Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Computer Applications in Science & Engineering (CASE)
Barcelona Supercomputing Center - BSC
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Generation of large-scale curved meshes for complex virtual geometries

Eloi Ruiz-Gironés with Xevi Roca

Tetrahedron VII Workshop

European Research Council
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Acknowledgements

- **Co-authors:**
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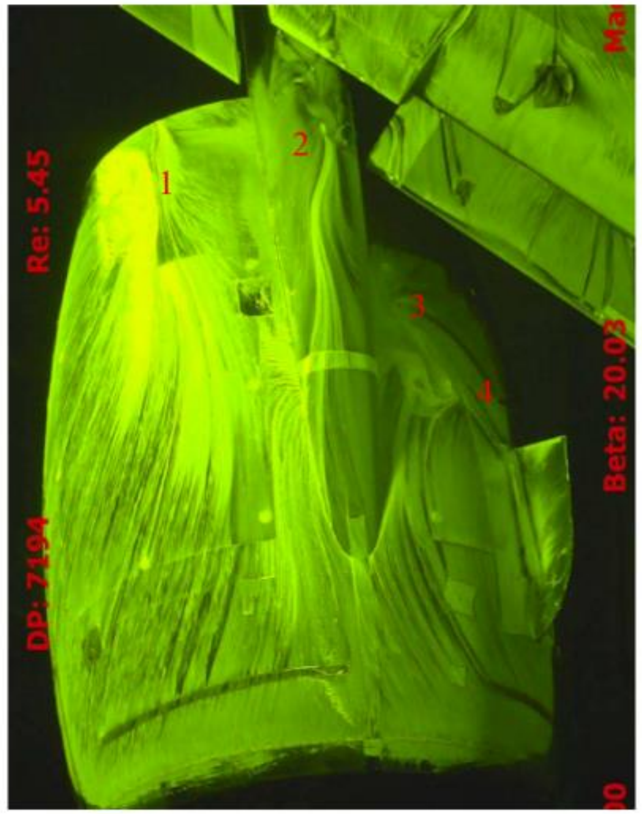
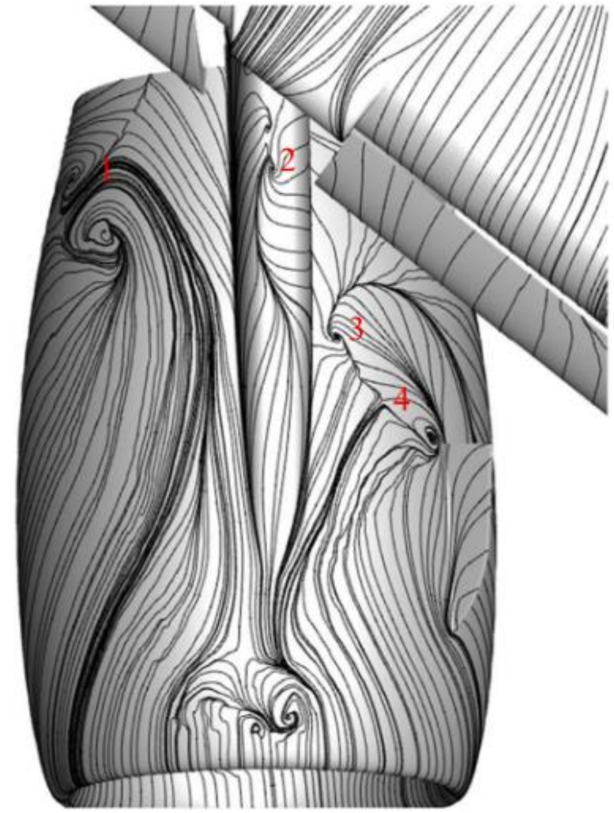
- **Simulations on our curved meshes:**
  - 4^{th} & 5^{th} HLPW high-order group
  - Z.J. Wang, University of Kansas, USA
  - Oriol Lehmkuhl, BSC, Spain

- **Computing hours:**
  - BSC
  - PRACE program

Motivation: Wind Tunnel vs Simulation

Wind tunnel data
(4th HLPW)
(NASA AIAA)





High-order simulation
(ZJ Wang AIAA'23)

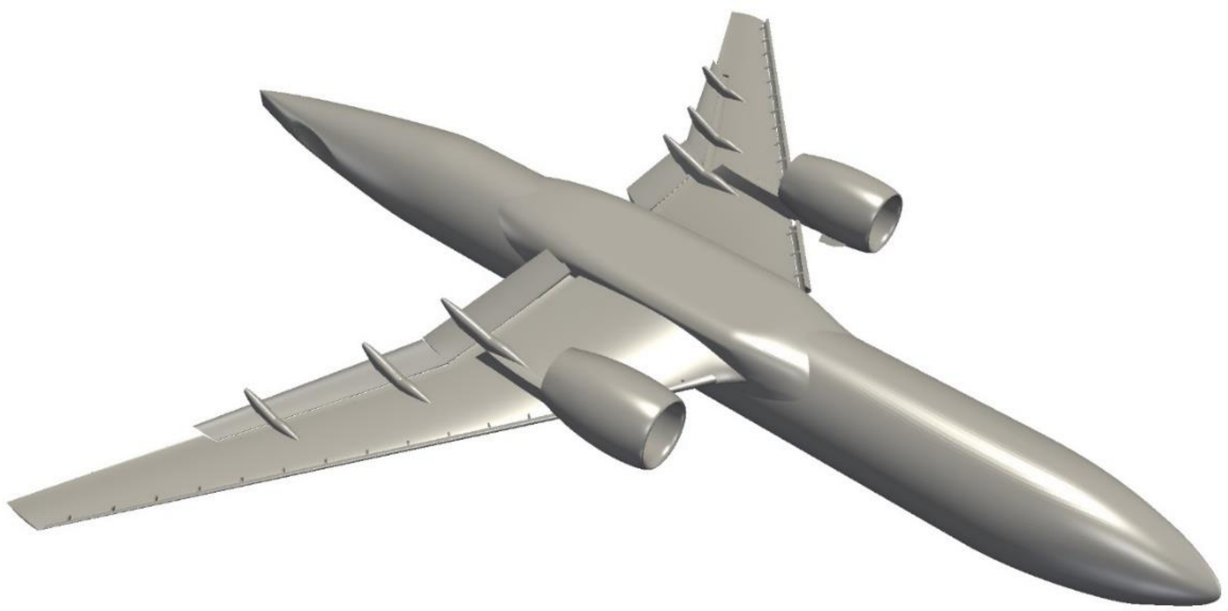
Unstructured high-order methods

- **Geometric flexibility:** using unstructured meshes
- **More accuracy:** with same #DOFs, less dissipation and dispersion

They require curved high-order meshes

- **Geometric error:** straight elements hamper simulation accuracy

Motivation: Curved Meshes for Flow Simulation



Large-scale curved meshes in complex virtual geometries

- **Approximate virtual CAD B-rep:** using curved elements
- **Mesh features:** small elements & size gradation, boundary layer...
- **Mesh quality:** facilitates solving the simulation problems

Mesh Curving Methods

Direct methods: Create curved mesh from scratch

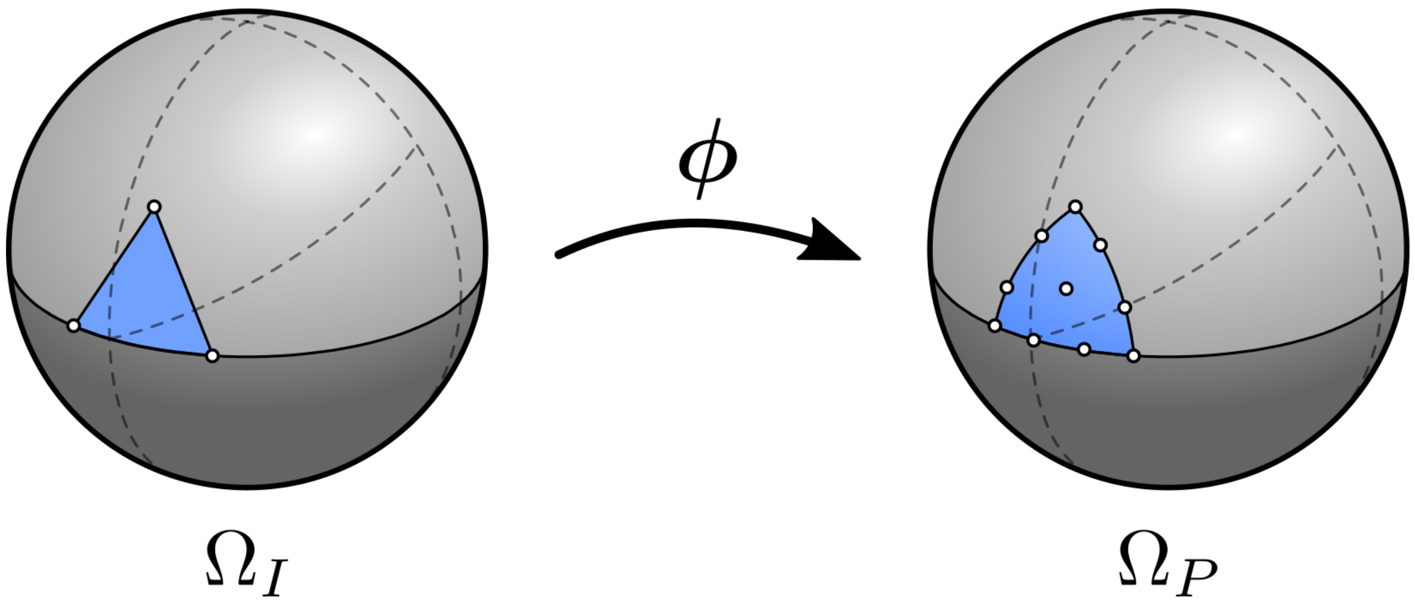
- Delaunay (Feng, Alliez, Busé, Delingette, Desbrun ToG'18)
- Advancing front (Mohammadi, Shontz IMR'21)

Indirect methods: Linear mesh generation + curving step

- **PDE-based**
  - Linear / non-linear elasticity
    (Persson, Peraire), (Xie, Poya, Sevilla, Hassan), (Turner, Moxey, Sherwin, Peiró)
  - Winslow (Fortunato, Persson), ...
- **Optimization-based**
  - Mesh distortion / quality (Tomov, Mittal, Kolev), (Karman),
    (Gargallo-Peiró, Ruiz-Gironés, Sarrate, Roca), (Feuillet, Loseille, Alauzet)...
  - Nodal displacement (Toulorge, Johnen, Lambrechts, Remacle), ...
  - Other quantities (Stees, Shontz), ...

