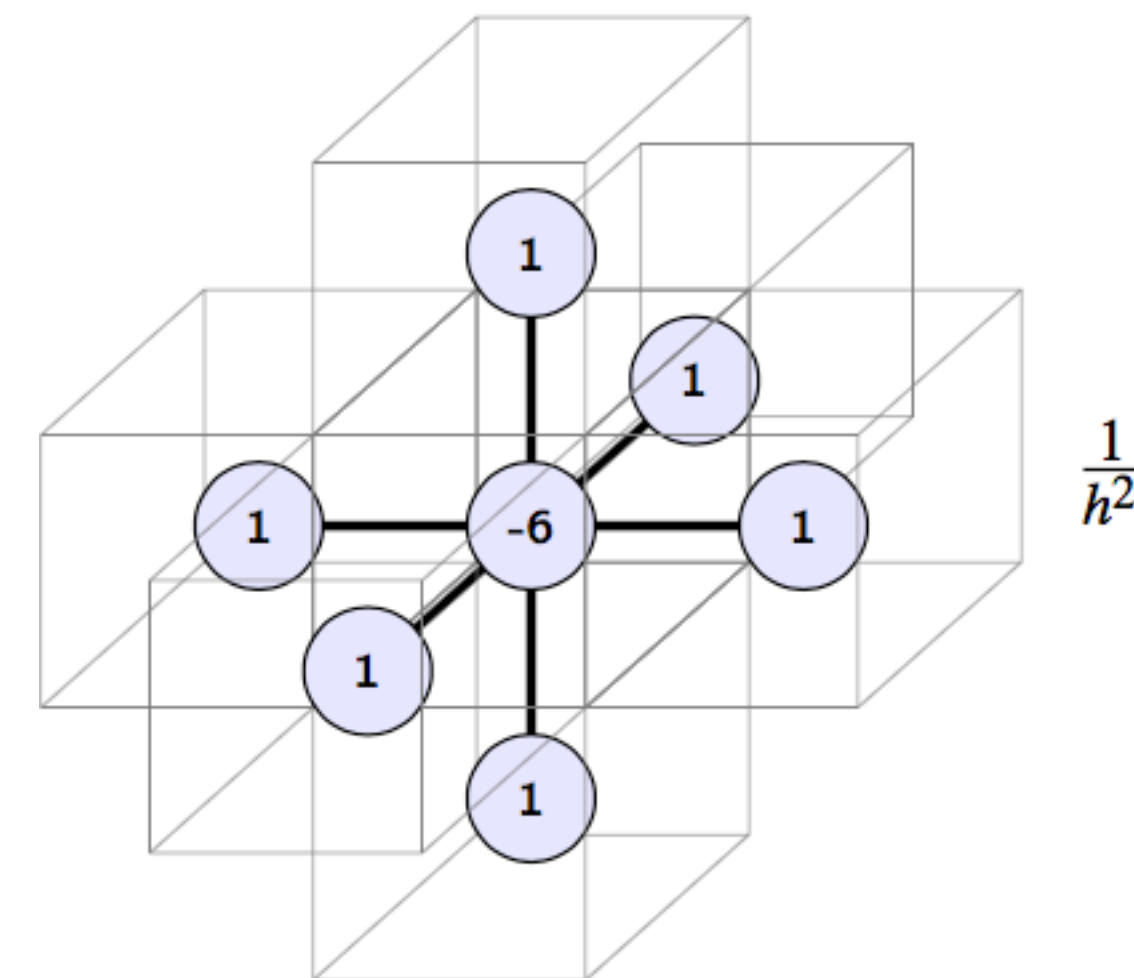
Key feature: Local information is spread immediately over whole domain!

Discretization with finite differences

5-point stencil in 2D



7-point stencil in 3D

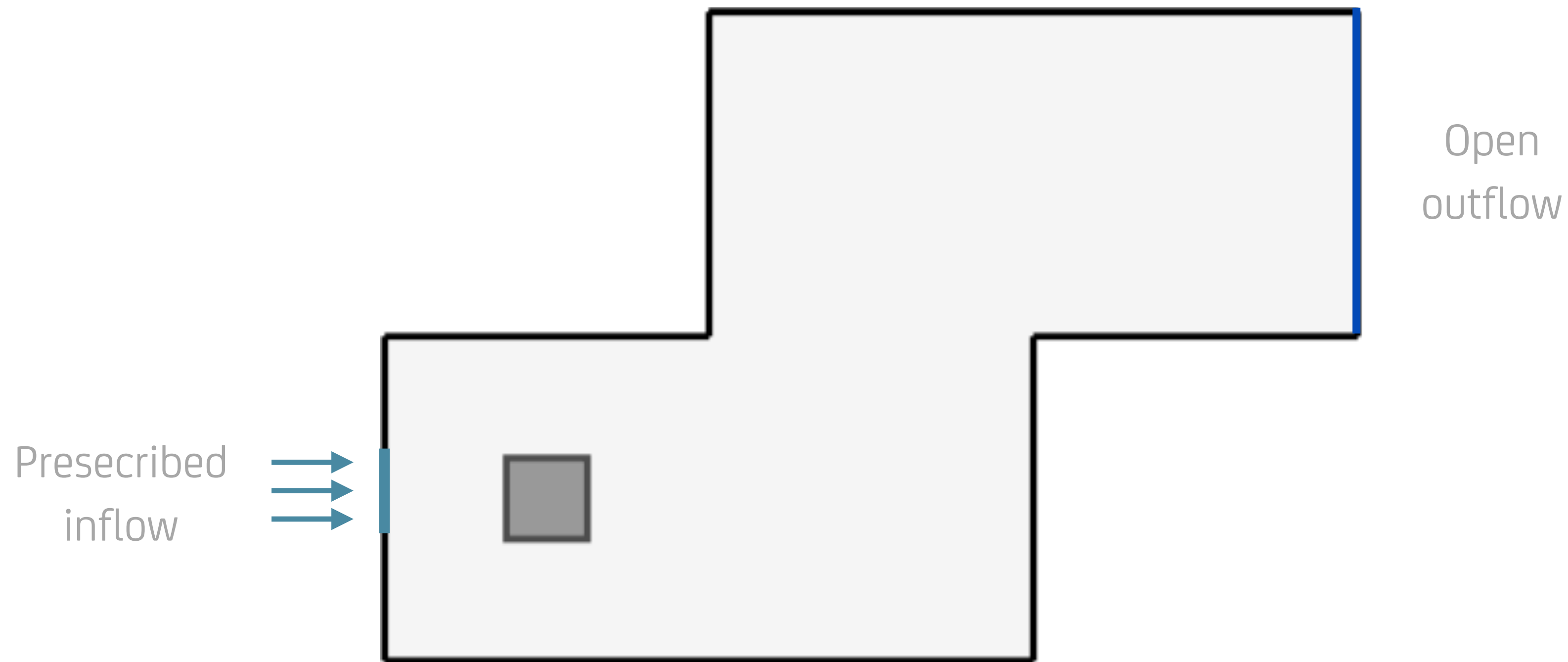


Pressure equation

Specifies physical relations between grid cells according to elliptic equation

Demo-case ,2D-pipe with obstruction‘

Simple example to explain the concepts



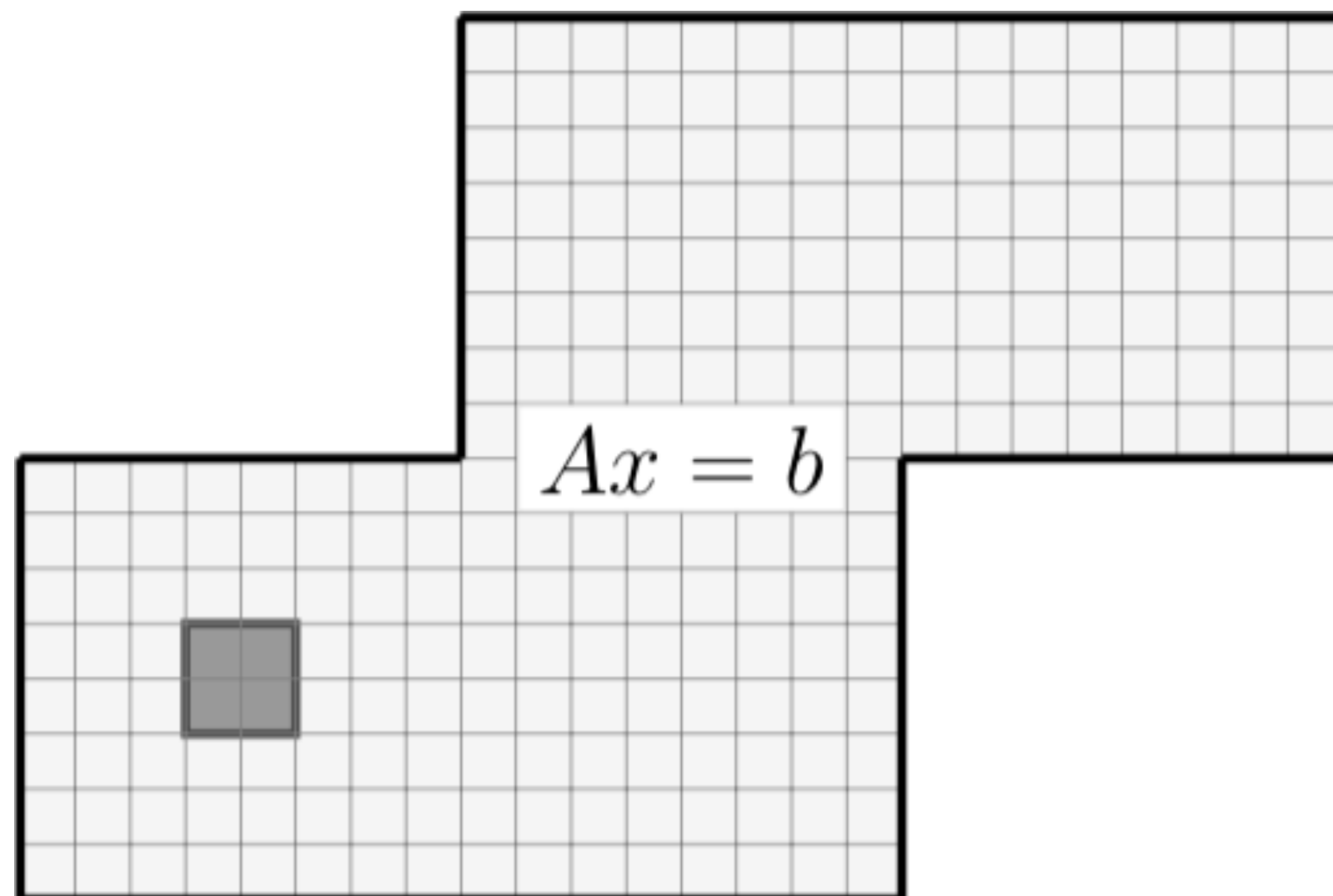
1

Pressure equation

Global versus local discretization

Global discretization

1 global matrix, 1 global right hand side vector



1

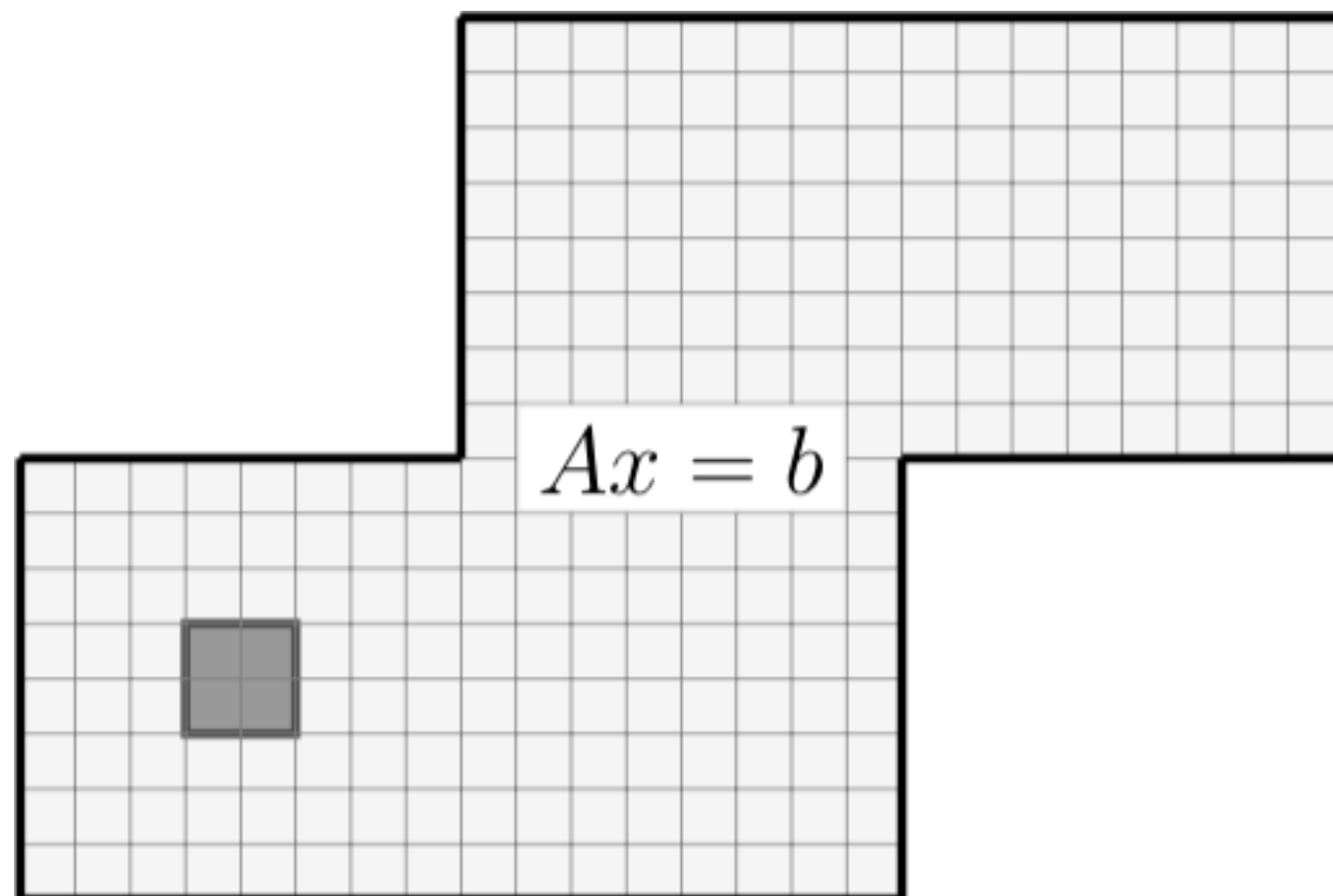
Pressure
equation

Global versus local discretization

1

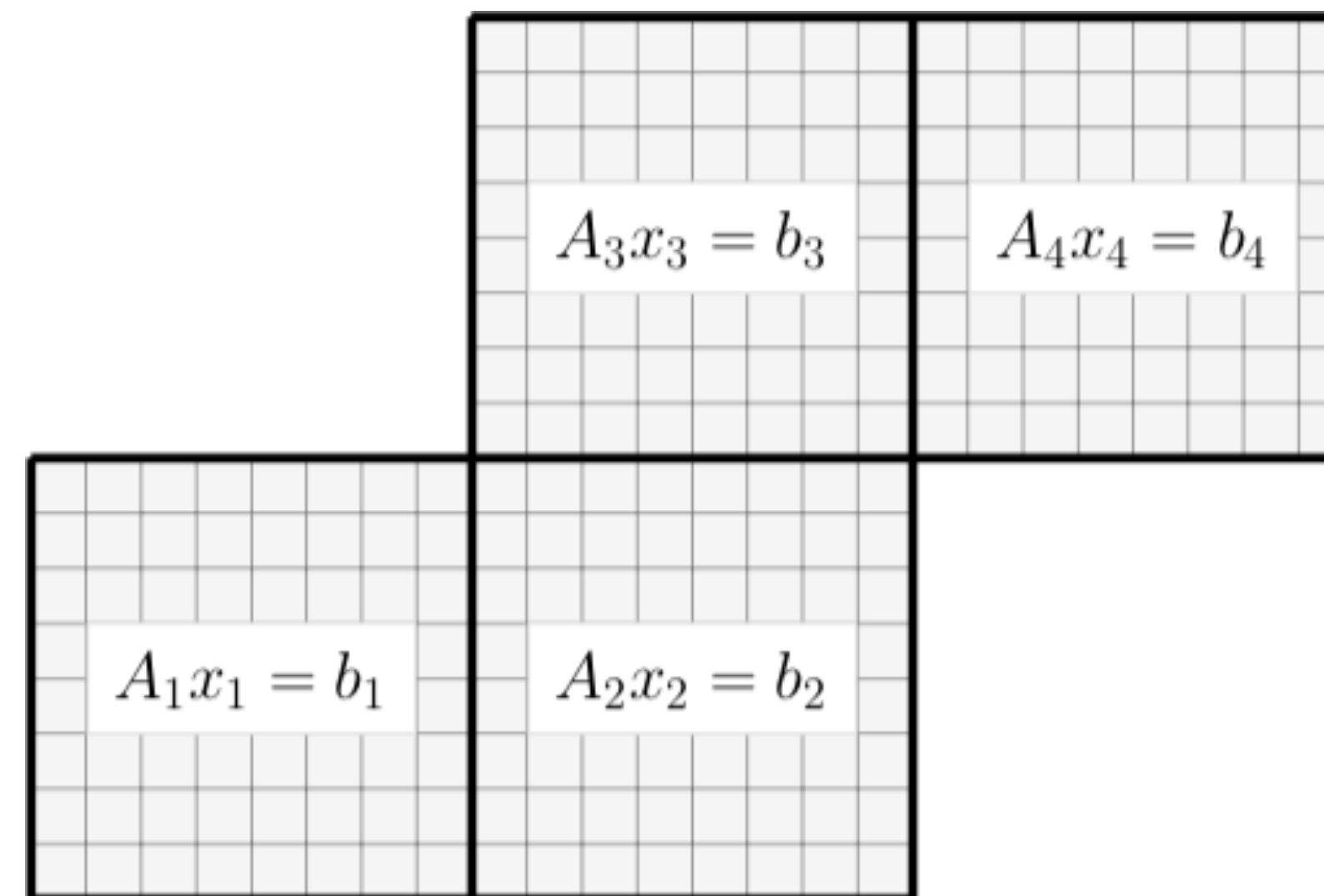
Global discretization

1 global matrix, 1 global right hand side vector



Set of local discretizations

M local matrices, M local right hand side vectors

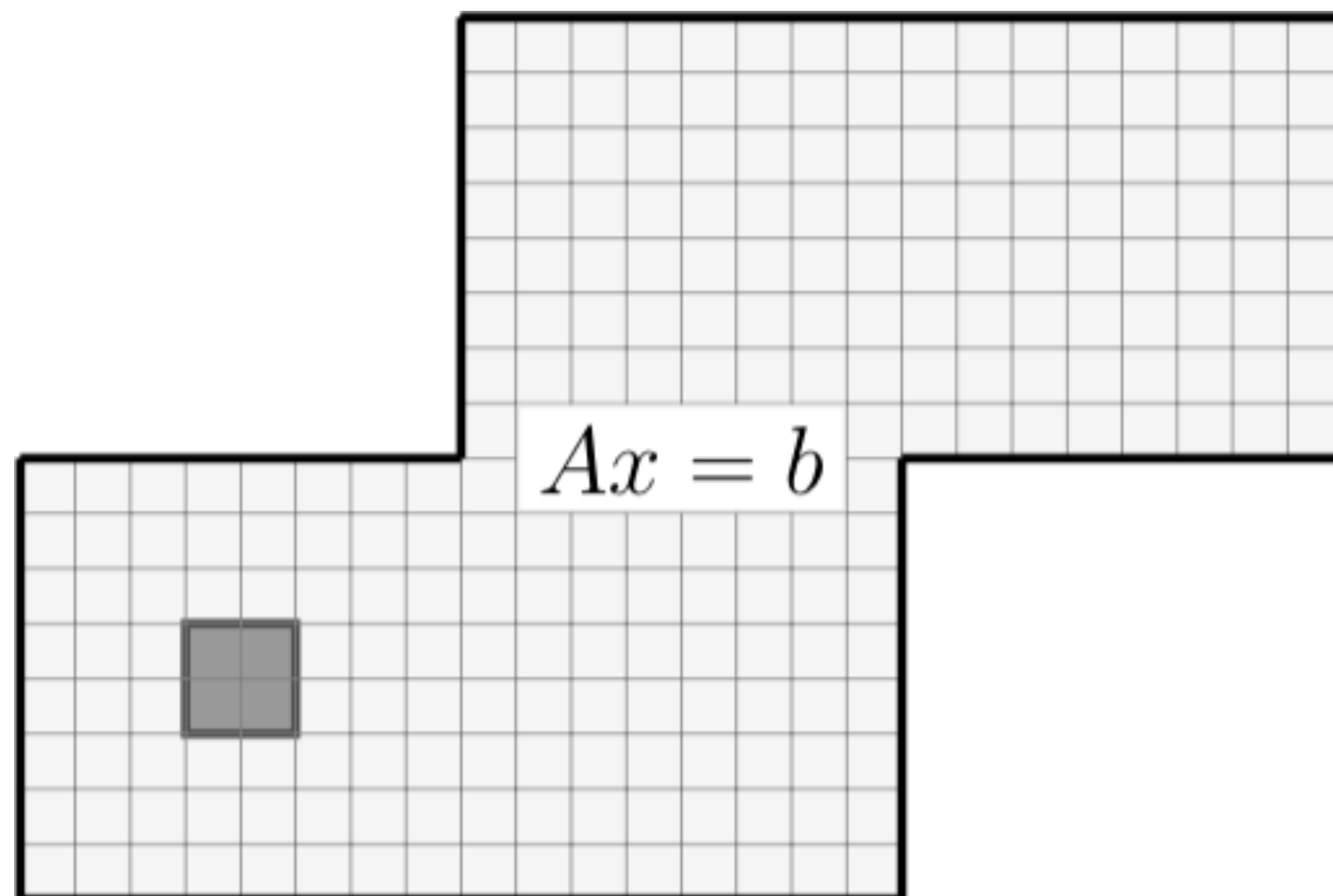


Pressure equation

Global versus local discretization

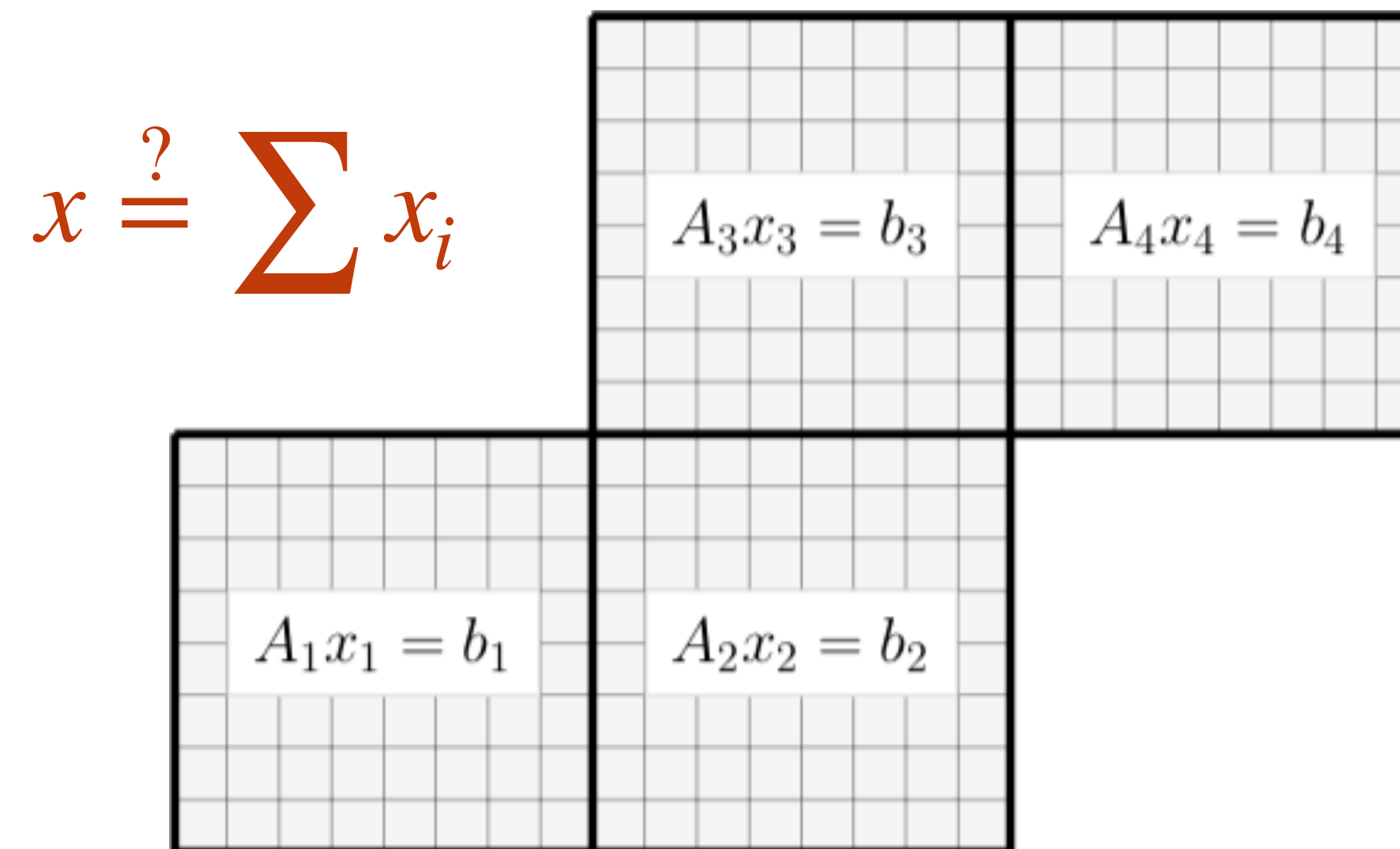
Global discretization

1 global matrix, 1 global right hand side vector



Set of local discretizations

M local matrices, M local right hand side vectors



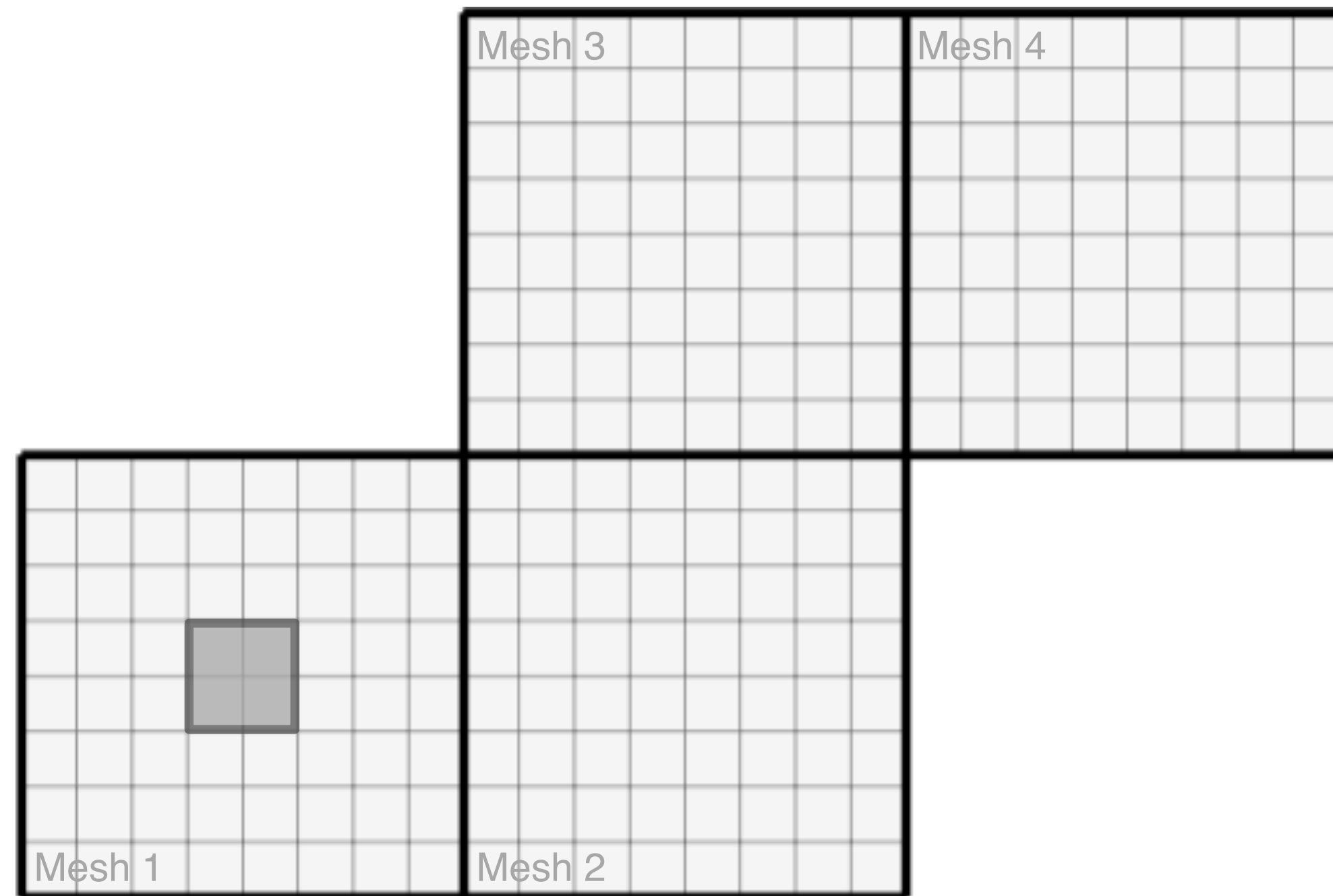
Pressure equation

Structured versus unstructured discretization

1

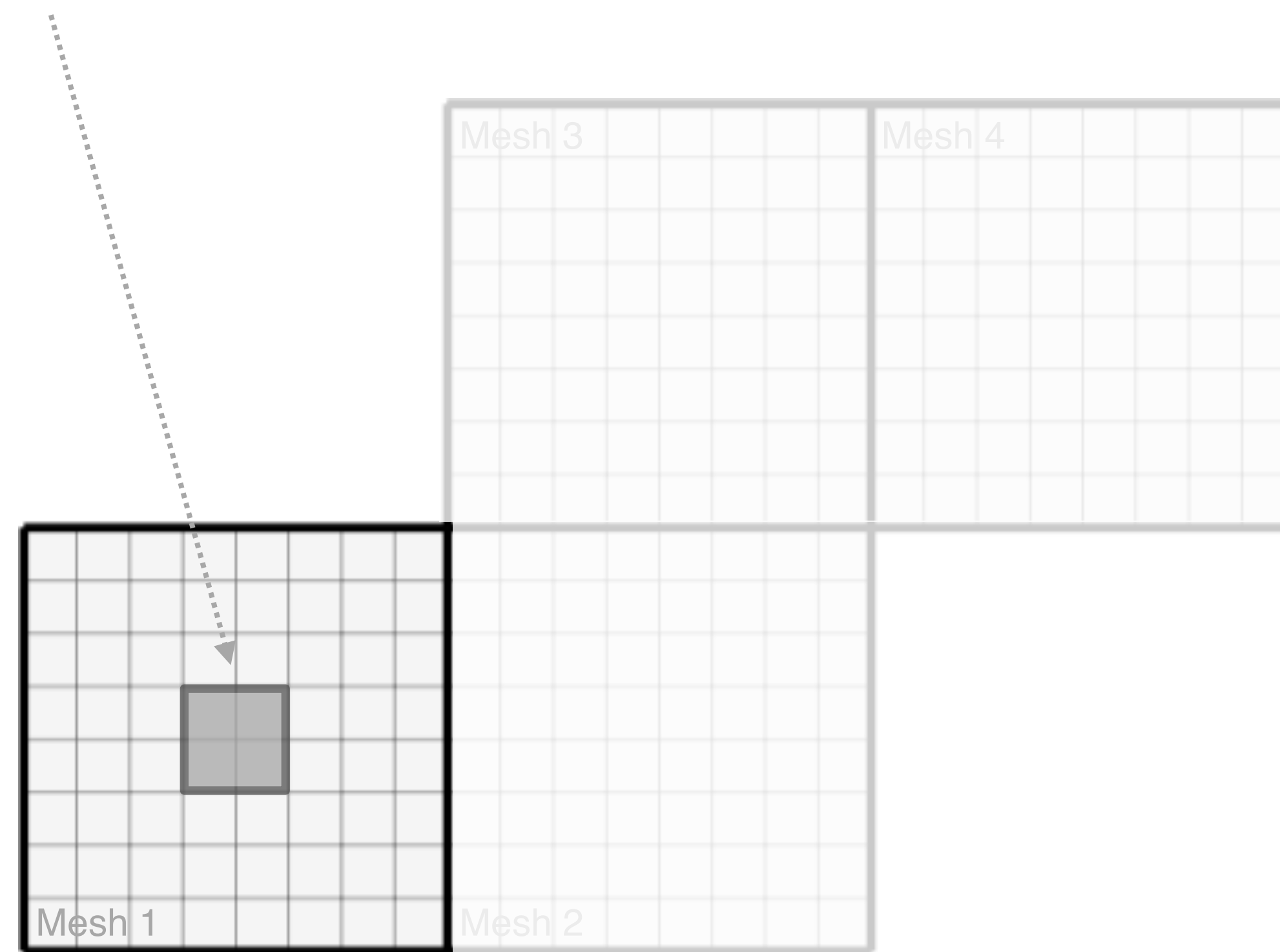
Pressure equation

There are different possibilities to discretize ...



