



Reaction-Diffusion Equation-based Topology Optimization: 3D Fluid-Structure System Design using FreeFEM-PETSc-Mmg

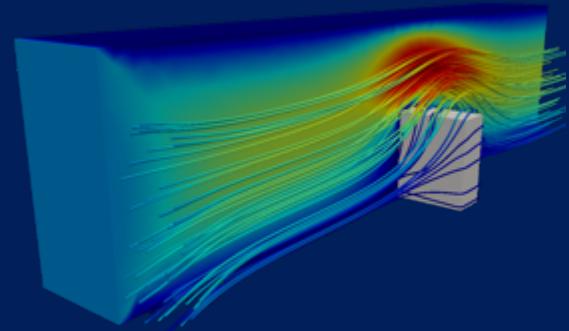
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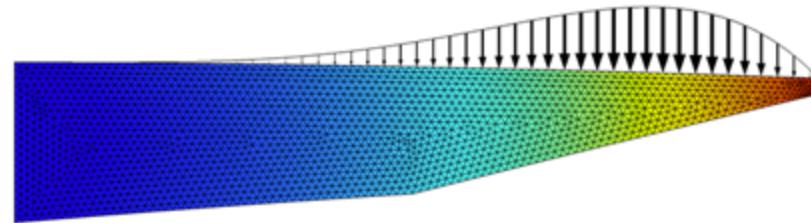
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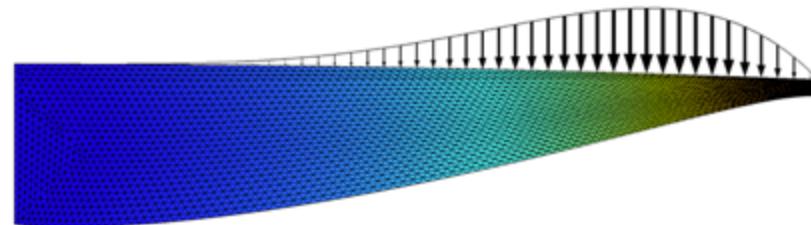
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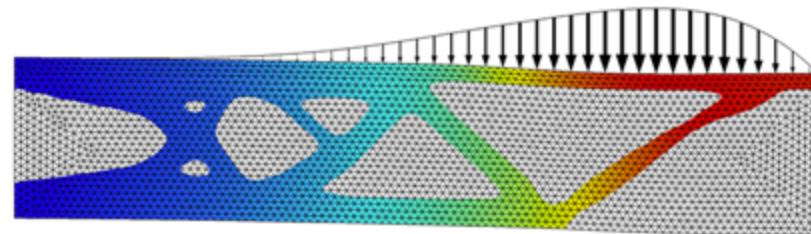
Introduction – Size, Shape, *Topology* optimization



Size optimization



Shape optimization



Topology optimization

Topology optimization (TO) is a mathematical method that optimizes material layout within a given design space, for a given set of loads, boundary conditions and constraints with the goal of maximizing the performance of the system. TO is different from shape optimization and size optimization in the sense that the design can attain any shape within the design space, instead of dealing with predefined configurations.

(Figure from COMSOL Multiphysics)