Outline

- Curving solution
- Complex geometry in parallel
- Large-scale distributed curving
- High-Lift Prediction Workshop

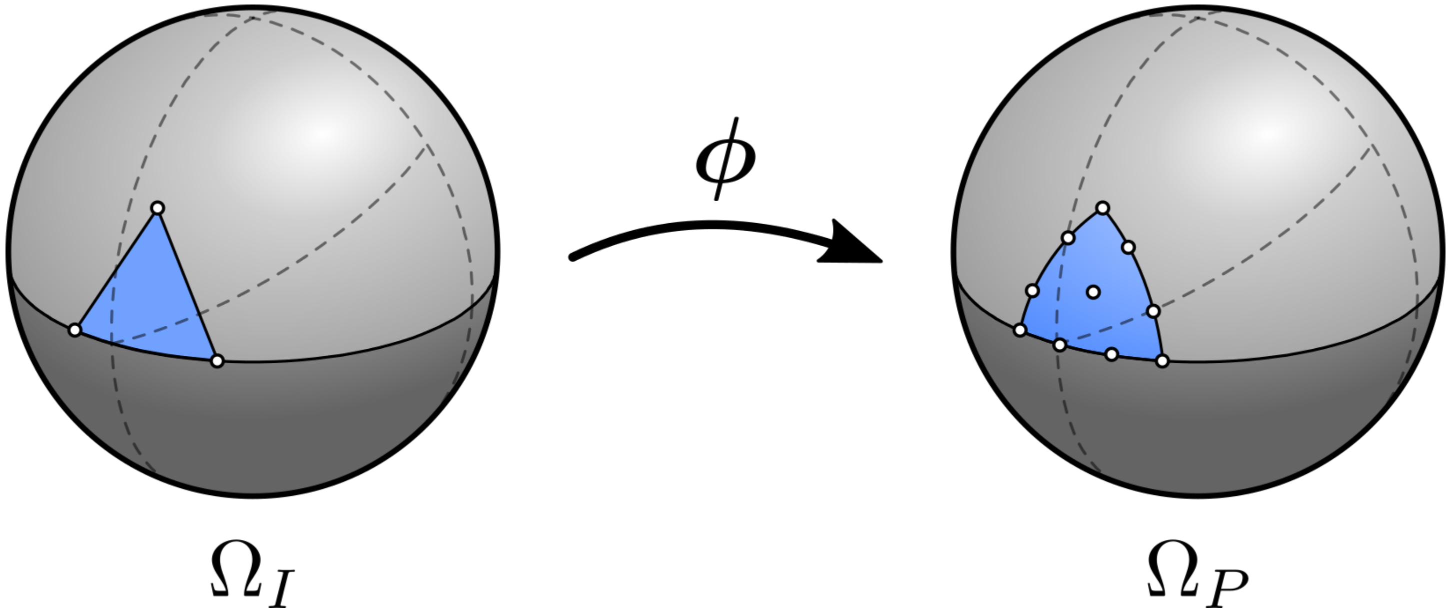


Curving Solution

(Ruiz-Gironés, Gargallo, Sarrate, Roca IMR'17 & CAD'19)
(Ruiz-Gironés, Roca IMR'18, IMR'19 & CAD'22)

- **Constrained optimization problem**
- **Continuous penalty**

Our Formulation : Constrained Optimization



$$M\boldsymbol{\phi} = \frac{|\boldsymbol{D\phi}|^2}{n\sigma_0(\boldsymbol{D\phi})^{2/n}}$$

(Knupp SIAM J. Sci. Comput.'01)
(Roca, Gargallo, Sarrate IMR'12)
(Gargallo, Roca, Peraire, Sarrate IJNME'15)

$$\min_{\boldsymbol{\phi}} ||M\boldsymbol{\phi}||^2_{\Omega_I}$$

constrained to:

$$\mathrm{T}\boldsymbol{\phi} = \boldsymbol{g}_D(\mathrm{T}\boldsymbol{\phi})$$

(Ruiz-Gironés, Roca, Sarrate CAD'16)
(Ruiz-Gironés, Gargallo, Sarrate, Roca IMR'17 & CAD'19)
(Ruiz-Gironés, Sarrate, Roca IMR'16)

(Ruiz-Gironés, Sarrate, Roca IMR'15 & JCP'21)

$$\boldsymbol{g}_D(\mathrm{T}\boldsymbol{\phi}) = \sum_{i=1}^{N} \pi_{\Omega_i}(\boldsymbol{x}_i)N_i$$

(Ruiz-Gironés, Roca IMR'18, IMR'19, CAD'22, AIAA'22)

Our Solution: Continuous Penalty Method

(Ruiz-Gironés, Roca IMR'18, IMR'19 & CAD'22)

Penalty method: Optimize several unconstrained problems

$$E_\mu(\boldsymbol{\phi}) = ||M\boldsymbol{\phi}||^2_{\Omega_I} + \mu||\mathrm{T}\boldsymbol{\phi} - \boldsymbol{g}_D(\mathrm{T}\boldsymbol{\phi})||^2_{\partial\Omega_I}$$

$$E_\mu : \mathcal{H}^1(\Omega) \longrightarrow \mathbb{R}$$

$$\boldsymbol{g}_D : \mathcal{L}^2(\partial\Omega) \longrightarrow \mathcal{L}^2(\partial\Omega)$$

Non-linear problem: volume & boundary

Fix-point iterative solver: Newton + backtracking line-search

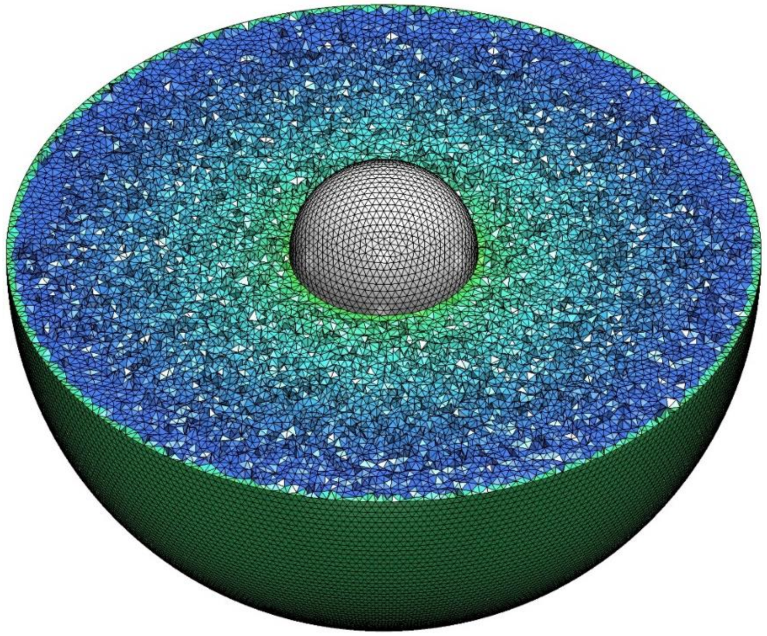
Compute target configuration

$$\boldsymbol{g}^k_D = \boldsymbol{g}_D(\mathrm{T}\boldsymbol{\phi}^k)$$

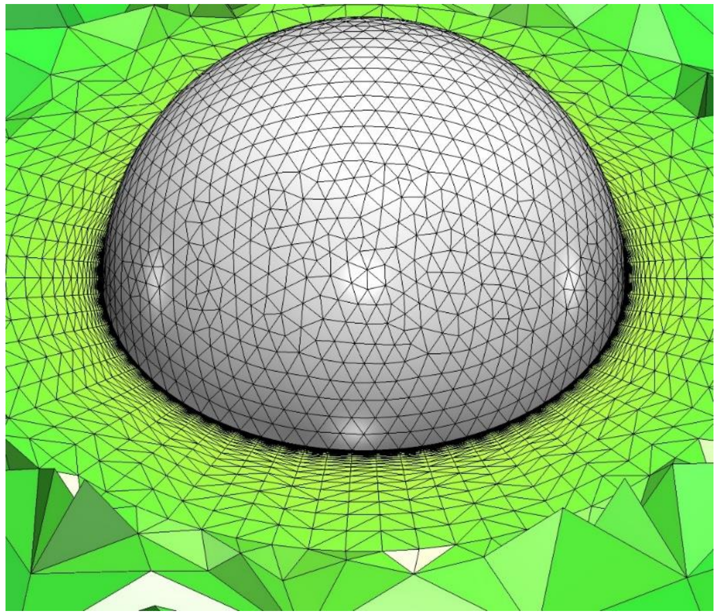
$$\boldsymbol{\phi}^{k+1} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\, E_\mu(\boldsymbol{\phi}, \boldsymbol{g}^k_D)$$

