Smart cloud collocation: a unified workflow from CAD to enhanced solutions

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Agenda

1. Introduction
2. Point collocation methods
3. CAD to smart cloud collocation
4. Stencil nodes selection
5. Parameter selection and solution improvement methods
6. Smart cloud adaptivity
7. Solution of collocation linear problems
8. Conclusions and perspectives

1. Introduction

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General

- Simulation tools are used to optimize system designs to:
  - ➢ increase the performance of a proposed design;
  - ➢ improve the reliability of a product;
  - ➢ lower manufacturing costs;
  - ➢ predict performance…

- The most popular and used methods are:
  - ➢ the finite element method ➔ used in the context of solid mechanics;
  - ➢ the finite volume method ➔ used in the context of computational fluid dynamics (CFD).

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What about point collocation methods ?

- Point collocation methods = strong form meshless method:
    - ➢ meshing complex domains can be extremely difficult;
    - ➢ modifying an existing mesh is challenging;
    - ➢ in case of modification of the computational domain, the generated mesh may no longer be appropriate.

Weak form meshless methods	Strong form meshless methods
• Element Free Galerkin (EFG); • Reproducing Kernel Particle Method (RKPM); • Meshless Local Petrov-Galerkin (MLPG); • Isogeometric Analysis (IGA).	• Moving Least Squares (MLS); • Generalized Finite Difference (GFD); • Radial Basis function Finite Difference (RBF-FD); • Discretization-Corrected Particle Strength Exchange (DC PSE).

What are the key steps to solve a problem with a collocation method ?

Domain definition

- CAD software
- Point cloud or mesh obtained from 3D scanner

Domain discretization

- Regular discretization
- Advancing front
- Triangulation

Stencil node selection

- Distance criteria
- Quadrant criteria
- …

Operator approximation

- GFD
- DC PSE
- MLS

Problem matrix assembly

- Boundary conditions
- Square matrix
- Not symmetric

Solution and post-processing

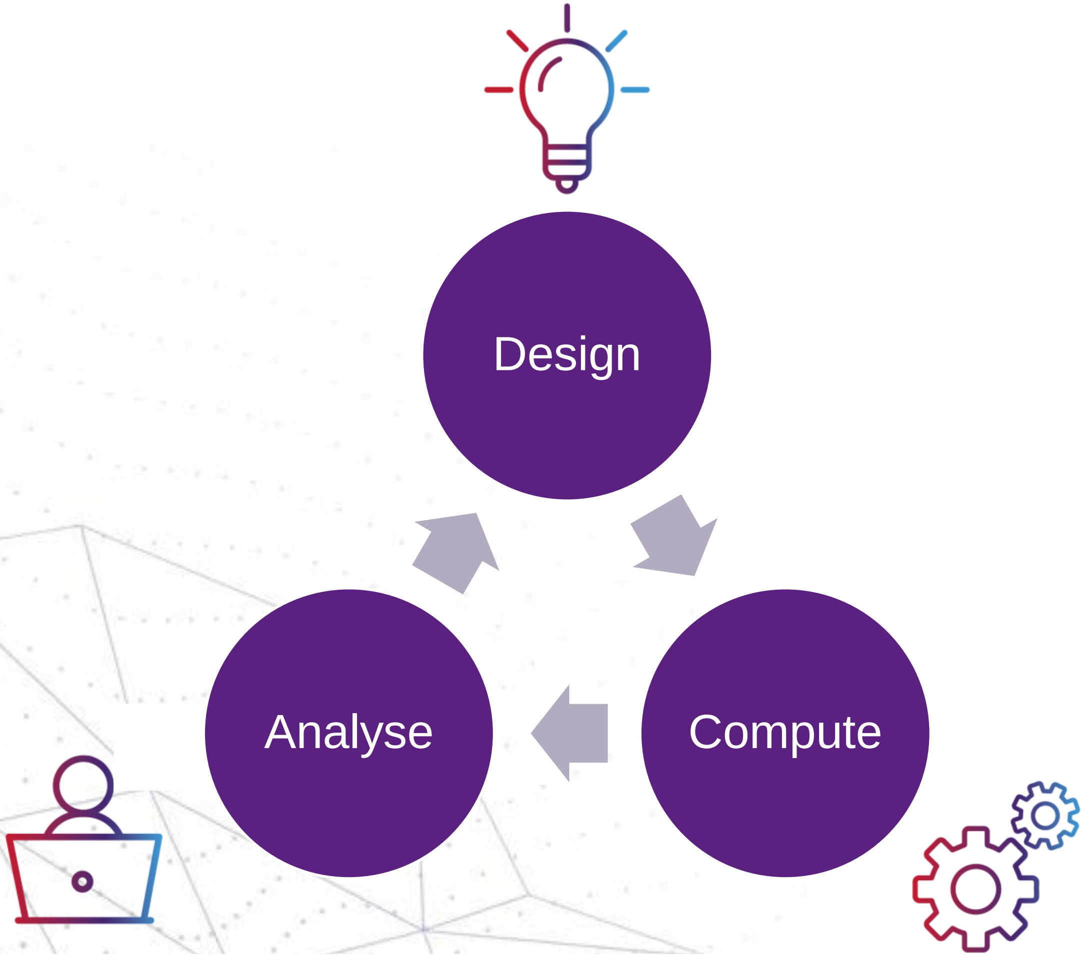
- Direct or iterative linear solvers
- System preconditioning

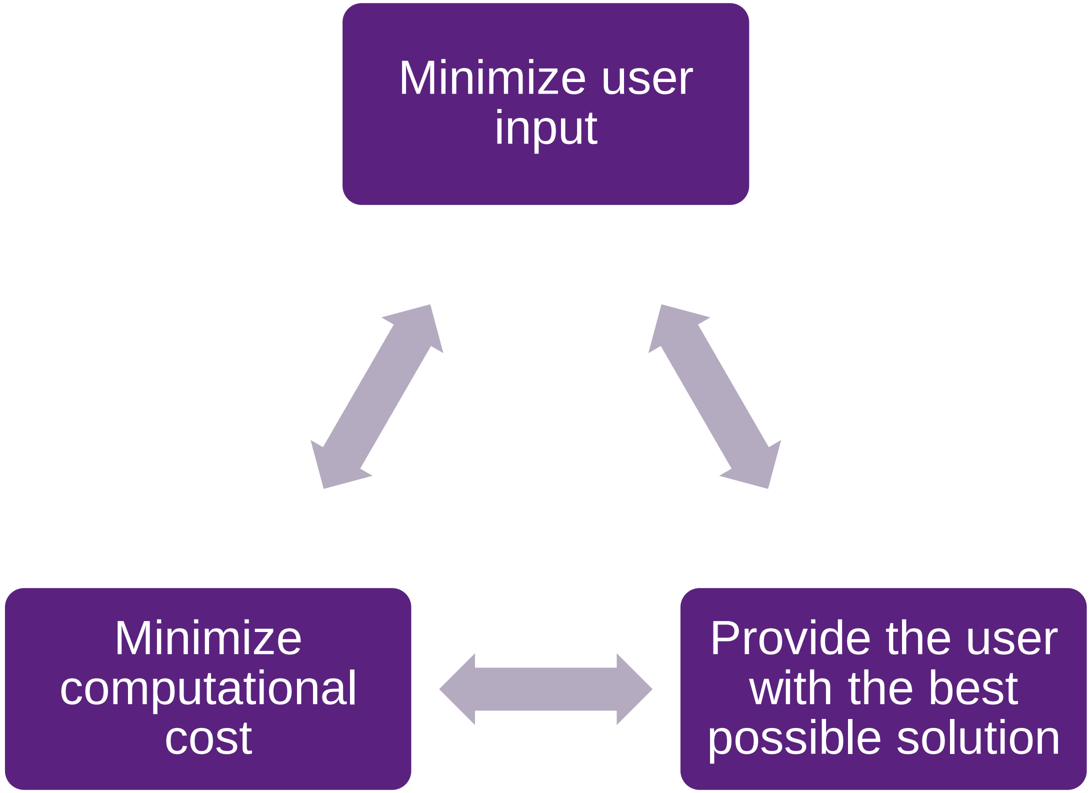
Point collocation methods: benefits and drawbacks

Benefits	Drawbacks
• Less constraints on domain discretization than element based methods; • Easy to implement; • Flexibility for domain refinement; • Collocation points can move in space.	• Domain integration is not readily possible; • Many parameters are involved; • System matrix denser and non-symmetric; • Convergence can be difficult to attain.

Scope and aim of the thesis (1/2)

Efficient design loop	Constraints





Scope and aim of the thesis (2/2)

- Linear elastic problems
  - 2D and 3D domains;
  - Smooth to singular solutions.

- Simplify the design workflow: from CAD to key engineering solutions
  - Start from a CAD file;
  - Determine a unique set of parameters applicable to most problems;
  - Improve the solution with schemes applicable to most problems;
  - Minimize computational cost;
  - Solve the linear system efficiently.

Thesis novelty and key references

Topic	Novelty	Key references
CAD to collocation	➢ Direct discretization from CAD; ➢ Exact surface normal vectors.	➢ T.J.R. Hughes et al. "Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement". In: Computer Methods in Applied Mechanics and Engineering 194.39-41 (Oct. 2005), https://doi.org/10.1016/j.cma.2004.10.008. ➢ OpenCASCADE: Open CASCADE Technology, 3D modeling & numerical simulation. https://dev.opencascade.org.
Stencil node selection	➢ Common algorithm for all the problems; ➢ Consideration of a threshold angle as part of the visibility criterion.	➢ T. Belytschko, Y.Y. Lu, and L. Gu. "Element-free Galerkin methods". In: International Journal for Numerical Methods in Engineering 37.2 (Jan. 1994). https://doi.org/10.1002/nme.1620370205. ➢ Pierre Alliez, Stéphane Tayeb, and Camille Wormser. "3D Fast Intersection and Distance Computation". In: CGAL User and Reference Manual. 5.0. CGAL Editorial Board, 2019. https://doc.cgal.org/5.0/Manual/packages.html#PkgAABBTree.
Discretization adaptivity	➢ Error indicators for point collocation methods; ➢ Smart cloud refinement based on CAD geometry.	➢ J.J. Benito et al. "An h-adaptive method in the generalized finite differences". In: Computer Methods in Applied Mechanics and Engineering 192.5-6 (Jan. 2003). https://doi.org/10.1016/s0045-7825(02)00594-7. ➢ J. Slak and G. Kosec. "Adaptive radial basis function–generated finite differences method for contact problems". In: International Journal for Numerical Methods in Engineering 119.7 (Apr. 2019). https://doi.org/10.1002/nme.6067.

2. Point collocation methods

T. Jacquemin et al. “Taylor-Series Expansion Based Numerical Methods: A Primer, Performance Benchmarking and New Approaches for Problems with Non-smooth Solutions”. Archives of Computational Methods in Engineering (Aug. 2019). https://doi.org/10.1007/s11831-019-09357-5.

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The Generalized Finite Difference (GFD) method (1/2)

- The Finite Difference method is the oldest method for solving PDEs numerically;
- A generalization of the method was proposed by Jensen in 1962;
- The method is based on a Taylor’s Series Expansion of the unknown field.