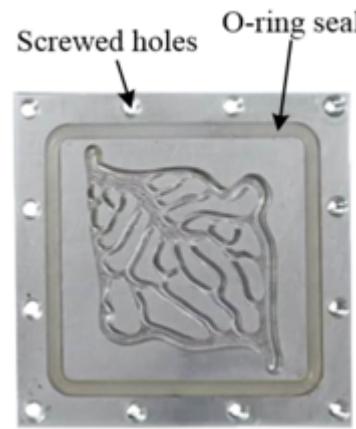
Introduction – Industrial application



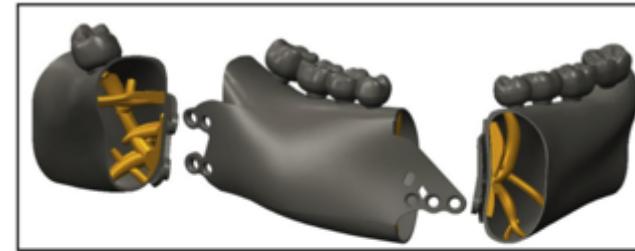
Qatar National Convention Center



Lei et al., 2018



Li et al., 2019



WBOS model



WBOS manufactured sample

Li et al., 2020



Aage et al., 2017

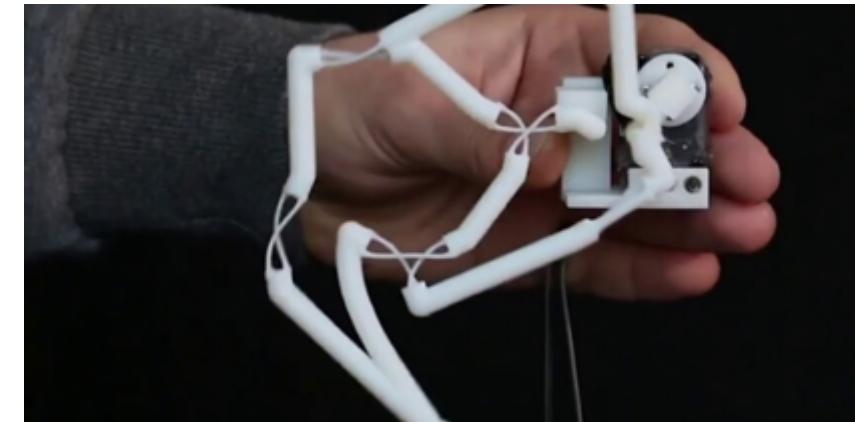


Figure cited from Sculpteo



Figure cited from Altair

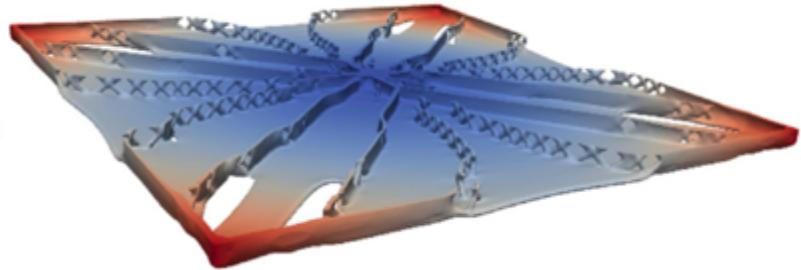
Introduction – 3D topology optimization



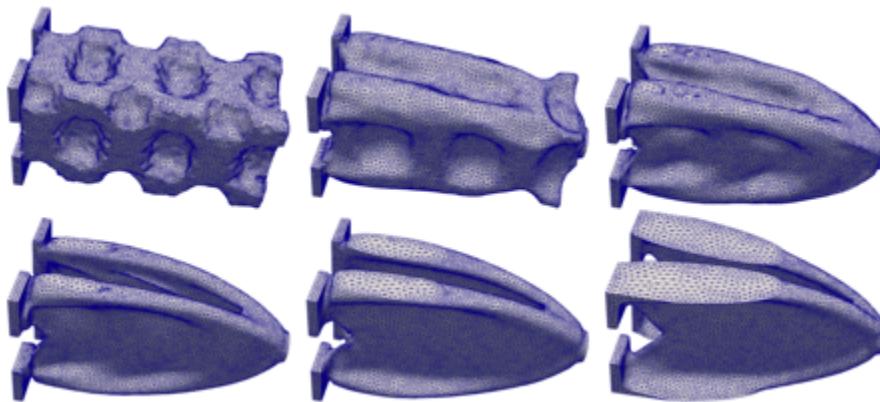
Aage et al., 2017



Liu et al., 2019



Liu et al., 2019



Feppon et al., 2020

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RDE based level-set method

Level-set update equation

Reaction equation

$$\begin{cases} \frac{\partial \phi}{\partial t} = -K \bar{F}' & \text{in } D \\ \phi = 0 & \text{on } \partial D \end{cases}$$

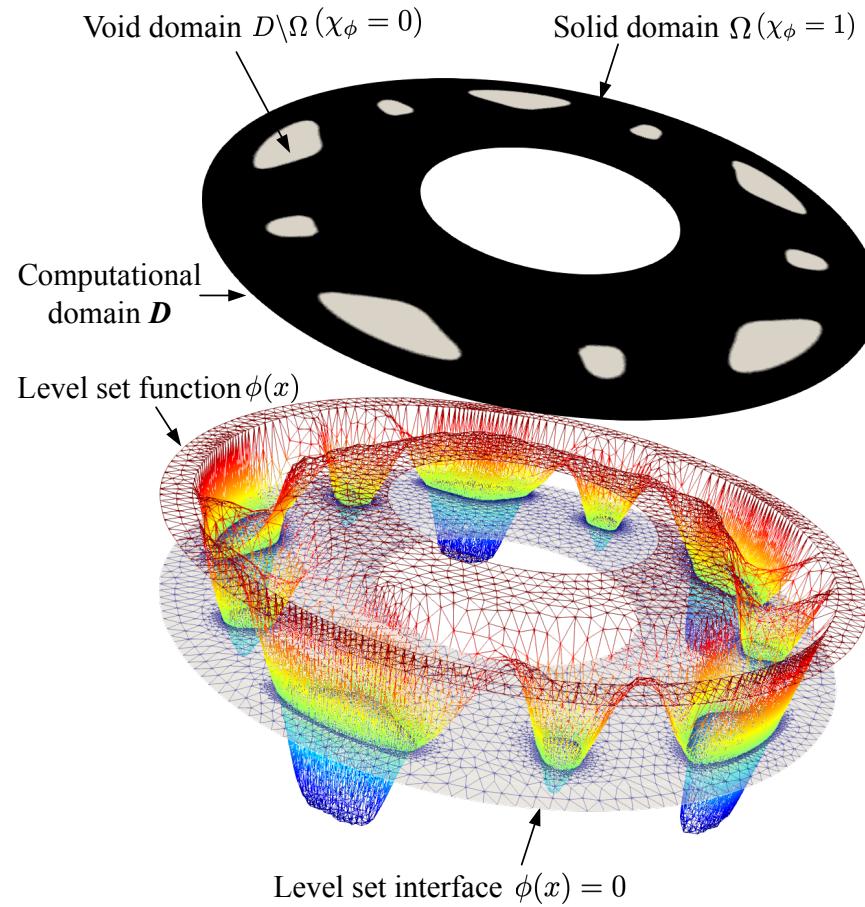
Reaction diffusion equation (Yamada et al.)