Structured versus unstructured discretization

... at cells inside and around a solid obstruction



1

Pressure
equation

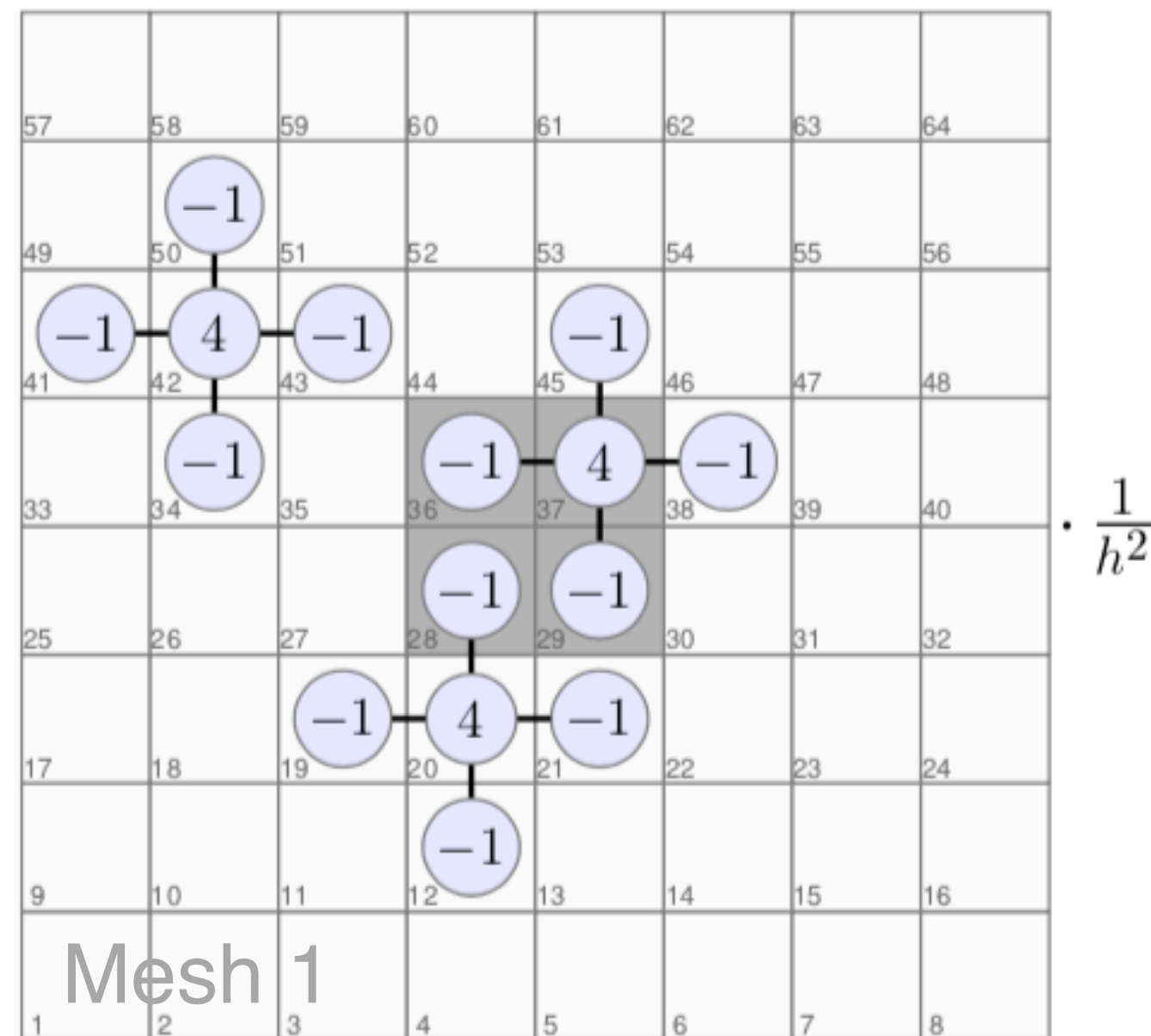
Structured versus unstructured discretizations

1

Pressure equation

Structured

Regular matrix stencils



Cells inside obstructions are **included**

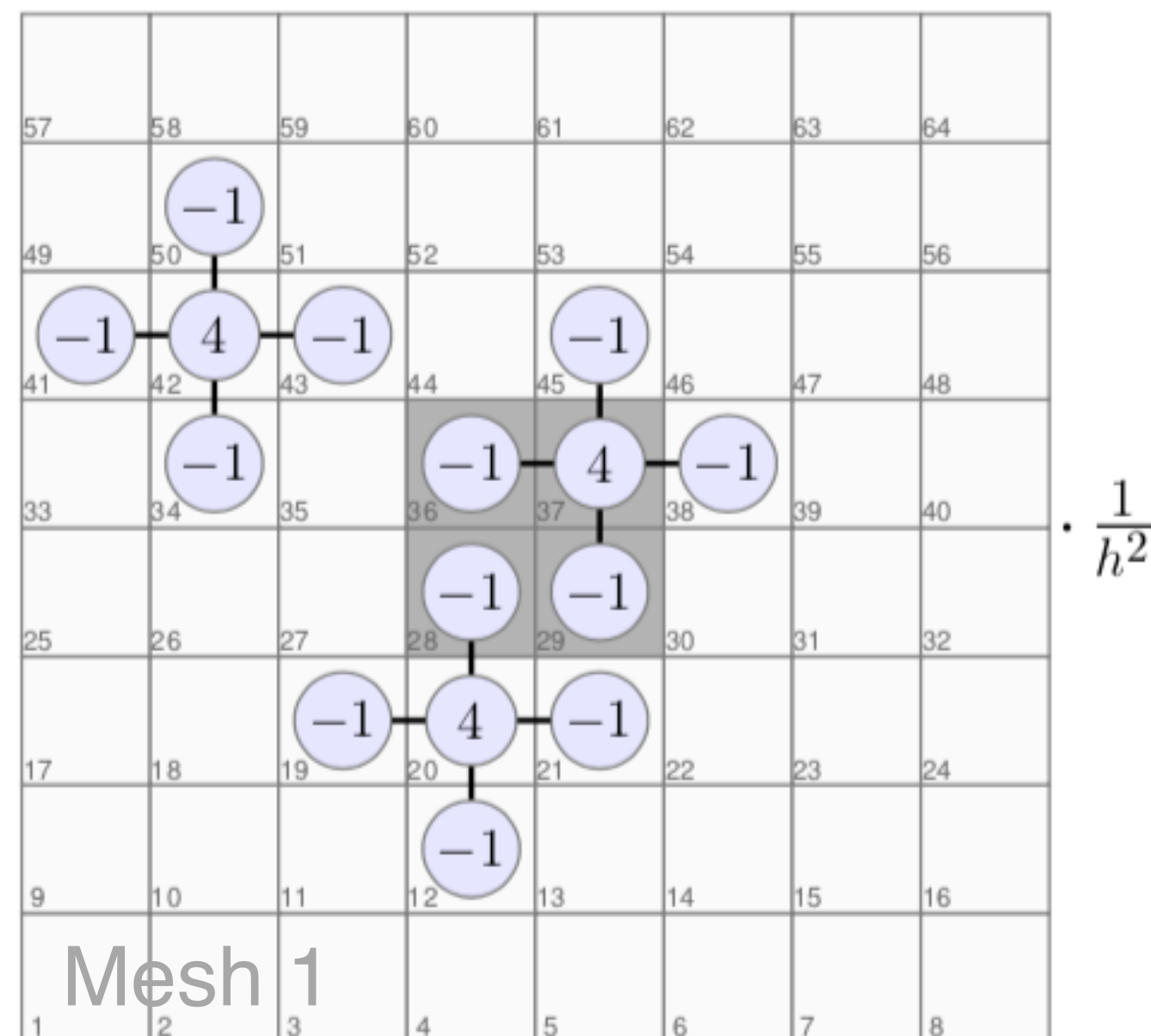
Structured versus unstructured discretizations

1

Pressure equation

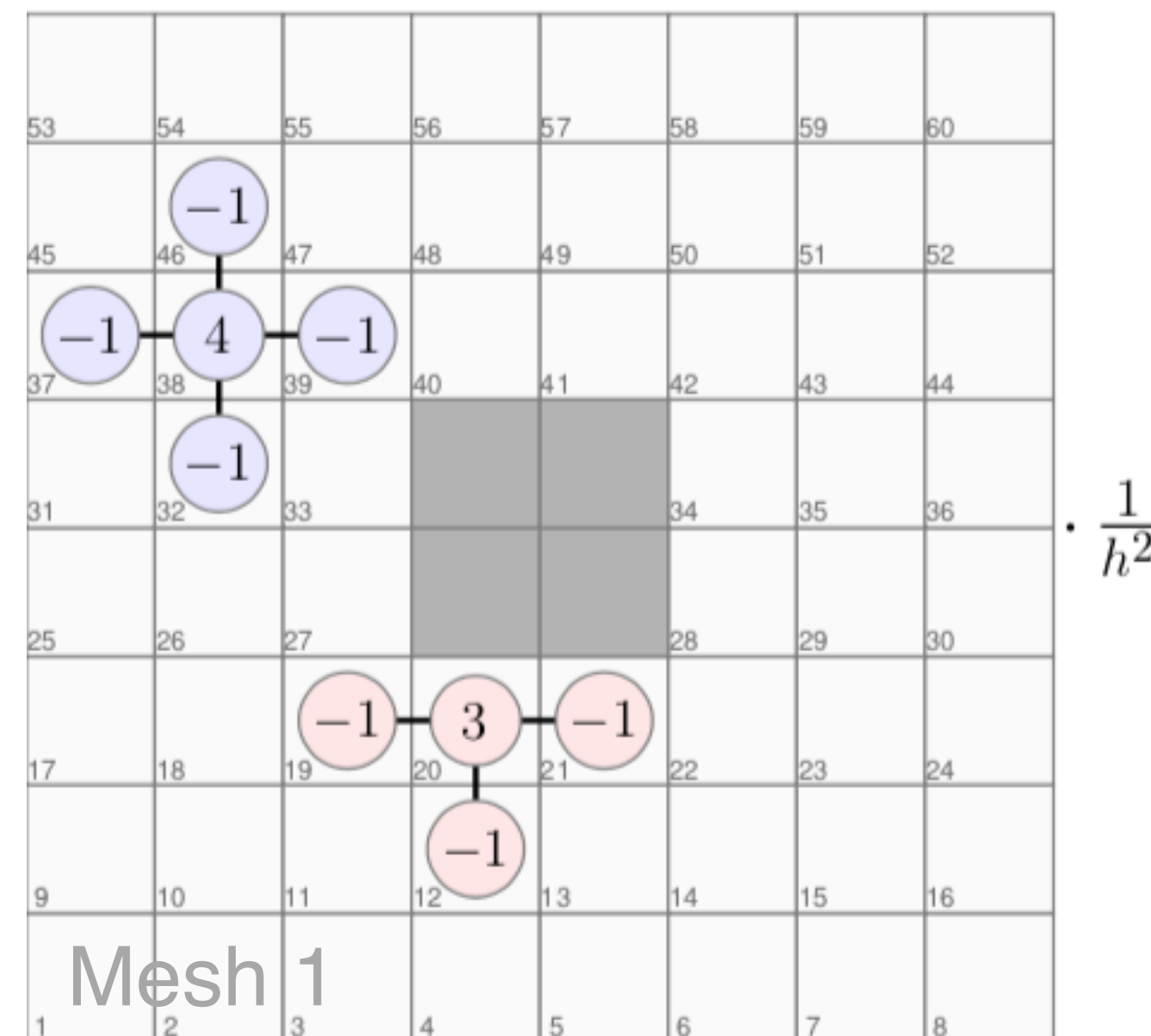
Structured

Regular matrix stencils



Unstructured

Irregular matrix stencils



Cells inside obstructions are **included**

Cells inside obstructions are **excluded**

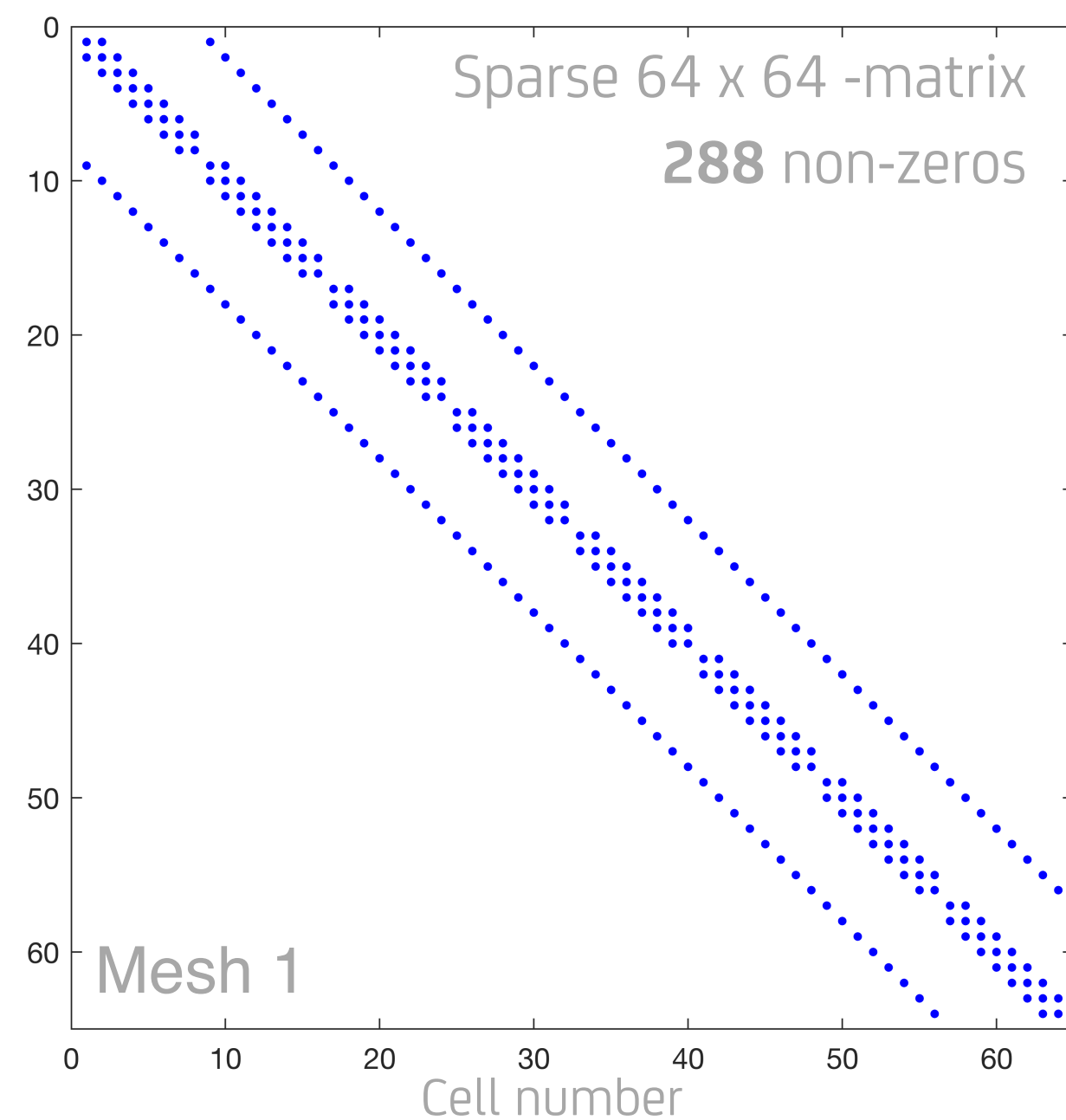
Regular versus irregular Poisson matrix

1

Pressure equation

Structured

Highly regular Poisson matrix A



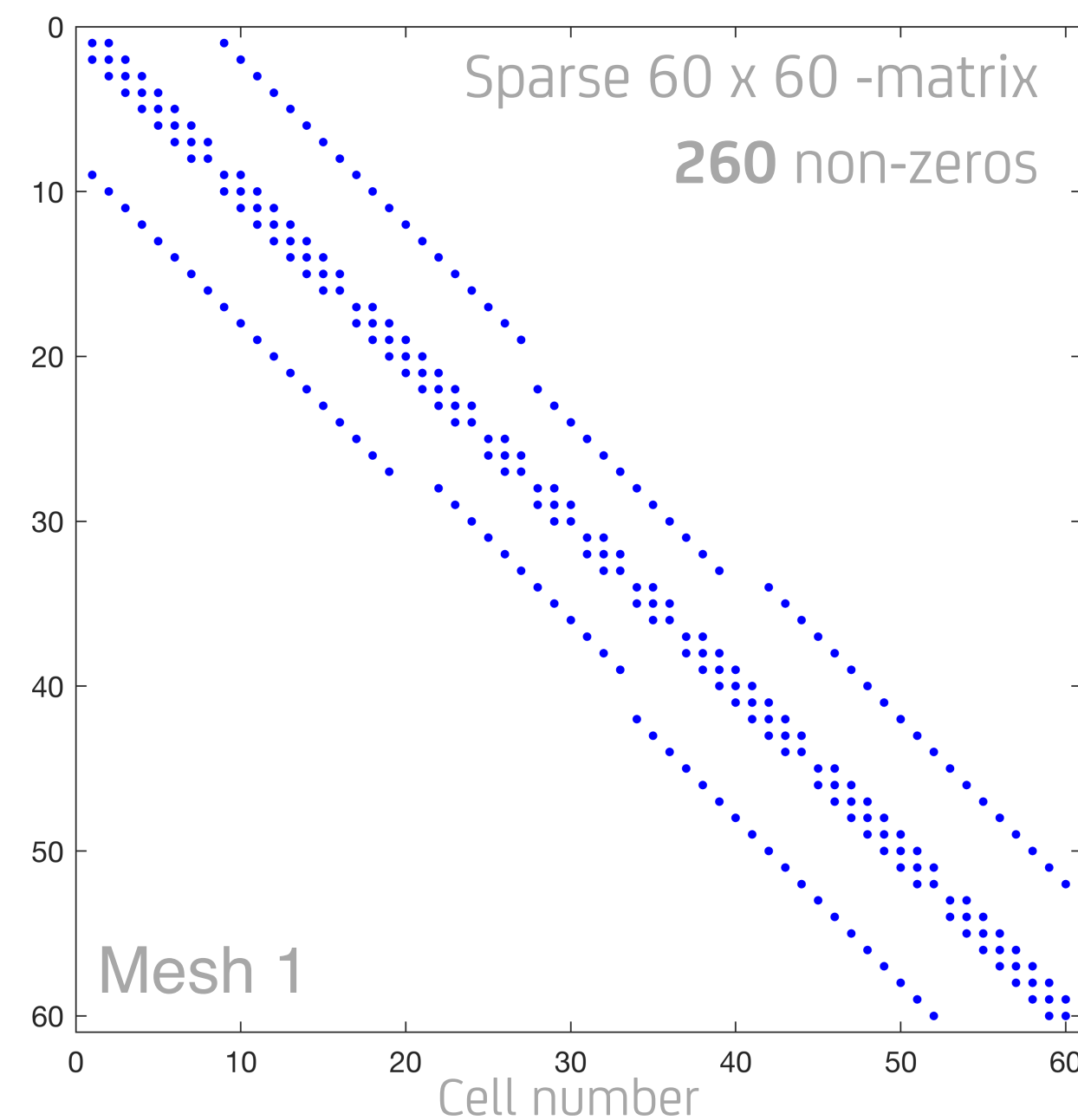
8x8 cells

Sparsity patterns

Highly optimized solvers usable (fast!)

Unstructured

Irregular Poisson matrix A



Need of more robust solvers (slower!)

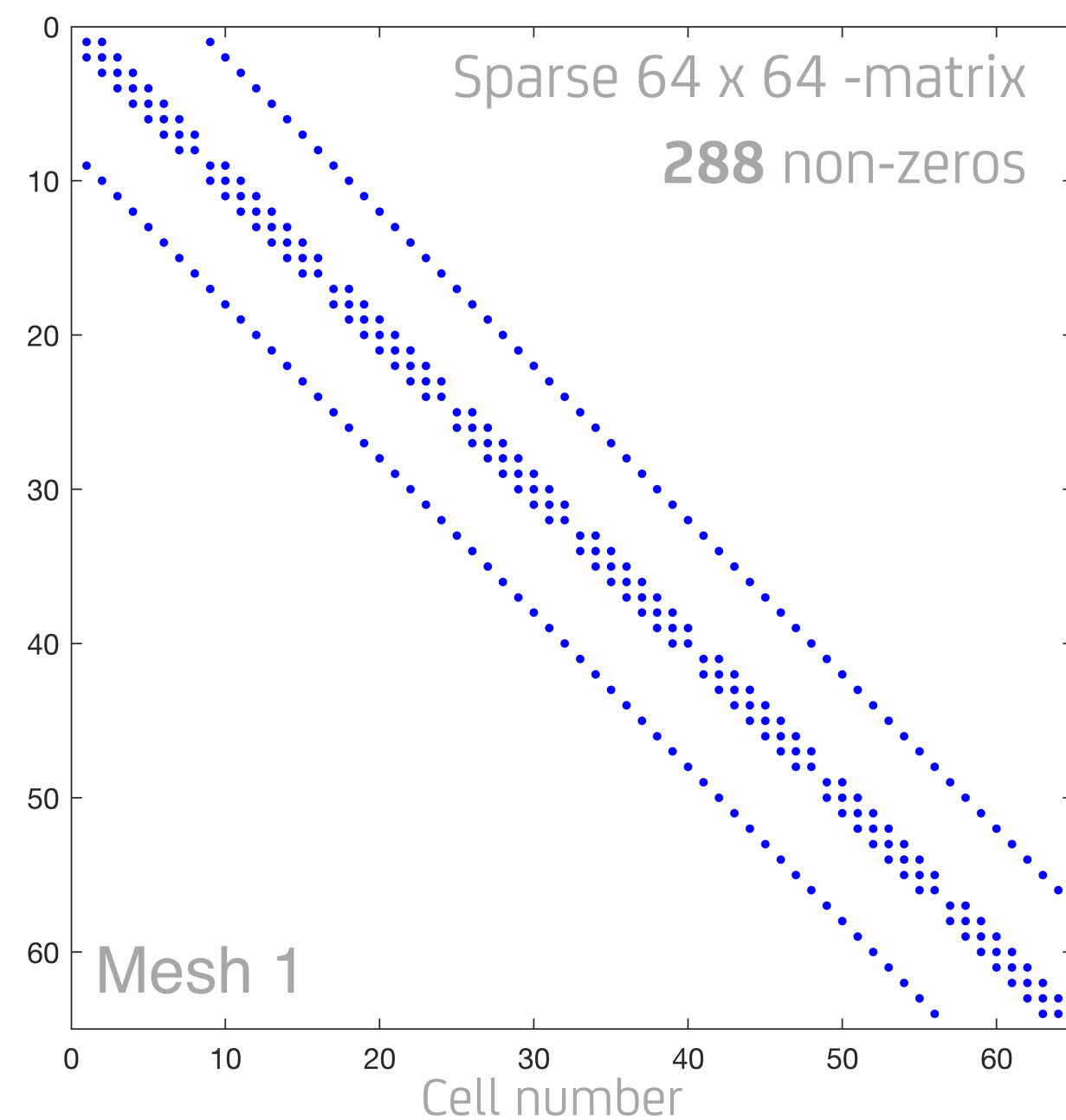
Regular versus irregular Poisson matrix

1

Pressure equation

Structured

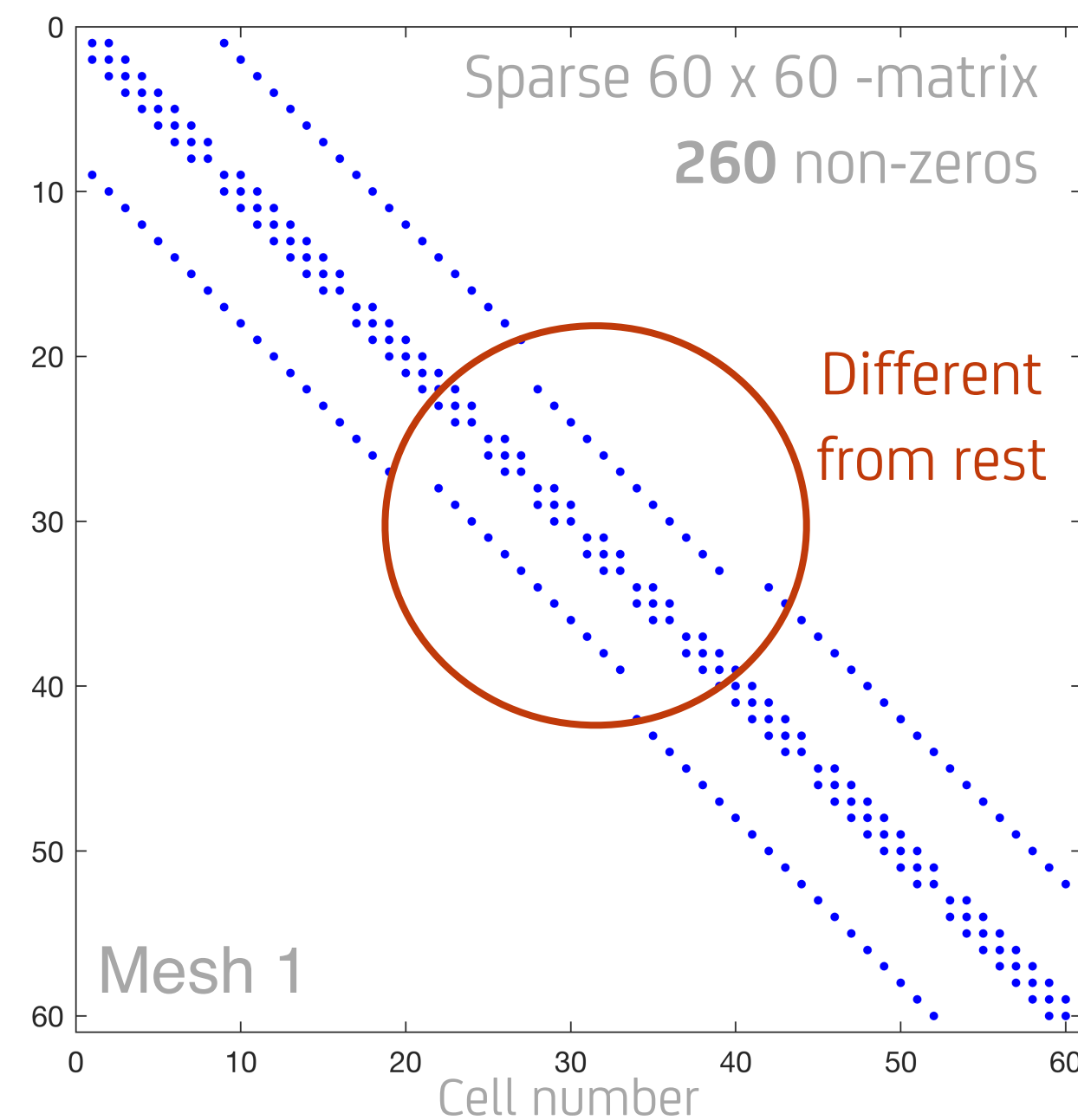
Highly regular Poisson matrix A



Highly optimized solvers usable (fast!)