Optimize mesh

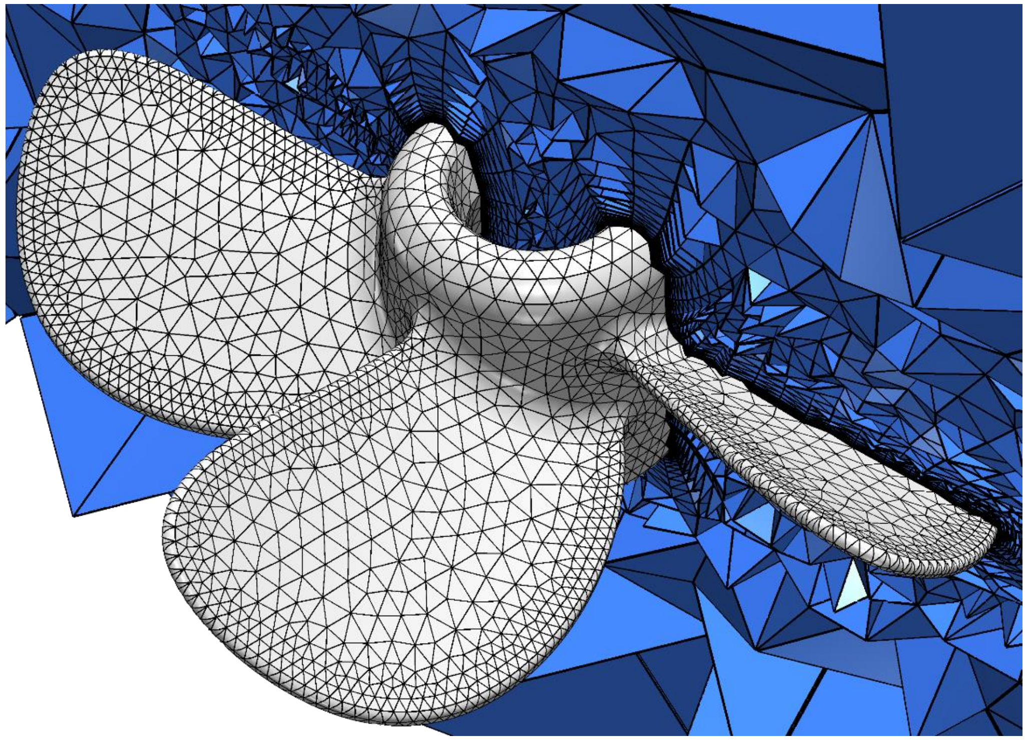
Example: Sample meshes



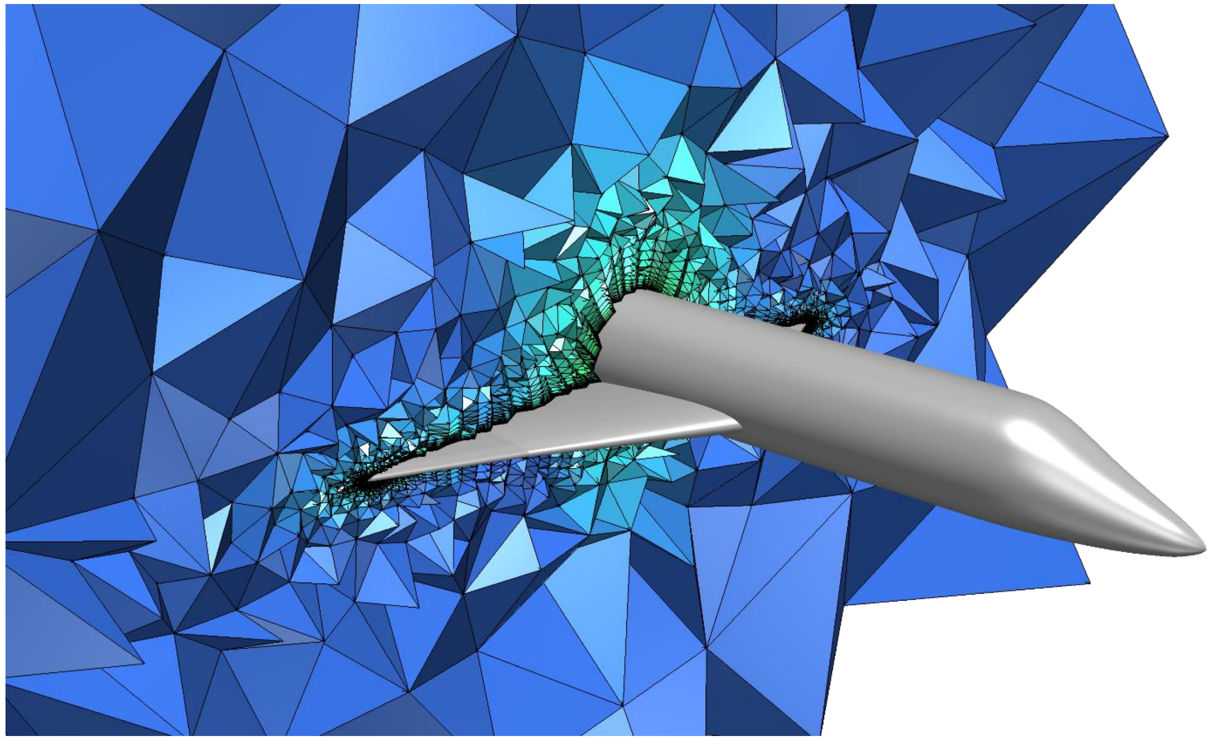
3.6M tets, p=4



0.7M tets, p=4
stretching $1:10^5$



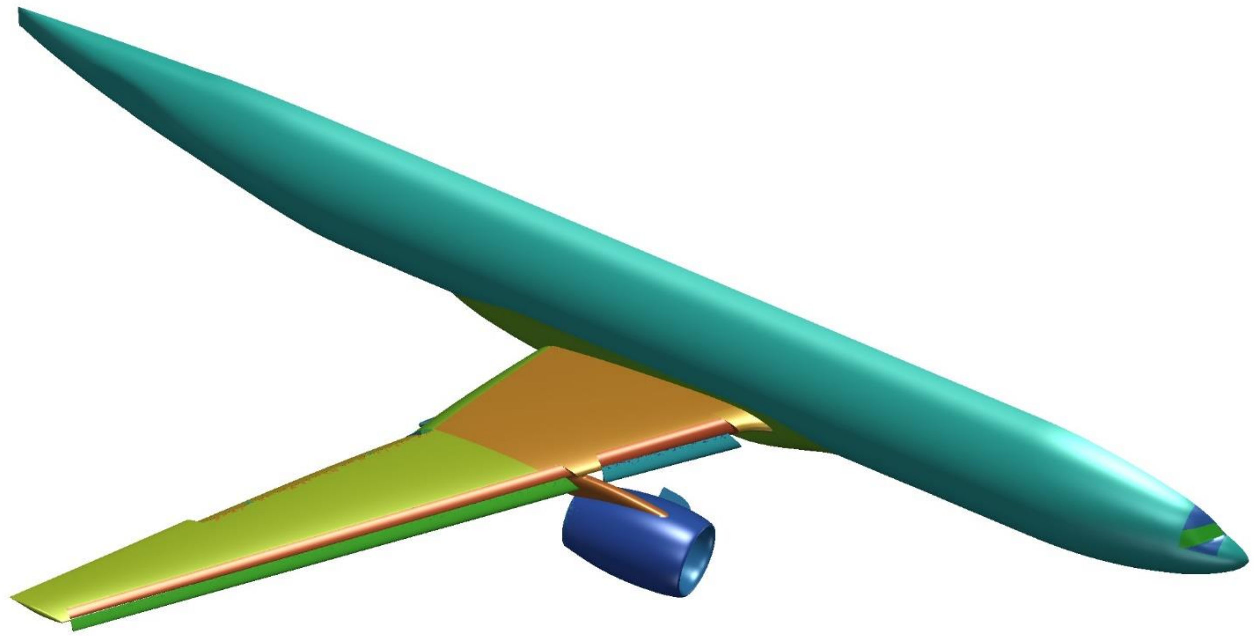
1.6M tets, p=3, stretching 1:750



4M tets, p=4, stretching 1:400

Features

- **Constrained optimization problem:**
  Minimize mesh distortion while approximating the virtual model
- **Mesh floats:**
  Mesh approximates the geometry
- **Mesh is always valid:**
  No need to introduce untangling
- **Virtual geometry aware:**
  Elements span several entities
- **Tight tolerances:**
  Fully converged meshes avoid element oscillations
- **Newton’s method with backtracking line-search:**
  Ensures quadratic convergence near solution



Complex geometry in parallel

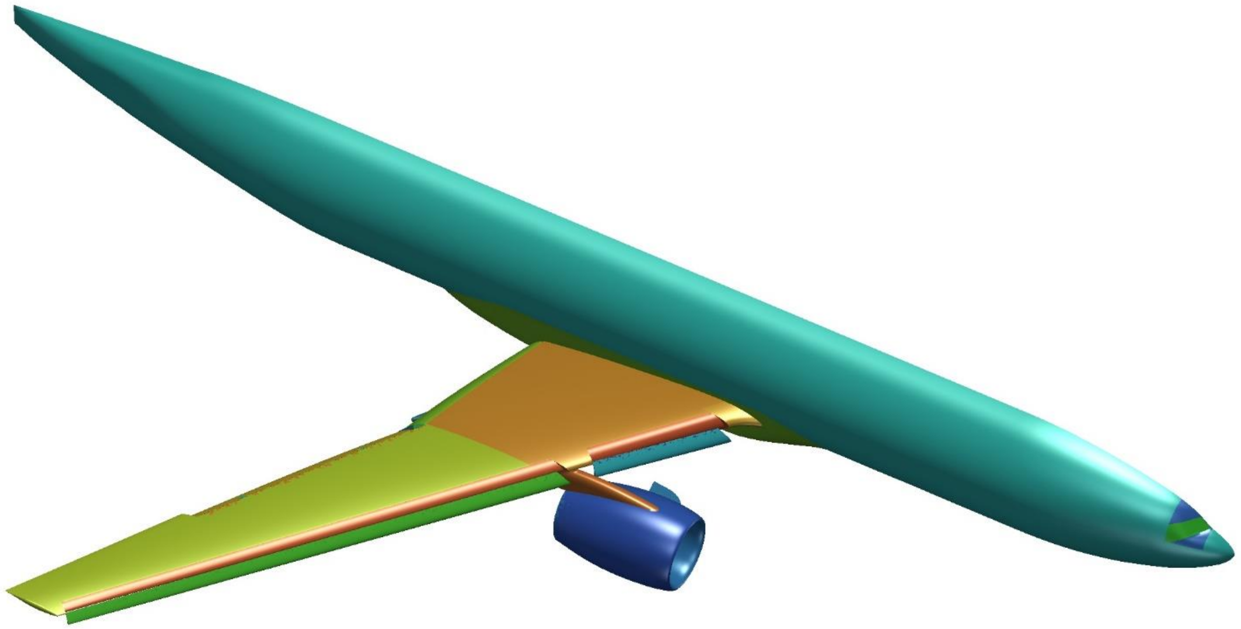
(Ruiz-Gironés, Roca IMR'18, IMR'19 & CAD'22)