$$\begin{cases} \frac{\partial \phi}{\partial t} = - \left(\tilde{C} \bar{F}' - \tau \nabla^2 \phi \right) & \text{in } D \\ \phi = 0 & \text{on } \partial D. \end{cases}$$

Using the finite difference method, semi-discretized in time as follows:

$$\begin{cases} \frac{\phi(t+\Delta t)}{\Delta t} - \tau \nabla^2 \phi(t + \Delta t) = -\tilde{C} \bar{F}' + \frac{\phi(t)}{\Delta t} & \text{in } D \\ \phi = 0 & \text{on } \partial D \end{cases}$$

“Ersatz material” method



Characteristic function

$$\chi_\phi = \begin{cases} 1 & \text{if } \phi \geq 0 \\ 0 & \text{if } \phi < 0 \end{cases}$$

Elasticity:

$$C_{\chi_\phi} = \chi_\phi C$$

Thermal:

$$\kappa_{\chi_\phi} = \chi_\phi \kappa$$

Fluid:

$$\alpha = \alpha_{\max} \frac{q(1-\chi_\phi)}{q+\chi_\phi}$$

•
•
•

RDE based level-set method

Level-set update equation

Reaction equation

$$\begin{cases} \frac{\partial \phi}{\partial t} = -K \bar{F}' & \text{in } D \\ \phi = 0 & \text{on } \partial D \end{cases}$$

A characteristic function is monotonically increase with level-set function:

$\phi = \phi(x)$ design variable

$\chi_\phi = \chi(\phi(x))$, $\frac{d\chi_\phi}{d\phi} \geq 0$ characteristic function.
assume that there is an optimization problem in which the Lagrangian is defined as:

$$\inf_{\chi_\phi \in \mathcal{X}} \mathcal{L} = \mathcal{L}(\chi_\phi).$$

The sensitivity with respect to the characteristic function

$$\bar{F}' = \frac{\delta \mathcal{L}(\chi_\phi)}{\delta \chi_\phi}.$$

Then the functional derivative of the Lagrangian with respect to the design variable (level set function)

$$\frac{\delta \mathcal{L}(\chi_\phi)}{\delta \phi} = \frac{\delta \mathcal{L}(\chi_\phi)}{\delta \chi_\phi} \frac{d\chi_\phi}{d\phi} = \bar{F}' \frac{d\chi_\phi}{d\phi}.$$

Using the Reaction equation as the time evolution equation:

Then, choose a time step, the variation of level-set function with the time step can be expressed as:

$$\delta \phi(t) = \phi(t + \Delta t) - \phi(t) \approx \frac{\partial \phi(t)}{\partial t} \Delta t = -K \bar{F}' \Delta t \quad \text{in } D.$$

Therefore, the variation of characteristic function with the time step can be expanded as:

$$\delta \chi_\phi(t) = \frac{d\chi_\phi(t)}{d\phi(t)} \delta \phi(t) = -K \bar{F}' \frac{d\chi_\phi(t)}{d\phi(t)} \Delta t.$$

Then the variation of Lagrangian with the time step can be rewritten as:

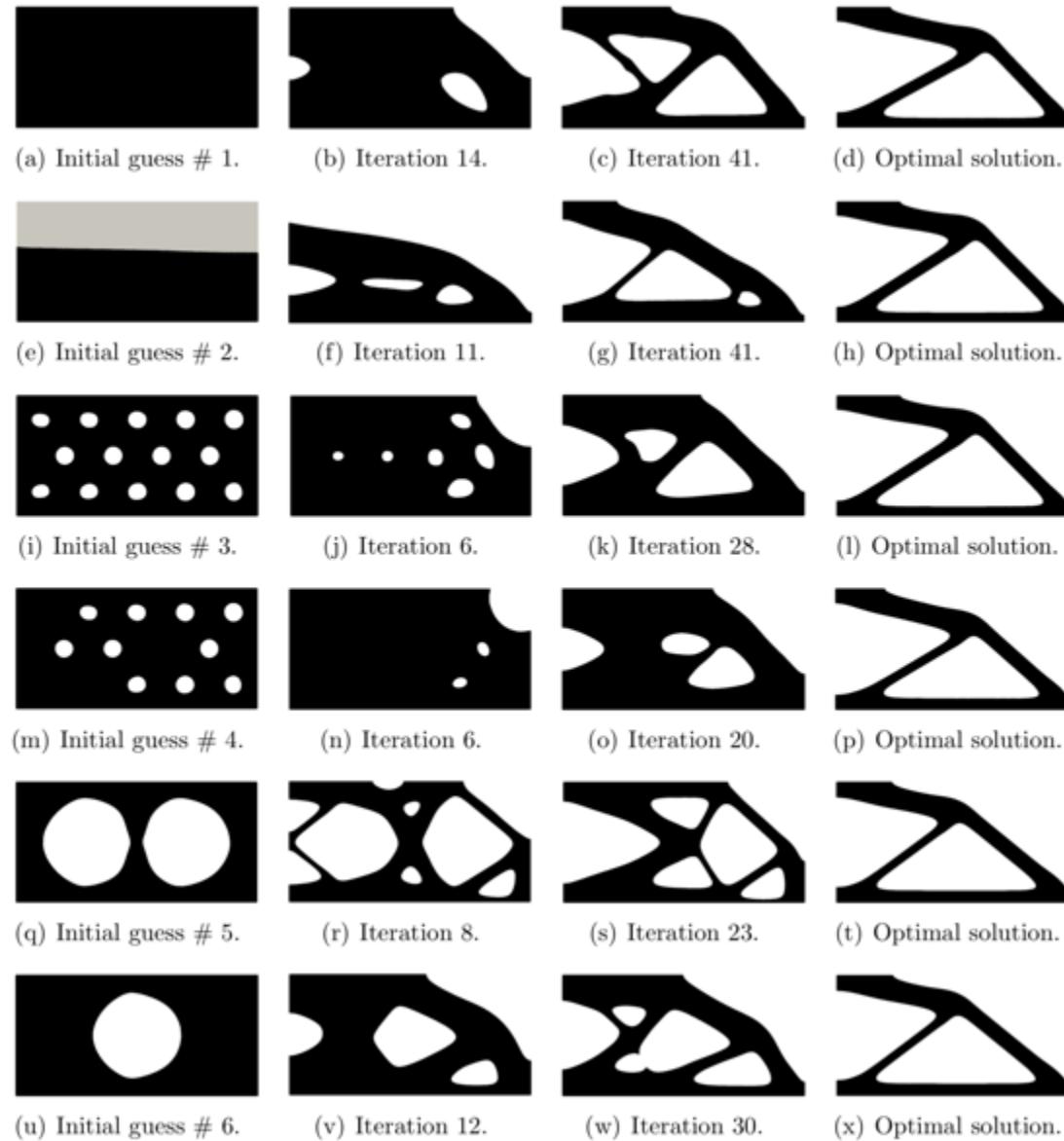
$$\begin{aligned} \delta \mathcal{L}(\chi_\phi(t)) &\equiv \mathcal{L}(\chi_\phi(t + \Delta t)) - \mathcal{L}(\chi_\phi(t)) = \mathcal{L}(\chi_\phi(t) + \delta \chi_\phi(t)) - \mathcal{L}(\chi_\phi(t)) \\ &= \int_D \bar{F}' \delta \chi_\phi(t) dD. \end{aligned}$$

Lagrangian monotonically decreases with the time evolution.

$$\delta \mathcal{L}(\chi_\phi(t)) \approx -K \Delta t \int_D (\bar{F}')^2 \frac{d\chi_\phi(t)}{d\phi(t)} dD \leq 0.$$