Unstructured

Irregular Poisson matrix A



Need of more robust solvers (slower!)

8x8 cells

Sparsity patterns

Current FDS pressure solver

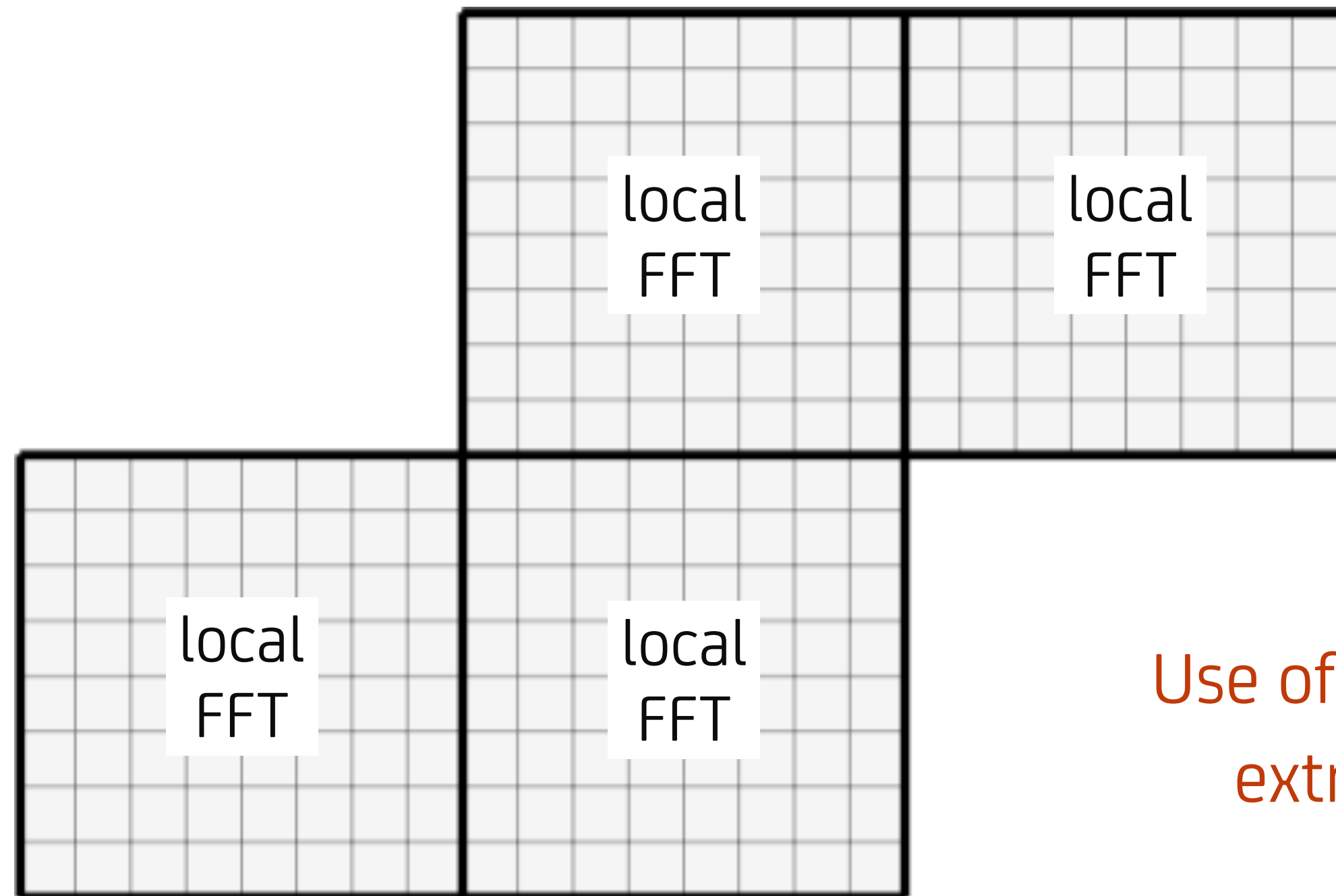
Mesh-wise FFT with pressure iteration

Mesh-wise FFT-solver

2

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

FFT
solver



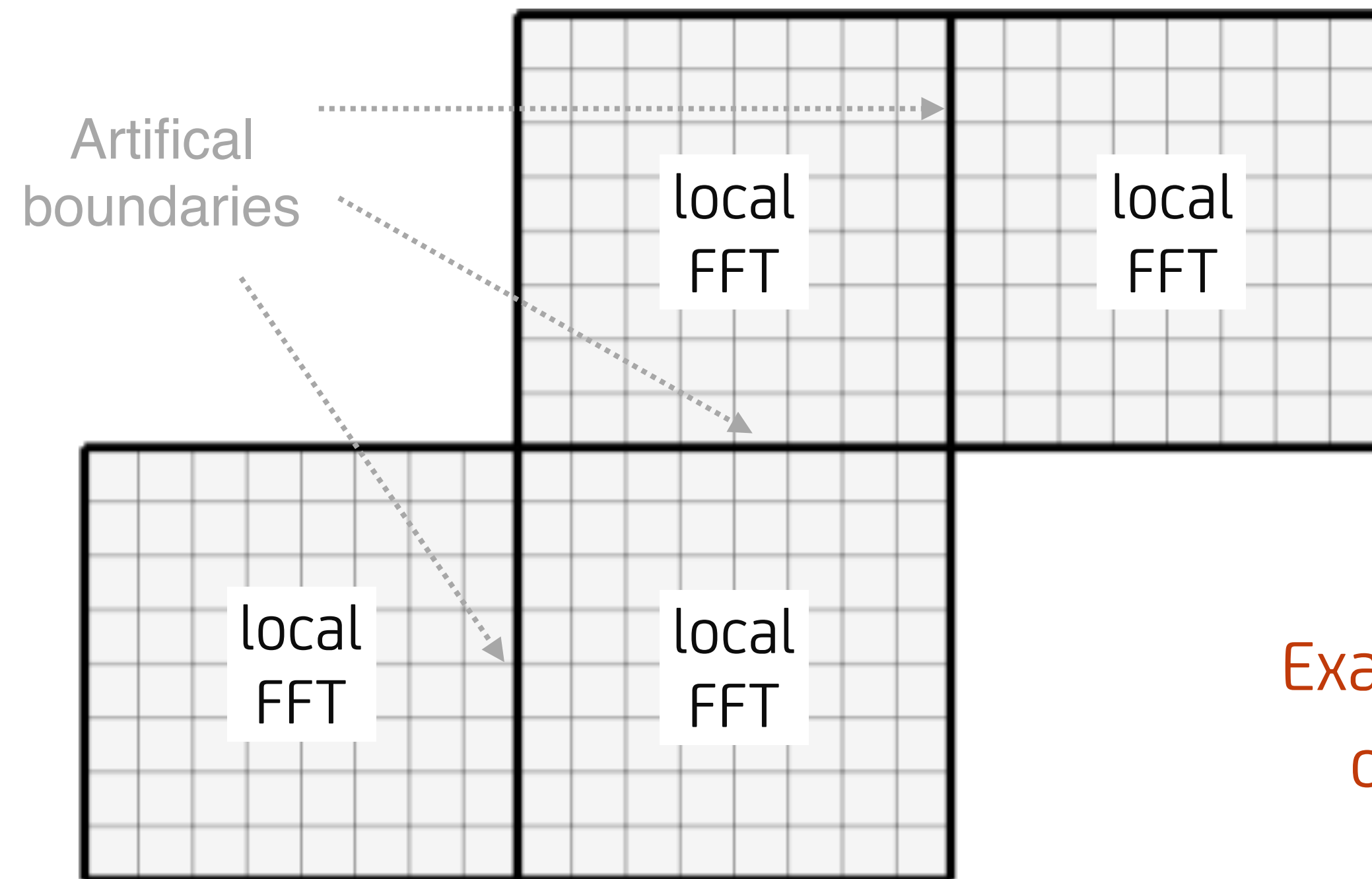
Use of optimized CRAYFISHPAK,
extremely fast and robust

Mesh-wise FFT-solver

2

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

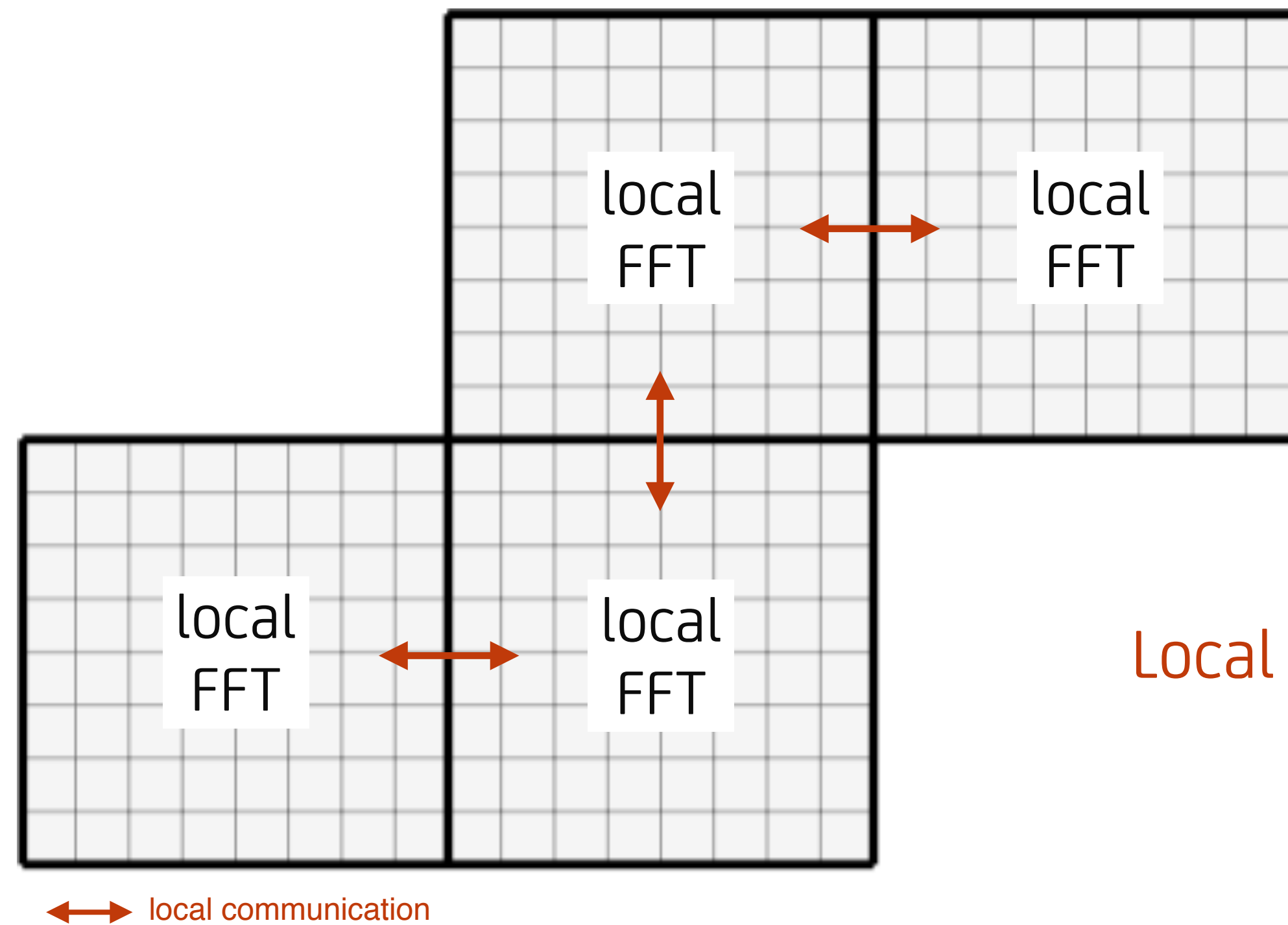
FFT
solver



Exact values not known,
only approximately

Mesh-wise FFT-solver

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



Local communication required
per FDS time step

2

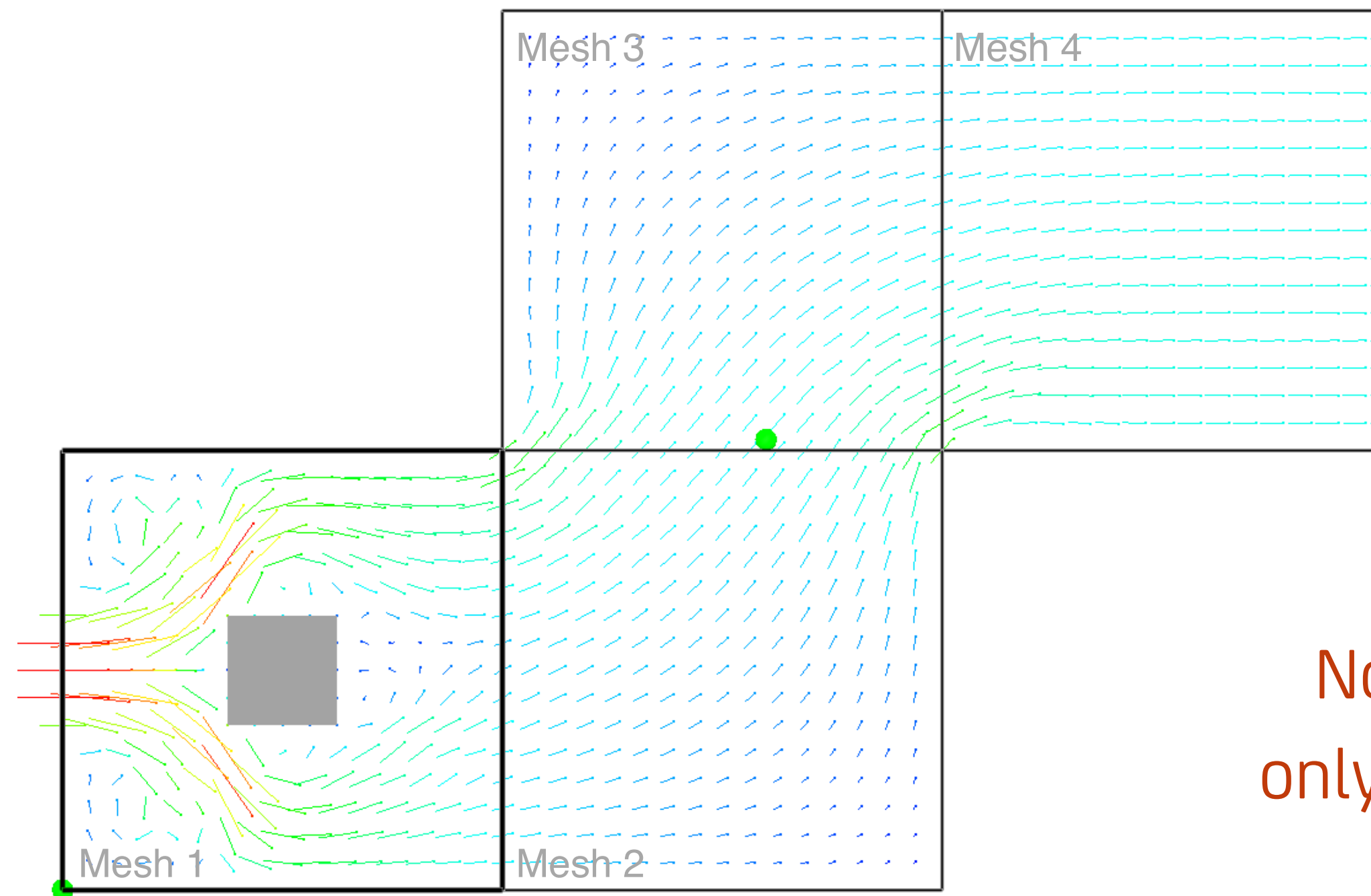
FFT
solver

Accuracy along mesh interfaces?

2

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

FFT
solver



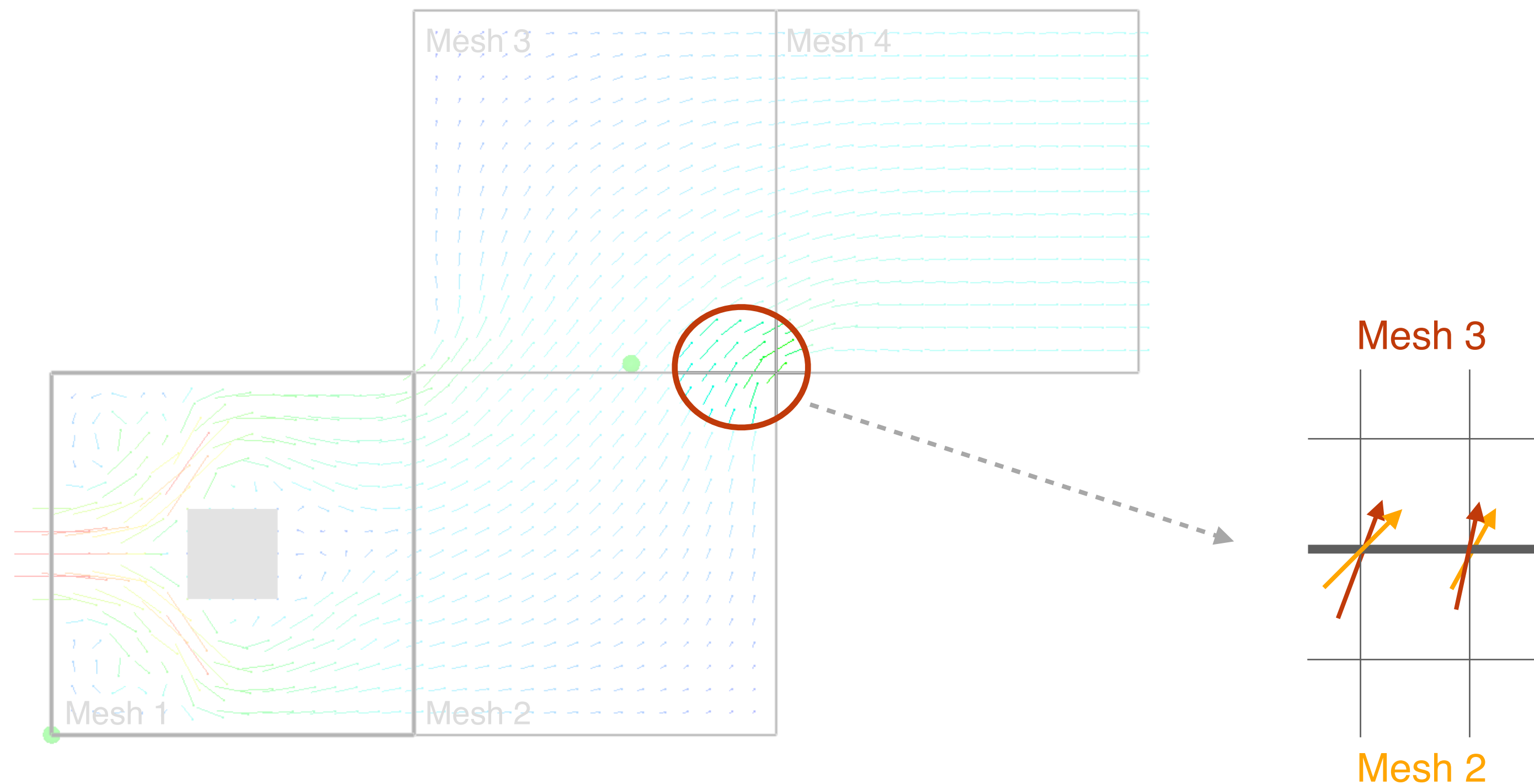
No global discretization,
only collection of local ones

Accuracy along mesh interfaces?

2

Local velocity components may be different along mesh interfaces

FFT
solver

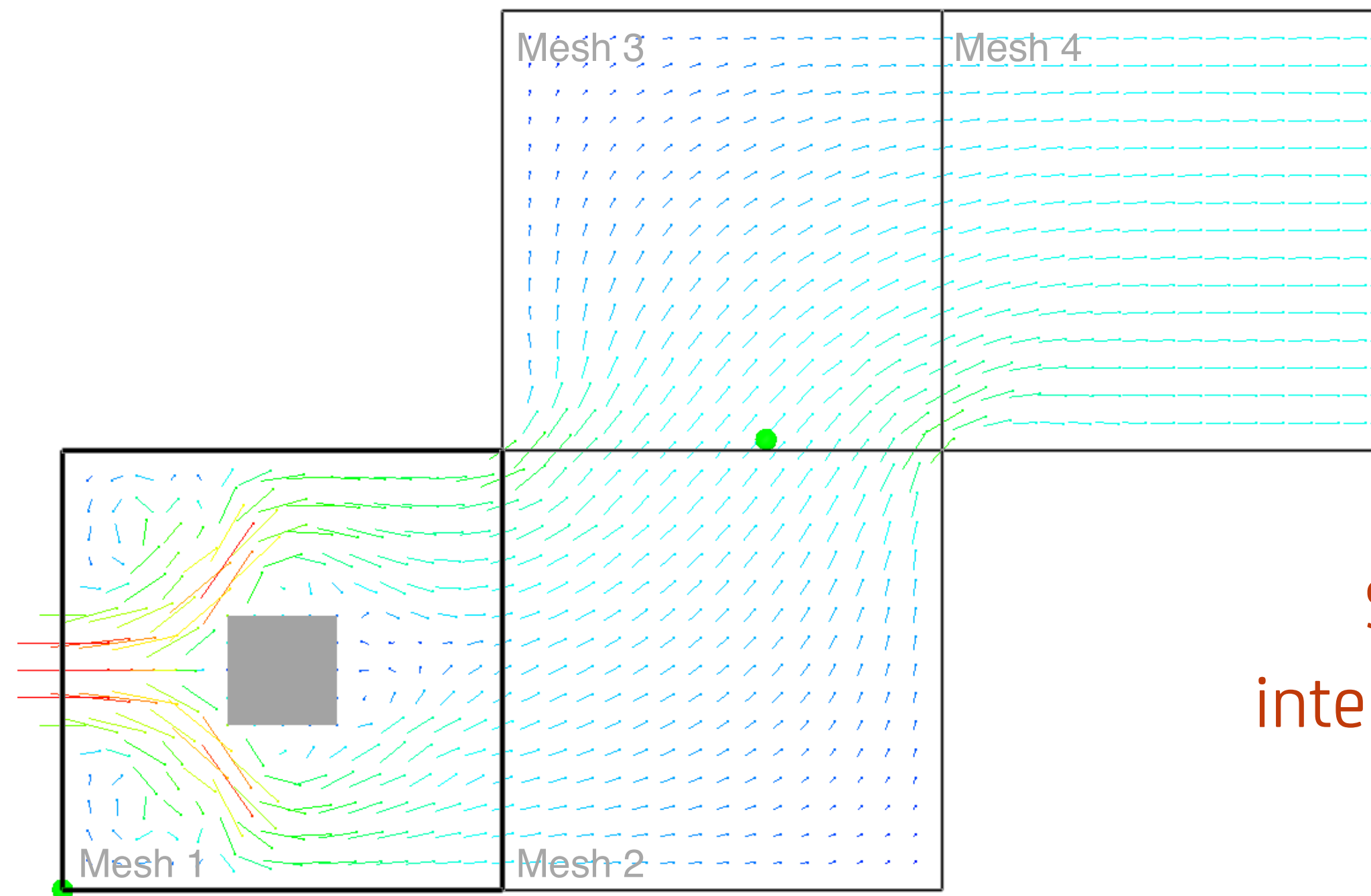


Accuracy along internal obstructions?

2

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

FFT
solver



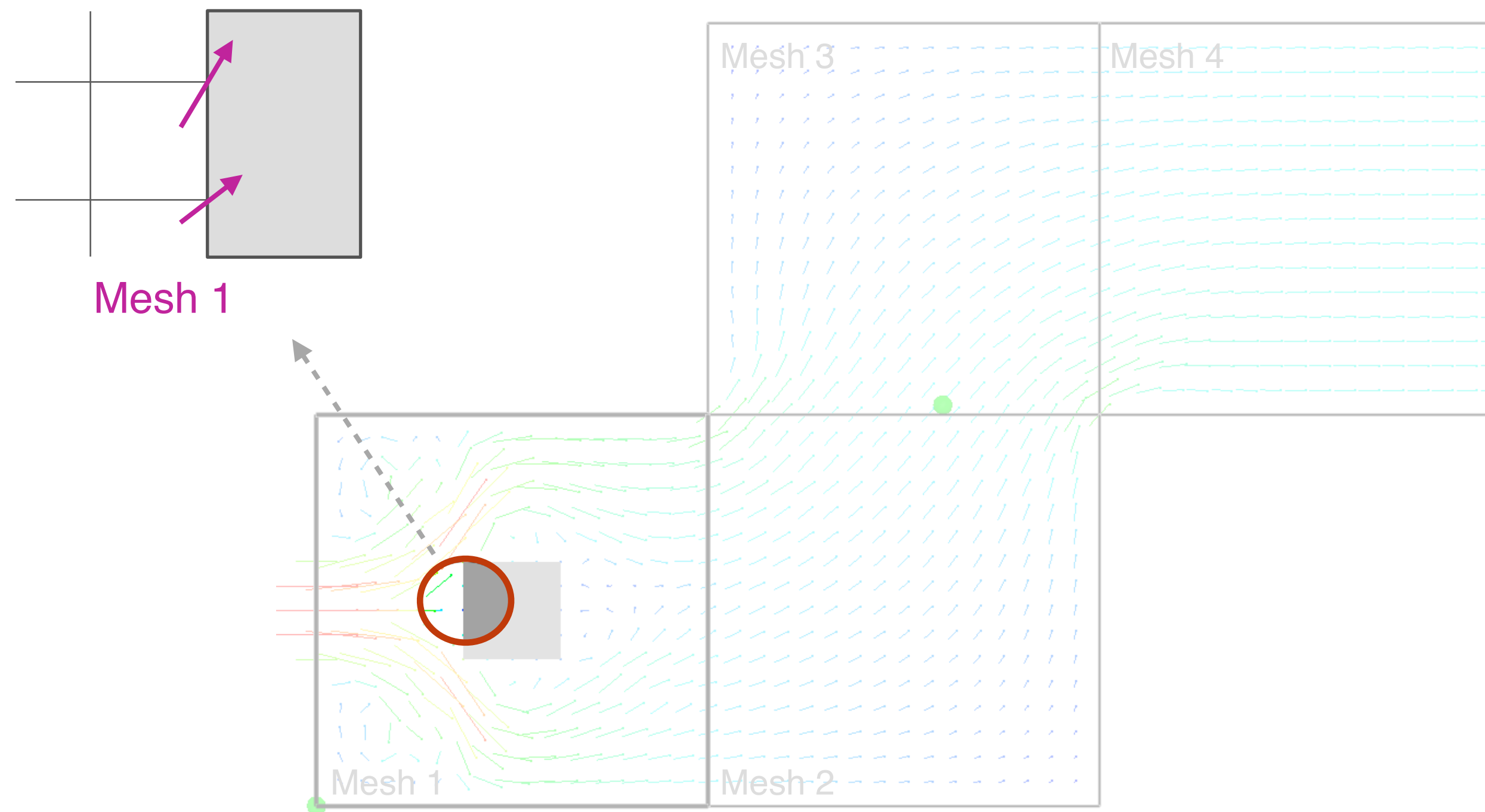
Structured grids only,
internal boundary conditions
cannot be specified

Accuracy along internal obstructions?