- In 2D, we have for $\boldsymbol{X_{pk}}$ close to $\boldsymbol{X_c}$:

$$f(\boldsymbol{X_{pk}}) = \sum_{i=0}^{+\infty}\sum_{j=0}^{+\infty}\left(\frac{\partial^{i+j} f(\boldsymbol{X_c})}{\partial^i x \partial^i y}\frac{(x_{pk}-x_c)^i}{i!}\frac{(y_{pk}-y_c)^j}{j!}\right)$$

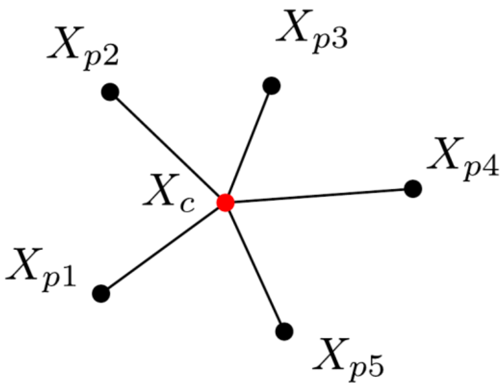
- The second order approximation is:

$$f_h(\boldsymbol{X_{pk}}) = f(\boldsymbol{X_c}) + (x_{pk}-x_c)\frac{\partial f(\boldsymbol{X_c})}{\partial x} + (y_{pk}-y_c)\frac{\partial f(\boldsymbol{X_c})}{\partial y} + \frac{(x_{pk}-x_c)^2}{2!}\frac{\partial^2 f(\boldsymbol{X_c})}{\partial^2 x}$$

$$+(x_{pk}-x_c)(y_{pk}-y_c)\frac{\partial^2 f(\boldsymbol{X_c})}{\partial x \partial y} + \frac{(y_{pk}-y_c)^2}{2!}\frac{\partial^2 f(\boldsymbol{X_c})}{\partial^2 y}$$

The Generalized Finite Difference (GFD) method (2/2)

- The equation can be written for five nodes in the vicinity of the collocation node;



- Knowing the field values at the collocation node and at the neighbouring nodes, the field derivatives can be approximated;

- To improve the robustness of the approximation more nodes than derivatives are selected. The functional $B_h(\boldsymbol{X_c})$ is minimized:

$$B_h(\boldsymbol{X_c}) = \sum_{k=1}^{m} w(\boldsymbol{X_{pk}} - \boldsymbol{X_c}) \Bigg[f(\boldsymbol{X_c}) - f(\boldsymbol{X_{pk}}) + (x_{pk} - x_c)\frac{\partial f(\boldsymbol{X_c})}{\partial x} + (y_{pk} - y_c)\frac{\partial f(\boldsymbol{X_c})}{\partial y} + \frac{(x_{pk} - x_c)^2}{2!}\frac{\partial^2 f(\boldsymbol{X_c})}{\partial^2 x} + (x_{pk} - x_c)(y_{pk} - y_c)\frac{\partial^2 f(\boldsymbol{X_c})}{\partial x \partial y} + \frac{(y_{pk} - y_c)^2}{2!}\frac{\partial^2 f(\boldsymbol{X_c})}{\partial^2 y} \Bigg]^2$$

The Discretization-Corrected Particle Strength Exchange (DC PSE) method

- The Taylor's series expansions is convoluted by a function η on a domain Ω_c associated to $\boldsymbol{X_c}$;

$$\int_{\Omega_c} f(\boldsymbol{X_{pk}})\eta(\boldsymbol{X_{pk}}-\boldsymbol{X_c})d\boldsymbol{X_{pk}} = \sum_{i=0}^{+\infty}\sum_{j=0}^{+\infty}\int_{\Omega_c} \frac{\partial^{i+j} f(\boldsymbol{X_c})}{\partial^i x \partial^j y}\frac{(x_{pk}-x_c)^i}{i!}\frac{(y_{pk}-y_c)^j}{j!}\eta(\boldsymbol{X_{pk}}-\boldsymbol{X_c})d\boldsymbol{X_{pk}}$$

- η is selected so that:

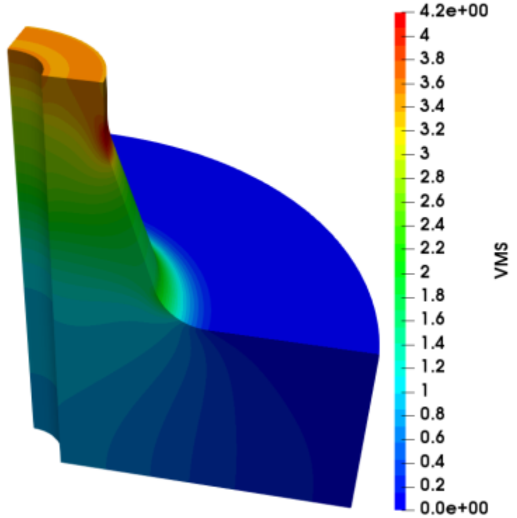
$$\frac{\partial^{i+j} f(\boldsymbol{X_c})}{\partial^i x \partial^i y} = \int_{\Omega_c} f_h(\boldsymbol{X_c})\eta(\boldsymbol{X_{pk}}-\boldsymbol{X_c})d\boldsymbol{X_{pk}} \simeq \sum_{k\in\Omega_c} f_h(\boldsymbol{X_c})\eta(\boldsymbol{X_{pk}}-\boldsymbol{X_c})$$

- η is the product of a correction function $K(\boldsymbol{X})$ and of a weight function $w(\boldsymbol{X})$;

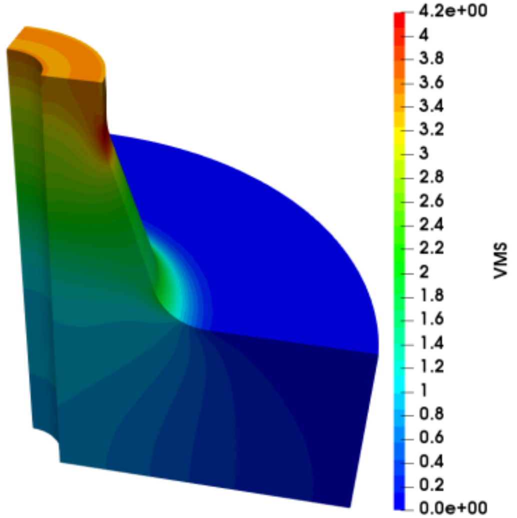
$$\eta(\boldsymbol{X}) = K(\boldsymbol{X})w(\boldsymbol{X})$$

- $K(\boldsymbol{X})$ is different for each derivative approximation.

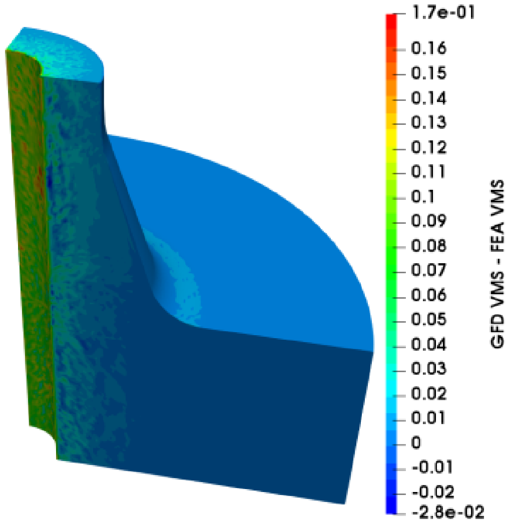
Some results

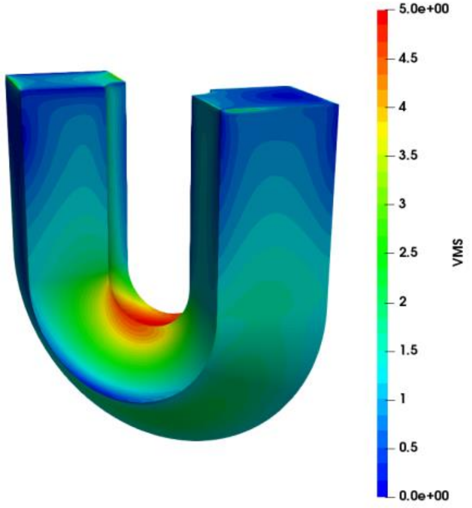


GFD solution

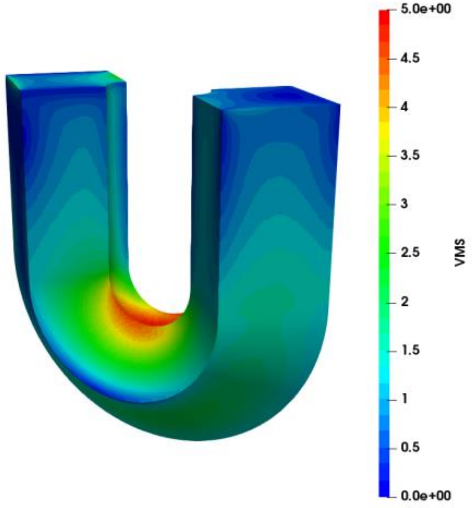


FEA solution

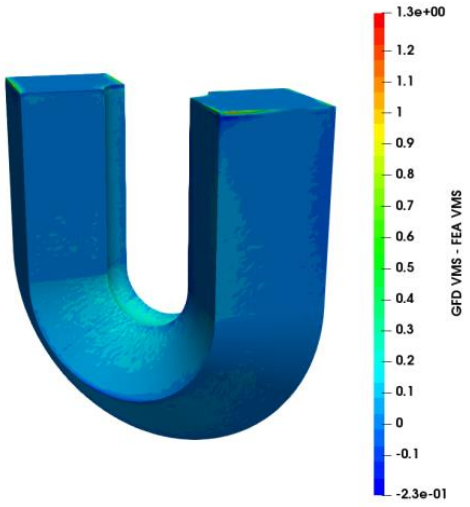


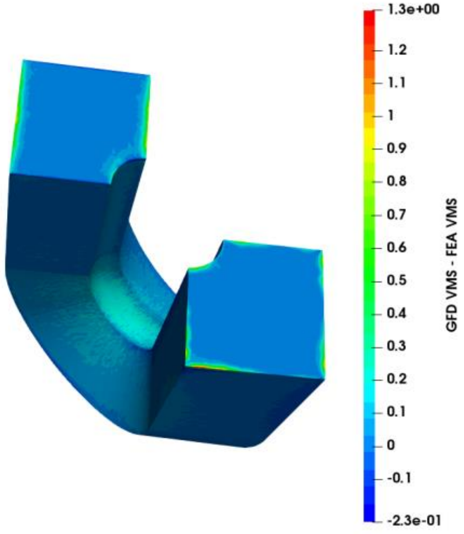


GFD solution



FEA solution





3. CAD to smart cloud collocation

CAD files, how are they composed ?

- Description of the boundary of the domain;
  - Topological and geometrical entities

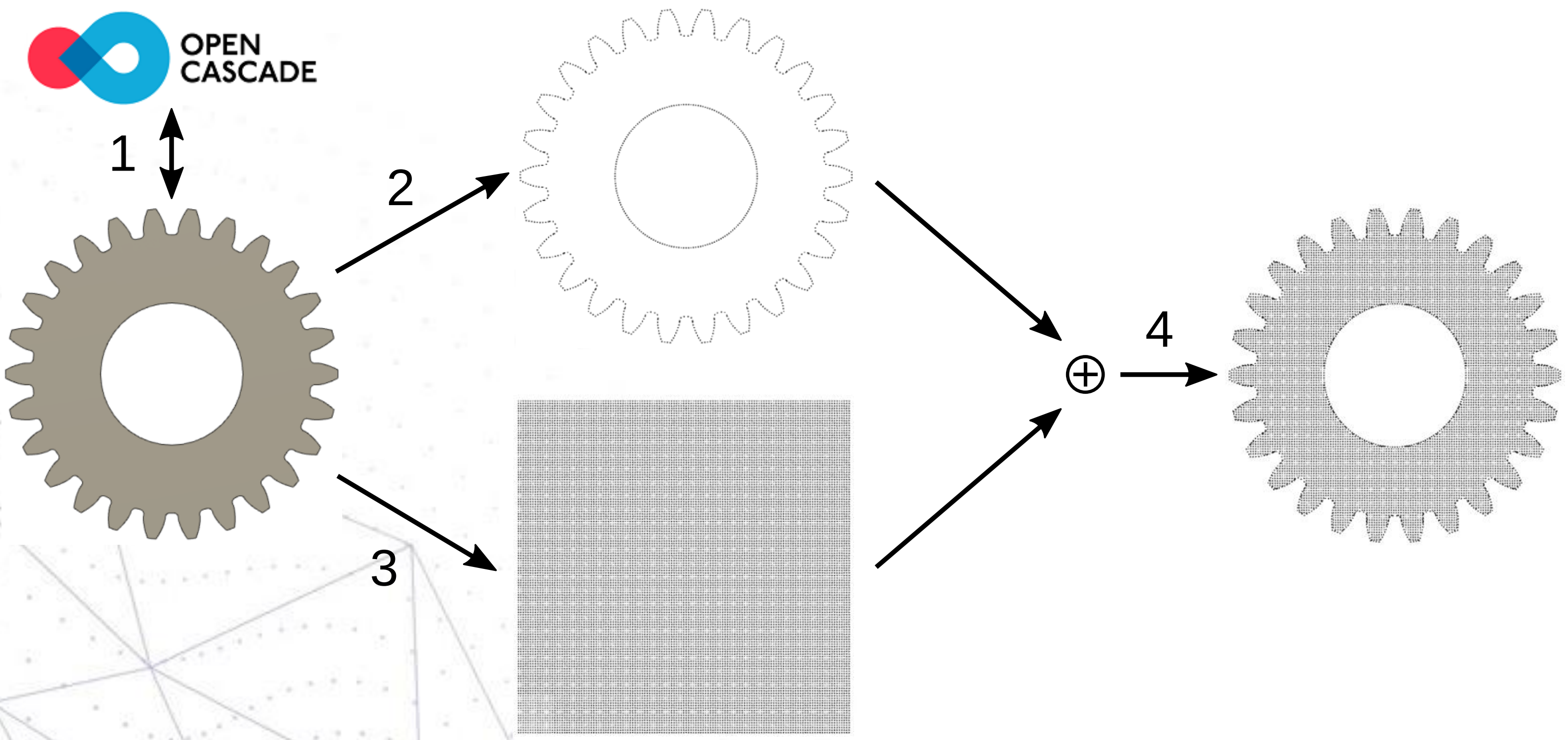
- Topology defines relationships between simple geometric entities;

- Topological entities:
  - solid;
  - shell;
  - face;
  - wire;
  - edge;
  - vertex.