(Ruiz-Gironés, Roca AIAA'22)

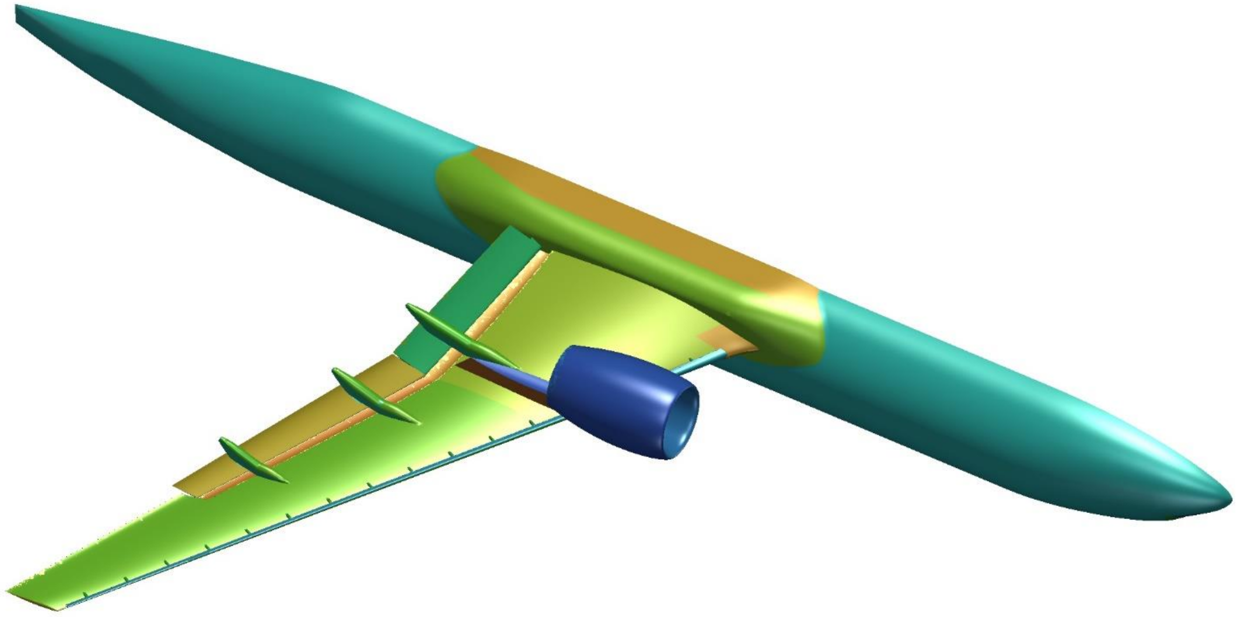
- **Virtual model**
- **Point projection**
- **Parallel distribution of input & output**

Virtual Model

- **Virtually join surfaces:** Simulation intent
- **Decouple CAD & mesh topologies:** one group for fuselage, wings, …
- **Surfaces:** From 415 original surfaces to 215 virtual surfaces



Virtual surfaces: top view

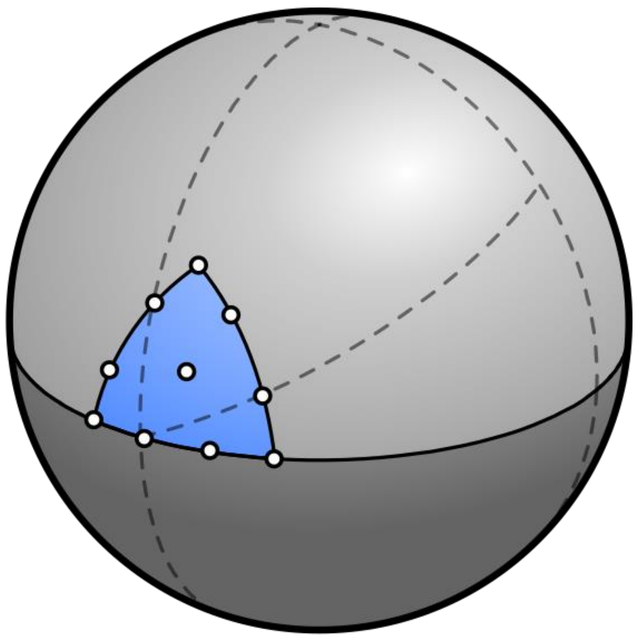


Virtual surfaces: bottom view

Point Projection onto Virtual Models

- **Projection onto virtual surface:**
  (Ruiz-Gironés, Roca IMR'18, IMR'19 & CAD'22)
  - Loop over the geometric surfaces

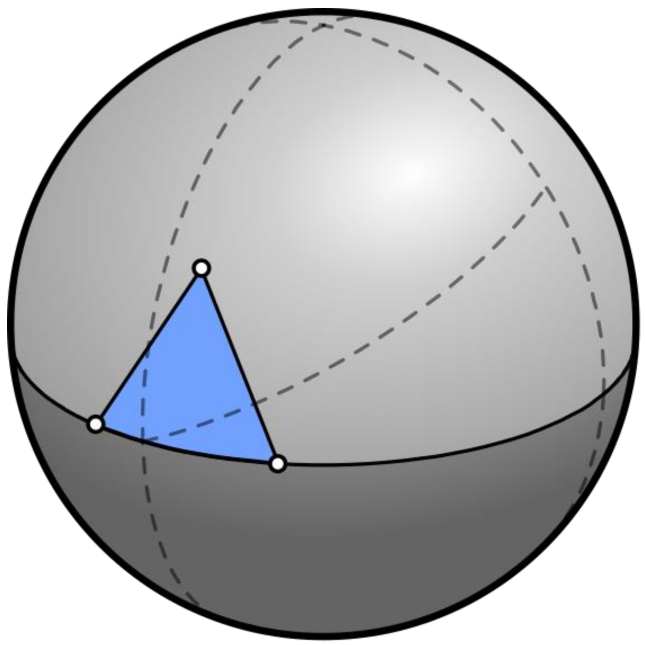
$$\Pi_{\mathcal{S}}(\mathbf{x}) = \arg\min_{\mathbf{y}\in\mathcal{S}} \|\mathbf{x}-\mathbf{y}\|$$



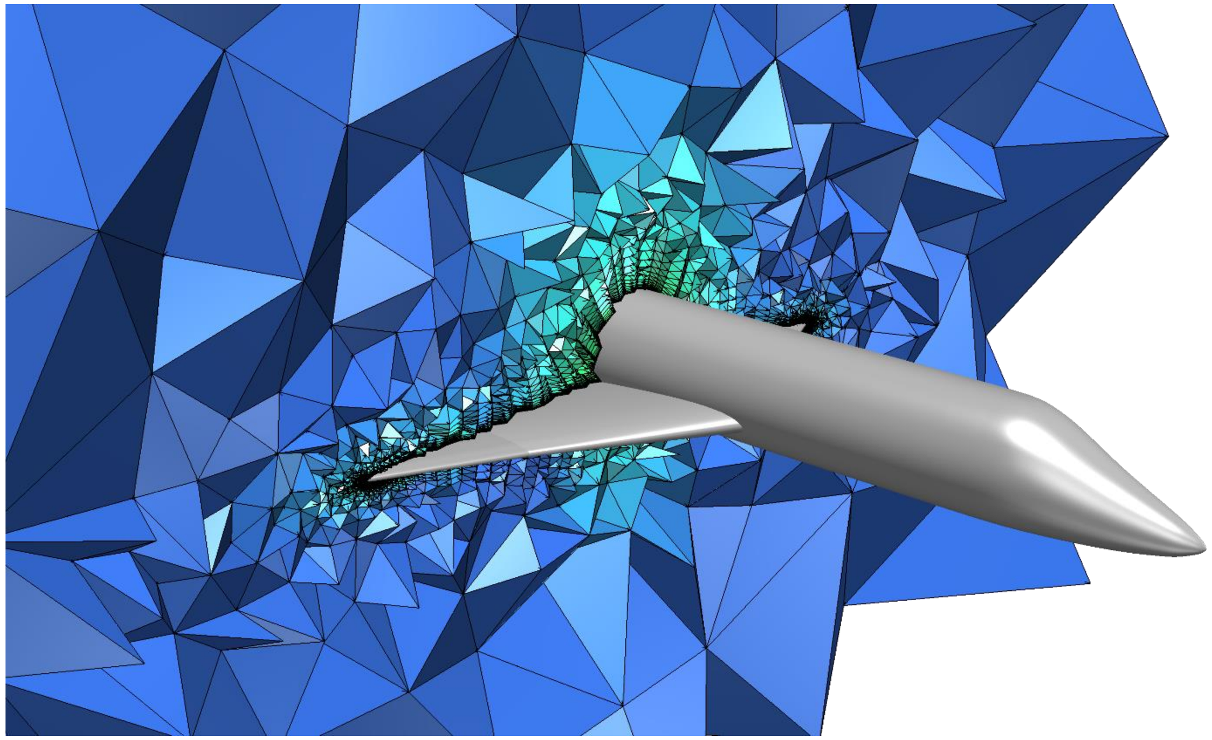
- **Projection onto virtual curve:** Dealing with surface gaps
  (Ruiz-Gironés, Roca AIAA'22)
  - Project the node in-between the surface gap

$$\Pi_{C}(\mathbf{x}) = \frac{1}{2}\left(\Pi_{\mathcal{S}_1}\left(\Pi_{\mathcal{S}_2}(\mathbf{x})\right) + \Pi_{\mathcal{S}_2}\left(\Pi_{\mathcal{S}_1}(\mathbf{x})\right)\right)$$

Parallel Distribution of input & output



- **Input data:**
  - Marked linear mesh
  - Virtual CAD model
- **Linear & high-order meshes:**
  - Each processor owns a set of elements and nodes
  - Each processor projects his boundary nodes
- **Virtual model:**
  - Each processor has a copy of the geometry
  - Easy to distribute, just read the CAD file
  - Processors have enough memory for this approach



Large-scale distributed curving

(Ruiz-Gironés, Roca IMR'19 & CAD'22)

- Reduce computational time
- Reduce memory footprint
- Reduce energy consumption

Lagrange Multiplier Approximation

- **In penalty method:** for μ large enough, Lagrange multiplier is like

$$\lambda \simeq -2\mu \left(\boldsymbol{T\phi} - \mathbf{g}_D(\boldsymbol{T\phi}) \right)$$