2

Velocity components may penetrate into the inner obstructions

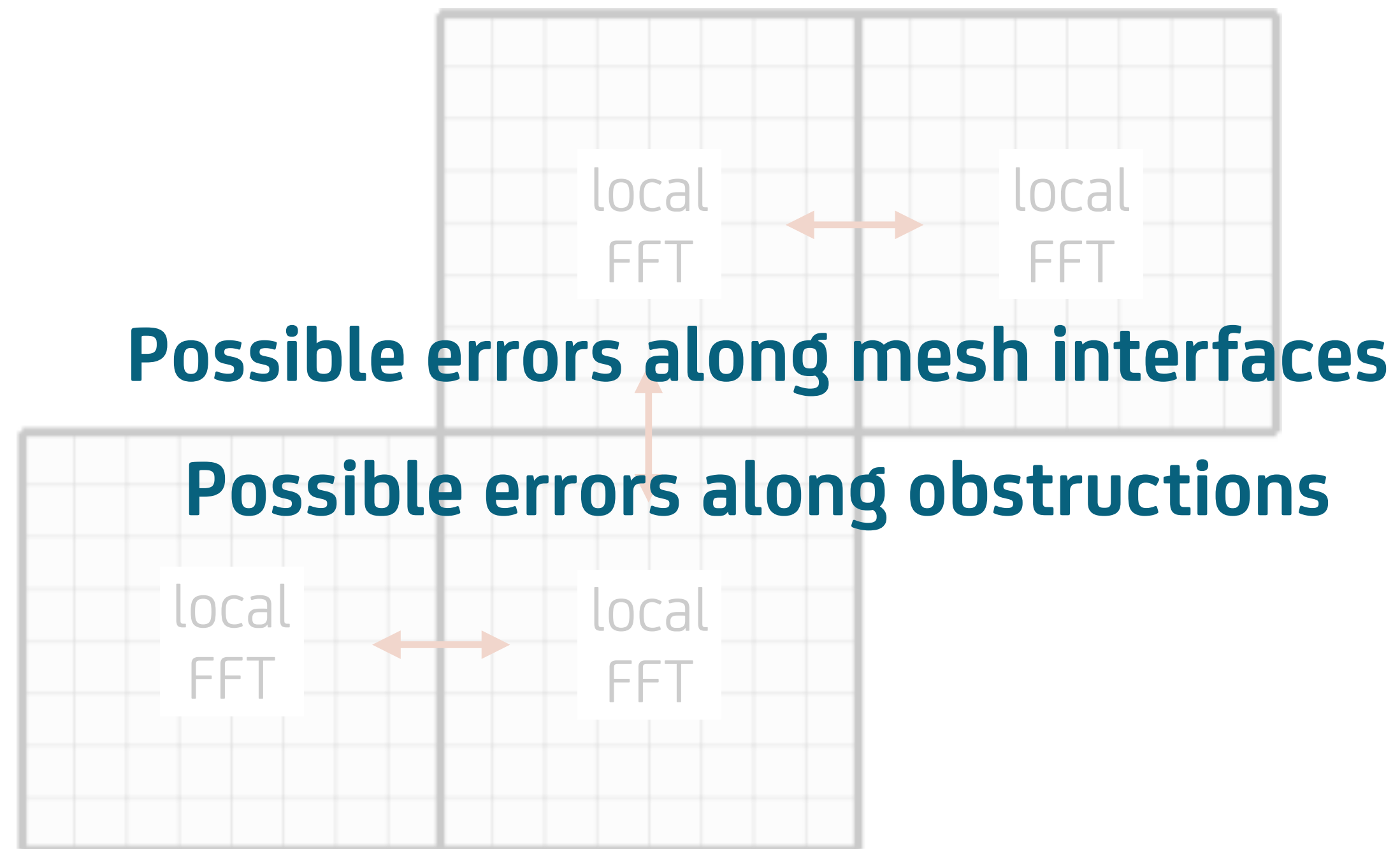
FFT
solver



Mesh-wise FFT-solver

2

FFT
solver



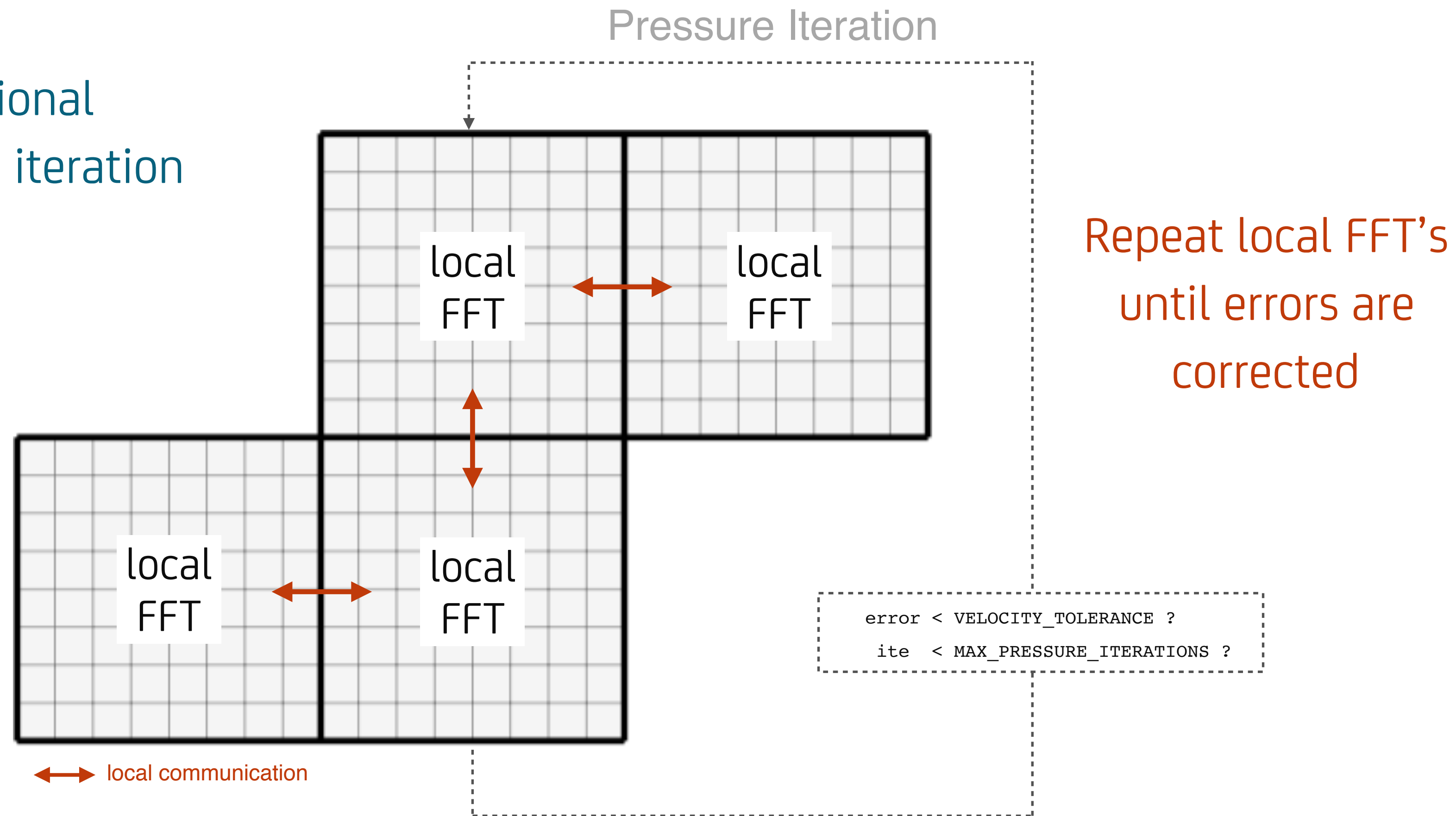
Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

Remedy:

Use additional
corrective iteration

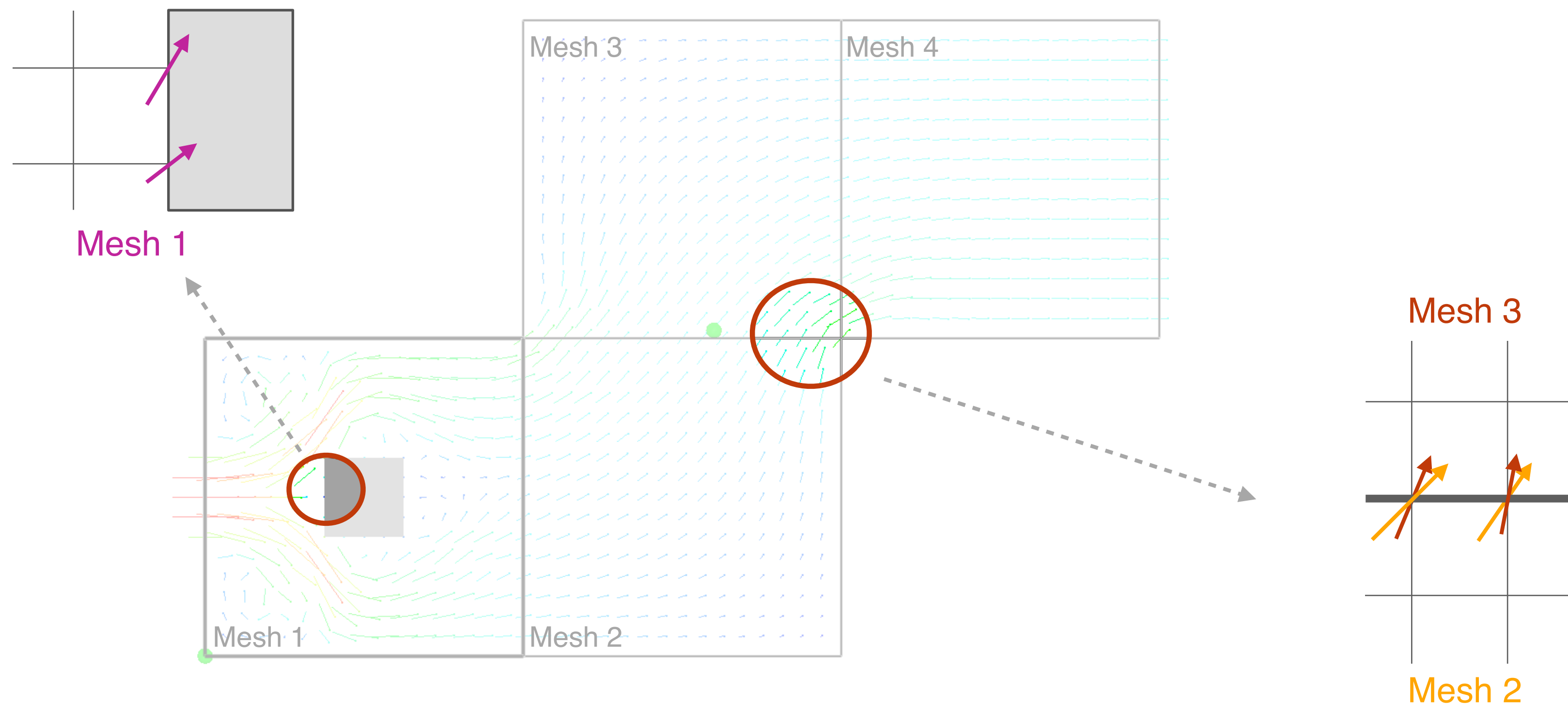


Mesh-wise FFT-solver with pressure iteration

2

Start iteration: Initial velocity errors

FFT
solver

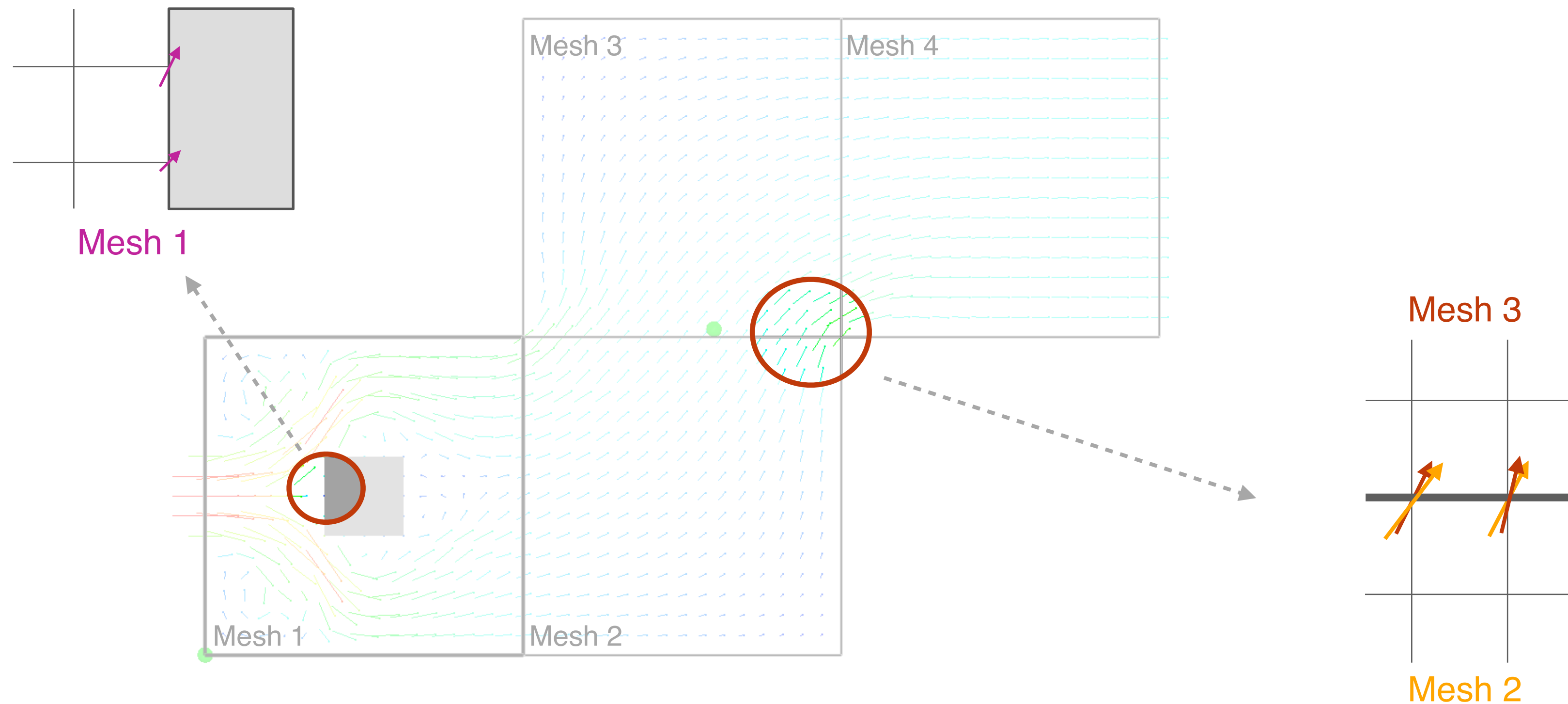


Mesh-wise FFT-solver with pressure iteration

2

Intermediate iteration: Velocity errors are reduced more and more

FFT
solver

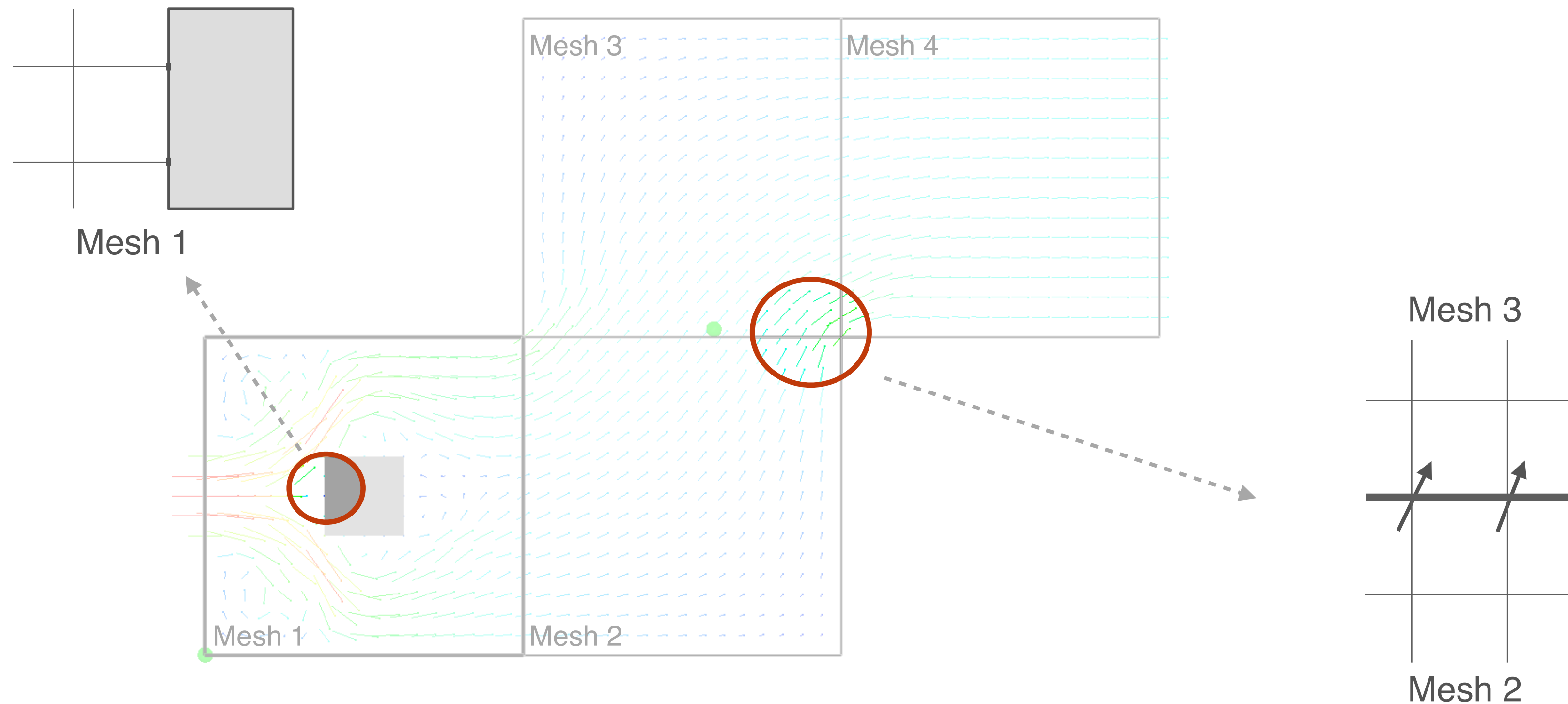


Mesh-wise FFT-solver with pressure iteration

2

End of iteration: Velocity errors are below specified tolerance

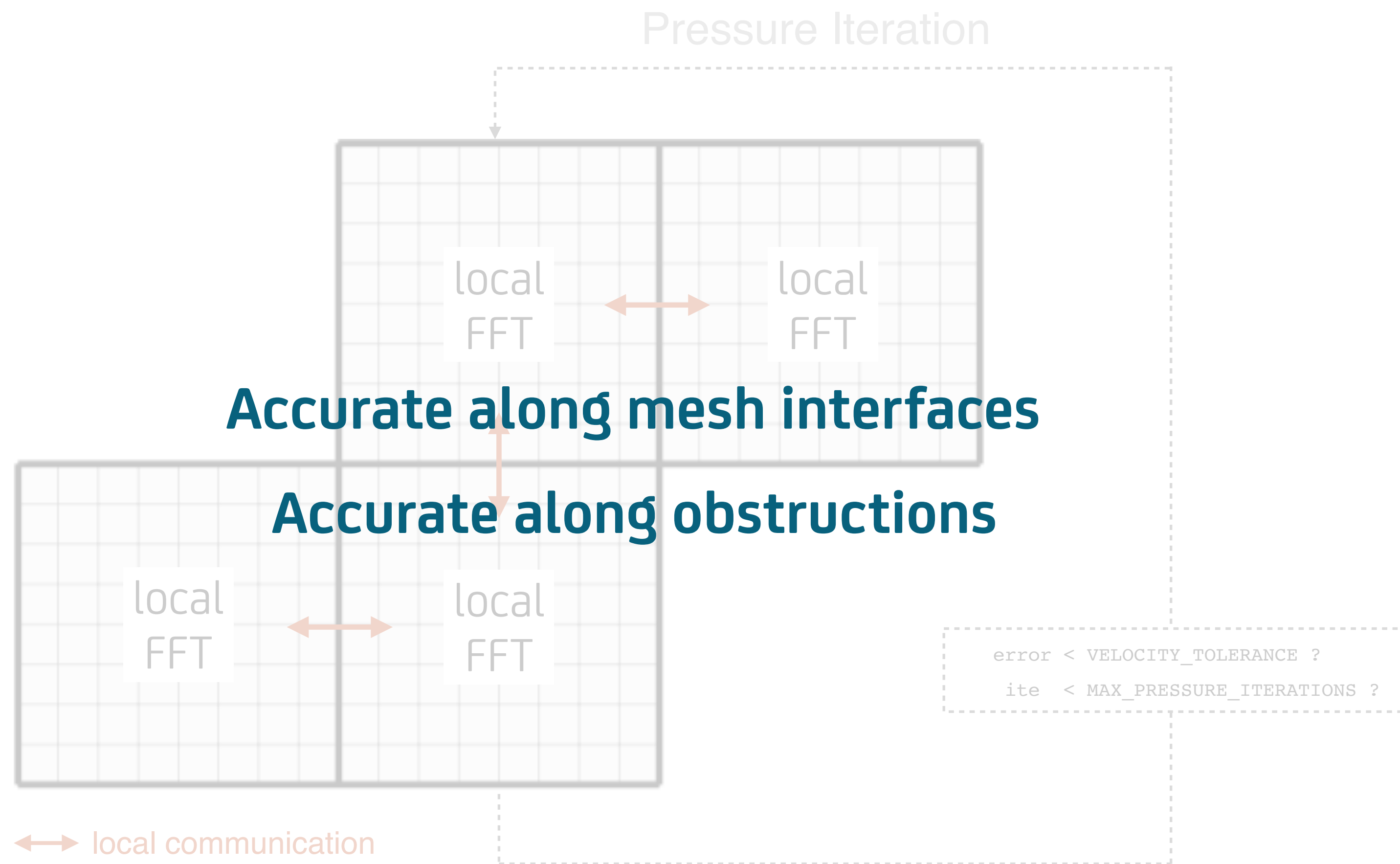
FFT
solver



Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

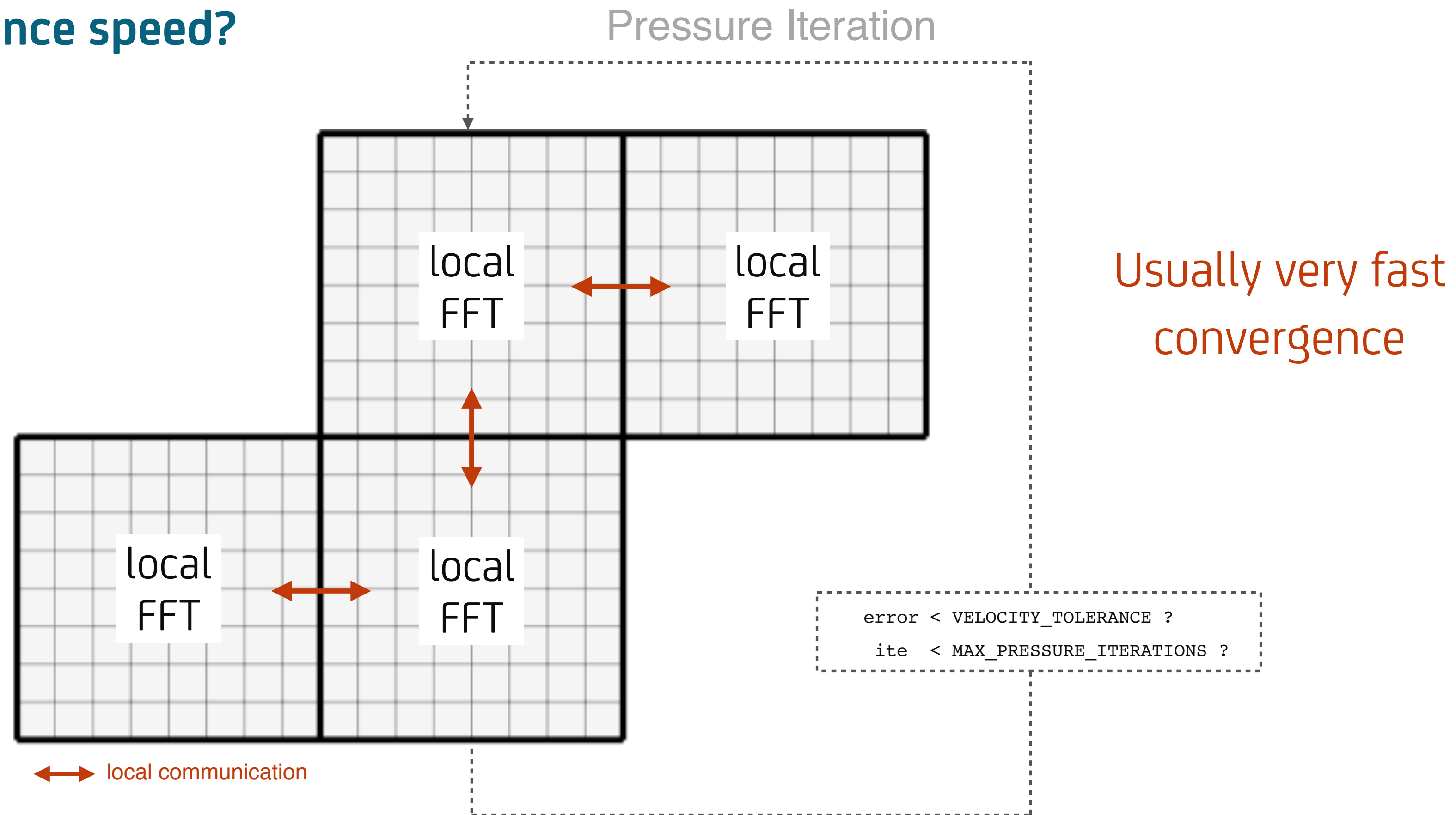


Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

Convergence speed?

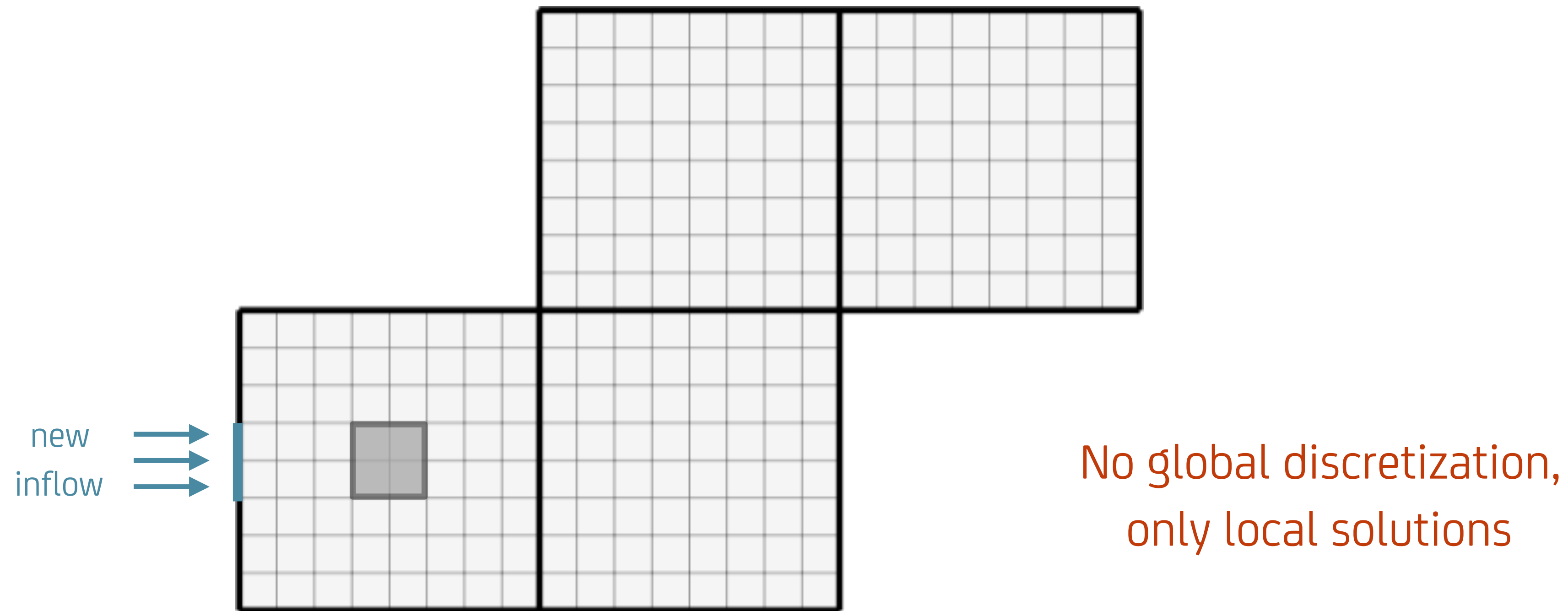


Mapping of the global flow of information?

2

Question: How quickly does new local information spread?