- Geometrical entities are:
  - surface;
  - curve;
  - vertex.

Domain discretization (1/2)

Key steps	Discretization parameters



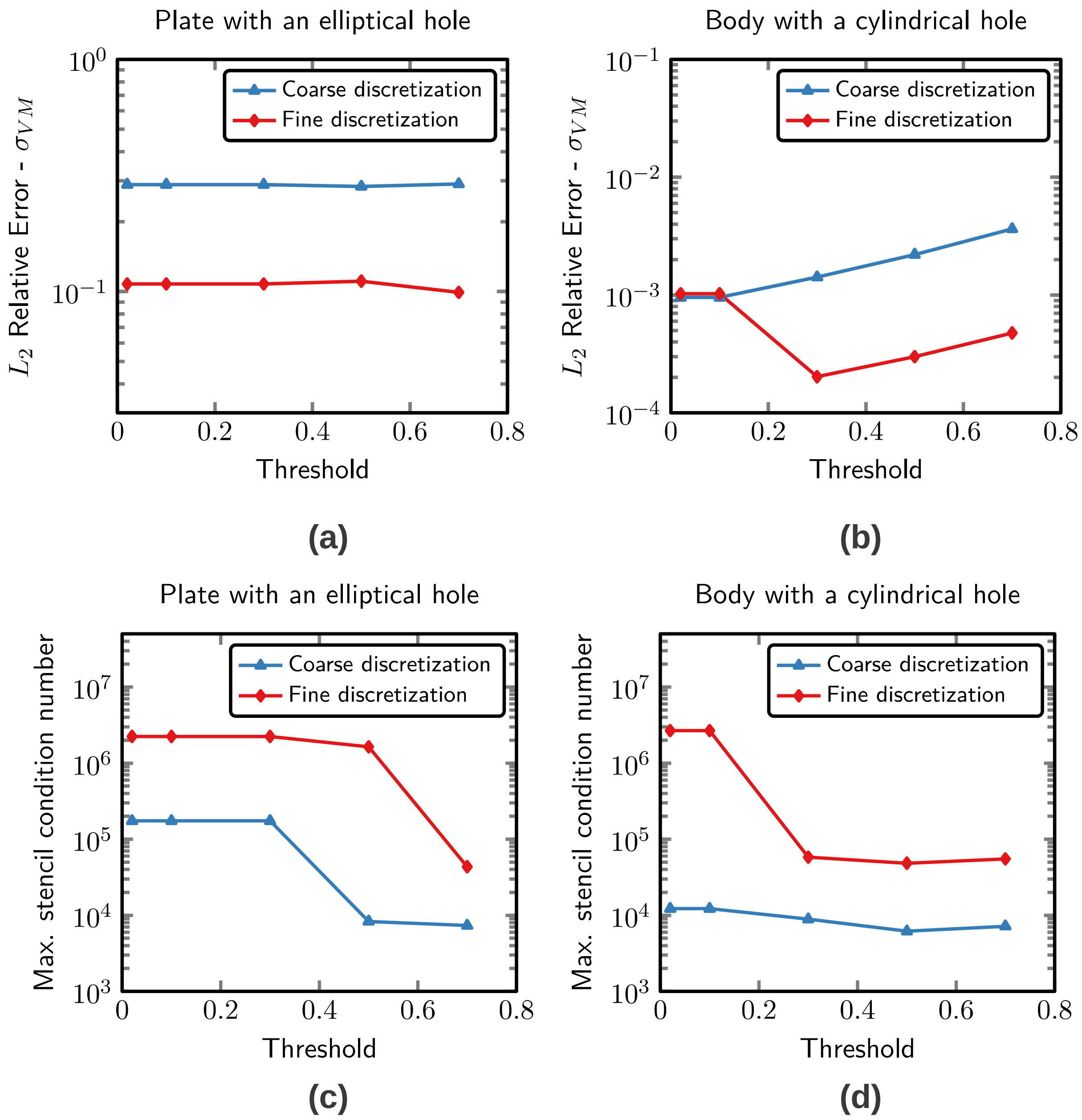
- characteristic lengths;
- regular node arrangement pattern;
- node removal threshold (fraction of the characteristic length).

Domain discretization (2/2)

- The selected discretization threshold impacts:
  - ➢ the error;
  - ➢ the stencil condition number.

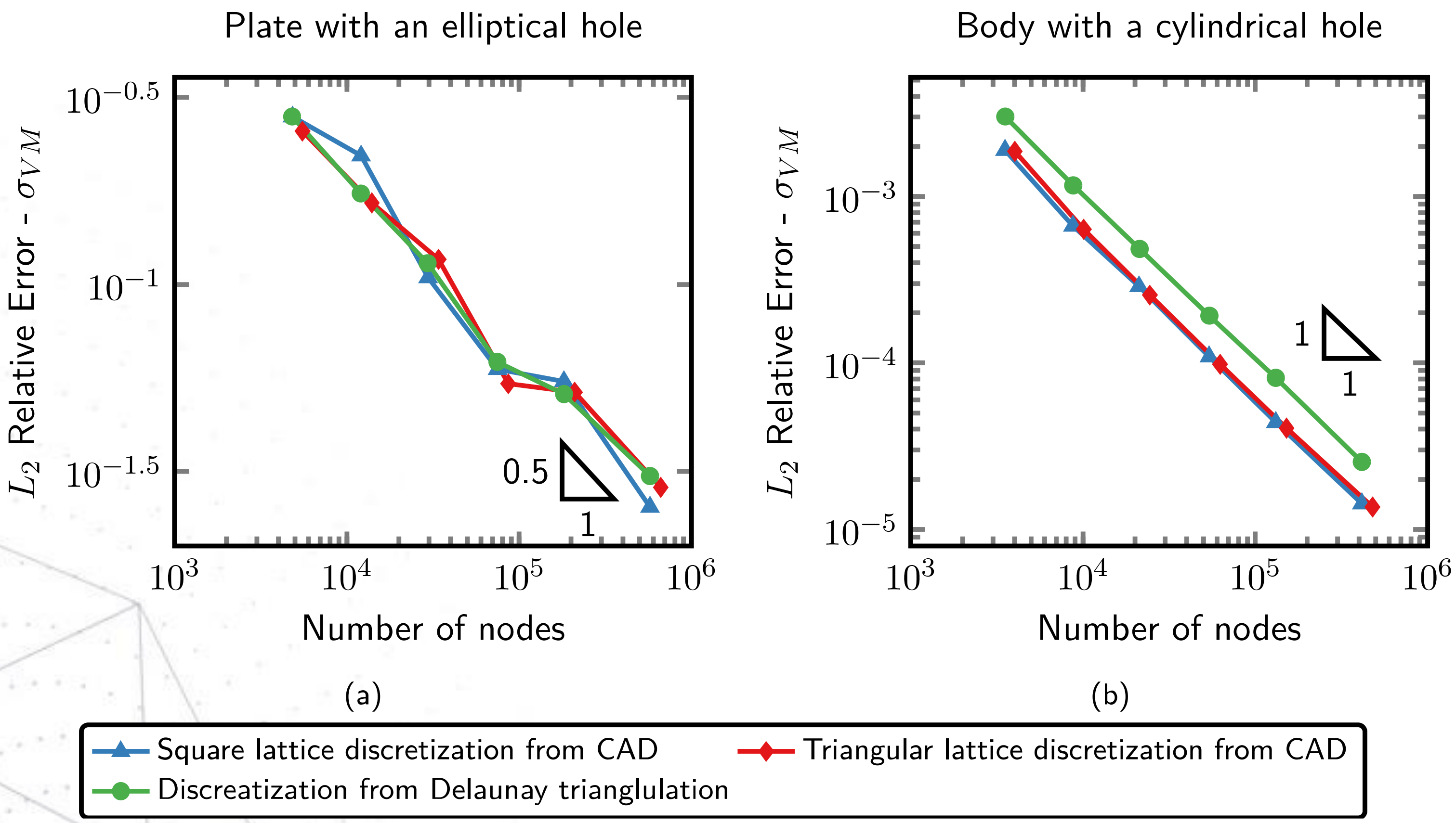
- The threshold of 0.3 leads to the lowest error:

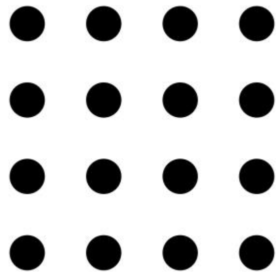
➔ selected threshold in this thesis.



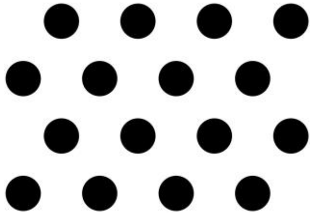
Domain discretization comparison

- Little impact of regular node arrangement pattern on the error.





Square lattice



Triangular lattice

4. Stencil nodes selection

T. Jacquemin et al. “Taylor-Series Expansion Based Numerical Methods: A Primer, Performance Benchmarking and New Approaches for Problems with Non-smooth Solutions”. Archives of Computational Methods in Engineering (Aug. 2019). https://doi.org/10.1007/s11831-019-09357-5.

T. Jacquemin and S.P.A. Bordas. “A unified algorithm for the selection of collocation stencils for convex, concave and singular problems”. International Journal for Numerical Methods in Engineering (Apr. 2021). https://doi.org/10.1002/nme.6703.

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Impact of the stencil size on the error (1/2)

- Small stencil may be inaccurate due to poor node arrangements;
- Large stencils tend to smooth the field too much.

➔ a compromise needs to be found.

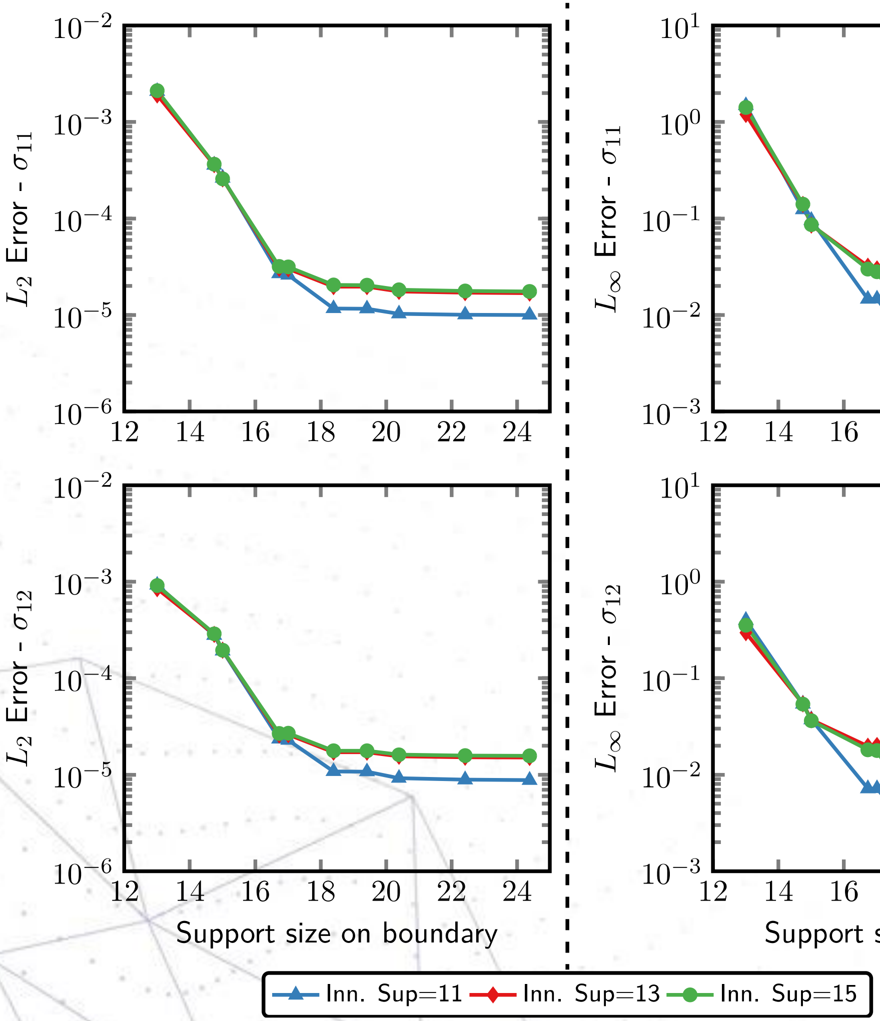
- Derivatives approximation are less accurate close to the boundary

➔ larger stencils may be required.