- **Function over the mesh boundary:**
  - When converging, doubling μ halves the constraint values

- **We use this to improve the solver:**
  - Given a target constraint norm, which μ we need?

p-Continuation: Less DOF's & Sparser Matrices

Idea: Use a lower degree solution as an initial approximation

Implementation:

- Increase polynomial degree when boundary constraint is *"good enough"*

$$\alpha \varepsilon^p < \varepsilon^{p+1}, \quad \varepsilon^p = \|\boldsymbol{T}\boldsymbol{\phi}^p - \mathbf{g}_D(\boldsymbol{T}\boldsymbol{\phi}^p)\|_{\partial \mathcal{M}_I}$$

- Approximate next penalty parameter using constraint norm

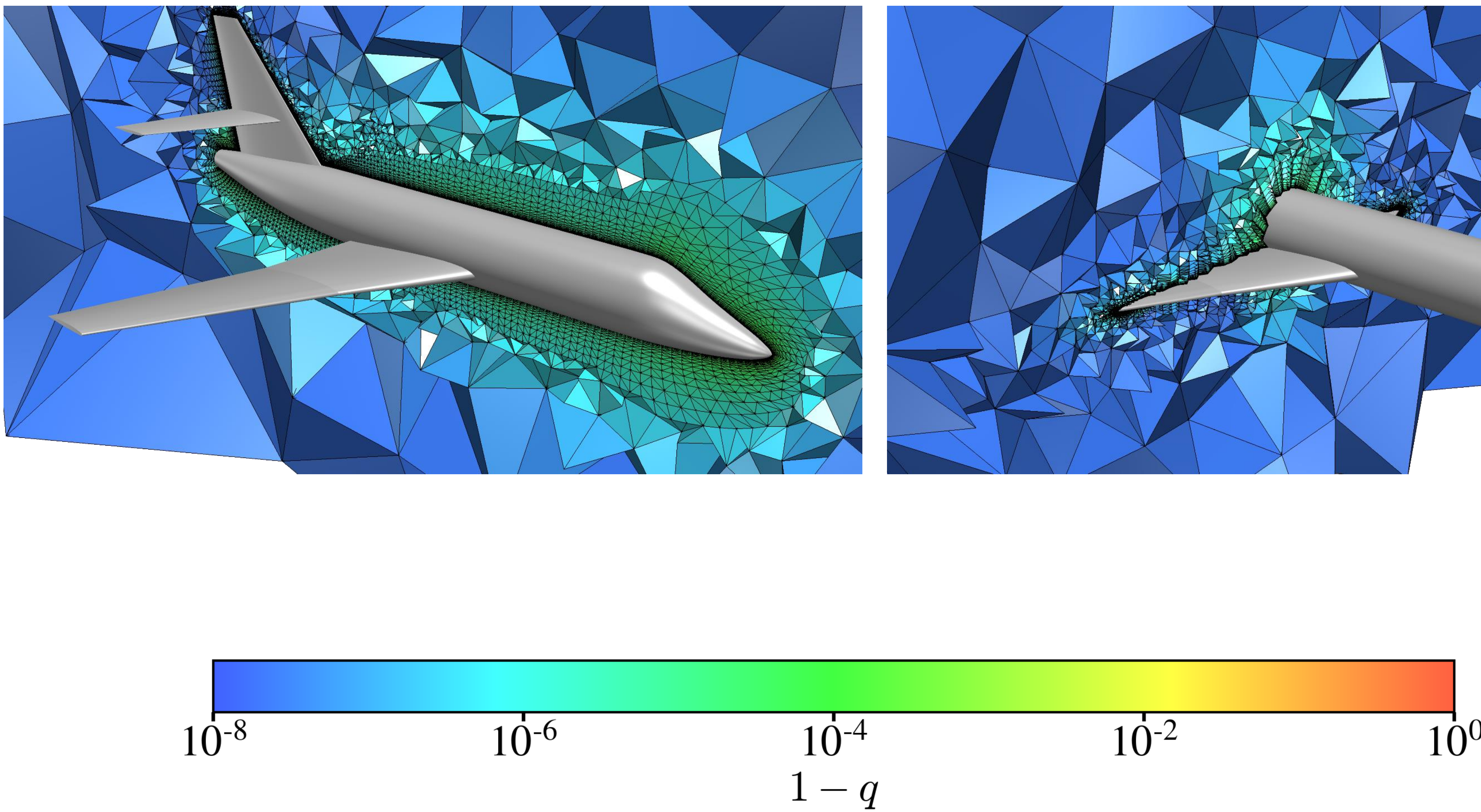
$$\mu^{p+1} = \mu^p \frac{\|\boldsymbol{T}\boldsymbol{\phi}^p - \mathbf{g}_D(\boldsymbol{T}\boldsymbol{\phi}^p)\|_{\partial \mathcal{M}_I}}{\|\boldsymbol{T}\boldsymbol{\phi}^{p+1} - \mathbf{g}_D(\boldsymbol{T}\boldsymbol{\phi}^{p+1})\|_{\partial \mathcal{M}_I}}$$

Examples

p-continuation: Falcon aircraft

Mesh: Degree 4, 4M elements, boundary layer stretching 1:400

Optimization: 2400 cores, RASDD(1) - SSOR(2)



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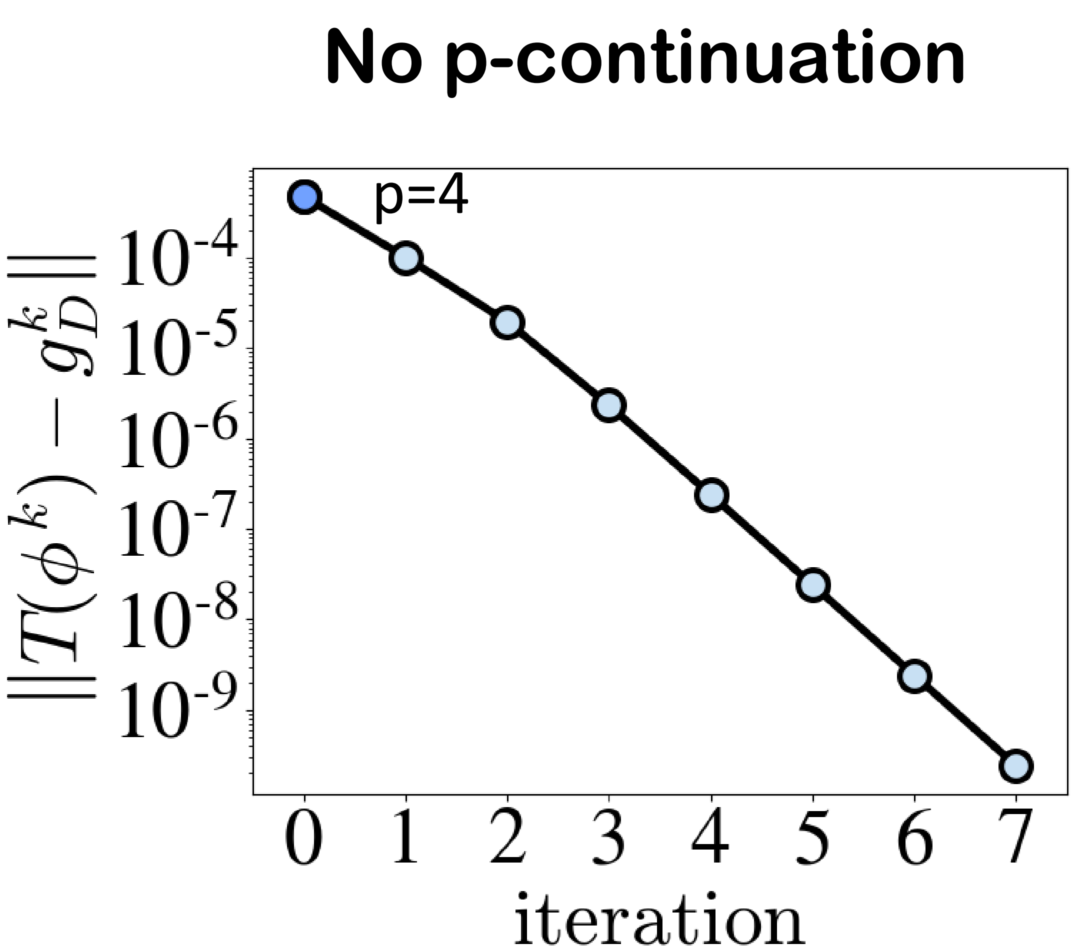