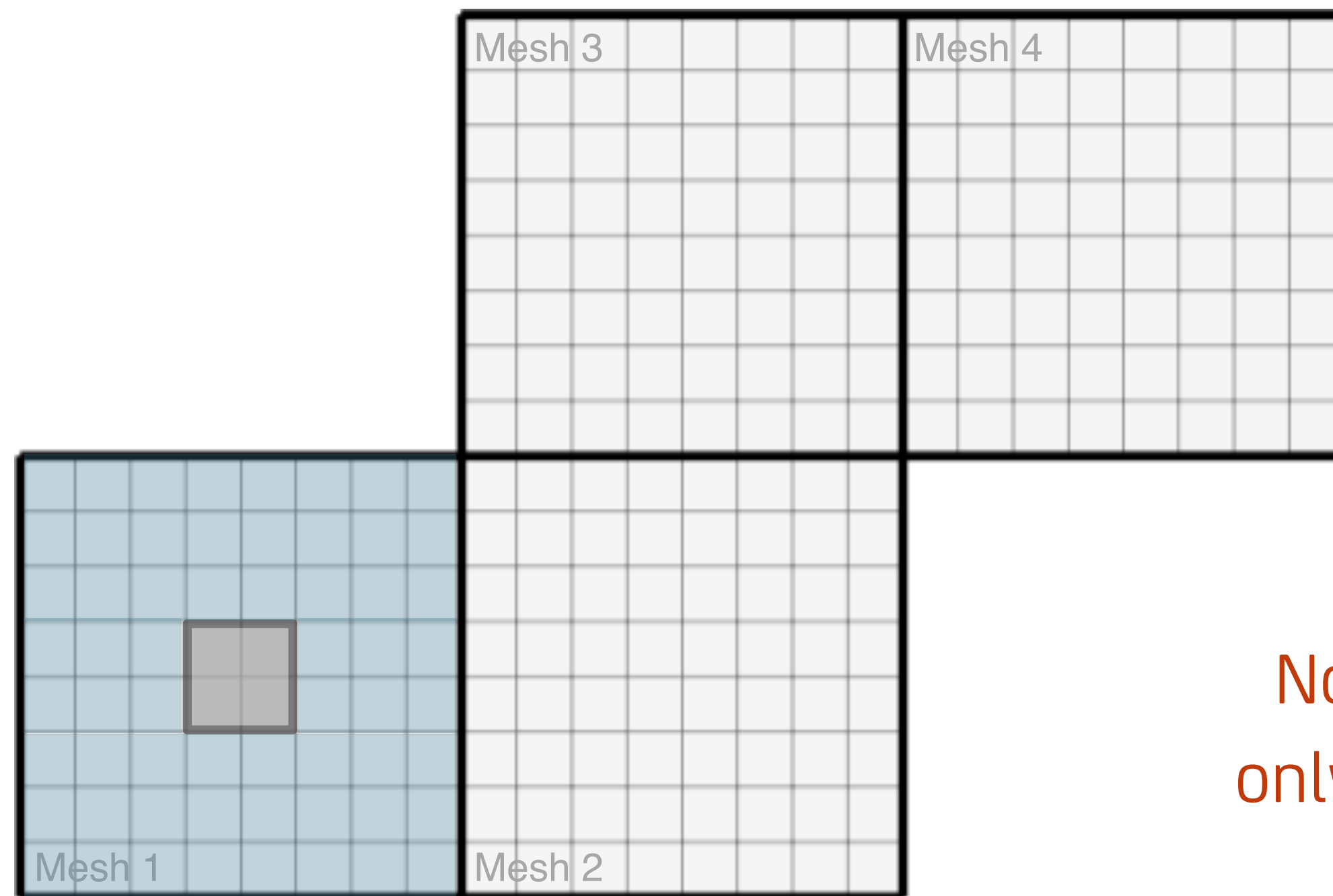
FFT
solver



Mapping of the global flow of information?

2

1. Cycle: Information reaches Mesh 1



No global data transfer,
only local communication

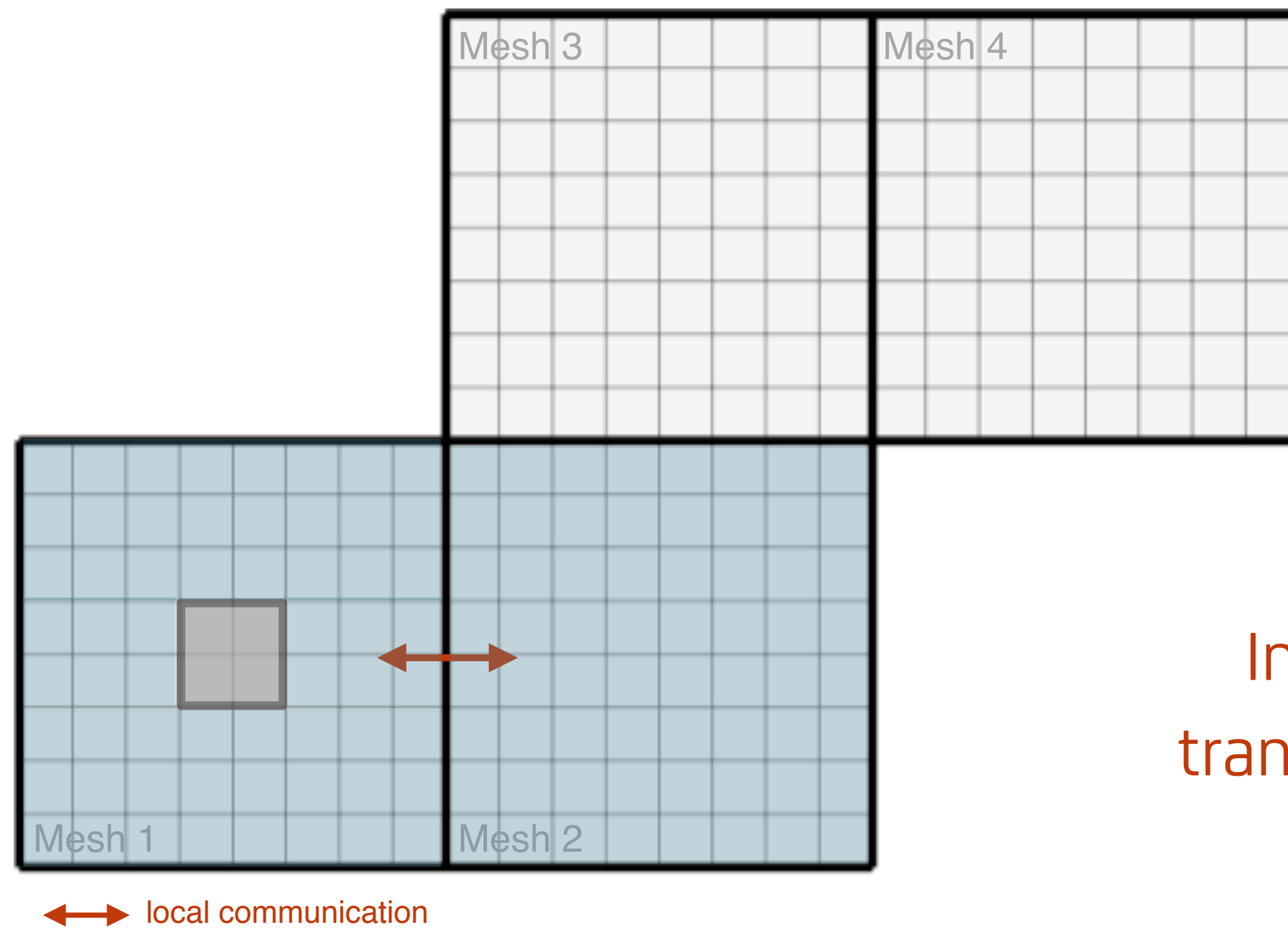
FFT
solver

Mapping of the global flow of information?

2

2. Cycle: Information reaches Mesh 2

FFT
solver



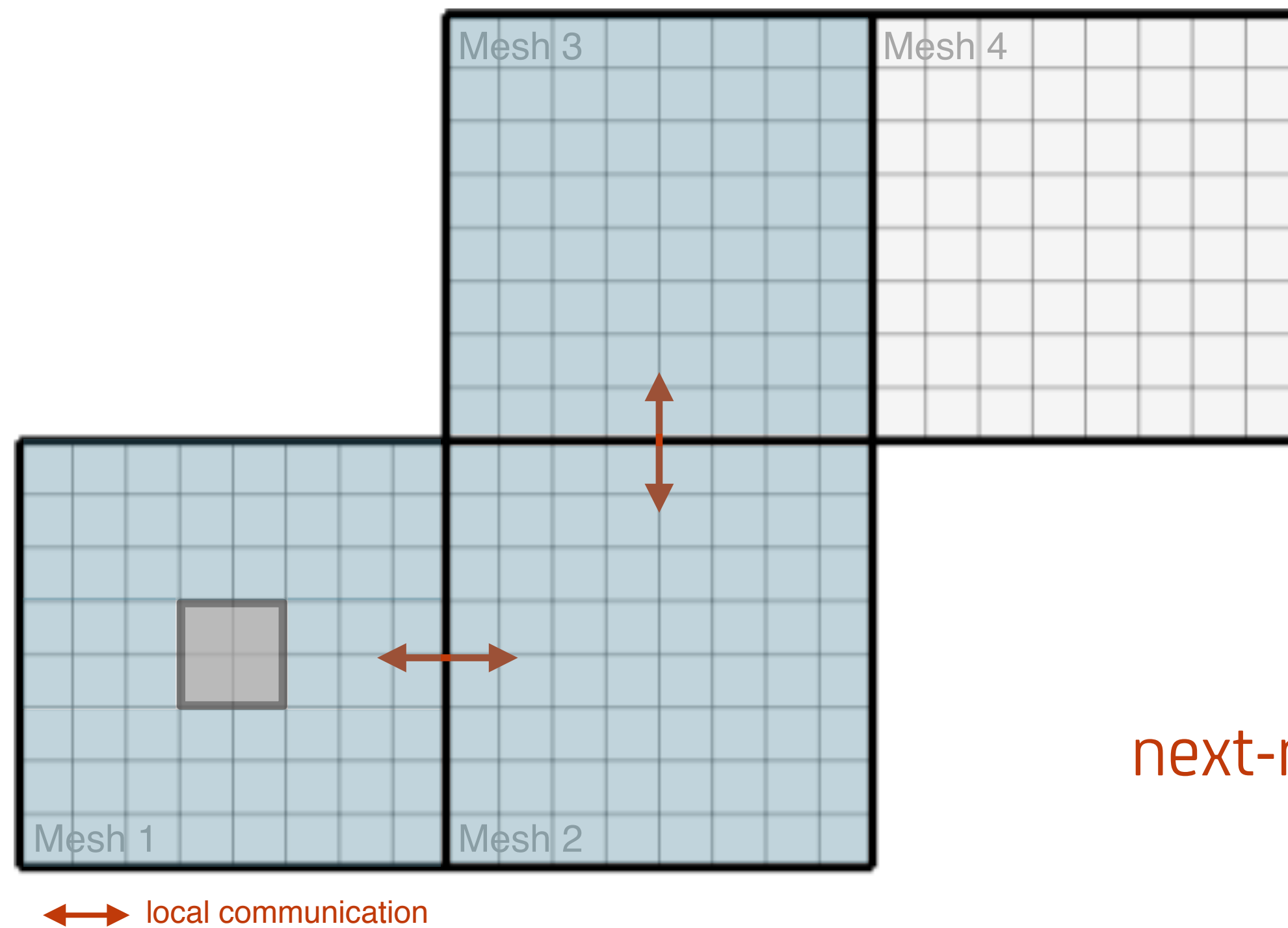
Information can only be transferred mesh-by-mesh ...

Mapping of the global flow of information?

2

3. Cycle: Information reaches Mesh 3

FFT
solver



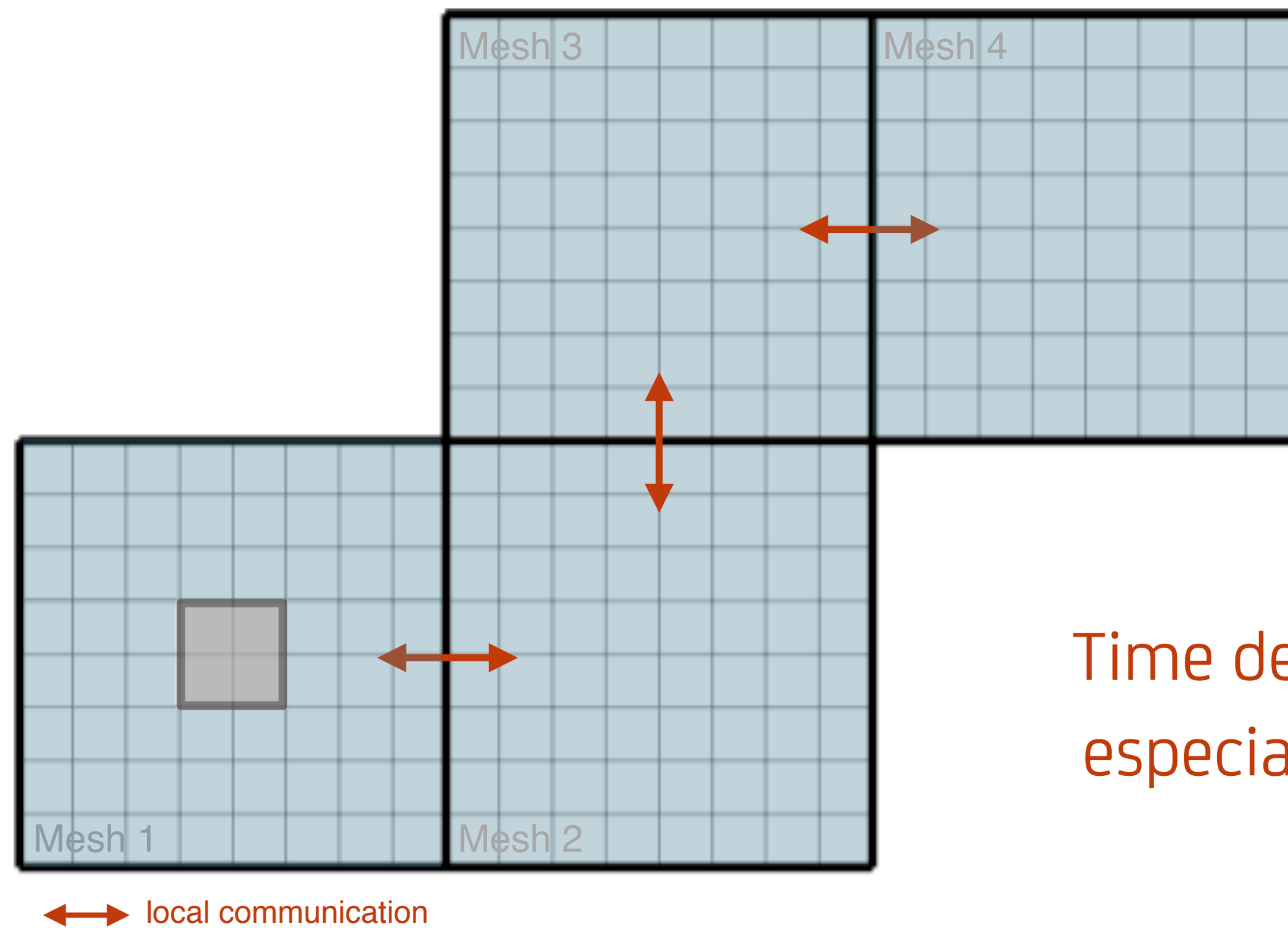
... successively using
next-neighbor communications

Mapping of the global flow of information?

2

4. Cycle: Information finally reaches Mesh 4

FFT
solver



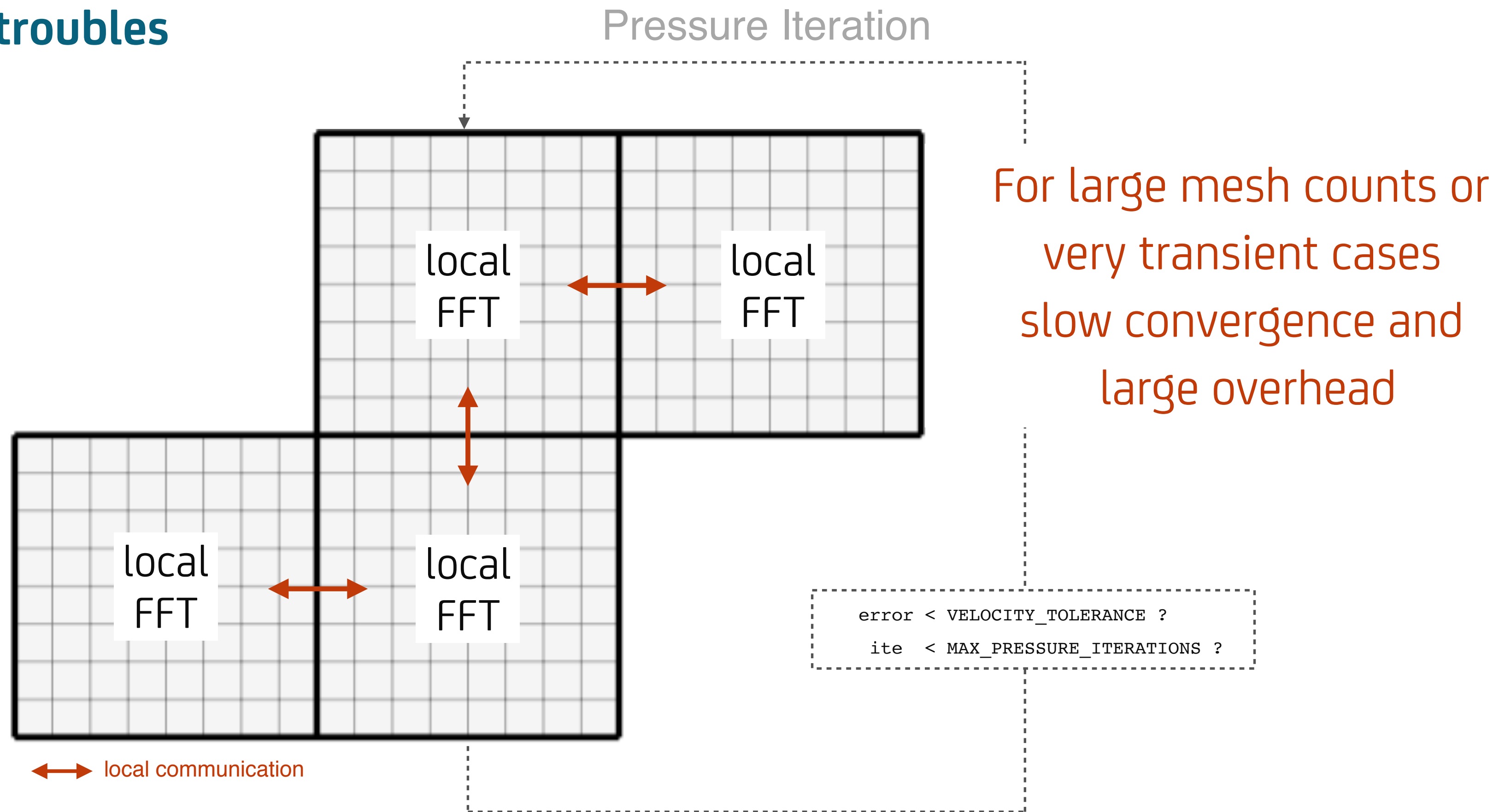
Time delay compared to 1-mesh,
especially for large mesh counts

Mesh-wise FFT-solver with pressure iteration

2

FFT
solver

Possible troubles



UGLMAT solver

Optimized parallel LU-decomposition

Alternative pressure solver UGLMAT

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

$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} L \end{bmatrix} \times \begin{bmatrix} U \end{bmatrix}$$

Parallel LU-decomposition

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

UGLMAT
solver

Alternative pressure solver UGLMAT

UGLMAT
solver

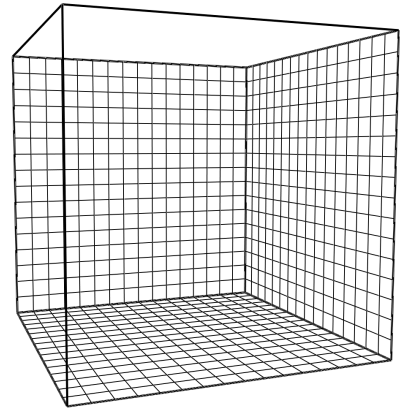
- **Global unstructured** discretization of whole domain
- Decomposition of global Poisson matrix A in lower and upper triangular matrices L and U

$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} L \end{bmatrix} \times \begin{bmatrix} U \end{bmatrix}$$

Accurate along mesh interfaces
Accurate along obstructions

Parallel
LU-decomposition

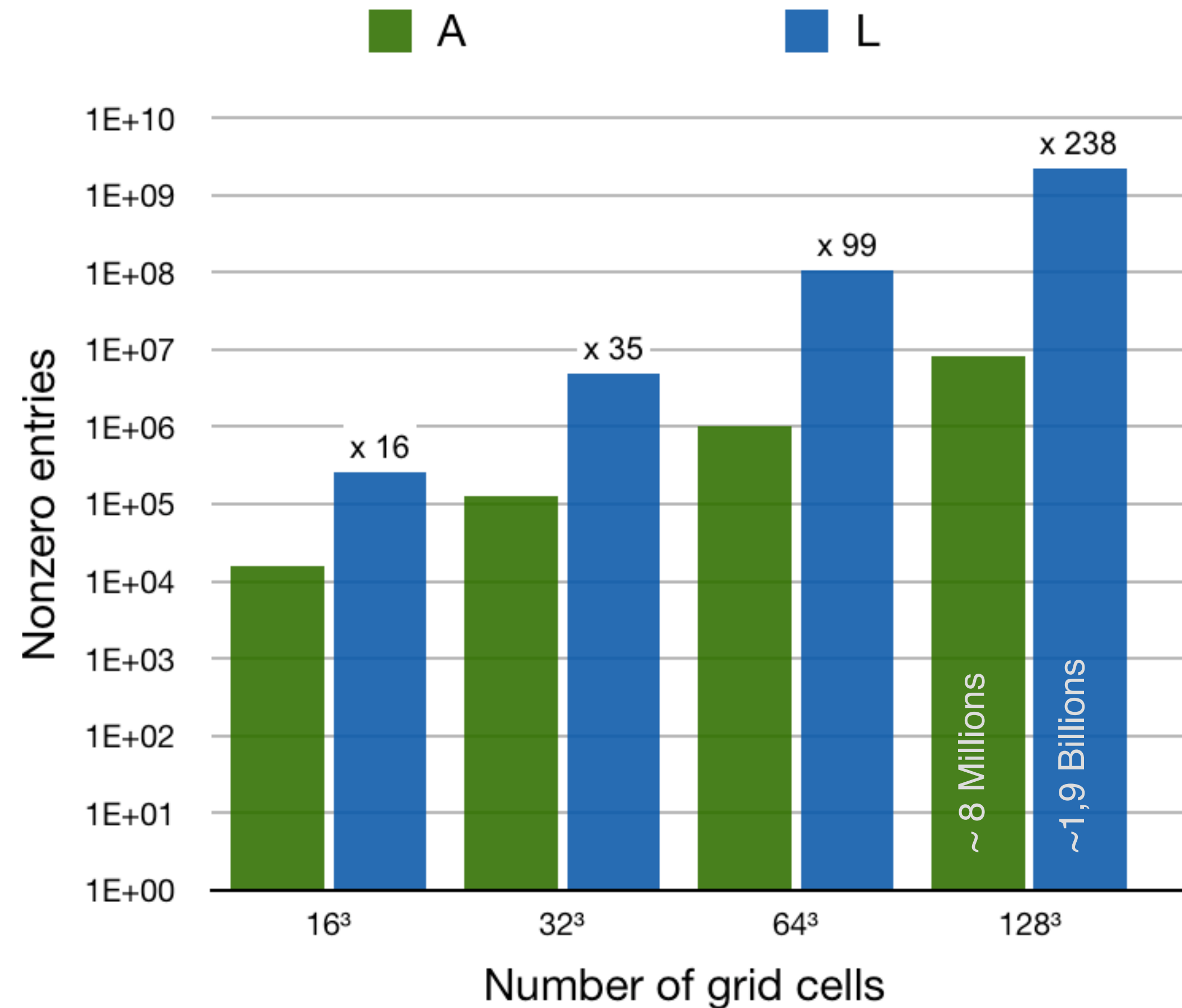
- Usage of optimized LU - solver from Intel Math Kernel Library (MKL)