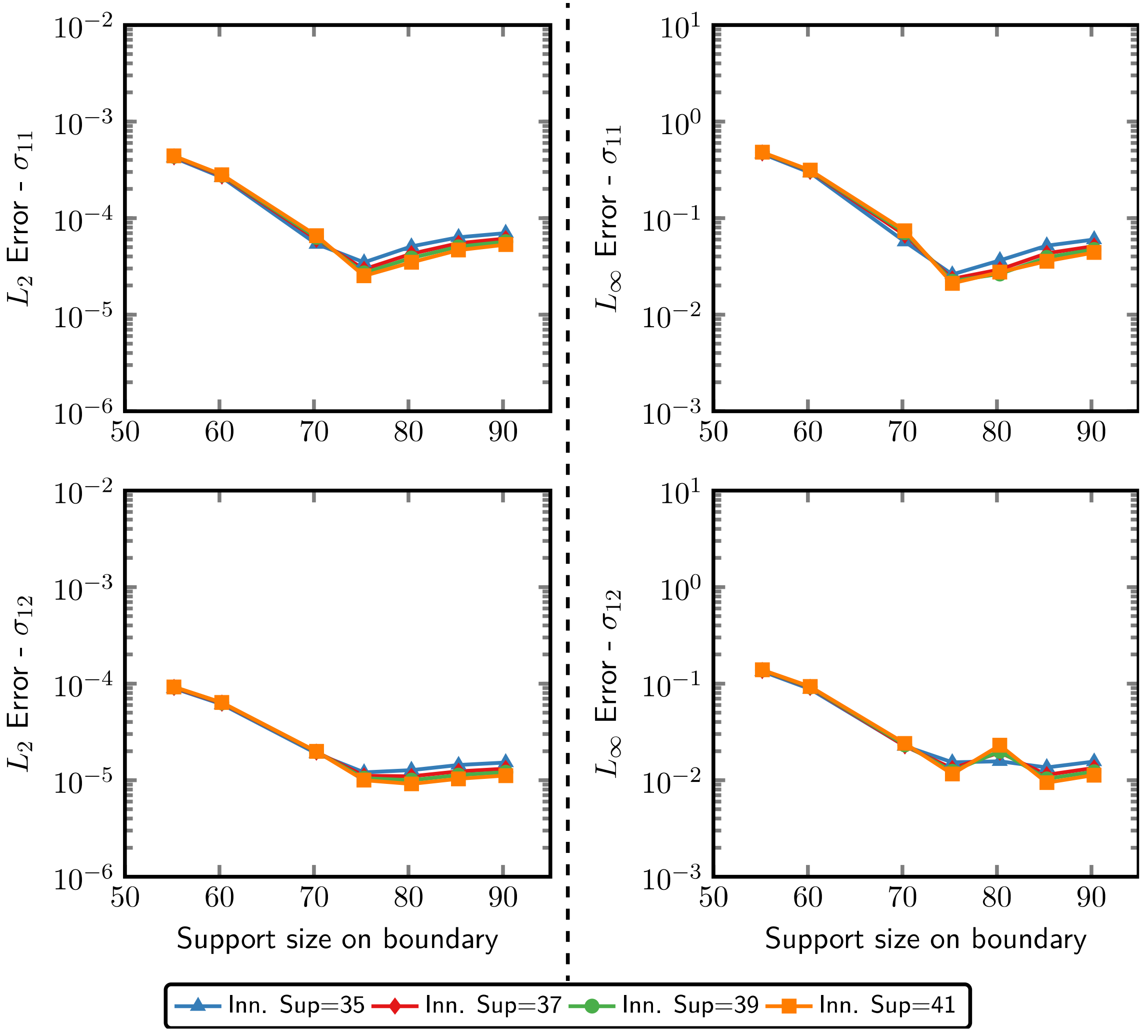
- The stencils are more balanced in the interior of the domain

➔ smaller stencils may be better.

Impact of the stencil size on the error (2/2)



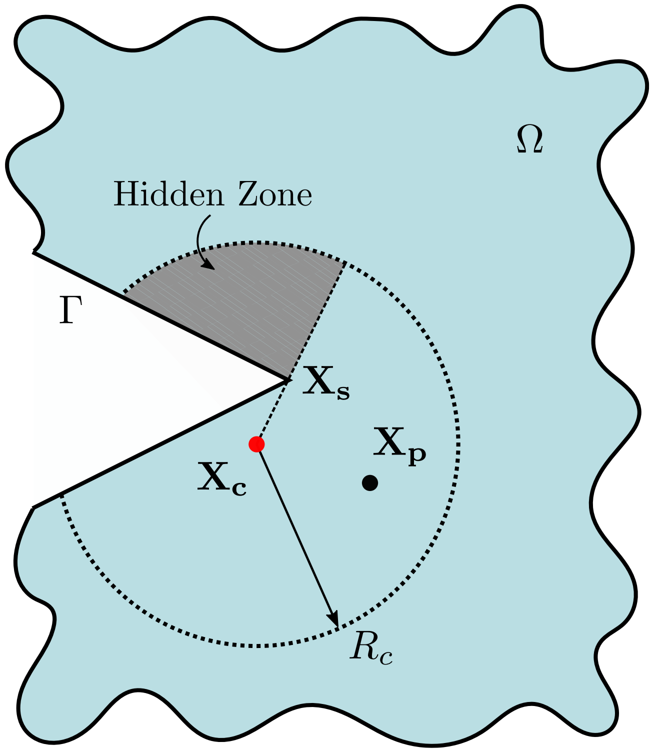
2D cylinder – GFD method



3D sphere – GFD method

Node selection close to a concavities

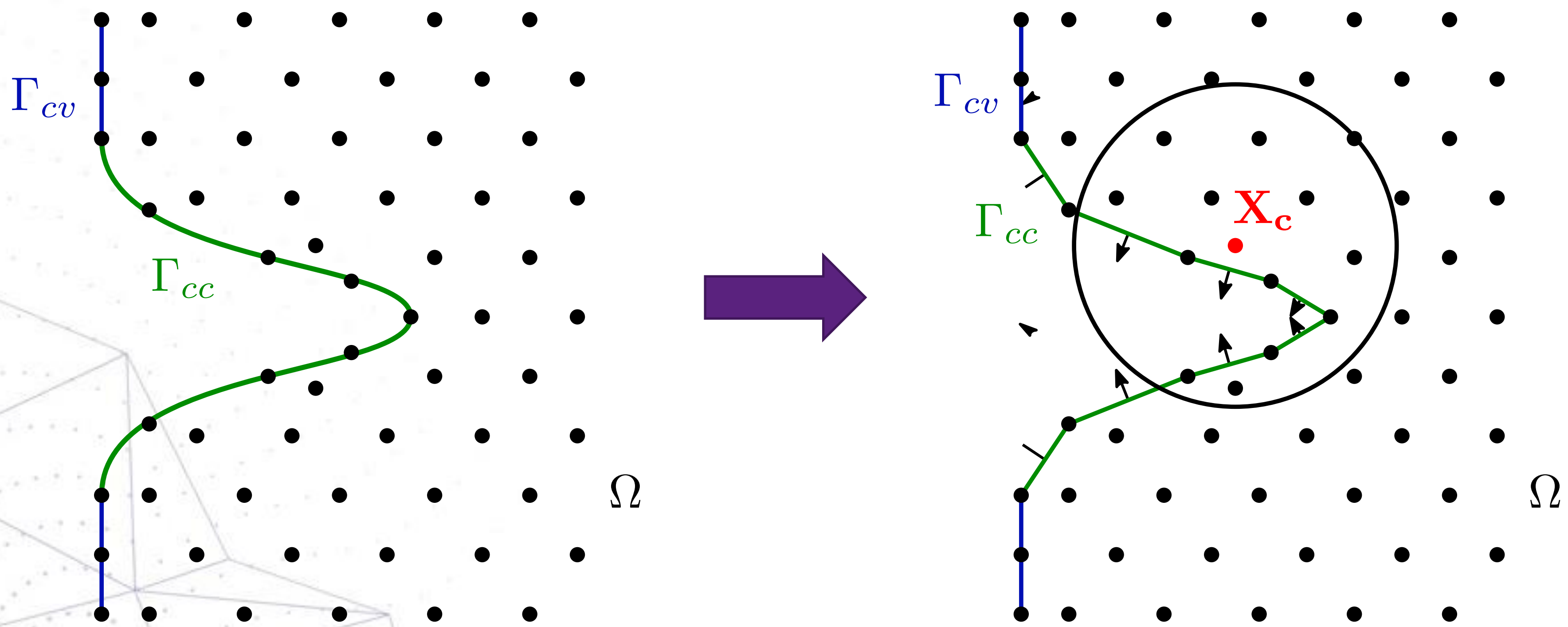
- The field should be sufficiently smooth over the collocation stencil;
- Close to singularities or concavities, the field is not smooth;
- The visibility criterion was introduced for singular problems;
- This criterion can be generalized to all the concave problems.



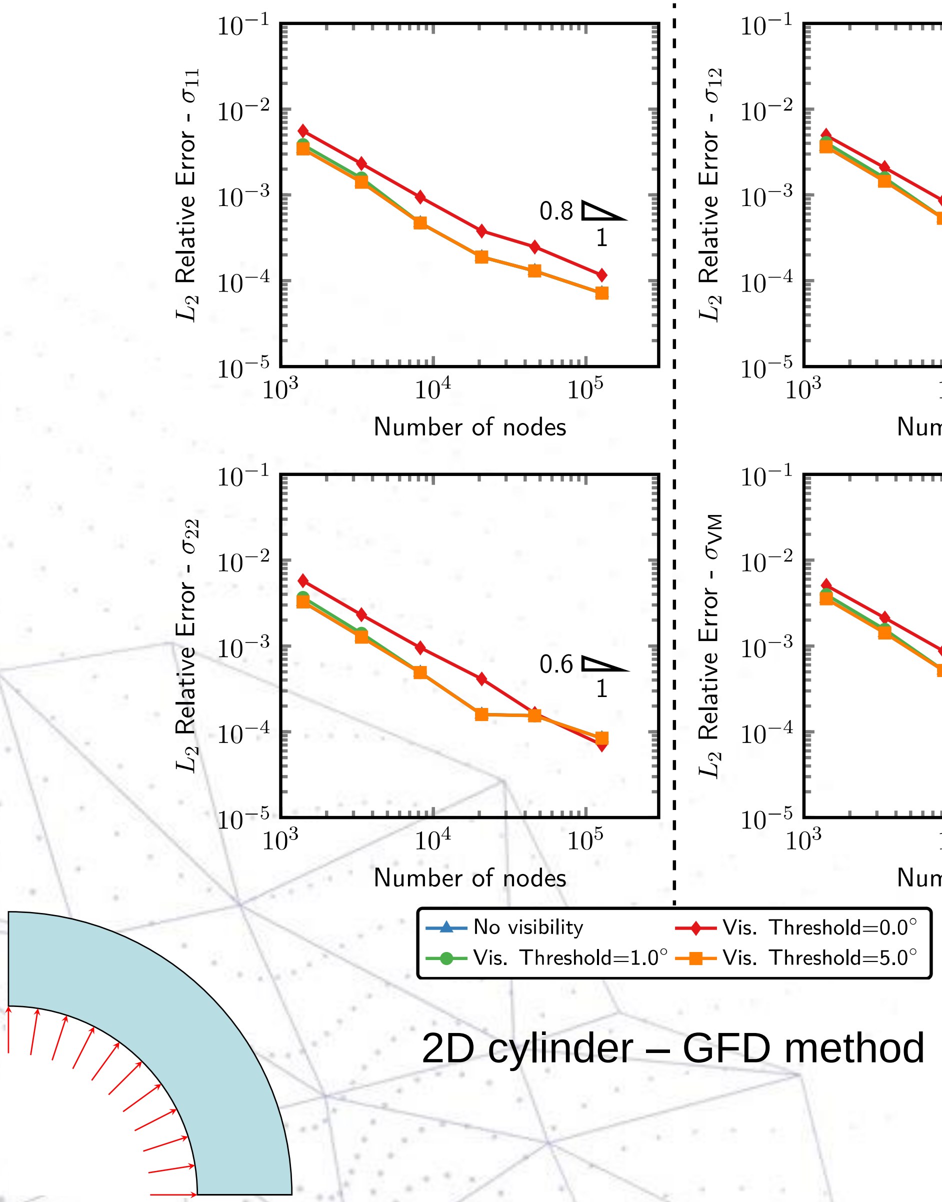
Visibility criterion principle

Generalized visibility criterion (1/2)