RDE based level-set method –Initial guess dependency

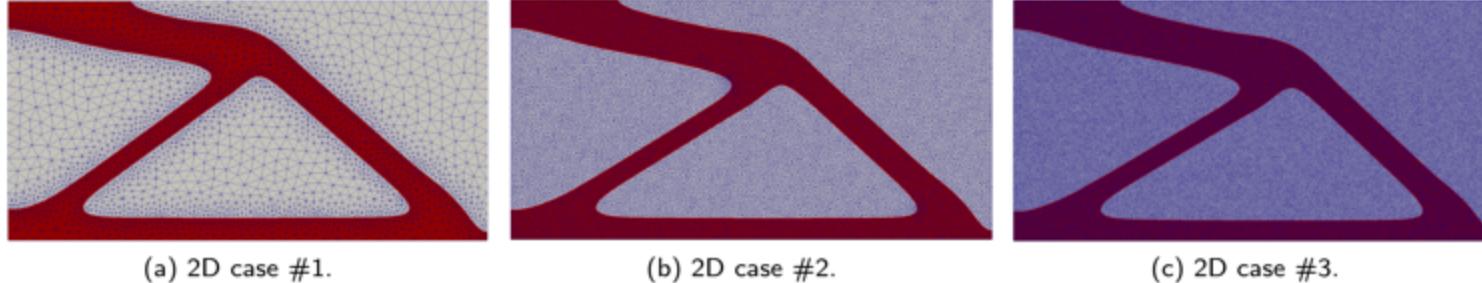
$$\begin{cases} \frac{\partial \phi}{\partial t} = - \left(\tilde{C} \bar{F}' - \tau \nabla^2 \phi \right) & \text{in } D \\ \phi = 0 & \text{on } \partial D. \end{cases}$$



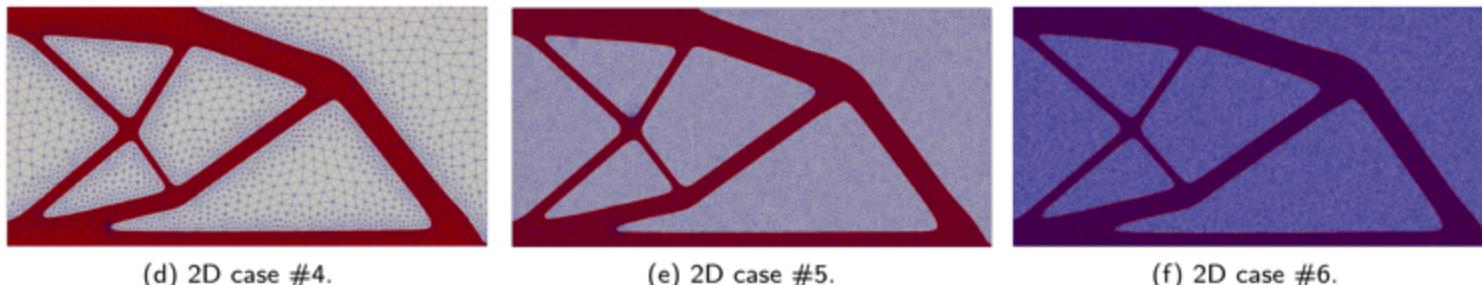
RDE based level-set method – Mesh dependency

$$\begin{cases} \frac{\phi(t+\Delta t)}{\Delta t} - \tau \nabla^2 \phi(t + \Delta t) = -\tilde{C} \bar{F}' + \frac{\phi(t)}{\Delta t} & \text{in } D \\ \phi = 0 & \text{on } \partial D \end{cases}$$

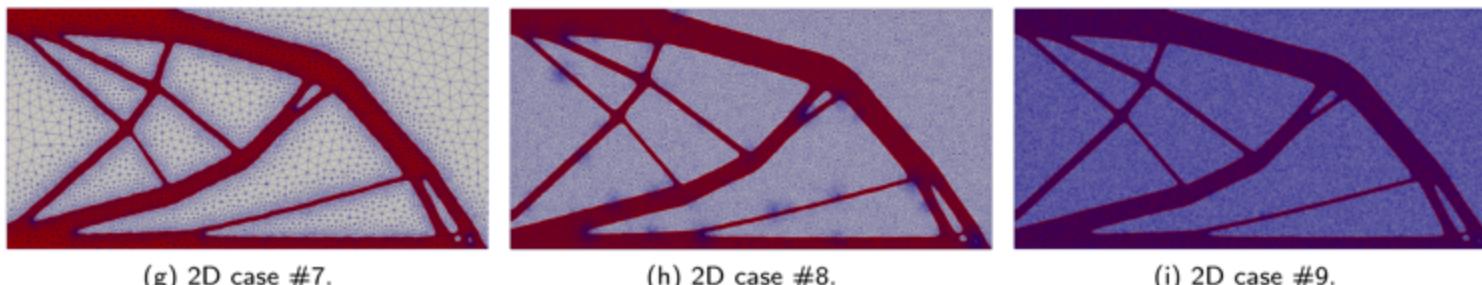
$\tau = 1 \times 10^{-4}$



$\tau = 1 \times 10^{-5}$



$\tau = 1 \times 10^{-6}$



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Body-fitted mesh adaption (Mmg)

Goals

Evolve an explicit mesh $\mathcal{T}_i \rightarrow \mathcal{T}_{i+1}$ of a specific value of an implicit level set function ϕ .