UGLMAT - Memory needs for 3D-cube

3

UGLMAT
solver



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

Huge memory requirements as grid is refined

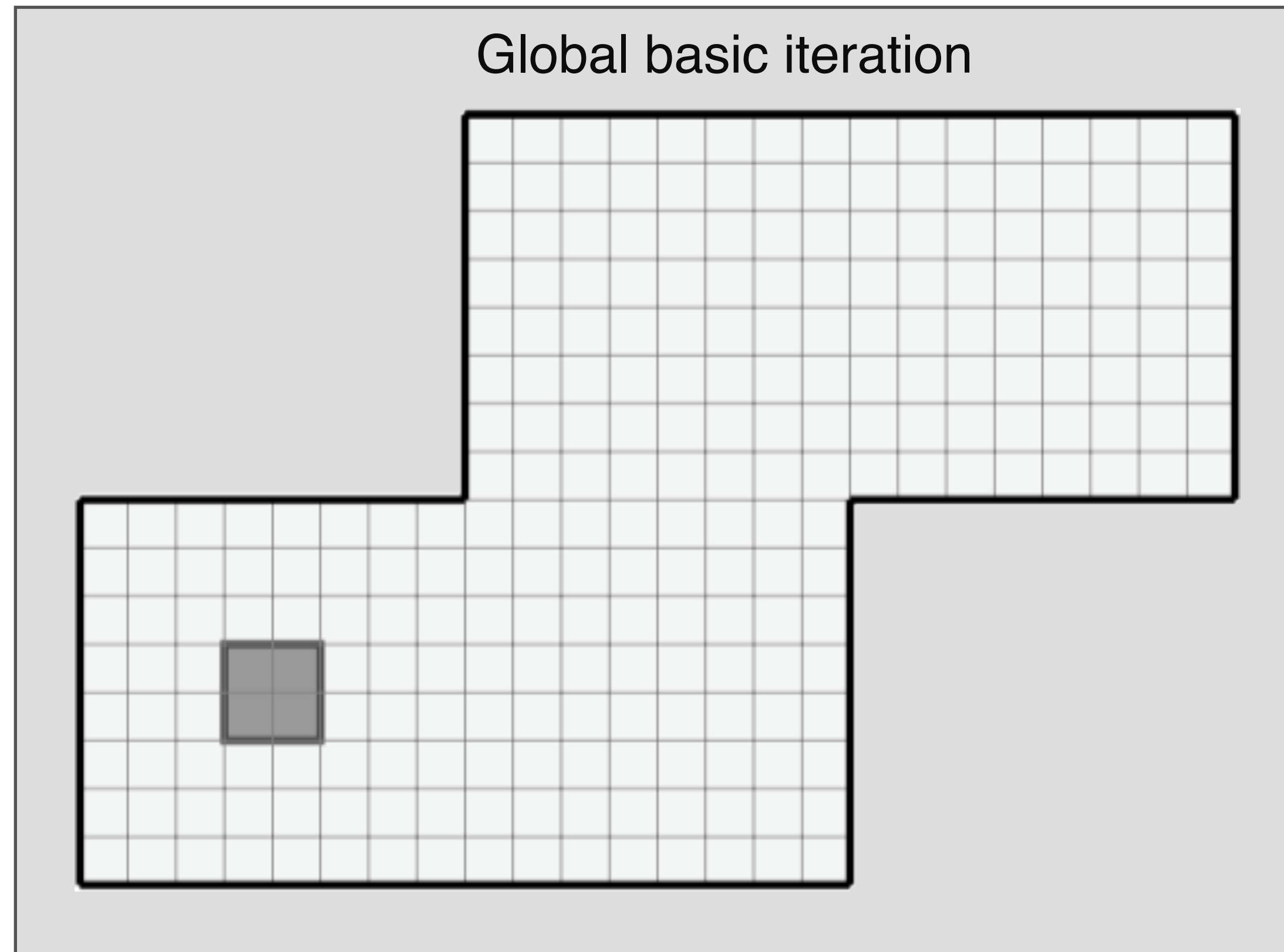
ScaRC

Scalable Recursive Clustering

ScaRC Core: Overall global iterative method

4

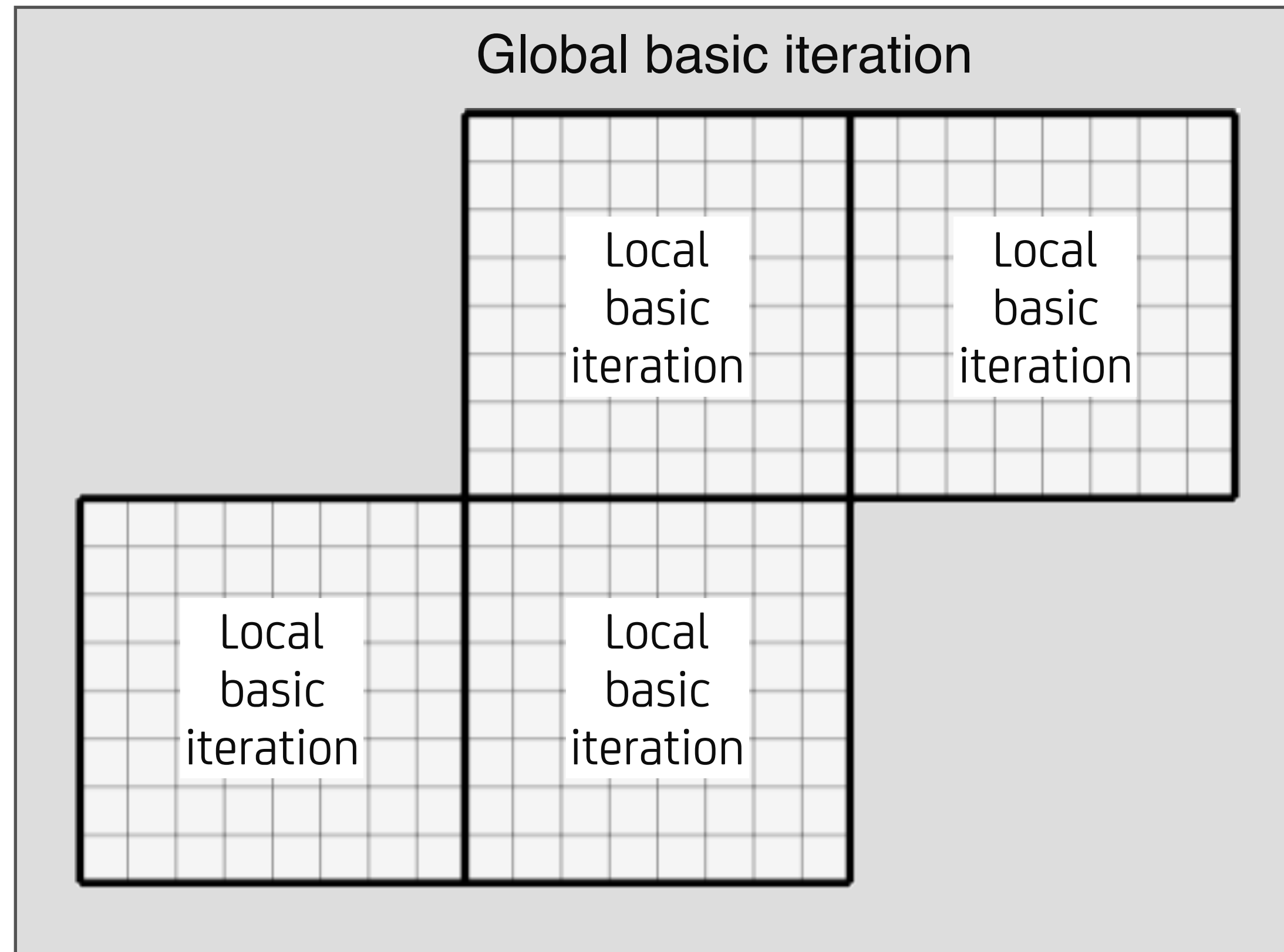
ScaRC
solver



**Global structured
discretization**

Data-parallel
iterative method for
global Poisson matrix

ScaRC Core: Additional local iterative methods

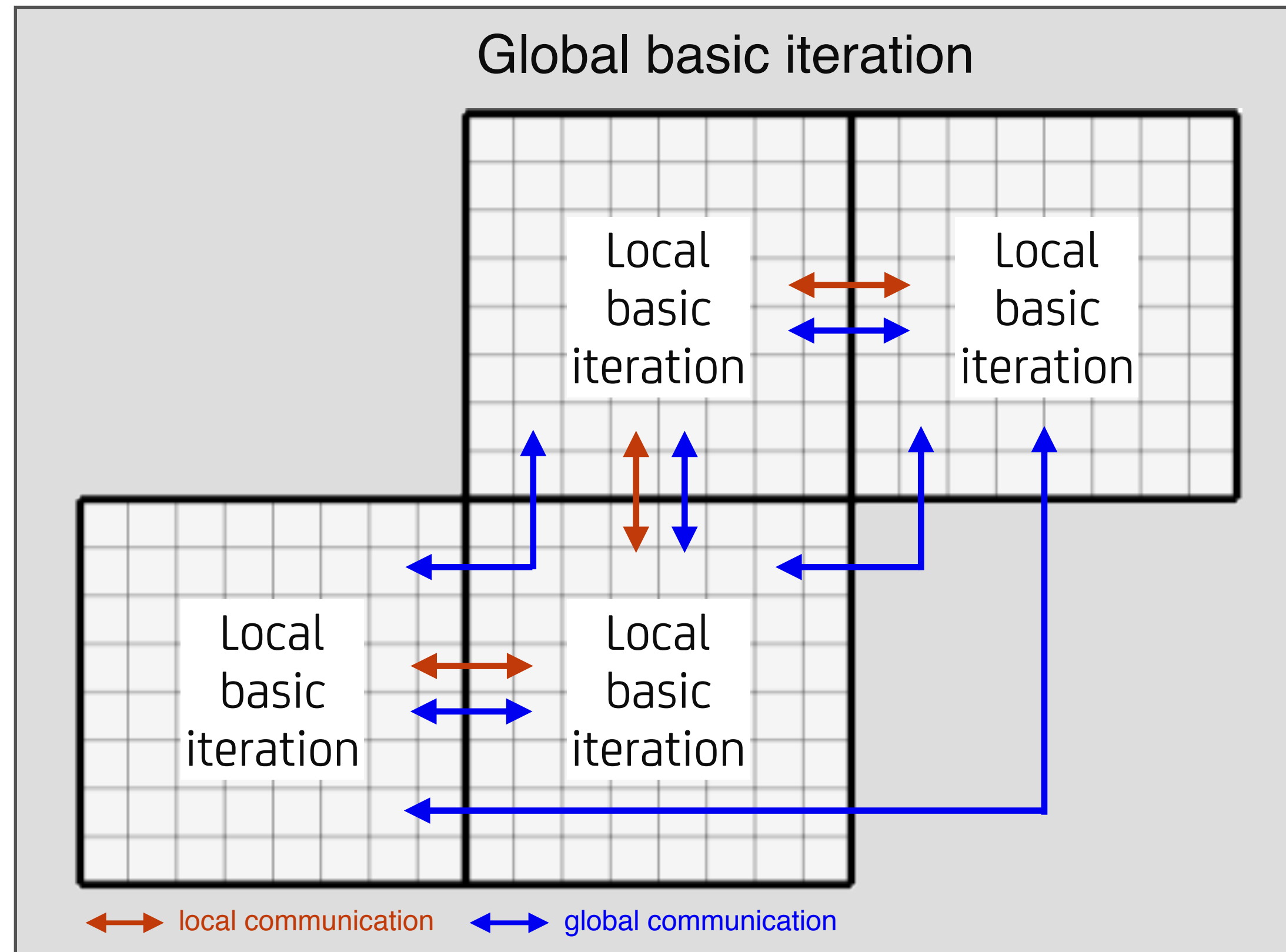


Not used as stand-alone solvers, but only as corrections to global solution

ScaRC Core: Local and global communication

4

ScaRC
solver



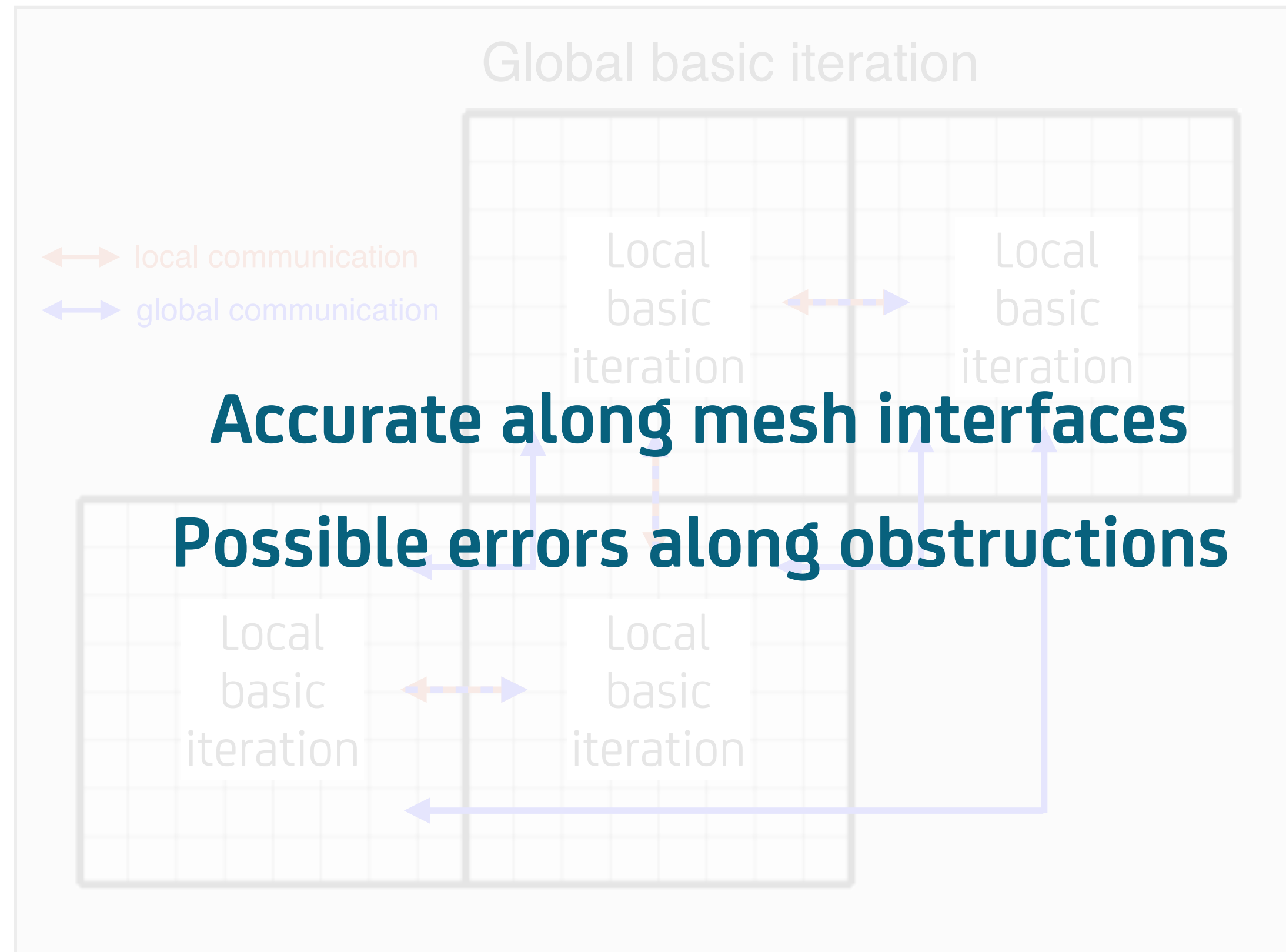
Local solvers offer
fine grid accuracy

Basic information transfer
is provided globally

ScaRC Core: Structured basic version

4

ScaRC
solver



Multiple variations of different techniques

4

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

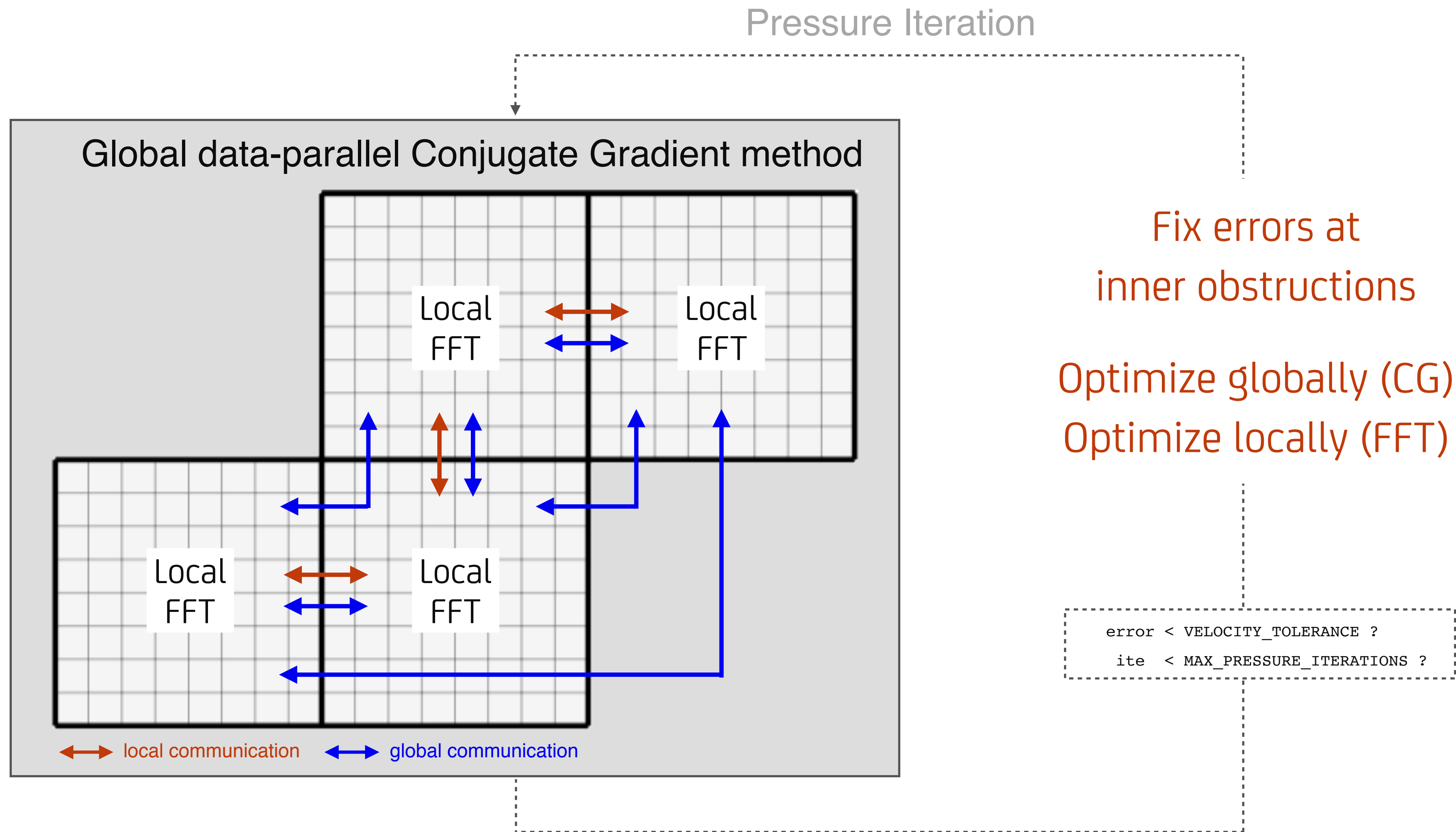
- Optimized FFT (CRAYFISHPAK) → Speed up local solutions in structured case
- Optimized LU (Intel MKL) → Speed up local solutions in unstructured case

ScaRC
solver

ScaRC-CG: Default for structured grids

4

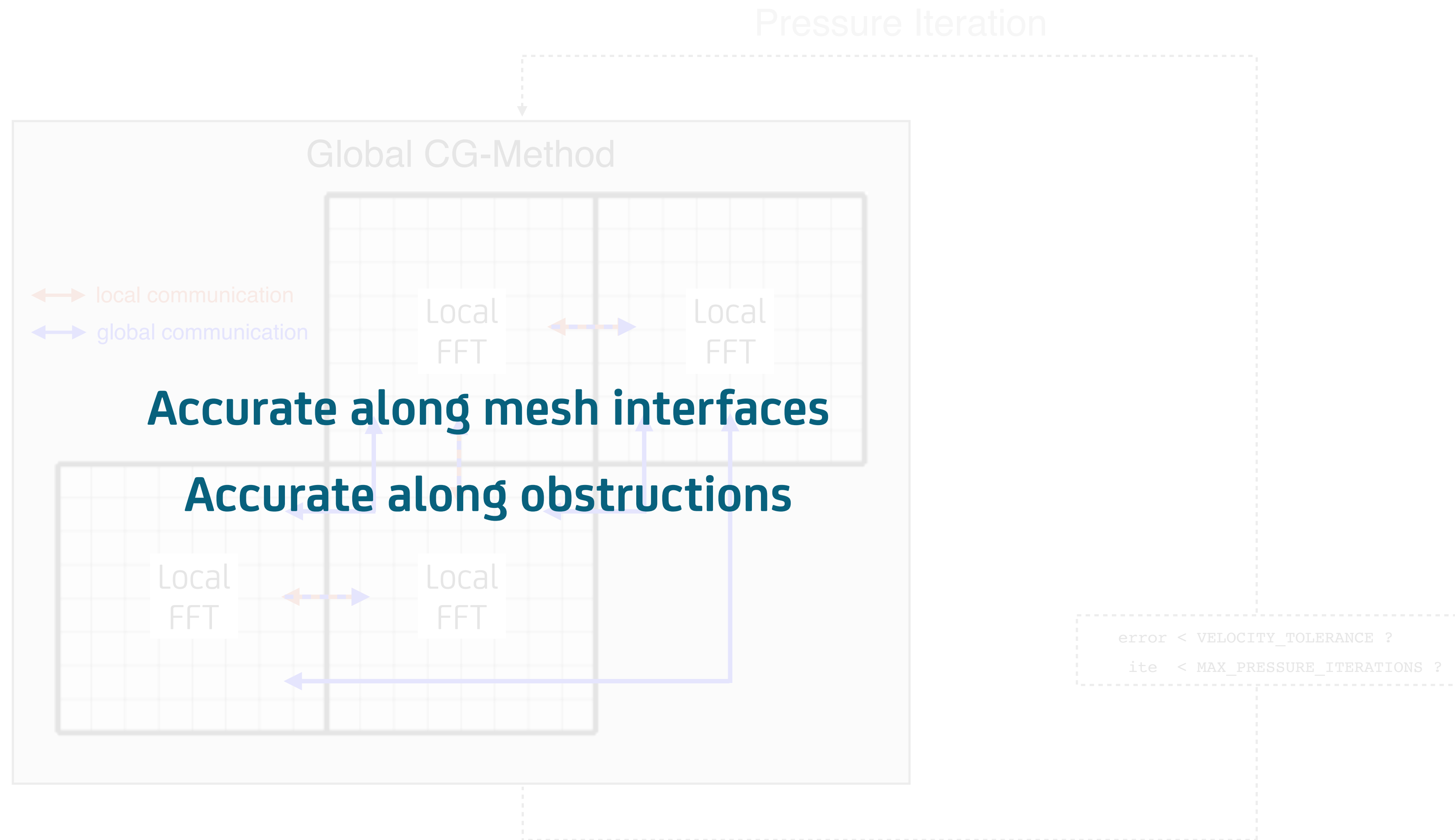
ScaRC
solver



ScaRC-CG: Default for structured grids

4

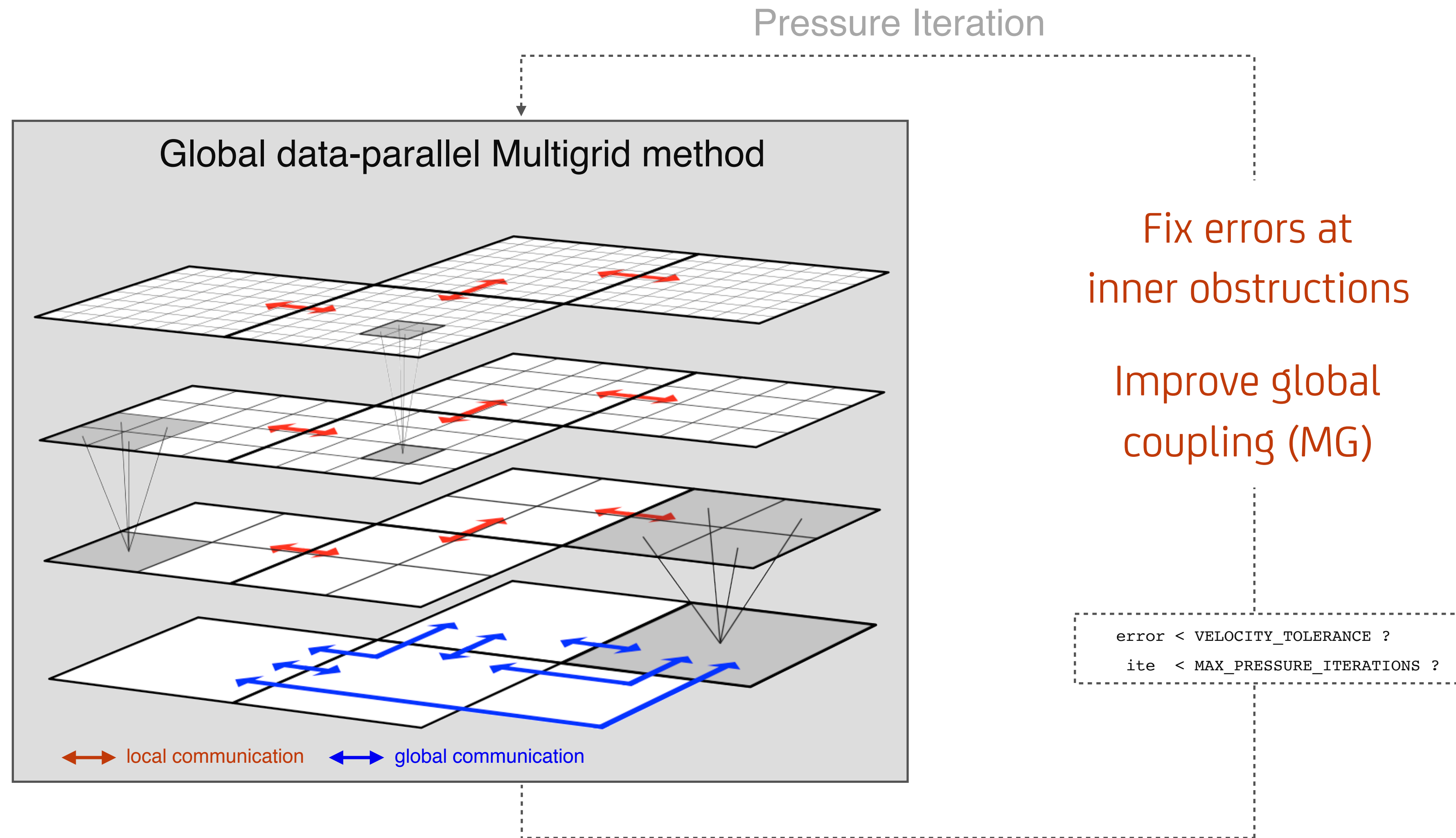
ScaRC
solver



ScaRC-MG: Alternative for structured grids

4

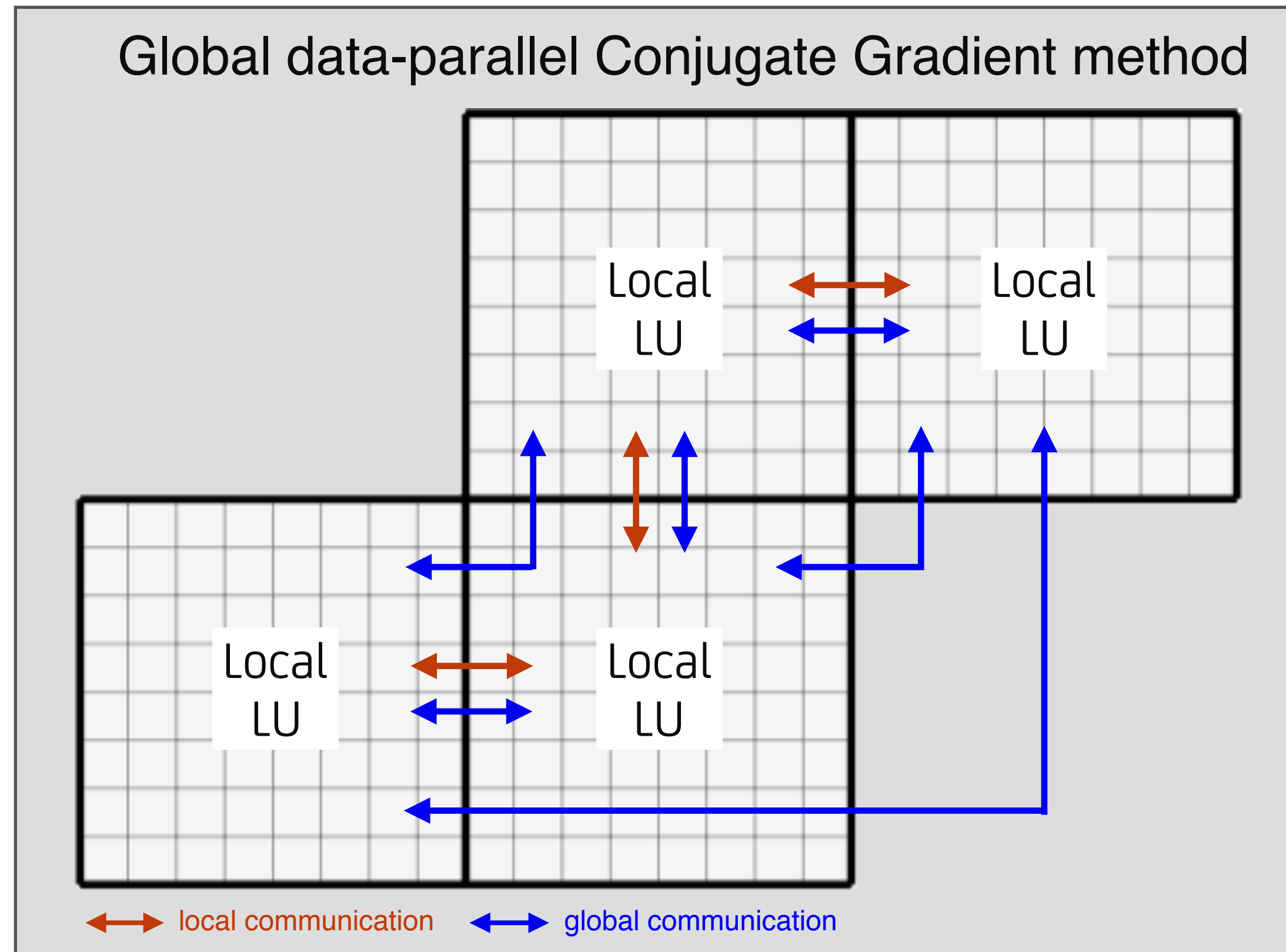
ScaRC
solver



UScaRC-CG: Default for unstructured grids

4

ScaRC
solver



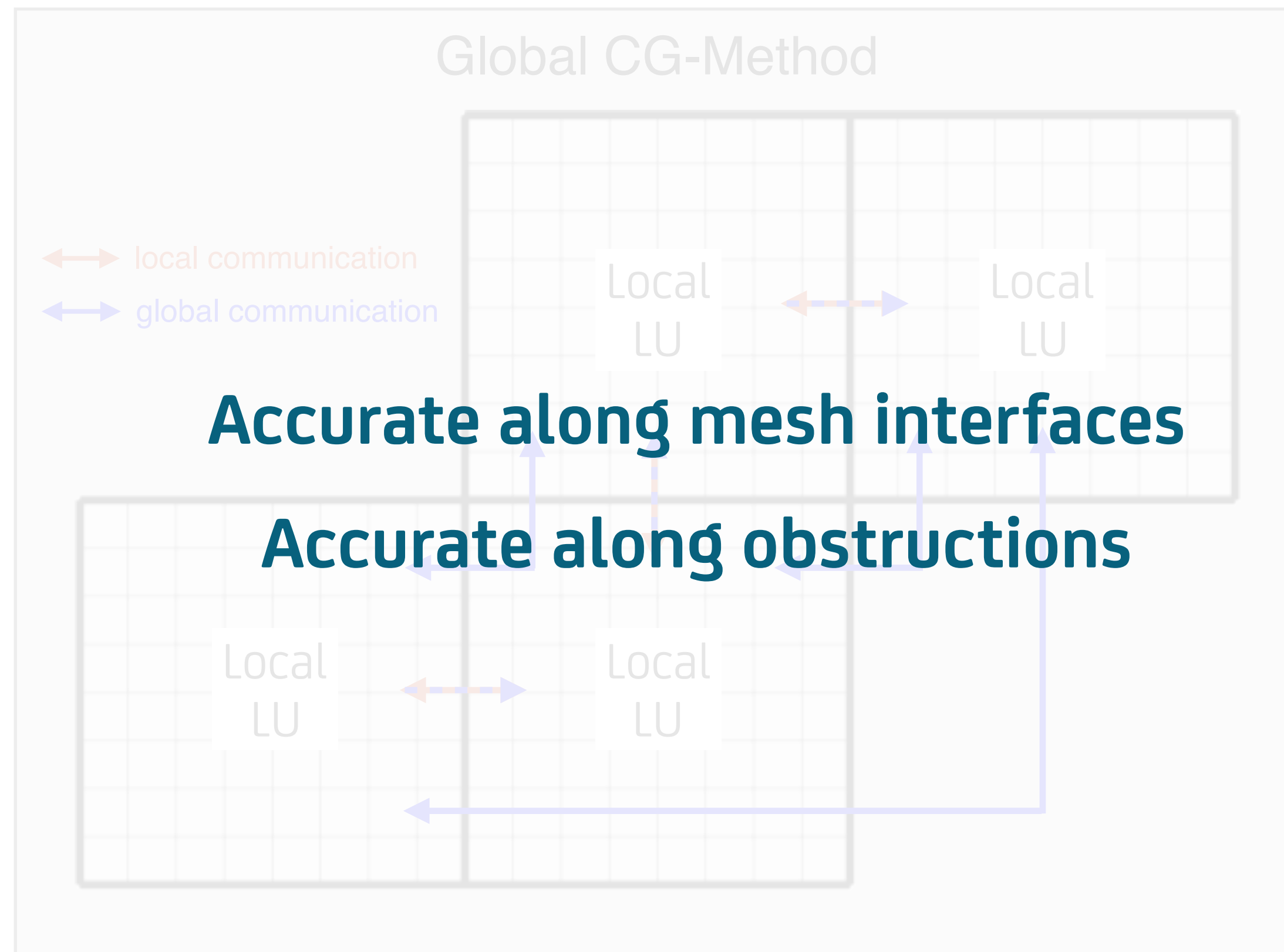
No need for
pressure iteration

Optimize globally (CG)
Optimize locally (LU)