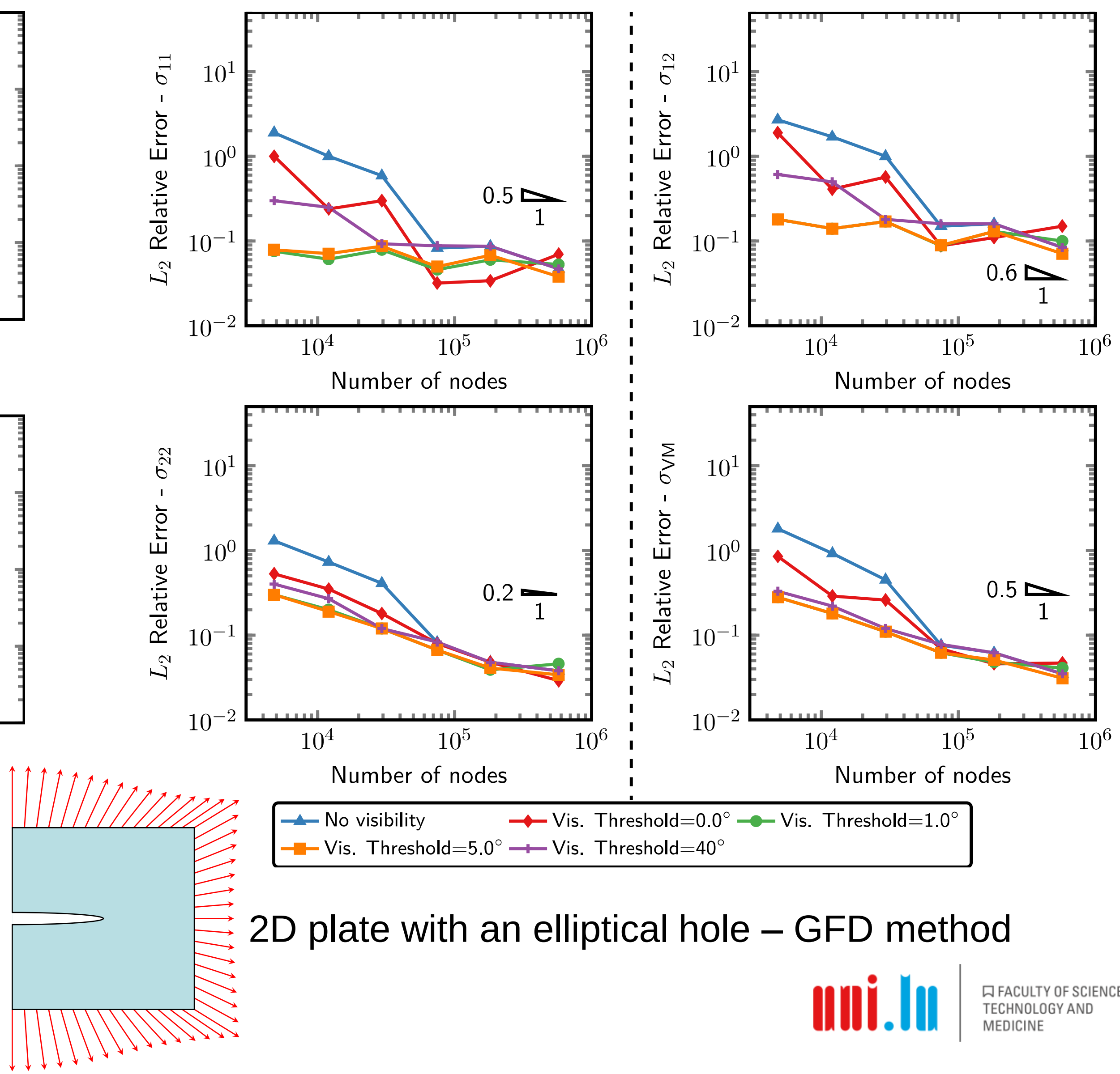
- Boundary elements are used in the concave regions;
- The normal vectors to these elements are computed;
- Determine is the segment connecting $\boldsymbol{X_c}$ to a support node intersects a boundary element;
- A threshold angle needs to be selected.



Generalized visibility criterion (2/2)



2D cylinder – GFD method



2D plate with an elliptical hole – GFD method

5. Parameter selection and solution improvement methods

T. Jacquemin et al. “Taylor-Series Expansion Based Numerical Methods: A Primer, Performance Benchmarking and New Approaches for Problems with Non-smooth Solutions”. Archives of Computational Methods in Engineering (Aug. 2019). https://doi.org/10.1007/s11831-019-09357-5.

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Parametric study

Parameter	GFD	DC PSE
Weight Function Type	4th order spline	Exponential
Weight Function Parameter	γ = 0.75	α = 1, ε = 0.30
Correction Function	N/A	Polynomial
Size of Inner Nodes Support (2D / 3D)	11 / 37	13 / 37
Size of Boundary Nodes Support (2D / 3D)	19 / 75	19 / 75

- 4^{th} order spline composed with a power function

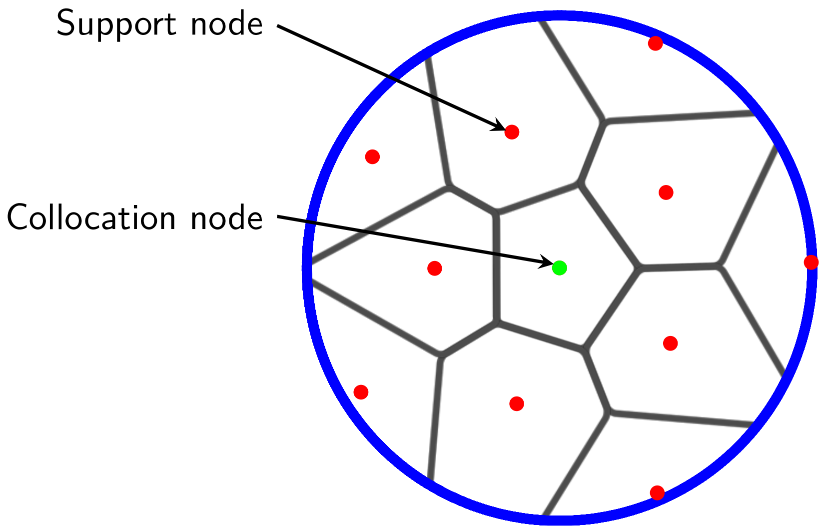
$$w(s) = \begin{cases} (1 - 6s^2 + 8s^3 - 3s^4)^\gamma & \text{if} \quad s \le 1 \\ 0 & \text{if} \quad s > 1 \end{cases}$$

- Exponential weight function

$$w(s) = \begin{cases} e^{-s^\alpha \varepsilon^{-2}} & \text{if} \quad s \le 1 \\ 0 & \text{if} \quad s > 1 \end{cases}$$

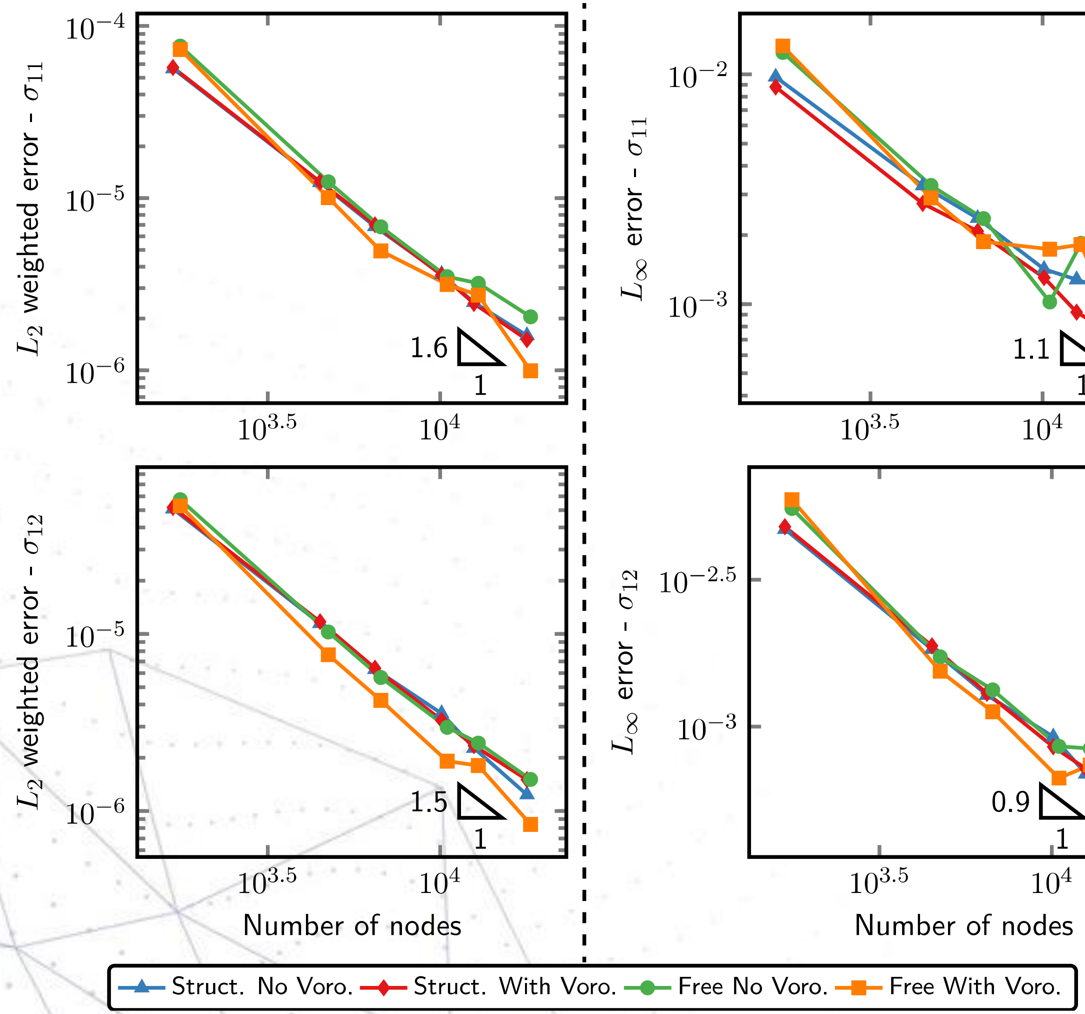
Voronoi diagrams and collocation methods (1/2)

- Voronoi diagram = partition of a domain in cells so that all the point of a cell are closer to the cell reference node than to any other node.