Step 1. Calculate design sensitivity \bar{F}' for the reaction source term. Choose a time step $\Delta t > 0$ and, on the current step computation mesh \mathcal{T}_i solve RDE. A new level-set field ϕ_{i+1} is obtained.

$$\begin{cases} \frac{\phi(t+\Delta t)}{\Delta t} - \tau \nabla^2 \phi(t + \Delta t) = -\tilde{C} \bar{F}' + \frac{\phi(t)}{\Delta t} & \text{in } D \\ \phi = 0 & \text{on } \partial D \end{cases}$$

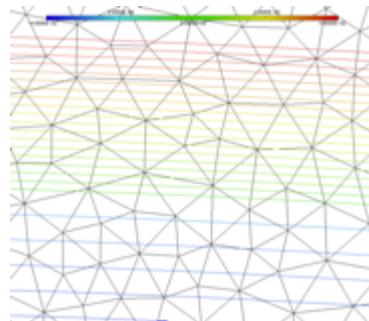
Step 2. Initialize the Mmg data structure, parse the mesh file and store the mesh in the Inria Medit format (.mesh).

Step 3. Roughly discretize the newly updated Ω_{i+1} into \mathcal{T}_i based on the zero-level-set of ϕ_{i+1}

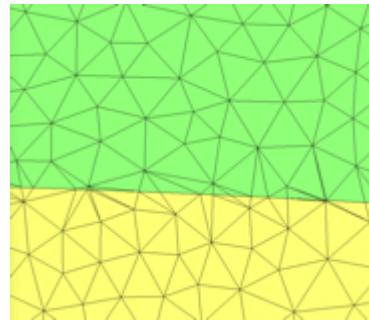
Step 4. Quality-oriented local mesh modification. (including split the edges that are “too long”, merge two endpoints of an edge, swap connectivities, etc.). Output a high-quality mesh \mathcal{T}_{i+1} for the next iteration.

(Algorithm proposed by Allaire, Dapogny, and Frey.) <https://www.mmgtools.org/>

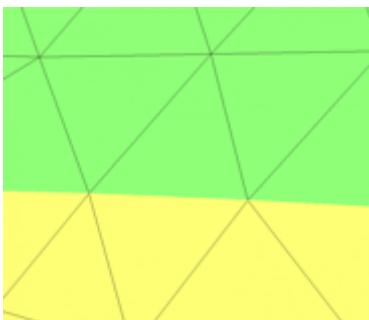
Dapogny, C., Dobrzynski, C., & Frey, P. (2014). Three-dimensional adaptive domain remeshing, implicit domain meshing, and applications to free and moving boundary problems. Journal of computational physics, 262, 358-378.



Nodal values of a level set function
(Step 1)