UScaRC-CG: Default for unstructured grids

4

ScaRC
solver



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

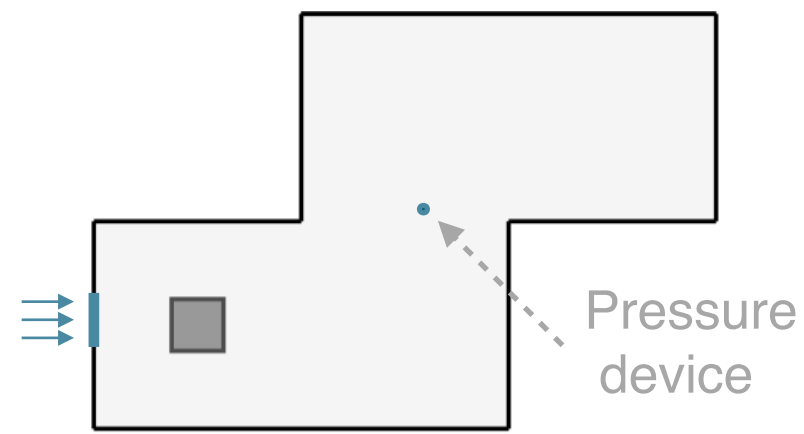
Verification & Validation

- run all pressure related verification tests
- start with validation tests

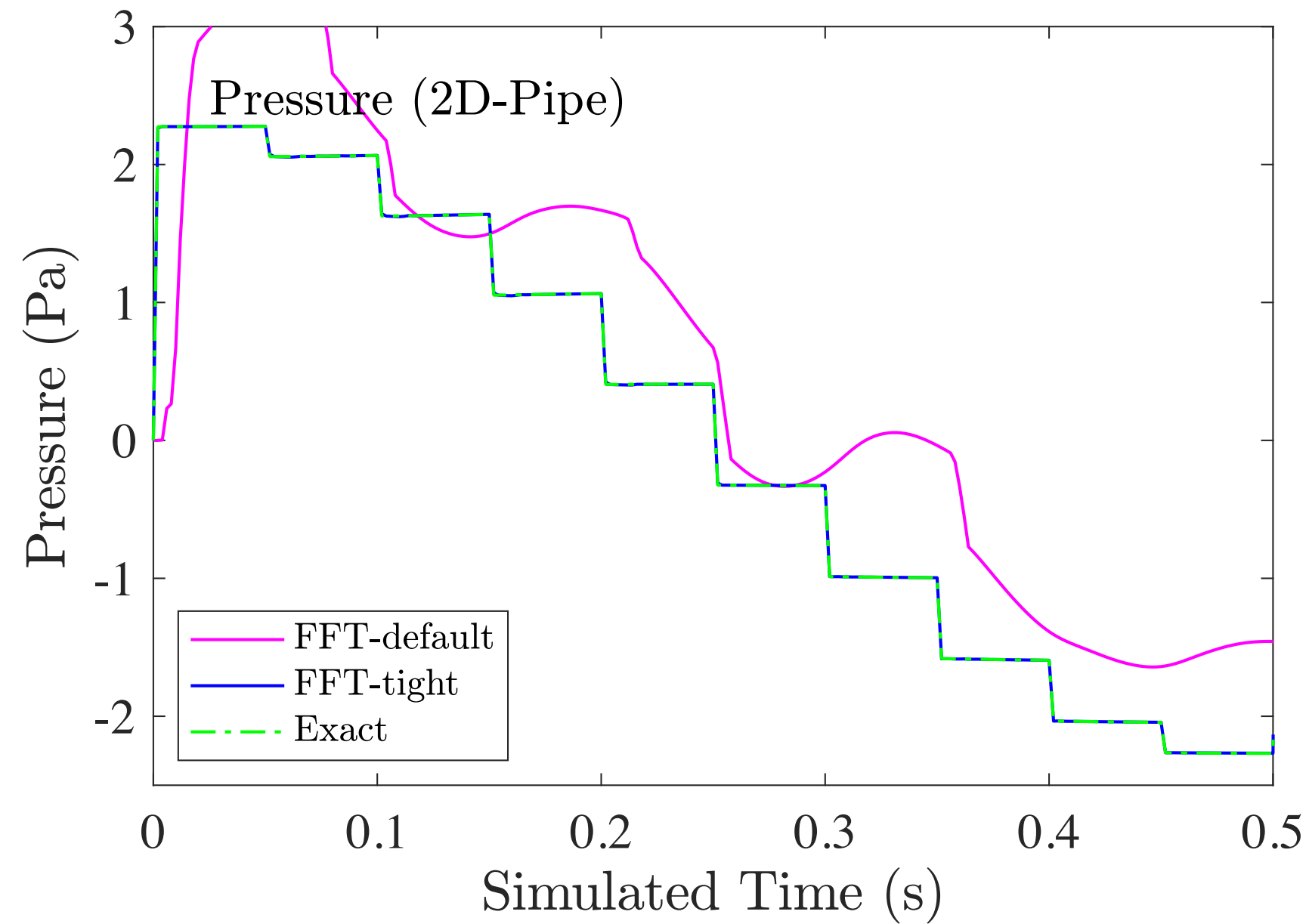
4

ScaRC
solver

Pressure trace for 2D-pipe

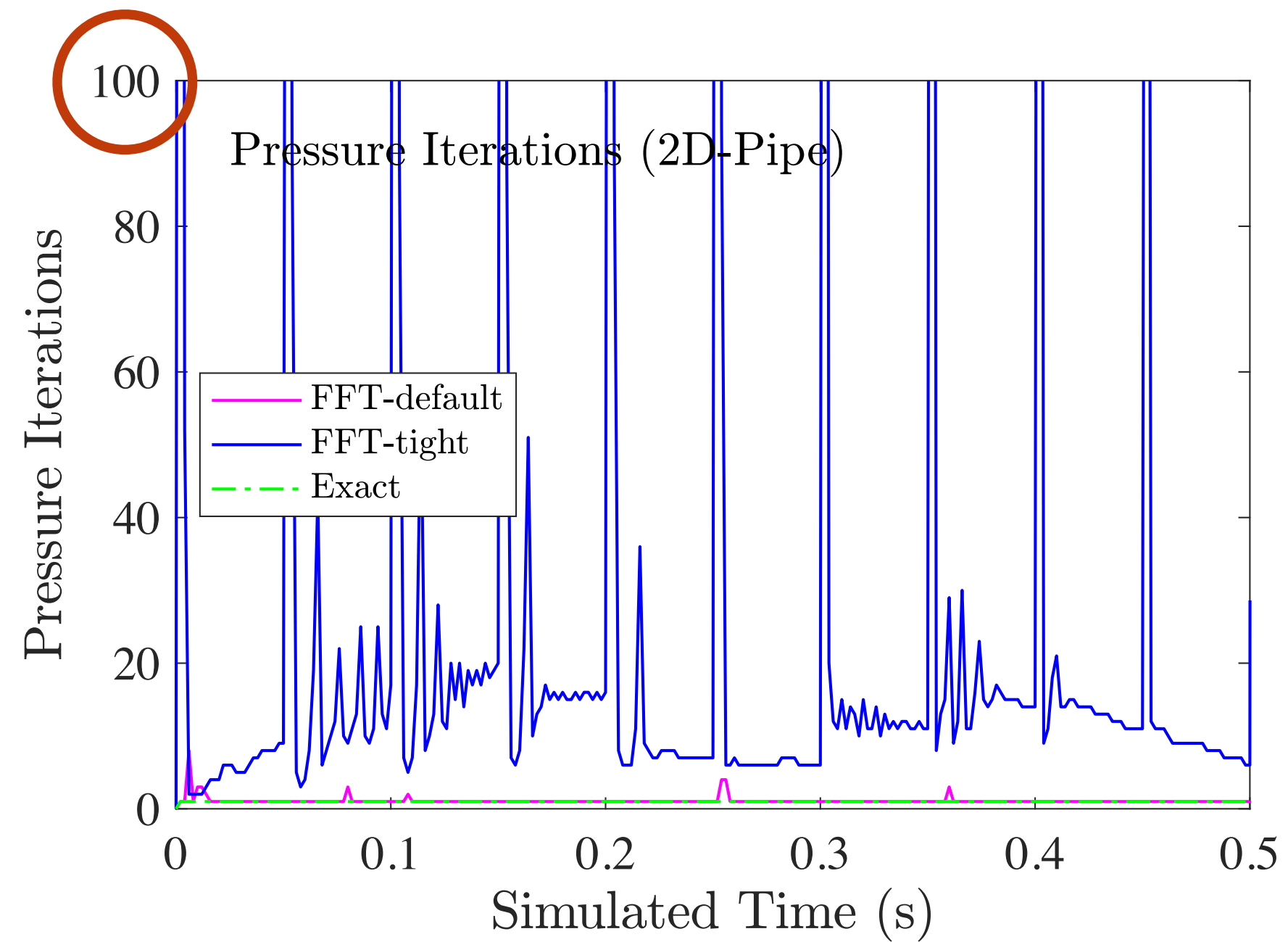


FFT default and tight (tol=10⁻⁵ m/s)



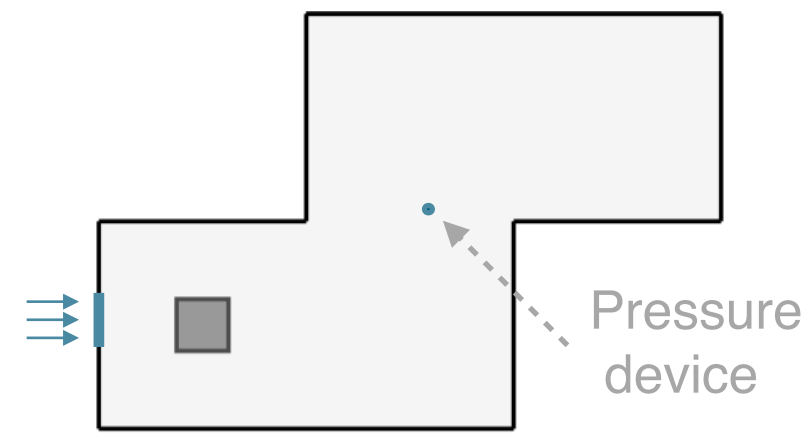
Only accurate for tight pressure iteration

Number of required pressure iterations

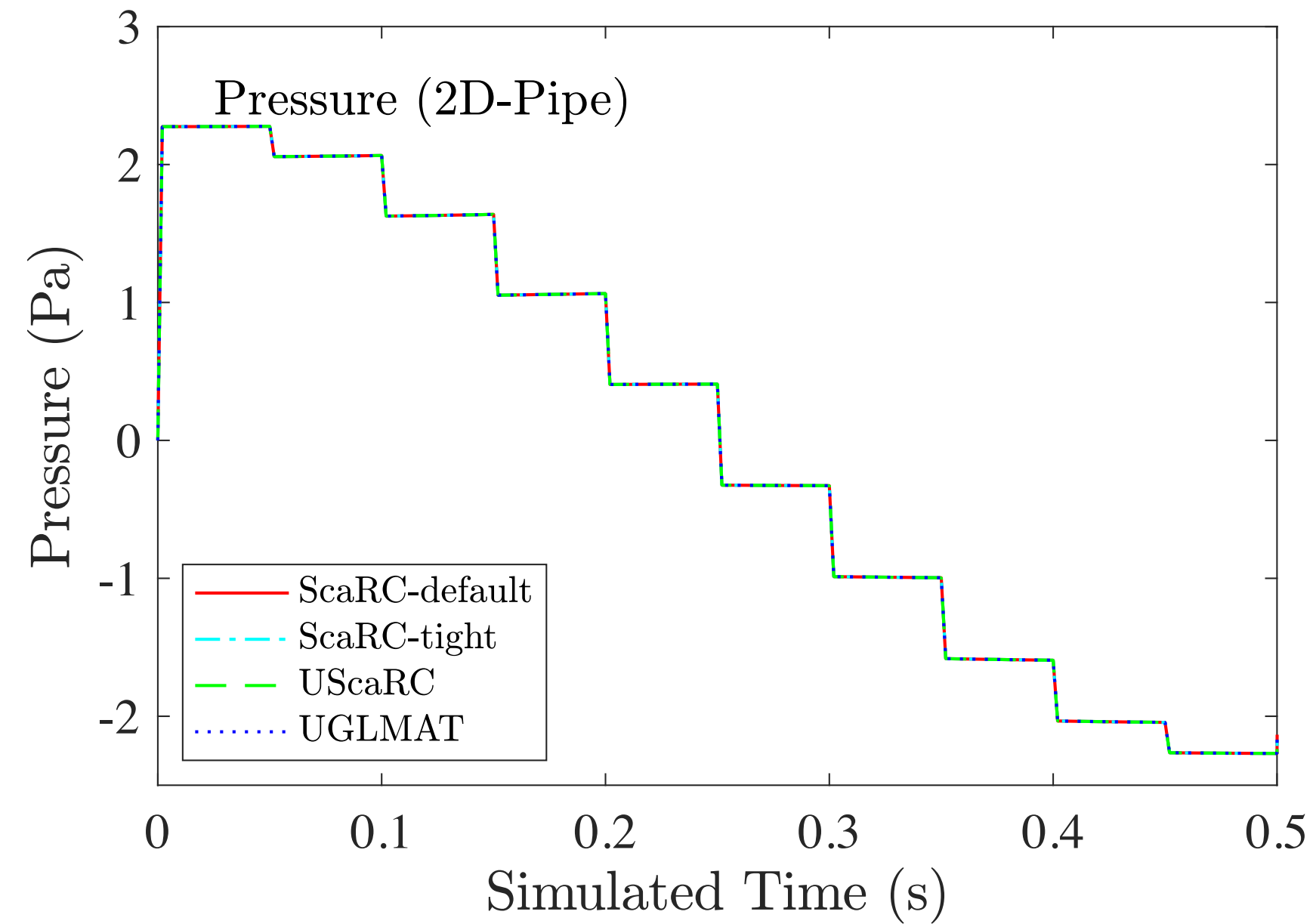


Increased number of pressure iterations (Ø 28)

Pressure trace for 2D-pipe

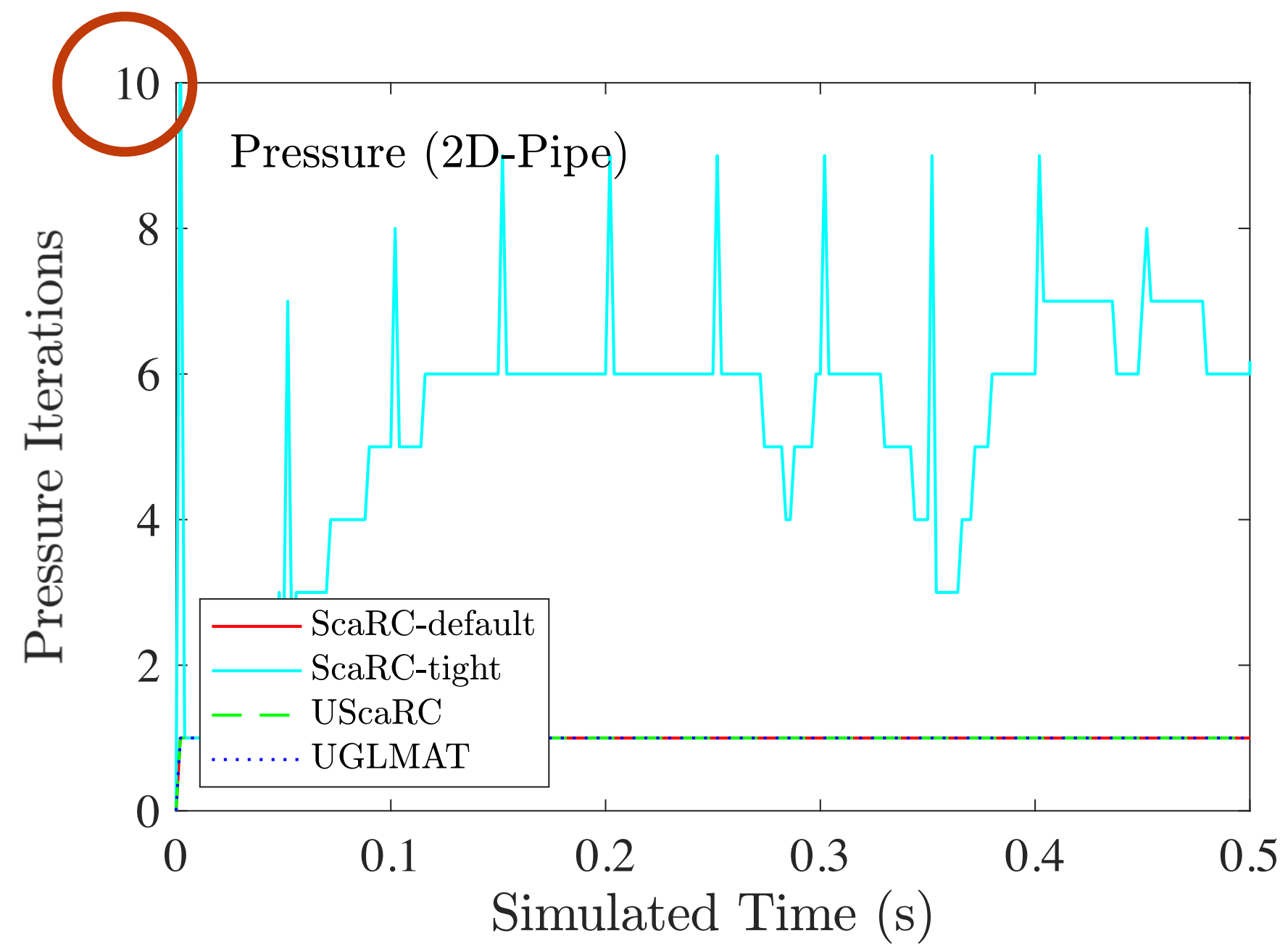


Different variants of ScaRC and UGLMAT



Accurate for all variants

Number of required pressure iterations



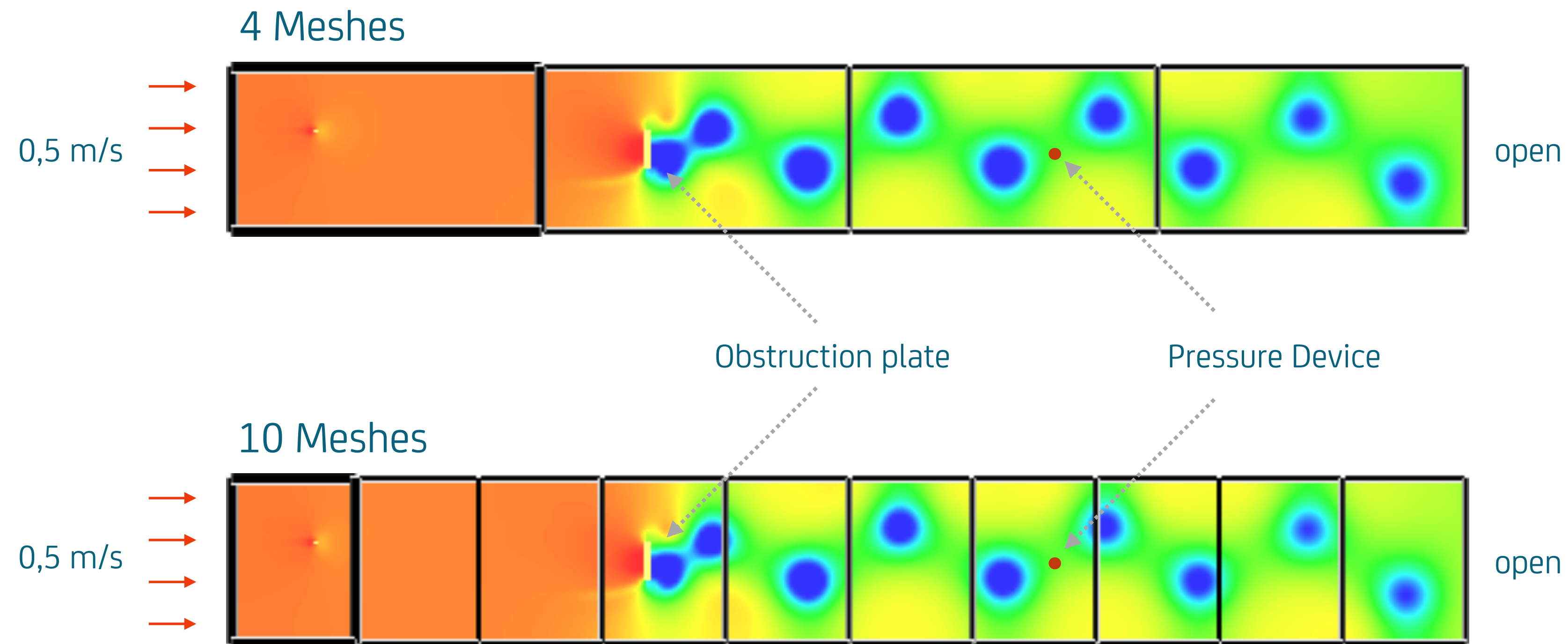
Less pressure iterations: 1 (default), max 9 (tight)