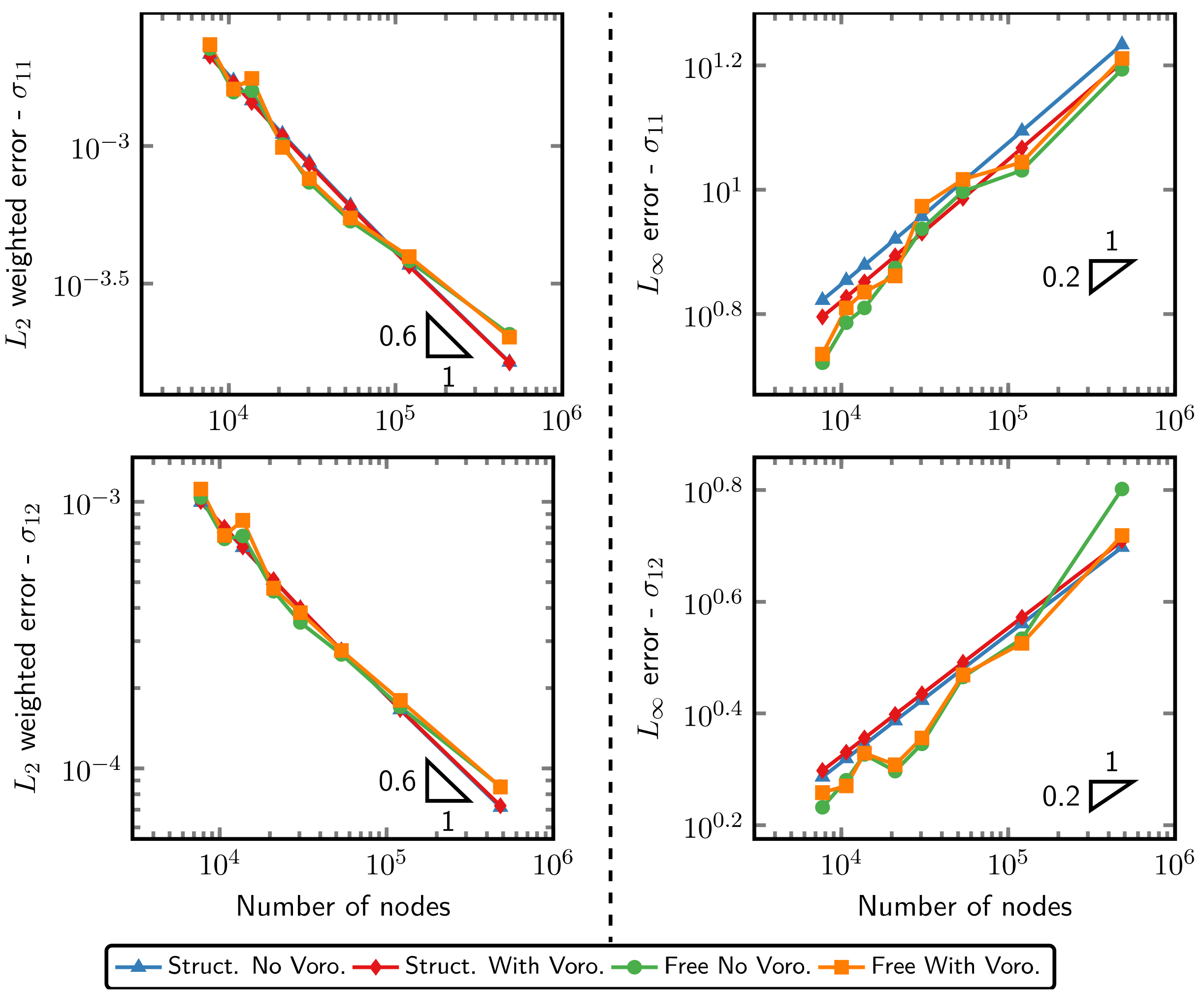


- Voronoi diagrams can be used to improve the solution:
  - GFD method:
    ➔ Assign a weight based on the “space” associated with each node.
  - DC PSE method:
    ➔ Improve the integration step.

Voronoi diagrams and collocation methods (2/2)



2D cylinder – GFD method



2D L-shape – GFD method

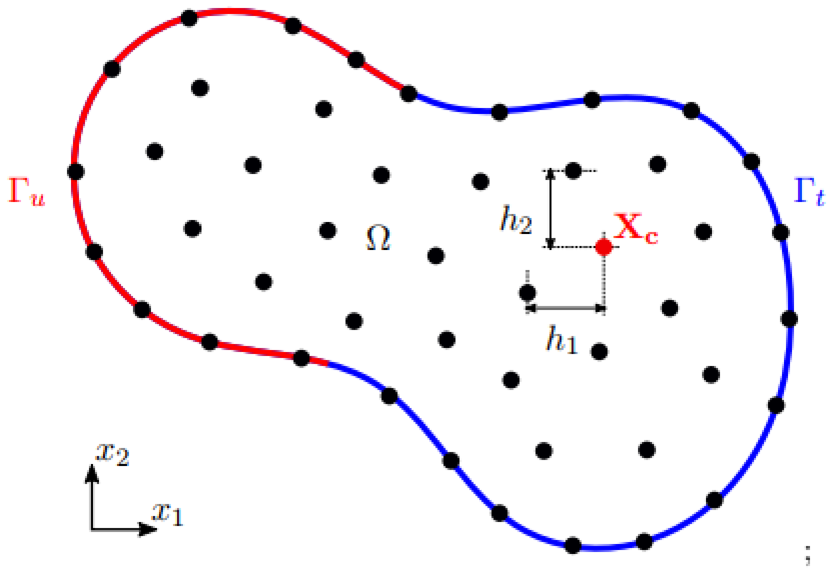
Stabilized form of PDE for collocation (1/2)

- PDE:

$$A(f) = 0 \quad \text{in} \quad \Omega$$
$$f - \bar{f} = 0 \quad \text{on} \quad \Gamma_u$$
$$B(f) = 0 \quad \text{on} \quad \Gamma_t$$

- Stabilized equations:

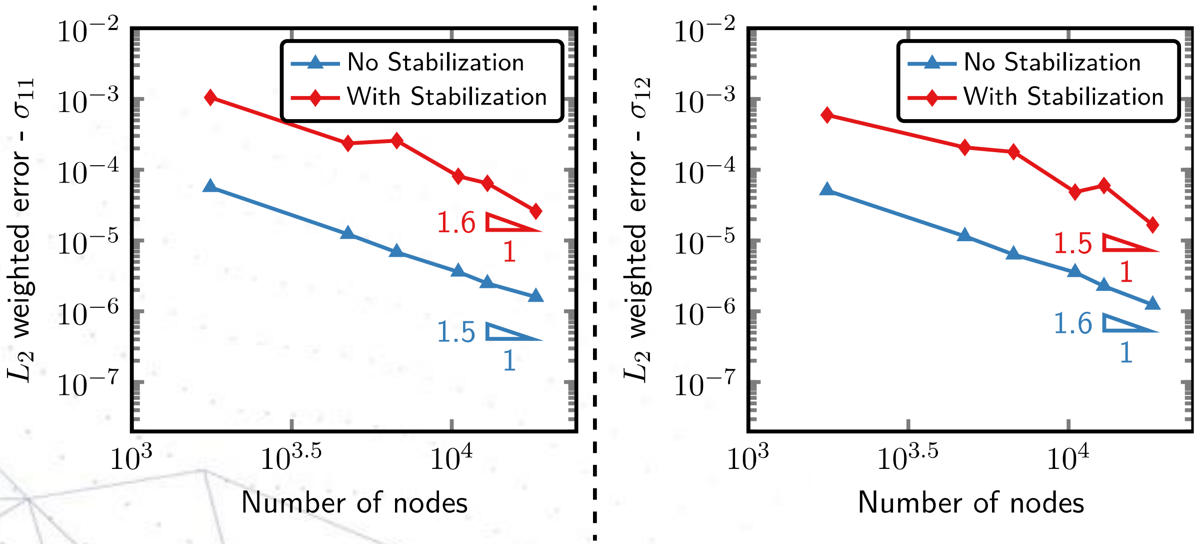
$$A(f) - \frac{1}{2}\sum_{j=1}^{m} h_j \frac{\partial A(f)}{\partial x_j} = 0 \quad \text{in} \quad \Omega$$
$$f - \bar{f} = 0 \quad \text{on} \quad \Gamma_u$$
$$B(f) - \frac{1}{2}\sum_{j=1}^{m} h_j n_j A(f) = 0 \quad \text{on} \quad \Gamma_t$$



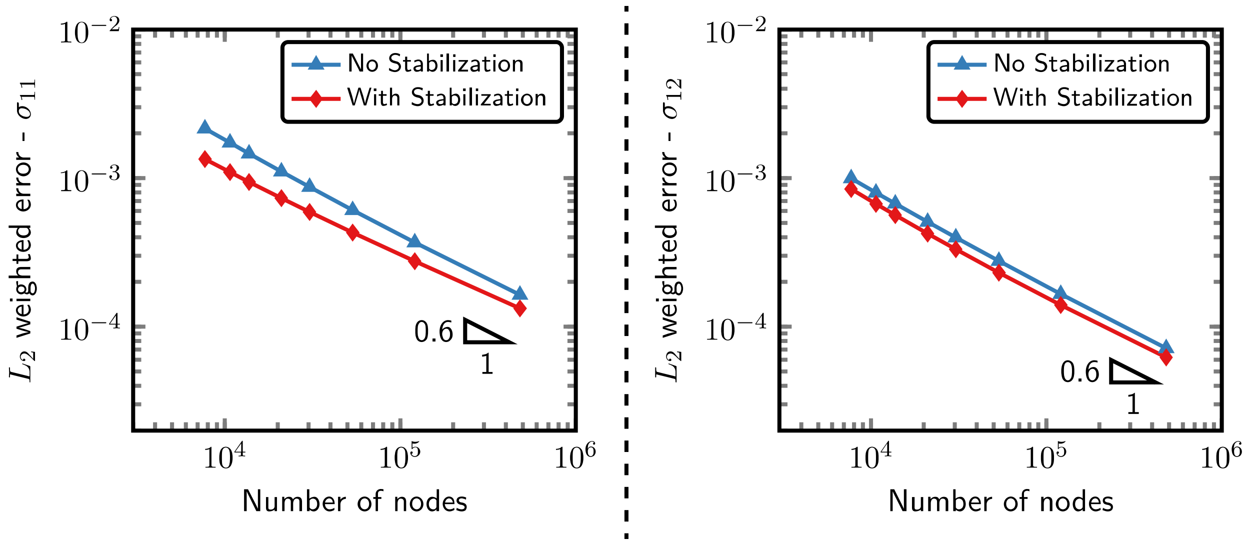
E. Onate. "Derivation of stabilized equations for numerical solution of advective-diffusive transport and fluid flow problems". Computer Methods in Applied Mechanics and Engineering (Jan. 1998). https://doi.org/10.1016/s0045-7825(97)00119-9.

Stabilized form of PDE for collocation (2/2)

- Stabilization of the boundary conditions only.



2D cylinder – GFD method



2D L-shape – GFD method

6. Smart cloud adaptivity

How to improve a given solution through adaptivity ?

- Error can be reduced locally through:
  - *h*-adaptivity ➔ local refinement of the discretization.
  - *p*-adaptivity ➔ increase of the approximation order.

- h-adaptivity involves placing new nodes at key locations of the domain:
  - Which areas of the discretization need to refined?
  - Where to place the new nodes?

Error indicators

ZZ-type error indicator	Residual-type error indicator

ZZ-type error indicator

- Computation of a “smooth” field in the vicinity of each collocation nodes.

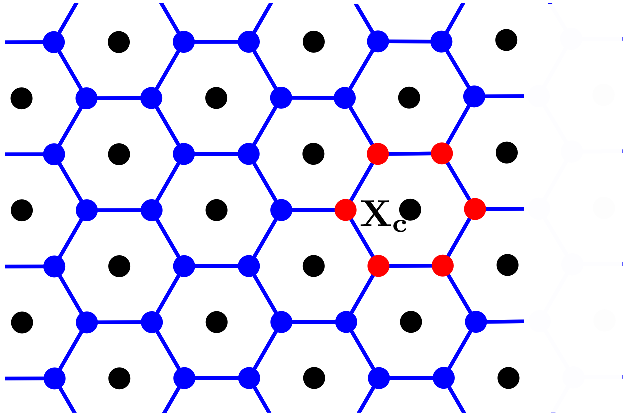
$$\sigma_{vM}^{s}(\boldsymbol{X},\boldsymbol{X_c}) = \boldsymbol{p}(\boldsymbol{X},\boldsymbol{X_c})^{\boldsymbol{T}}\boldsymbol{a}(\boldsymbol{X_c})$$

$$B_h(\boldsymbol{X_c}) = \sum_{k=1}^{m} w(\boldsymbol{X_{pk}} - \boldsymbol{X_c})\left[\boldsymbol{p}(\boldsymbol{X},\boldsymbol{X_c})^{\boldsymbol{T}}\boldsymbol{a}(\boldsymbol{X_c}) - \sigma^{c}(\boldsymbol{X_{pk}})\right]^2$$

➔ $e(\boldsymbol{X_c}) = |\sigma^{c}(\boldsymbol{X_c}) - \sigma^{s}(\boldsymbol{X_c})|$

Residual-type error indicator

- Computation of the residual of the PDE in the vicinity of each collocation node (corners of Voronoi cells).