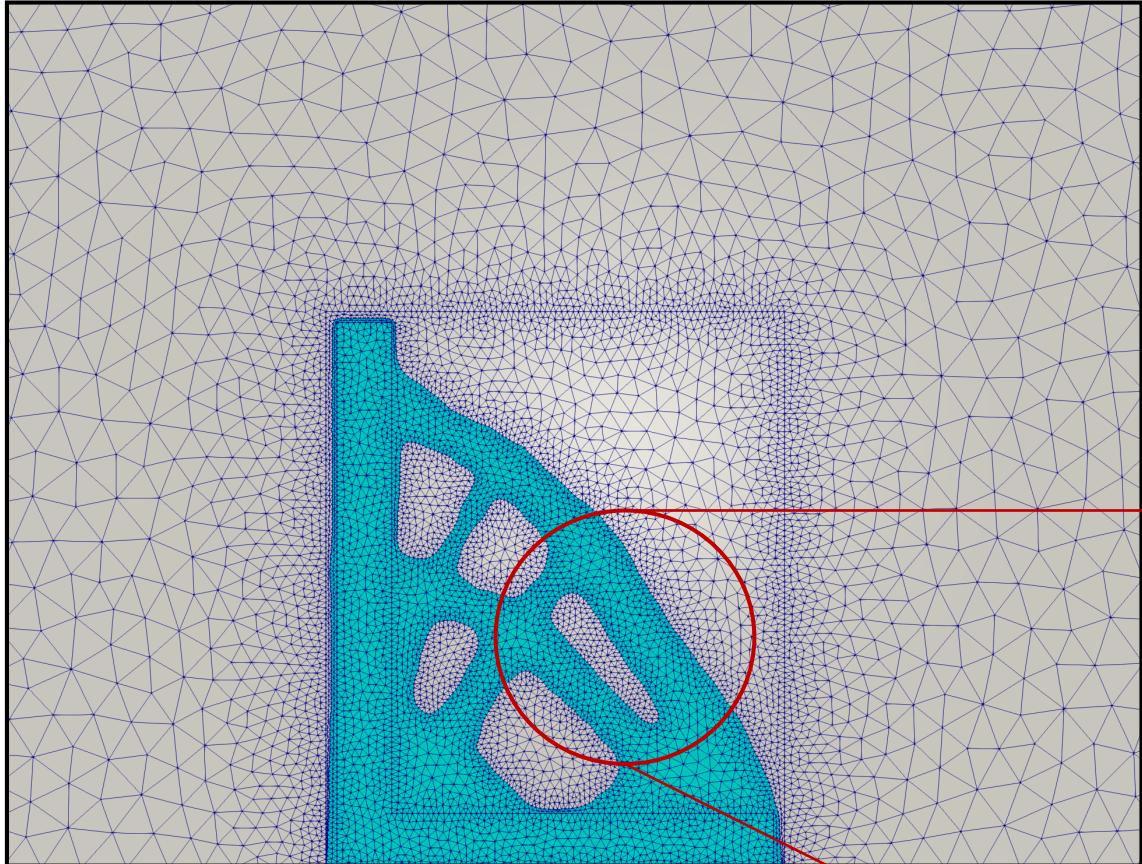


Temporary mesh after the level-set
discretization **(Step 3)**



Output mesh **(Step 4)**

Body-fitted mesh adaption (Mmg)

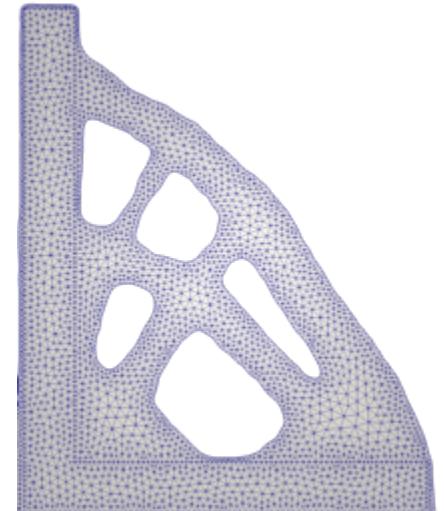


What can we set?

1. Max./Min. element edge size of GLOBAL domain
2. Max./Min. element edge size along ZERO-LEVEL-SET interface
3. Ratio between the length of two adjacent edges

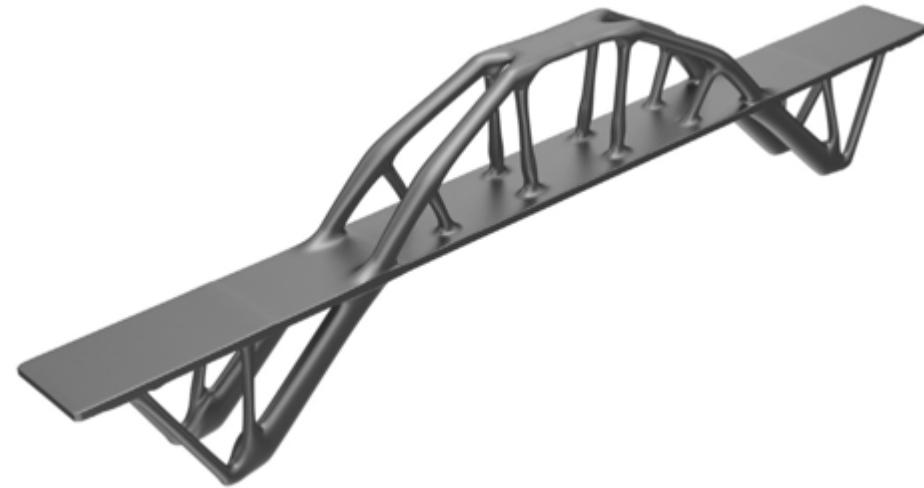
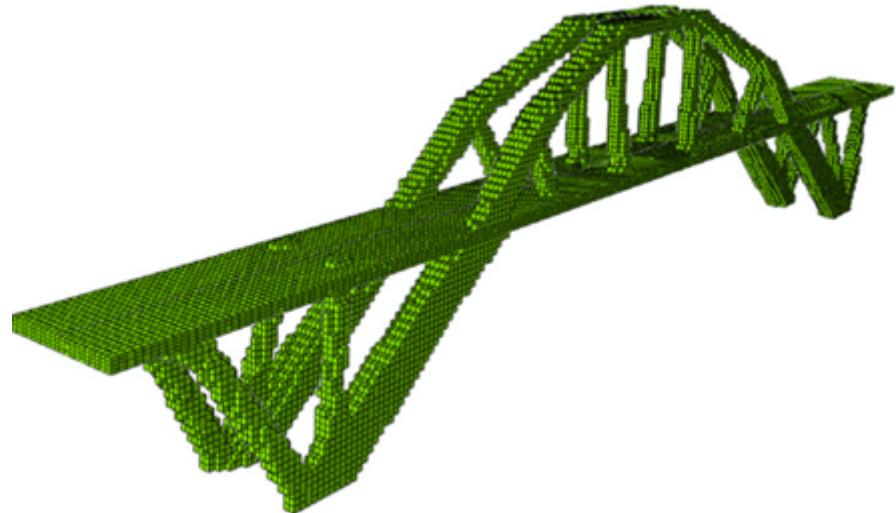
What can we achieve?