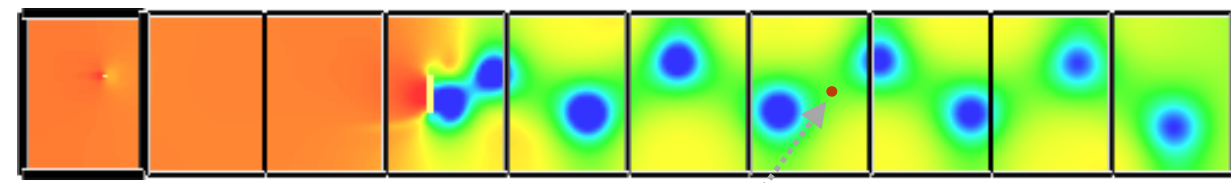
Verification case: Karman vortex street

4

dancing_eddies

ScaRC
solver

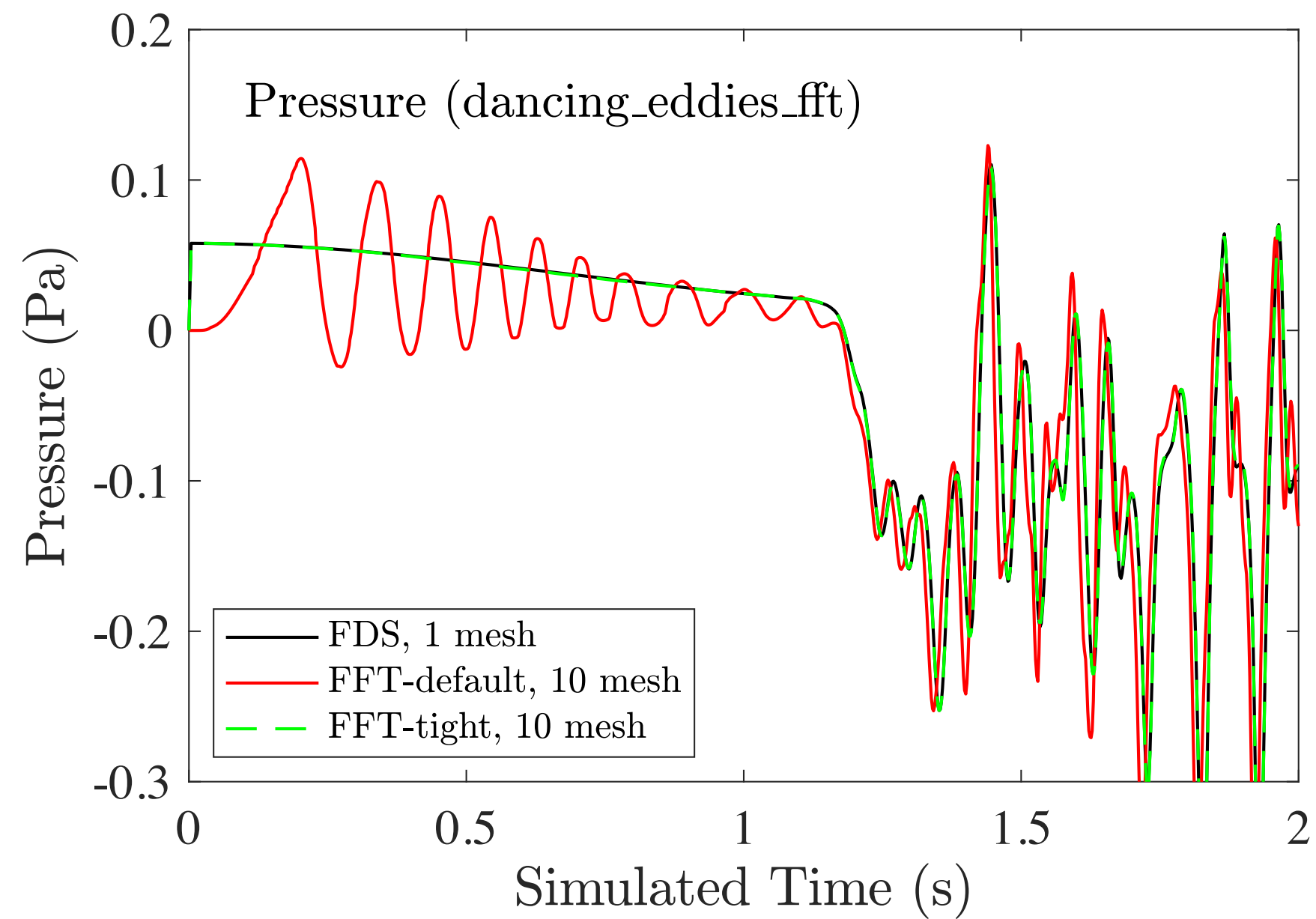




Pressure Device

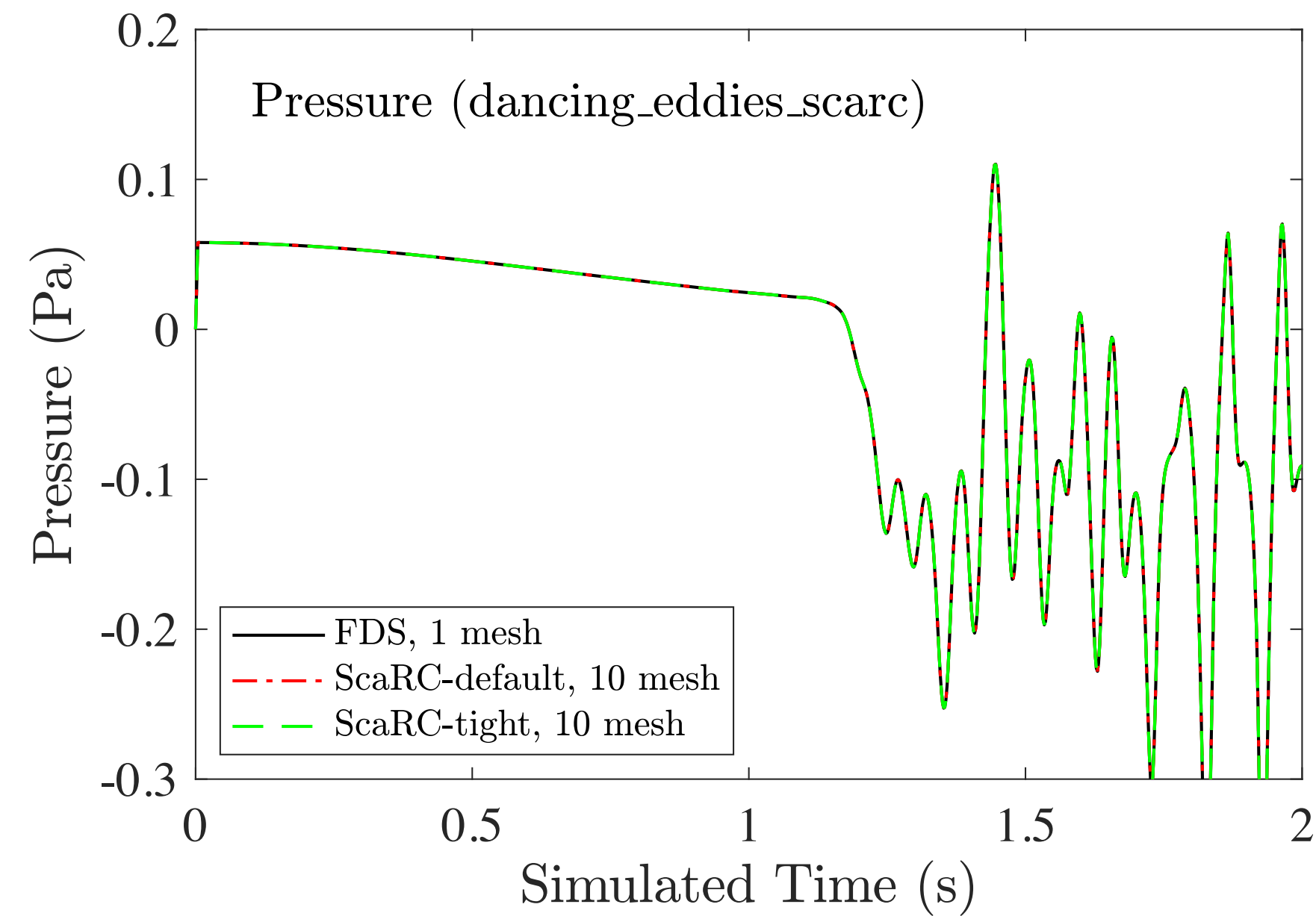
Pressure trace 10-mesh case

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



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

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



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

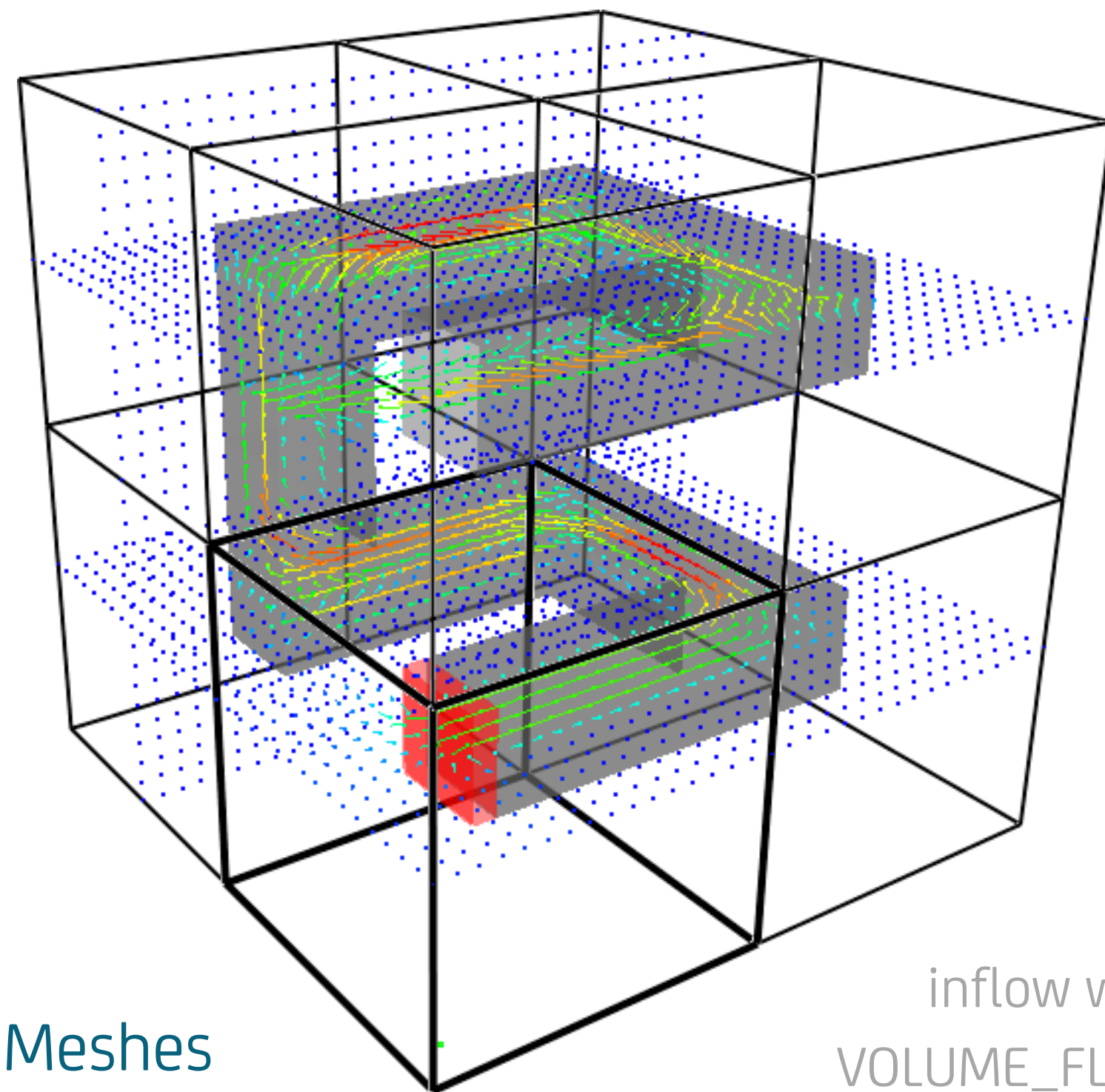
ScaRC
solver

Verification Case: Flow through a channel

4

duct_flow

ScaRC
solver

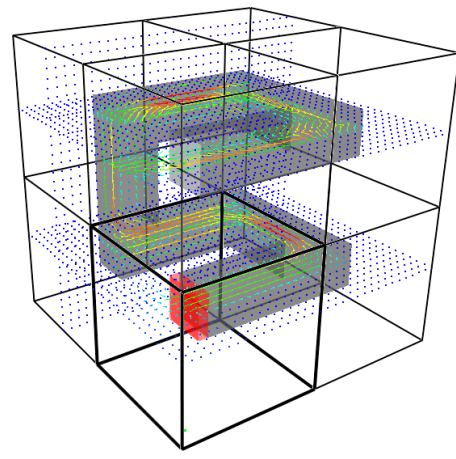


Many internal obstructions
which cause frequent
changes of flow direction

8 Meshes

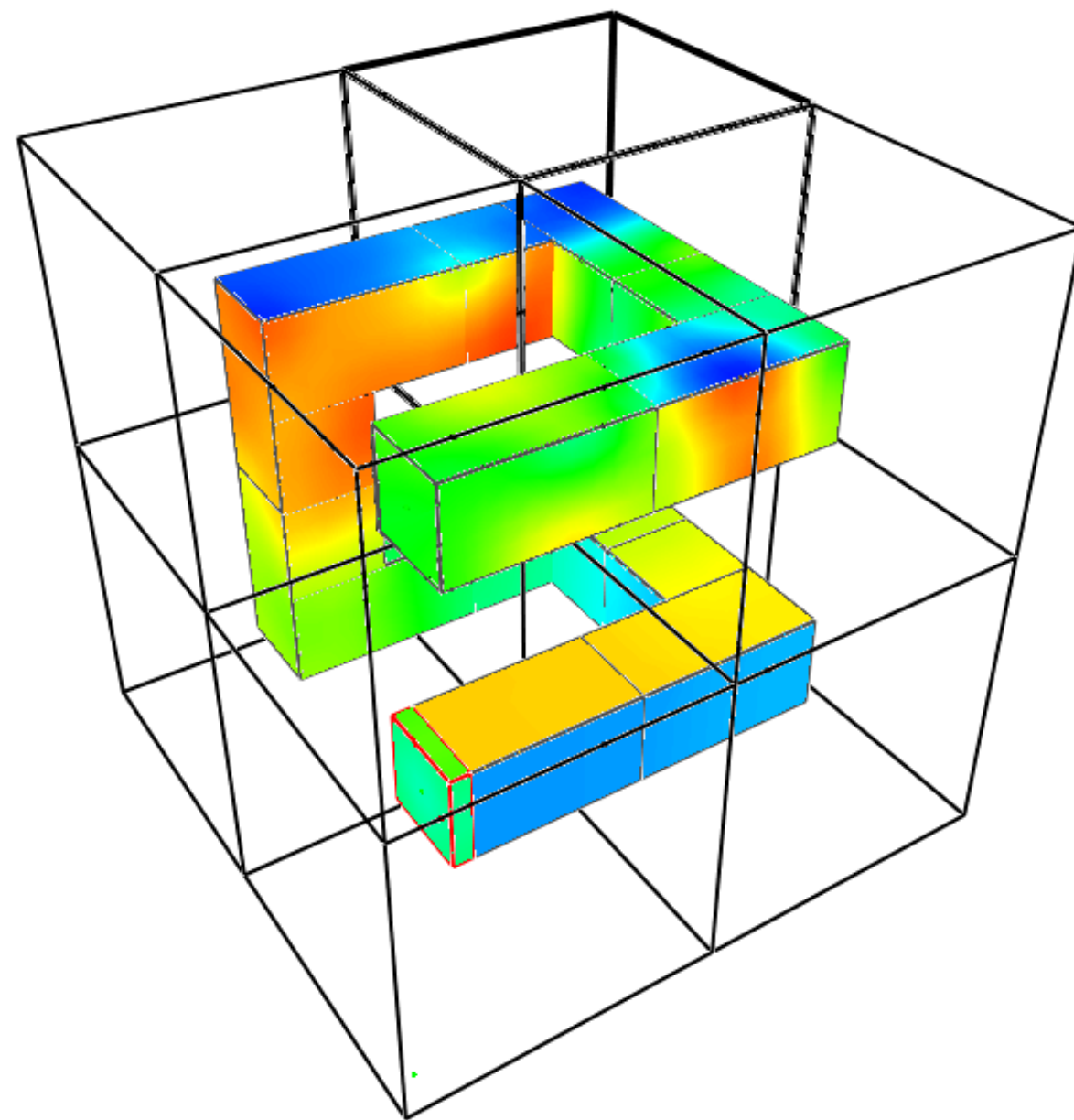
inflow with
VOLUME_FLOW = 1

Velocity error along channel



Structured

FFT and ScaRC (tol=10⁻³ m/s)



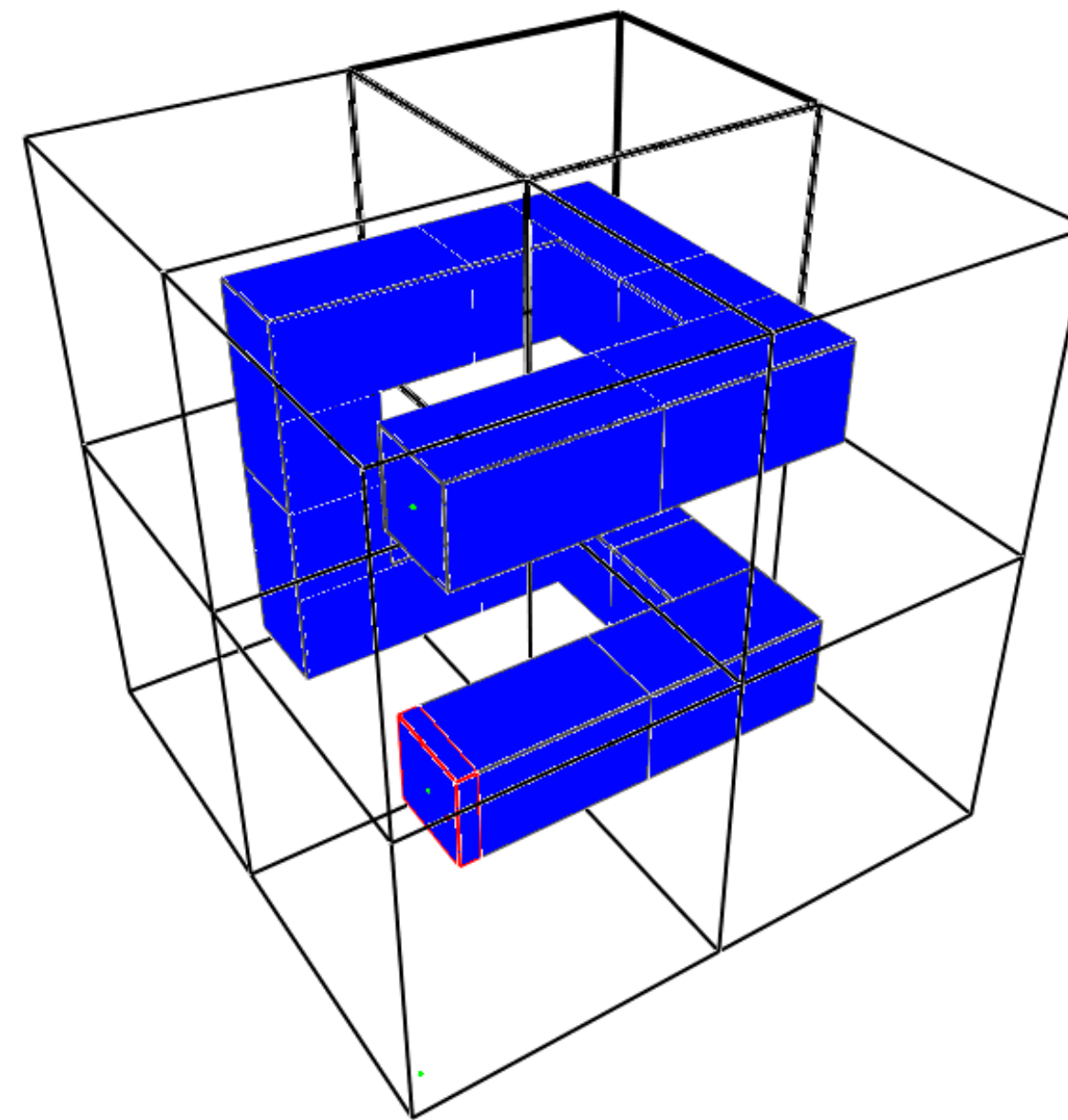
Bndry
err
m/s
*10⁻⁴



Time: 43.8

Unstructured

UGLMAT, UScaRC



Bndry
verr
m/s



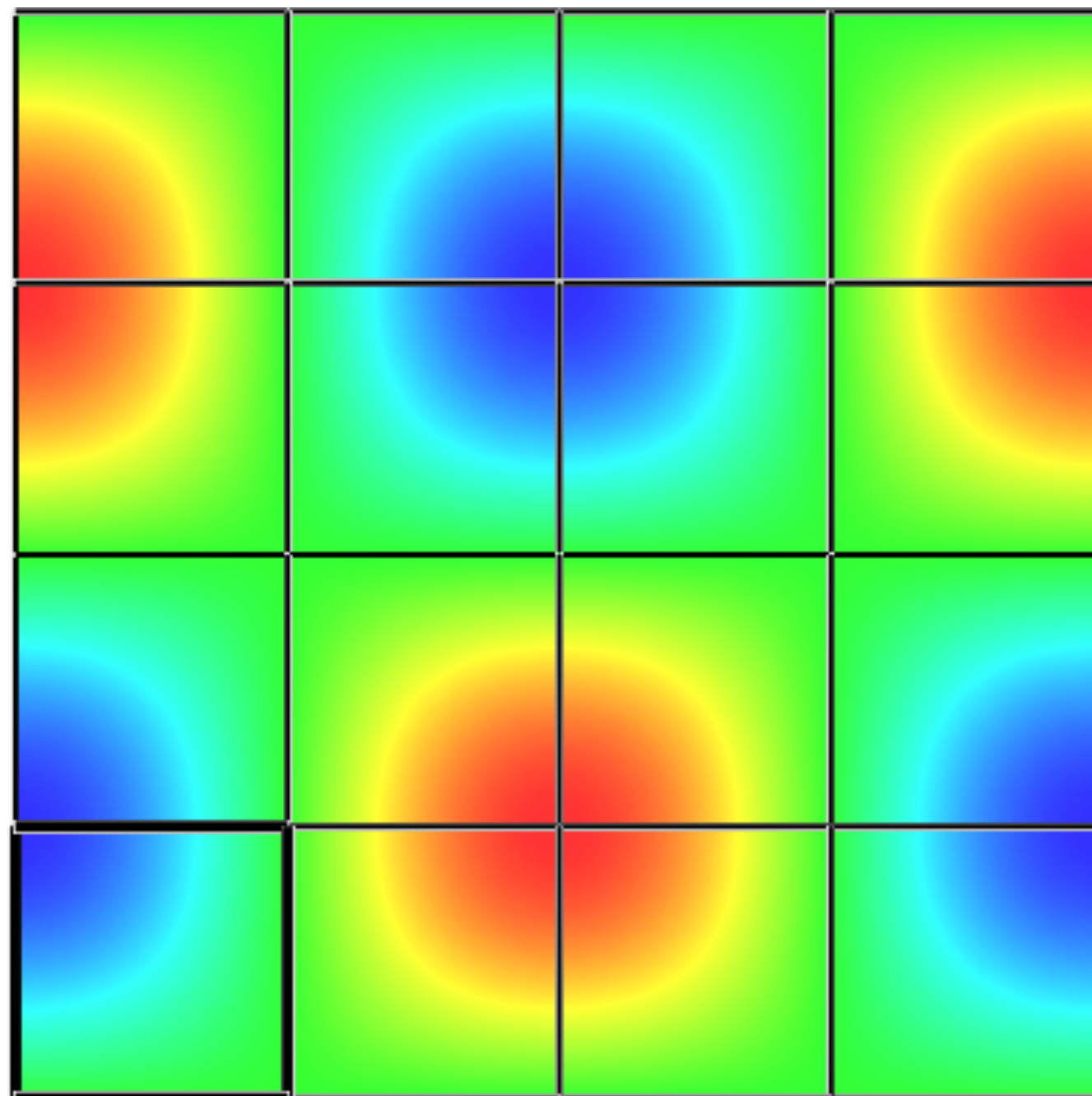
Time: 43.8

Verification cases: Periodic boundaries

4

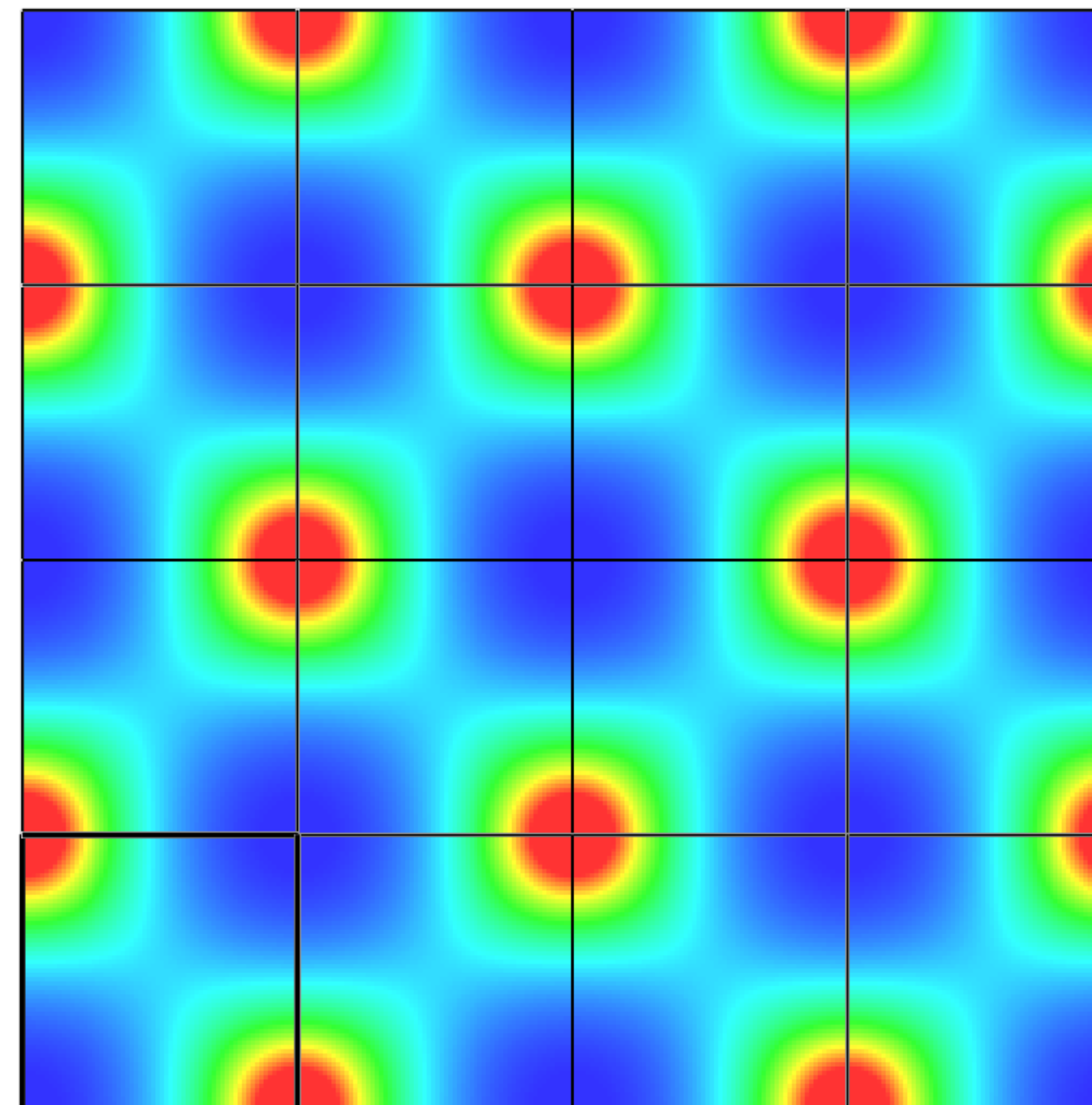
NS_Analytical_Solution

u - component velocity



shunn3

mixture fraction Z



ScaRC
16 meshes

Preserves
periodic
behavior

ScaRC
solver



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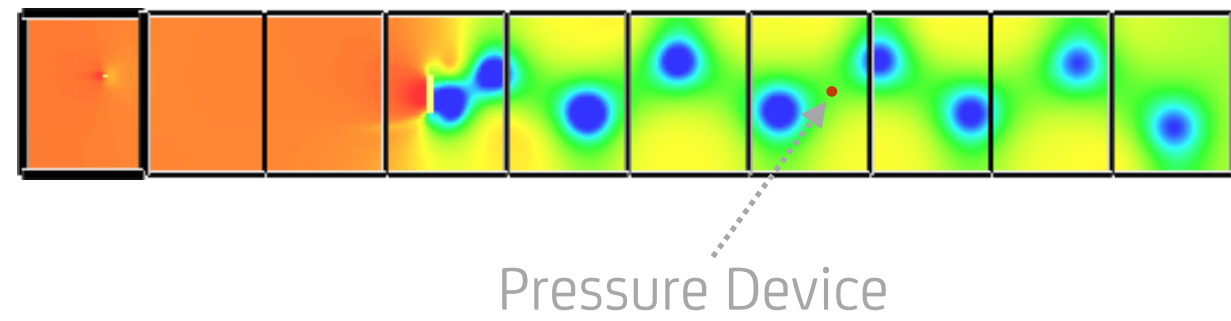
Summary

4

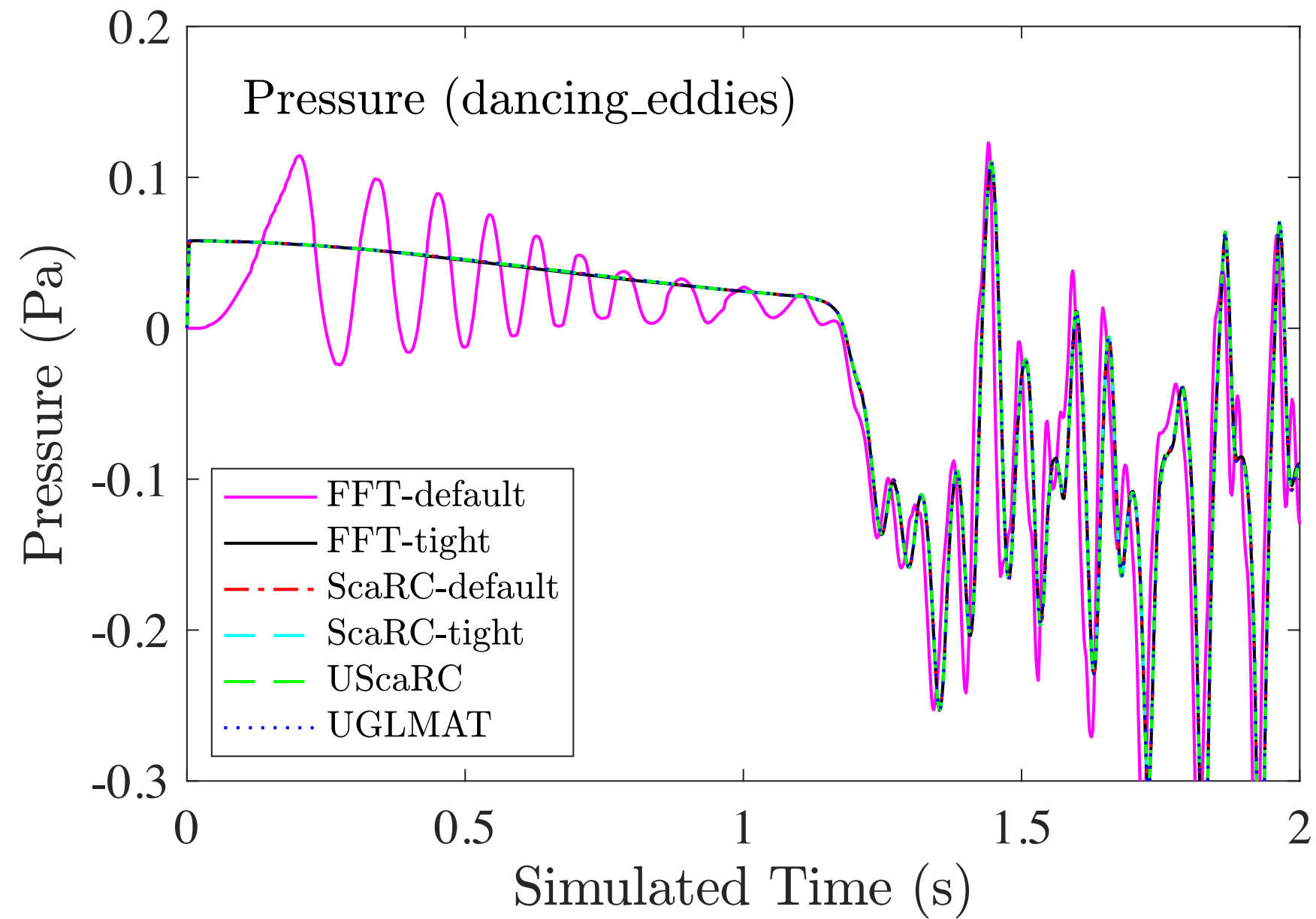
ScaRC
solver

Discretization	Solver	Pressure iteration
Structured	FFT	Internal obstructions & Mesh interfaces
	ScaRC	Internal obstructions
Unstructured	UScaRC	-
	UGLMAT	-

Pressure iterations

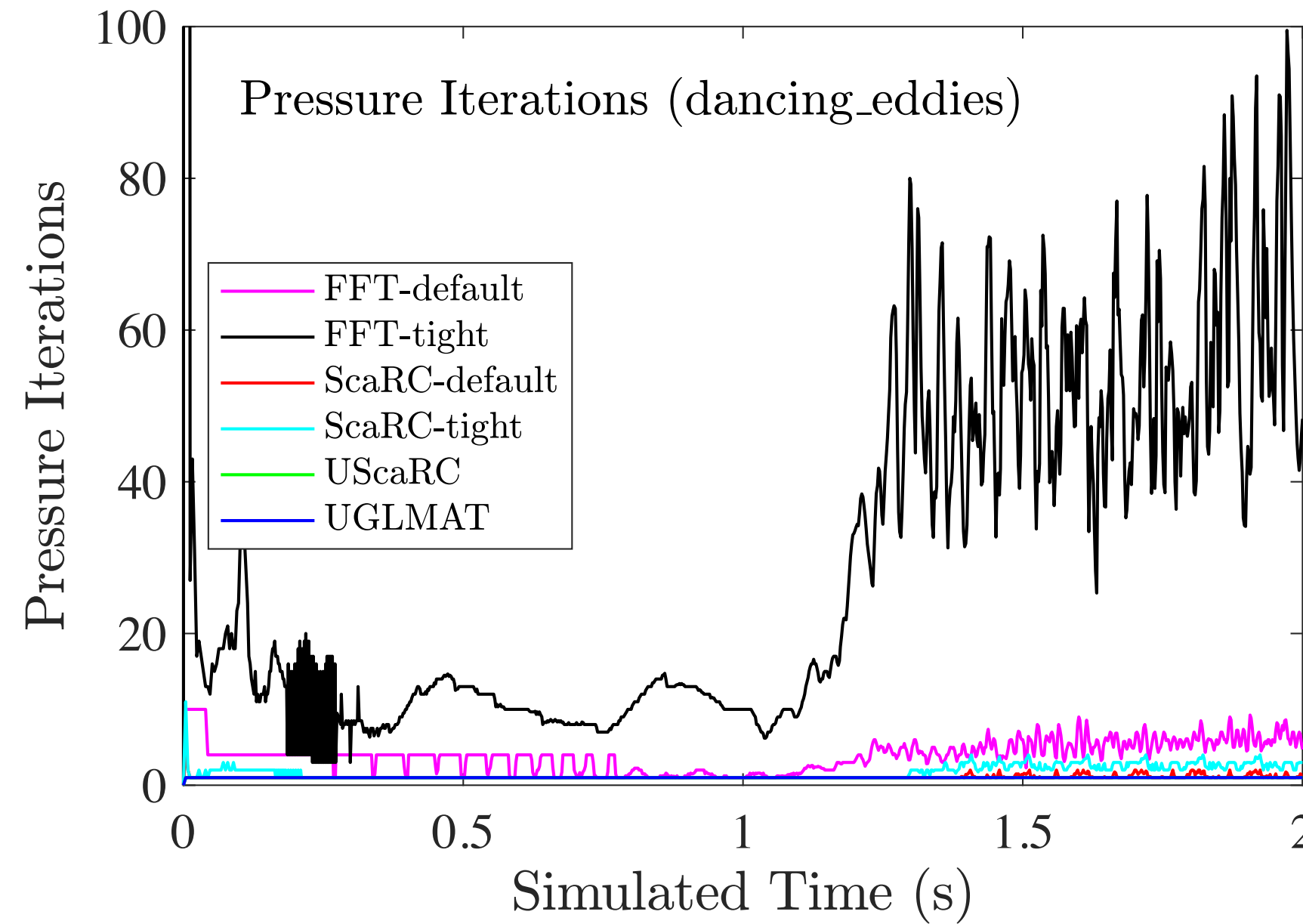


Pressure trace in upper device



Only accurate for tight pressure iteration

Number of required pressure iterations



Pressure iteration causes additional effort