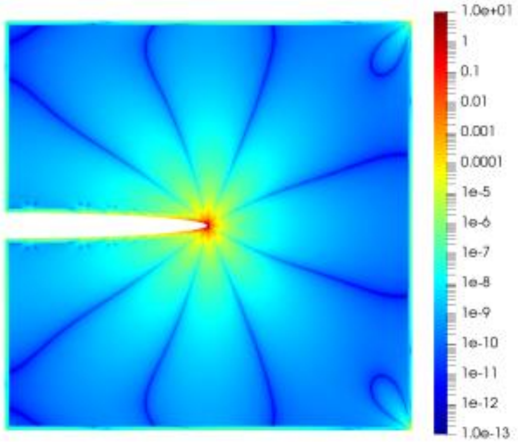
➔ $e(\boldsymbol{X_c}) = \frac{1}{m}\sum_{i=1}^{m}|\boldsymbol{\nabla}.\boldsymbol{\sigma}(\boldsymbol{X_{vi}}) + \boldsymbol{b}(\boldsymbol{X_{vi}})|$

Impact of discretization on error indicator

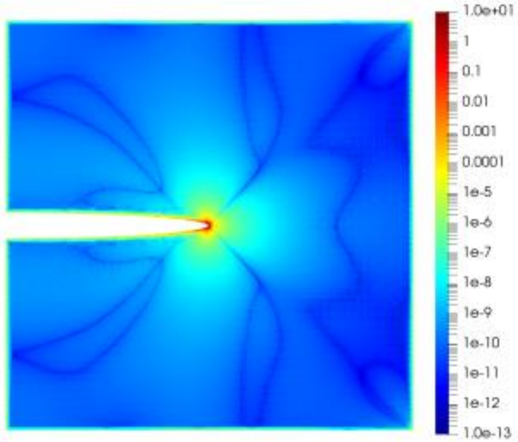
ZZ-type error indicator	Residual-type error indicator

ZZ-type error indicator

- The error pattern is affected by the regular discretization pattern



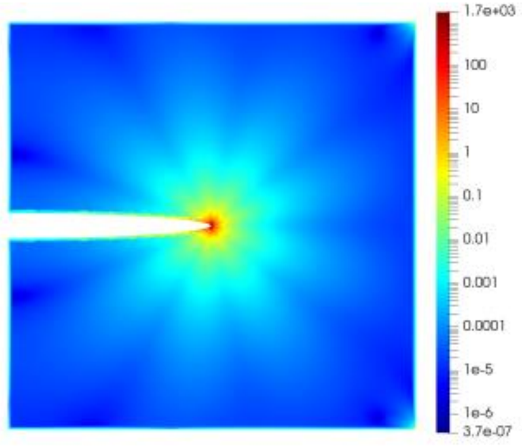
Square lattice



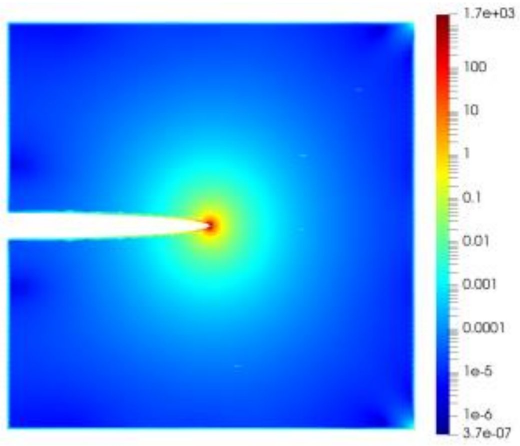
Triangular lattice

Residual-type error indicator

- The discretization pattern has little impact on the error pattern

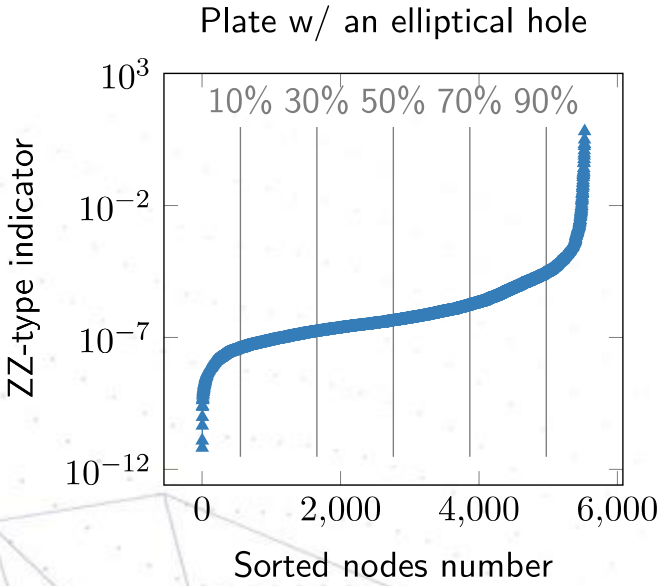


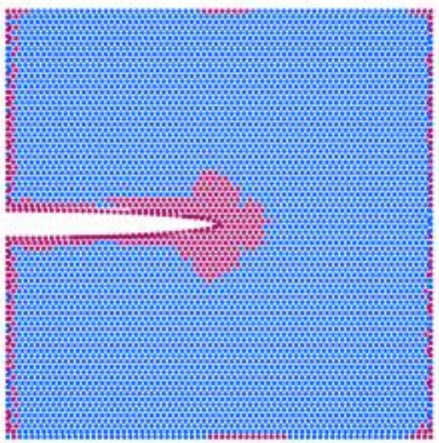
Square lattice



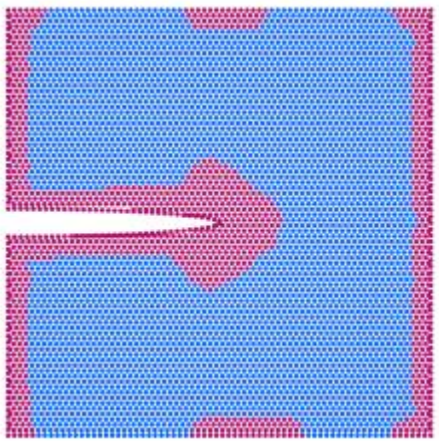
Triangular lattice

Identification of the refinement areas and placement of new nodes

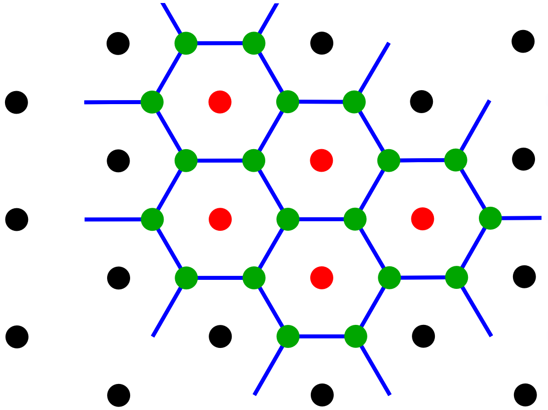




10% of the nodes of highest error



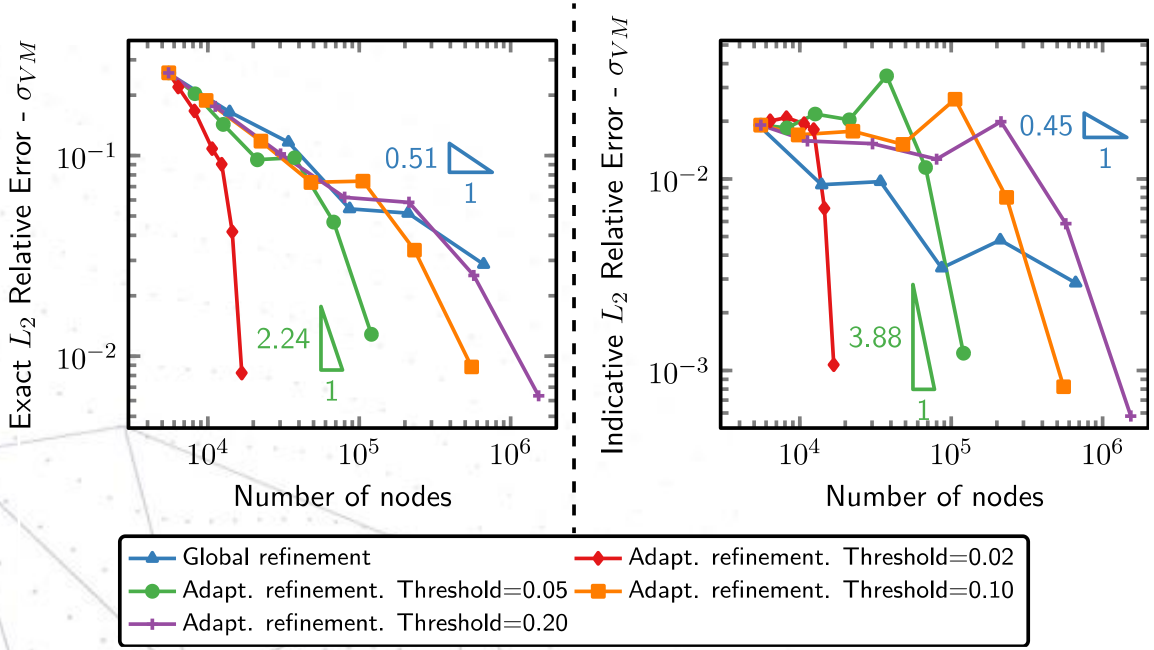
10% of the nodes of highest error + associated stencil nodes



Placement of new nodes at the corners of Voronoi cells

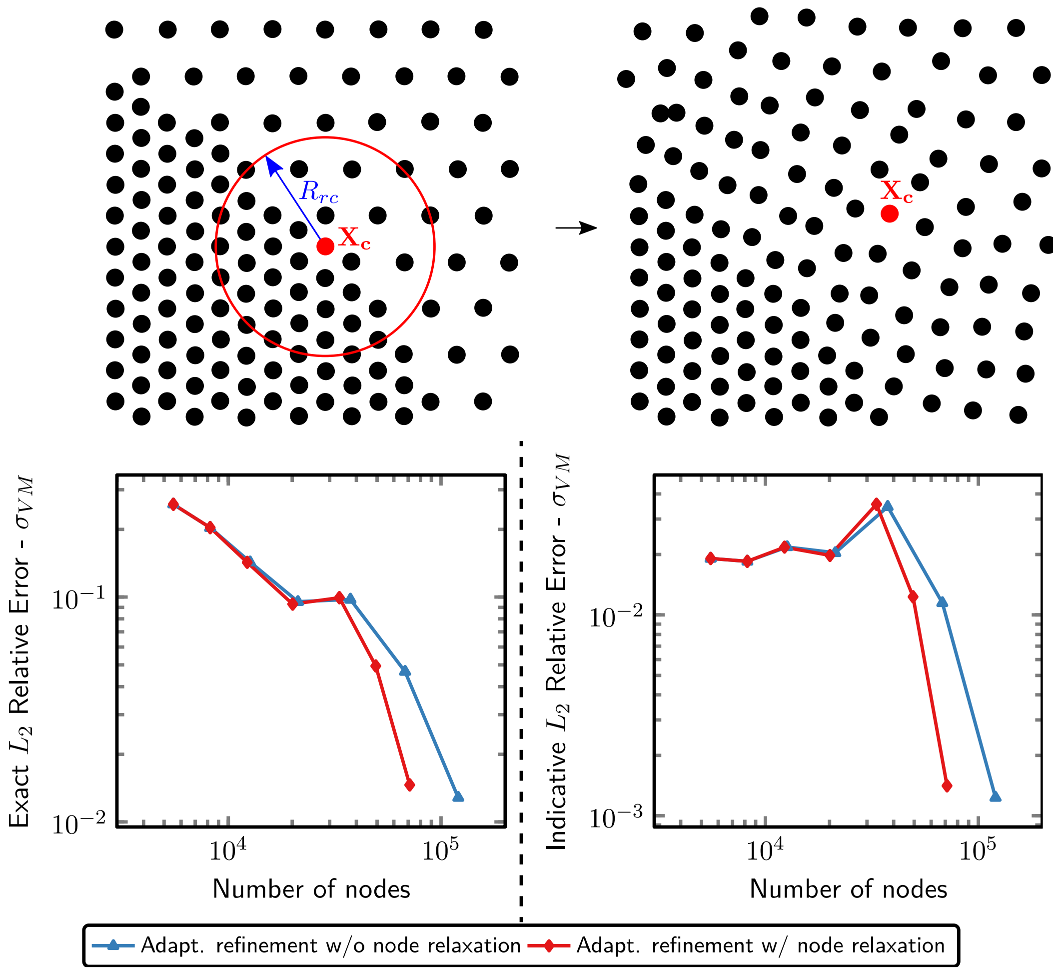
Refinement threshold and node relaxation