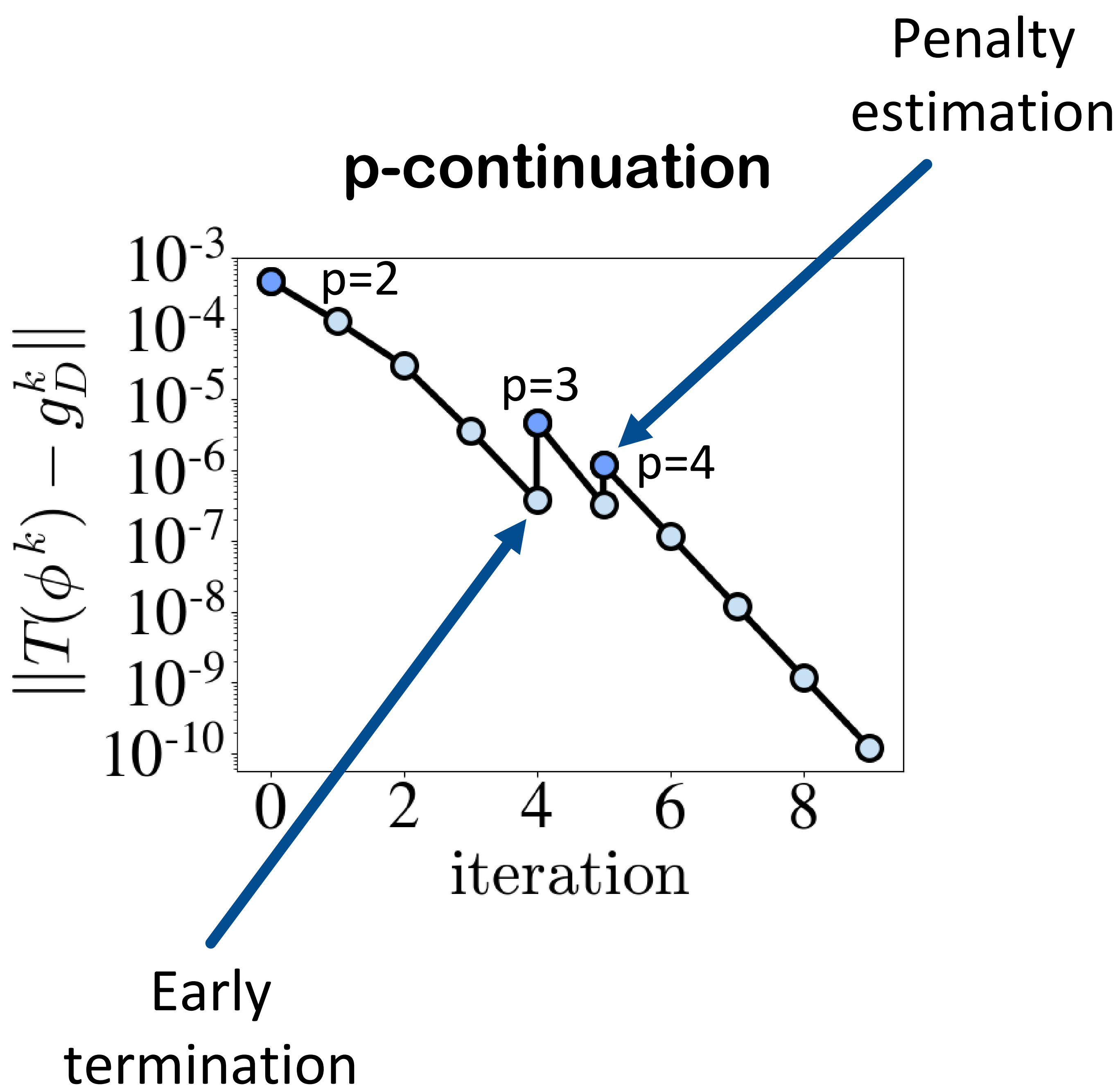

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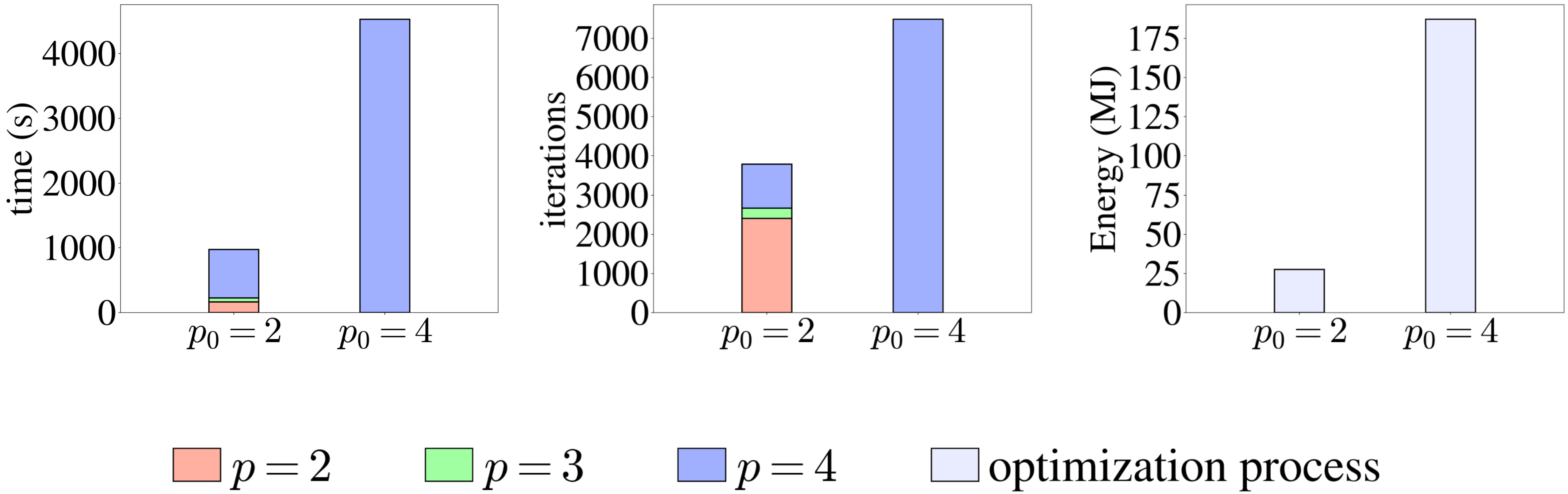


p-continuation technique allows:

- 4 times reduction in time
- 8 times reduction in energy

Penalty Estimation: Less non-linear problems

Optimal penalty parameter

$$\mu^* = \mu_k m^* = \mu_k 1.01 \frac{\varepsilon^*}{\varepsilon_k}$$

Convergence indicator

$$s_k = \frac{\mu_{k-1}}{\mu_k} \frac{\varepsilon_{k-1}}{\varepsilon_k} \qquad e_k = \max\{s_k, 1/s_k\} - 1$$