Impact of node selection threshold

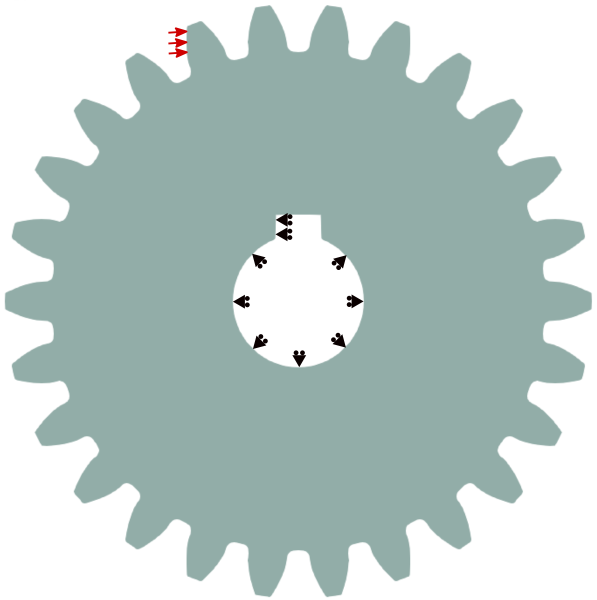
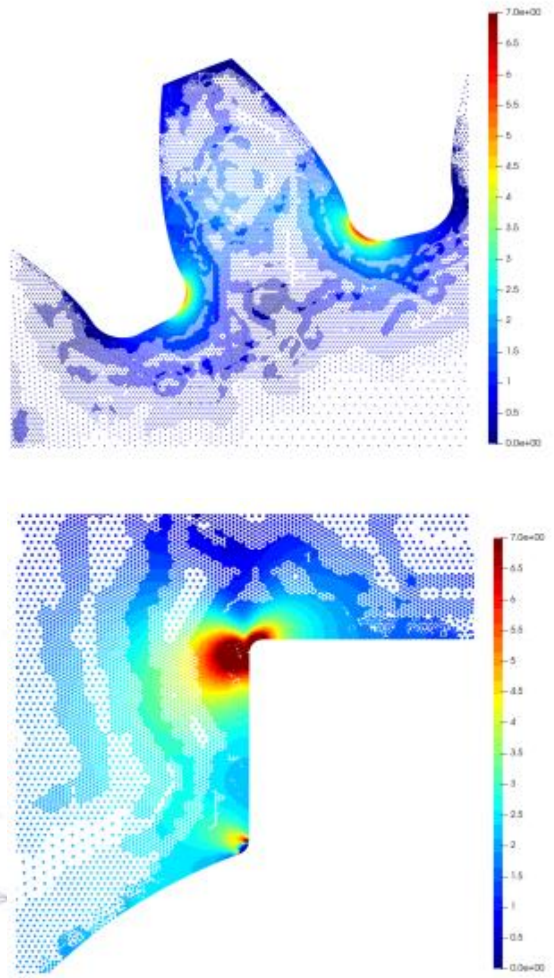
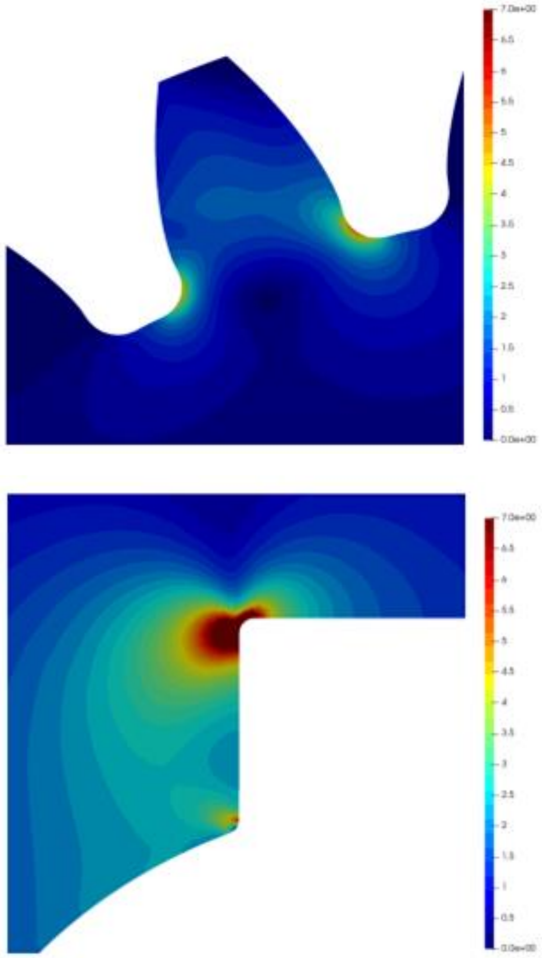


2D plate with an elliptical hole – GFD method

Impact of node relaxation



Some results

Model	Adaptive smart cloud collocation (4 iterations)	Very fine FEA
		
	143,763 nodes – $h_{min} \cong 0.018$	132,665 nodes – $h \cong 0.15$

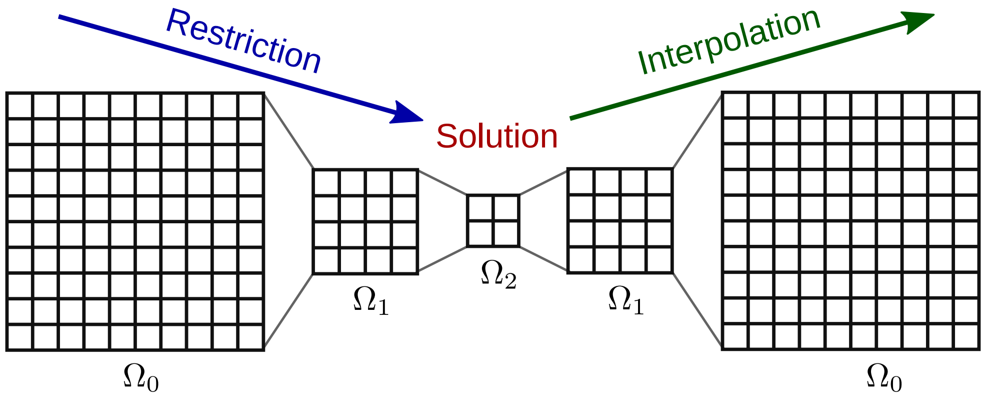
7. Solution of collocation linear problems

Linear problem solution for point collocation

- Direct solvers;
- Iterative solvers;
  - Necessity of robust matrix preconditioning to speed-up convergence;
  - Jacobi preconditioner:
    - ➔ most simple preconditioner;
    - ➔ appropriate for greatly diagonal dominated systems.
  - ILU preconditioner;
    - ➔ easy to set-up;
    - ➔ robust.
  - AMG (Algebraic Multigrid) preconditioner:
    - ➔ complex to set-up;
    - ➔ great performance can be achieved.

Multigrid methods and AMG preconditioners

- Two main forms of multigrid methods:
  - ➢ Geometric Multigrid Methods;
  - ➢ Algebraic Multigrid Methods.
- Restriction and interpolation operators are built differently.

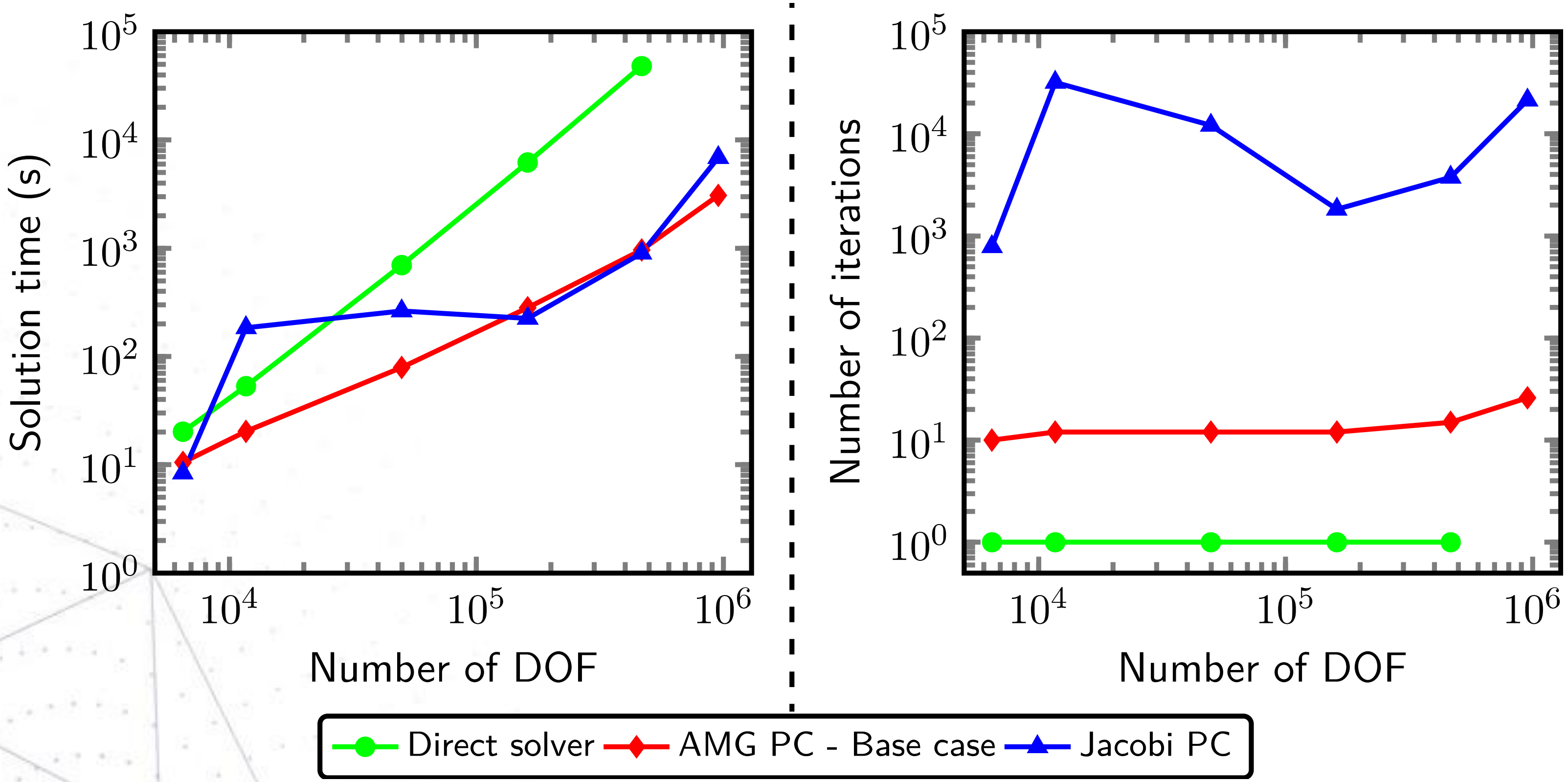


Concept of multigrid methods

- BoomerAMG (*hypre*) is a state of the art AMG preconditioner. It relies on many parameters such as :
  - ➢ Number of AMG cycles;
  - ➢ Number of sweeps;
  - ➢ Coarsening strategy;
  - ➢ Number of aggressive coarsening levels;
  - ➢ Aggressive coarsening threshold.

Comparison of solution methods

- Problem of a 3D sphere under internal pressure – GFD method.



8. Conclusions and perspectives

Main conclusions

CAD to smart clouds

- direct generation of colloc. model from CAD files;
- contain all information of the CAD geometry.

Stencil node selection

- larger stencils for boundary nodes:
  ➔ error reduction;
- generalized visibility criterion:
  ➔ effective with a threshold angle.

Voronoi diagrams and stabilization methods

- Voronoi diagrams or stabilization methods do not always lead to an error reduction.

Smart cloud adaptivity

- ZZ-type and residual-type error indicator:
  ➔ succeed in identifying the zones of large error;
  ➔ are not good error estimators;
- smart cloud *h*-adaptivity:
  ➔ faster convergence to the exact solution.

Solution of collocation linear problems

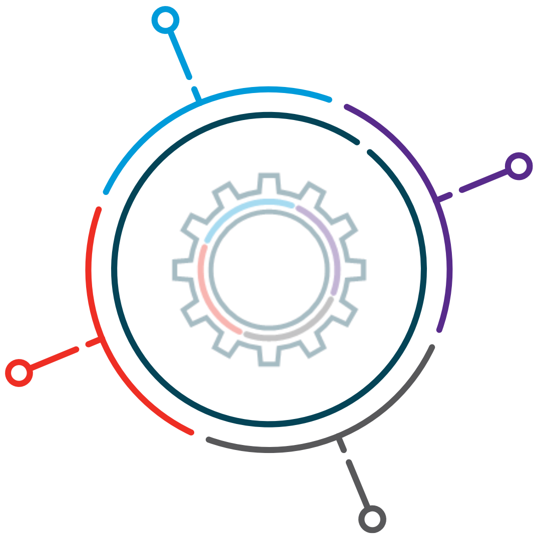
- AMG preconditioners are powerful but rely on many parameters;
- ILU preconditioners are robust and simple to use.

Perspectives

Point cloud adaptivity to modified geometries

Smart cloud simplification

Multigrid preconditioner based on PDE



Anisotropic point clouds

Robust error estimator

Solve directly point clouds

Intrinsic or extrinsic enrichment

Q&A

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