Next penalty parameter

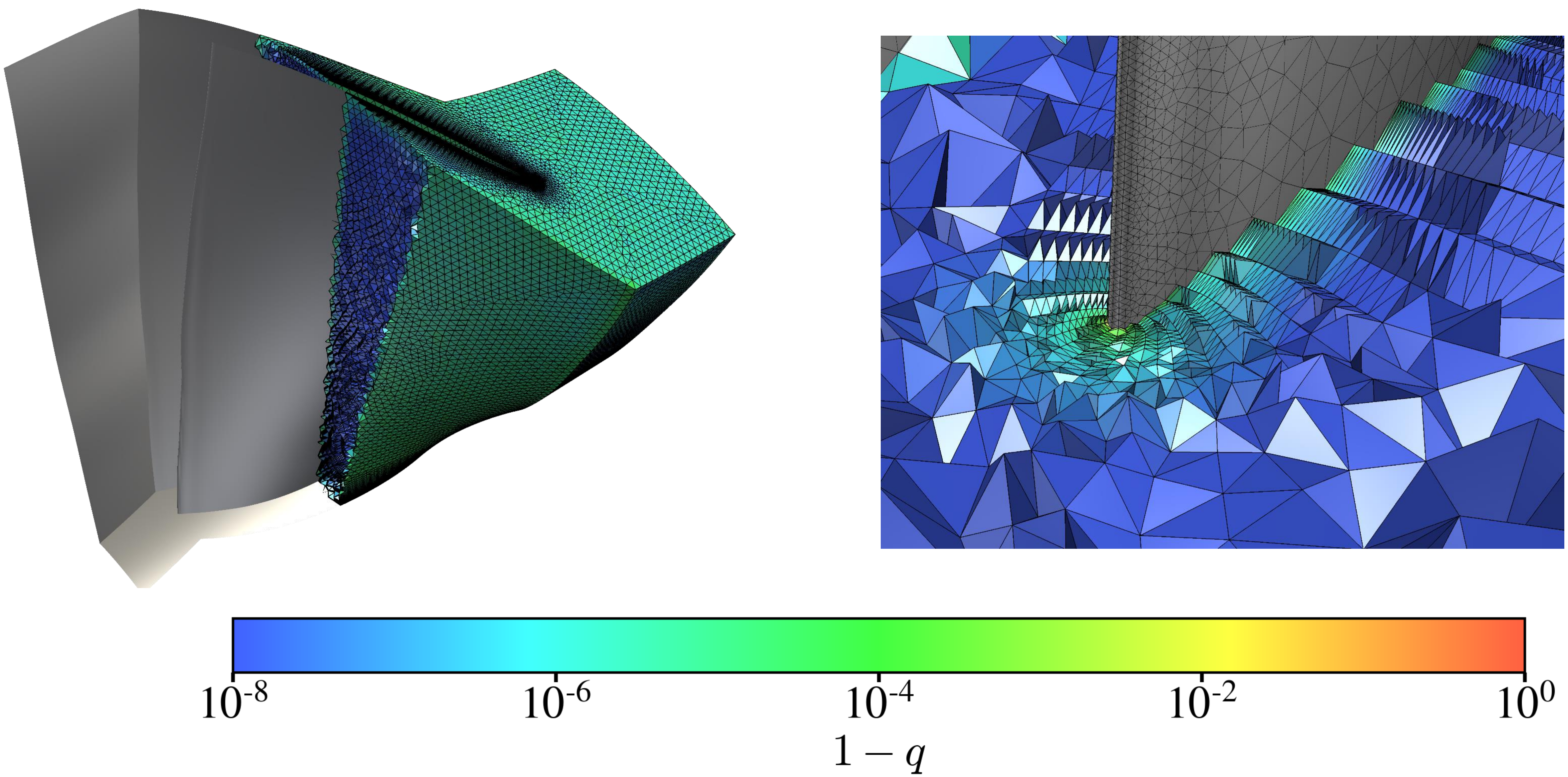
$$m_k = \max\{10, 1/e_k\}$$

$$\mu_{k+1} = \mu_k \min\{m^*, m_k\}$$

Example: Periodic Mesh for the Rotor 67

Set periodic condition in target boundary

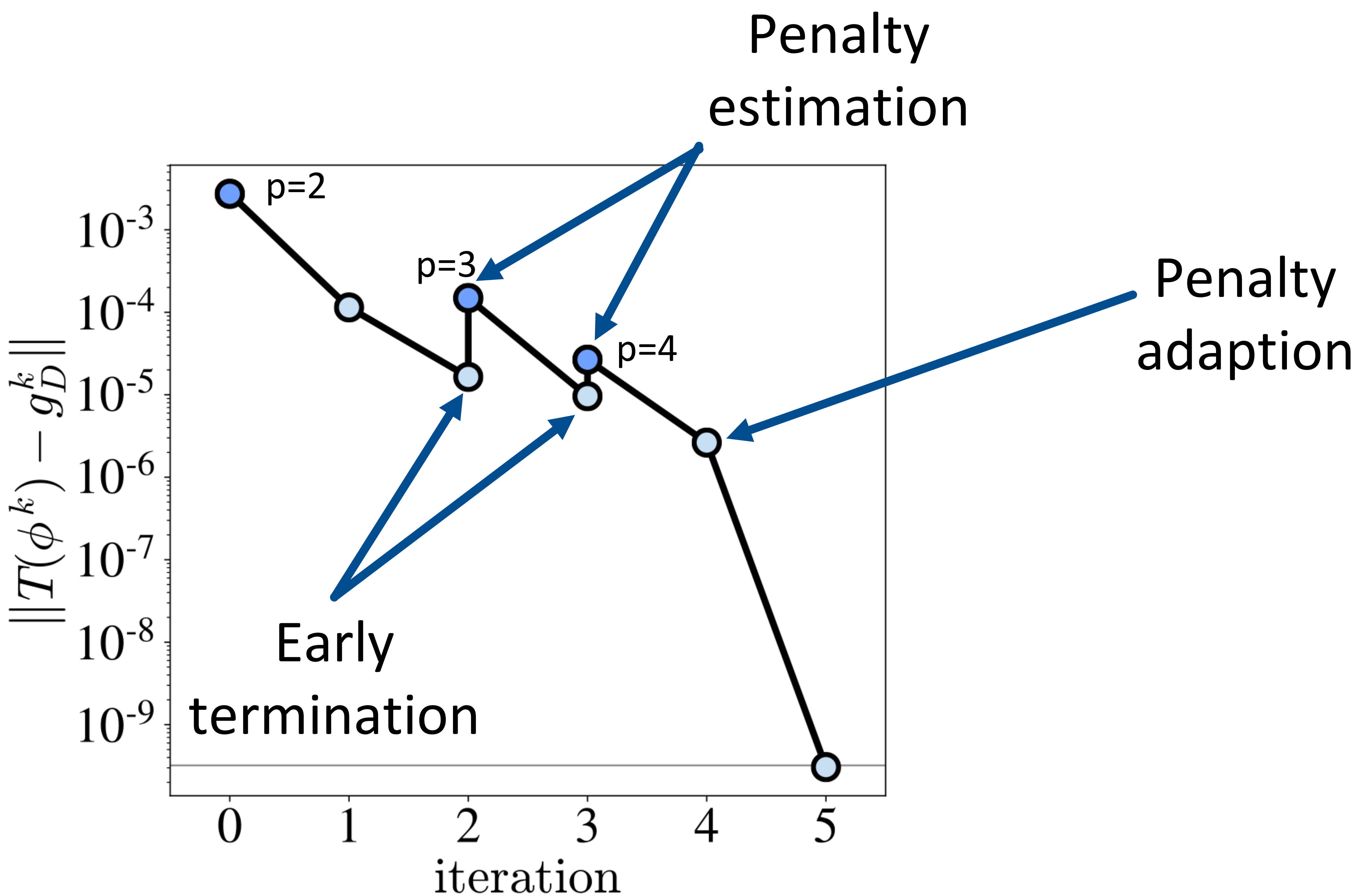
- **Mesh:** p=4, 3.6M elements, boundary layer stretching 1:25
- **Optimization:** 768 cores, 52 minutes, 31.5MJ
- **Metrics:** minQ = 0.987, avg_dist = $1.5 \cdot 10^{-8}$, max_dist = $2.91 \cdot 10^{-5}$



Example: Periodic Mesh for the Rotor 67

Periodic mesh: Impose periodic boundary condition

Mesh: p=4, 3.6M elements, boundary layer stretching 1:25



Forcing Term: Less Linear Iterations

Adapt linear solver tolerance: From loose to tight tolerance

Track the progress of the optimization: use boundary constraint

$$t_k = \frac{\log\left(\frac{\varepsilon_0}{\varepsilon_k / m_k}\right)}{\log\left(\frac{\varepsilon_0}{\varepsilon^*}\right)}$$

Linear solver tolerance

$$\delta = {\delta_{\text{loose}}}^{1-t_k} \cdot {\delta_{\text{tight}}}^{t_k}$$

Pre-conditioned GMRES: 3 Times Less Memory

- Separate the linear problem in smaller blocks: x, y, z coordinates

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_{1,1} & \mathbf{H}_{1,2} & \mathbf{H}_{1,3} \\ \mathbf{H}_{2,1} & \mathbf{H}_{2,2} & \mathbf{H}_{2,3} \\ \mathbf{H}_{3,1} & \mathbf{H}_{3,2} & \mathbf{H}_{3,3} \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix}$$

- Block-based SOR and forward substitution

$$\begin{pmatrix} \mathbf{H}_{1,1} & \mathbf{0} & \mathbf{0} \\ \mathbf{H}_{2,1} & \mathbf{H}_{2,2} & \mathbf{0} \\ \mathbf{H}_{3,1} & \mathbf{H}_{3,2} & \mathbf{H}_{3,3} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1^{l+1} \\ \mathbf{x}_2^{l+1} \\ \mathbf{x}_3^{l+1} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} - \begin{pmatrix} \mathbf{0} & \mathbf{H}_{1,2} & \mathbf{H}_{1,3} \\ \mathbf{0} & \mathbf{0} & \mathbf{H}_{2,3} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1^{l} \\ \mathbf{x}_2^{l} \\ \mathbf{x}_3^{l} \end{pmatrix}$$

- Each block: GMRES preconditioned with RASDD(1)+SSOR(2)
- Store the 3 diagonal blocks and use matrix-free products for the rest
- 3 iteration of block-SOR, $\delta_{pre} = \delta^{1/2}$

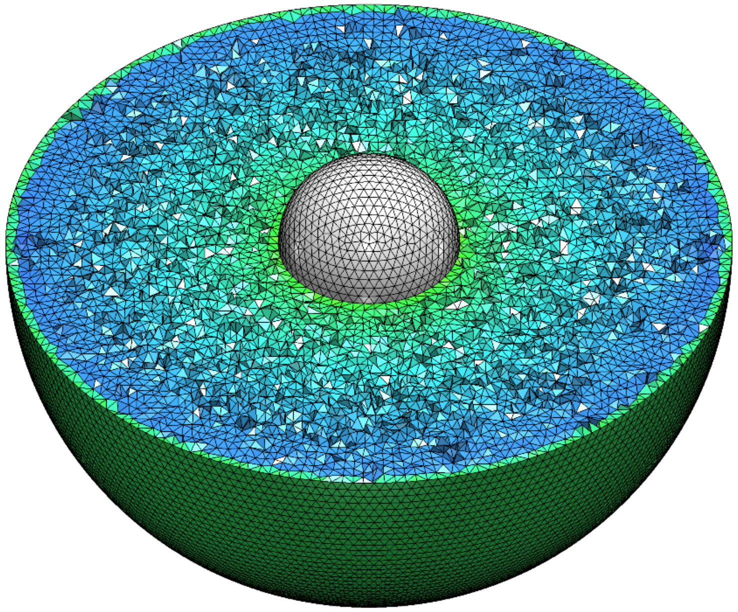
Example: Influence of the improvements

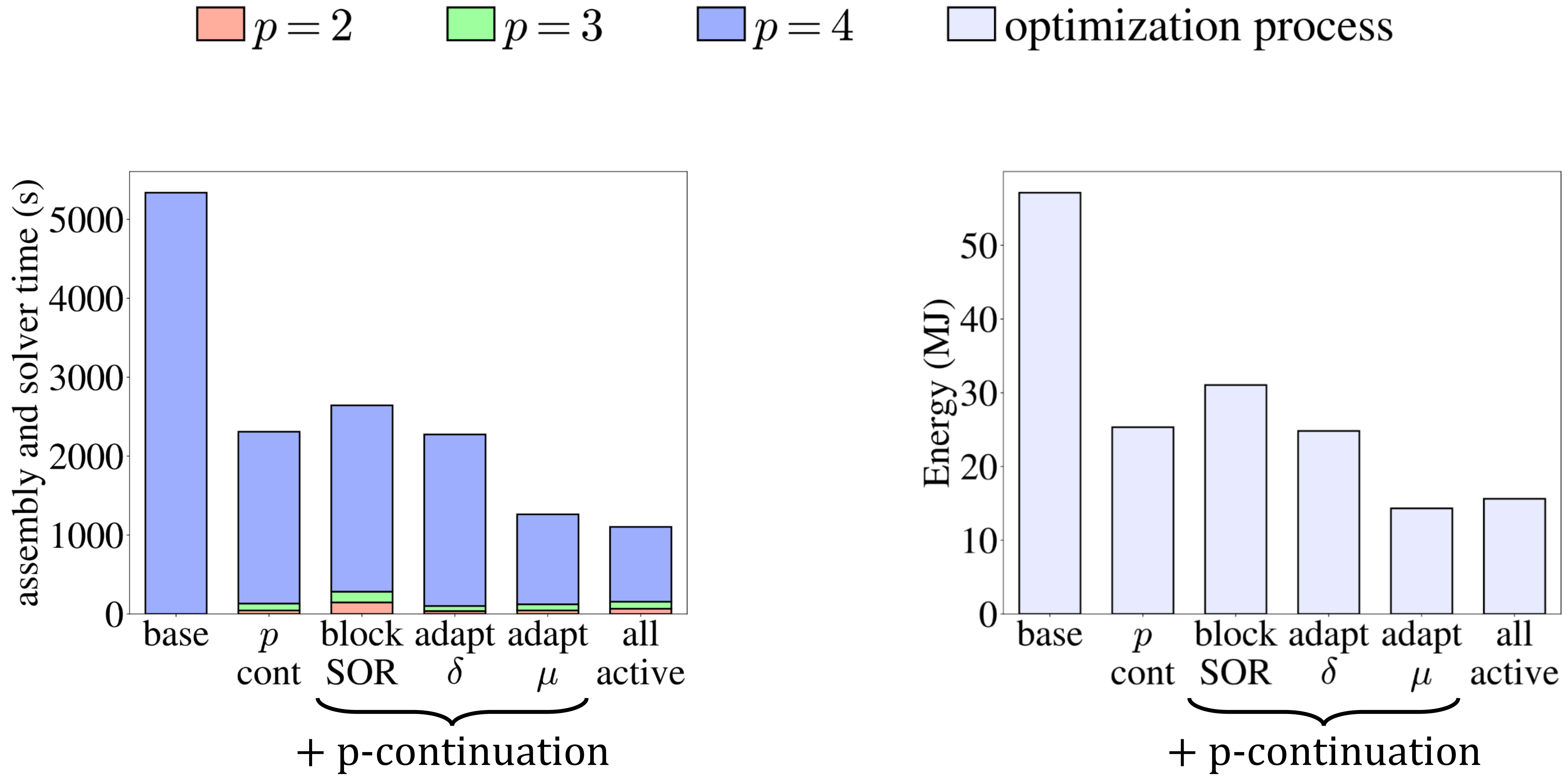
Uniform Mesh for a sphere

Isotropic mesh

1.44M elements, p=4

768 processors





Distributed Solver: Concluding Remarks

- **Key Improvements:**
  - p-continuation
  - Penalty parameter adaption
  - Block-SOR pre-conditioner
  - Forcing term (only for p=2)

- **Improvements**:
  - Decrease time and energy: 4 times
  - Decrease memory footprint: 3 times

3 times larger meshes with the same resources

High-Lift Prediction Workshop

(Ruiz-Gironés, Roca AIAA'22)

- Pre-process
- Post-process
- Software, libraries, and languages

HLPW: Pre-processing for curving-friendly inputs

- **Setup the simulation intent:** repair geometry & virtual model

- **Linear mesh generation:**
  - **Element size:** Simulation and geometry accuracy
  - **Curving:** curving-friendly mesh leads to easy curving process

- **Convert sequential inputs to parallel inputs**
  - Sequential inputs are bottlenecks
  - Create a hdf5 parallel input

HLPW: Check curved mesh and create output file

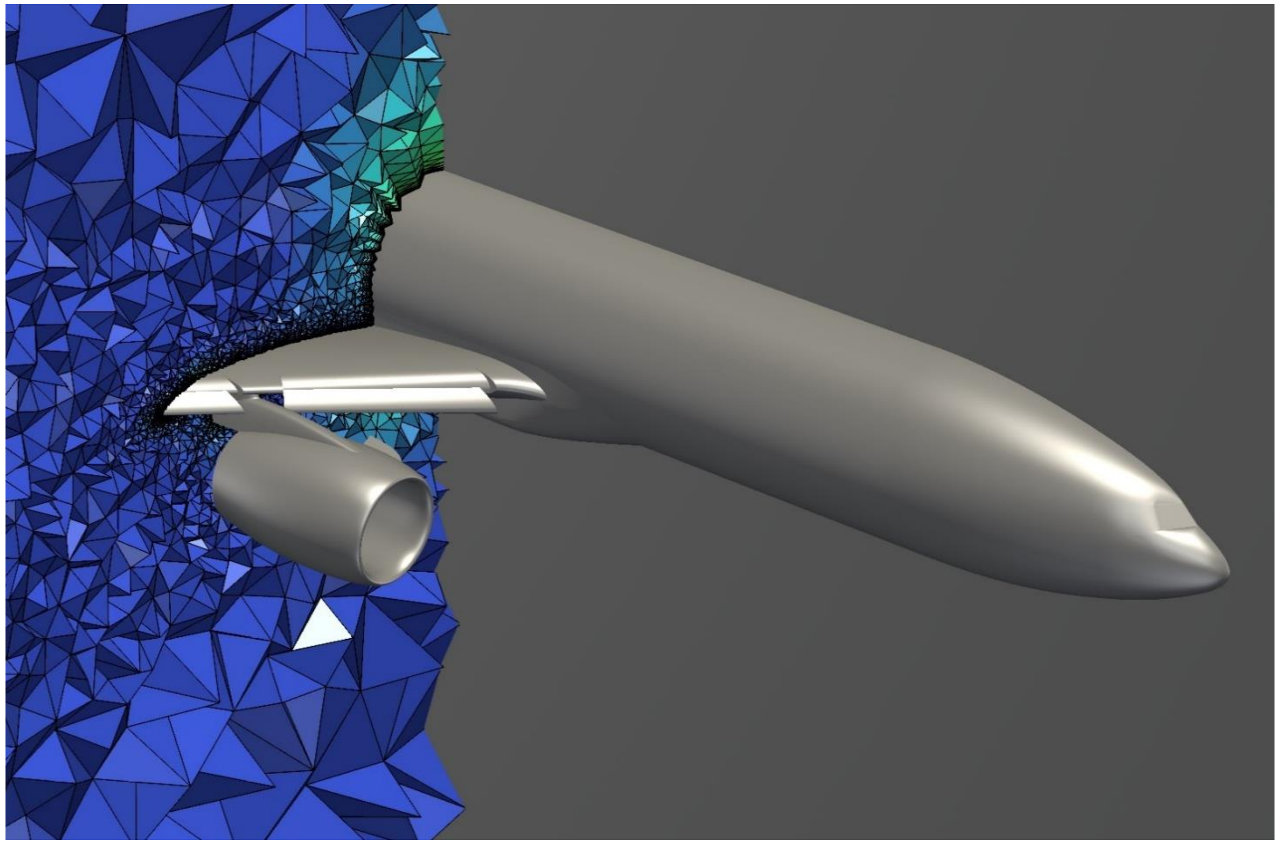
- **Mesh validity and quality:** Numeric validation
- **Visual inspection:** Paraview in distributed parallel
  Locate low-quality and low-accuracy elements
- **Curving iterative process:**
  Remesh low-quality and low-accuracy elements
- **Create output file:** python wrapper of cgns library

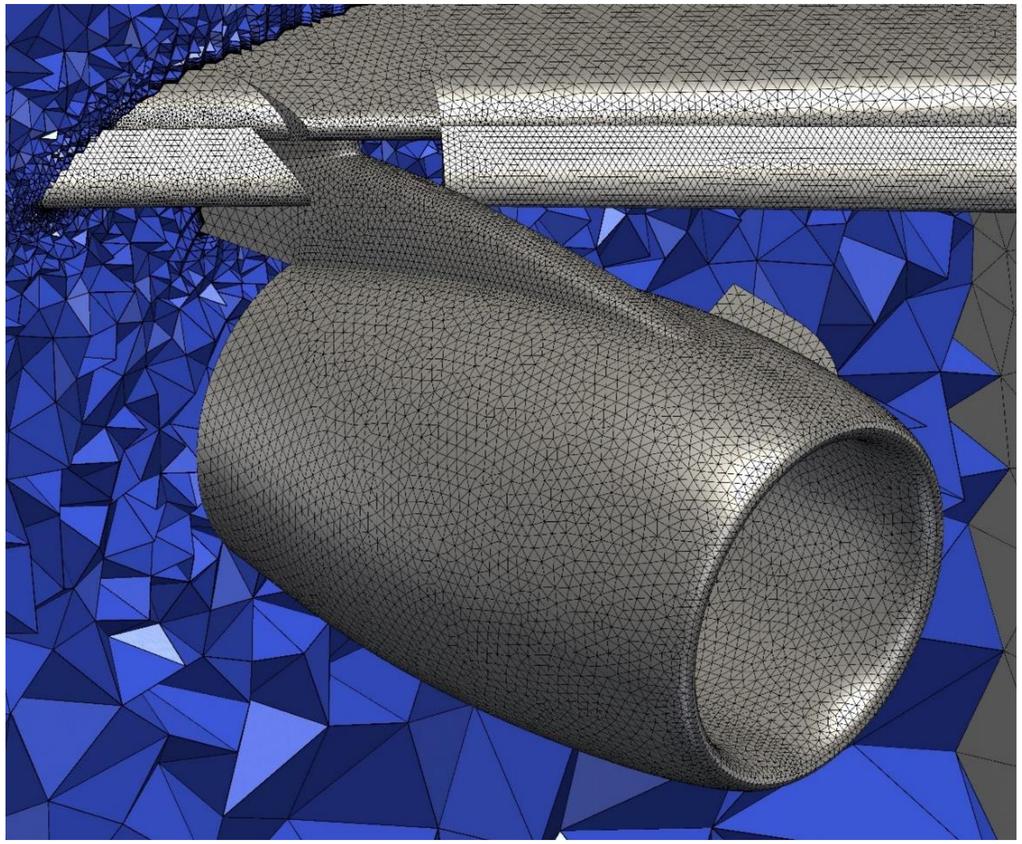
HLPW: Software, Libraries and Languages

- **Virtual model & linear mesh:** Pointwise
- **Distributed solver:** our python implementation with FEniCS library
- **CAD engine:** our python wrapper of Project Geode / OpenCASCADE
- **Linear solver library:** petsc4py interface to PETSc
- **Distributed parallel solver:** running on MareNostrum 4
- **Visualization:** distributed parallel Paraview
- **cgns output:** our python wrapper of cgns library

Example: CRM-HL of the 4^{th} HLPW

- **Mesh:** p=2 & p=3, 8M elements, boundary layer stretching 1:250
- **Accuracy:** relative to aircraft length $\sim 10^{-7} - 10^{-6}$
- **Computational resources:** 768 processors
  - p = 2 → 12 minutes
  - p = 3 → 48 minutes





Our meshes provided the best match with experimental results

(ZJ Wang AIAA'22)

Our Participation in HLPW: Concluding Remarks

- **Preparing curving-friendly inputs takes days** (human labor)
  - Tune the virtual model & linear mesh → Iterative process
  - Curving-friendly inputs → High-quality mesh in a short time

- **Mesh curving for the CRM-HL takes minutes** (computing wall time)
  - We generate larger meshes than the CFD community wants to run
  - Curving is a steady-state problem with less unknowns than CFD

- **You can try our meshes!**
  - Free to download in the 4^{th} & 5^{th} HLPW websites

Our meshes provided the best match with experimental results

Summary & Conclusions

Summary & conclusions: Large-Scale Curving

- **Mesh curving constrained formulation:**
  - Always numerically valid
  - Optimal quality
  - Approximates target geometry
  - Tightly converged
- **Complex geometry in parallel:** mesh approximates virtual geometry
- **Large-scale curving:** 3 times larger meshes on thousands of cores
- **High-lift prediction:** Our meshes lead to best match with experiments

Our curving enables high-fidelity simulations on complex geometries

Thank you for your attention!

European Research Council
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