1. High resolution boundary
2. Coarse mesh in void domain -->save computational cost

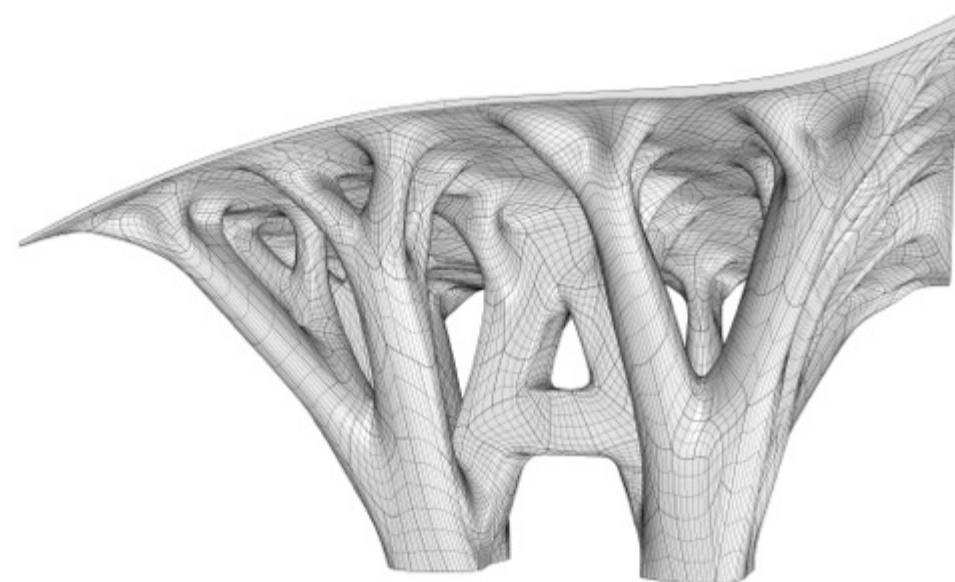
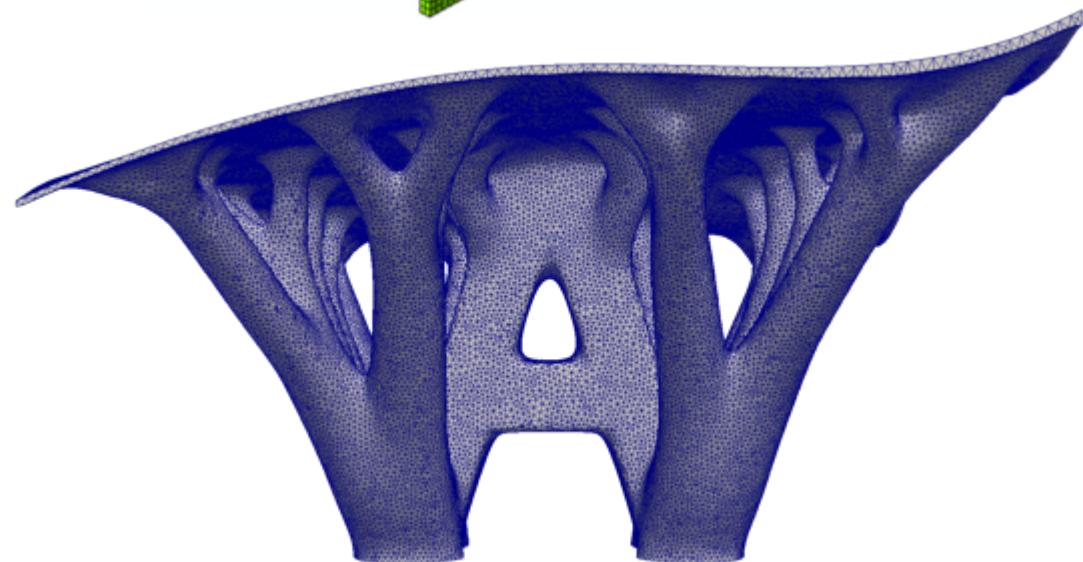


Body-fitted mesh adaption (Mmg)

B-Reps conversion (Mesh → CAD)



(He et al., 2020)



(Our result)

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Numerical implementation

- **FreeFEM is used for the discretization of PDEs.**

After decomposing an initial mesh using a graph partitioner package like METIS, the distributed assembly of the weak forms of Equations is performed by FreeFEM.

- **PETSc is used for the linear algebra backend.**

The resulting discrete linear systems are passed over to PETSc. They are solved using multigrid preconditioners, GAMG for Lamé and *hypre* for RDE, etc.

Augmented Lagrangian preconditioner for large-scale nonlinear problem. (Moulin et al., 2019)

<https://github.com/prj-/moulin2019al>.

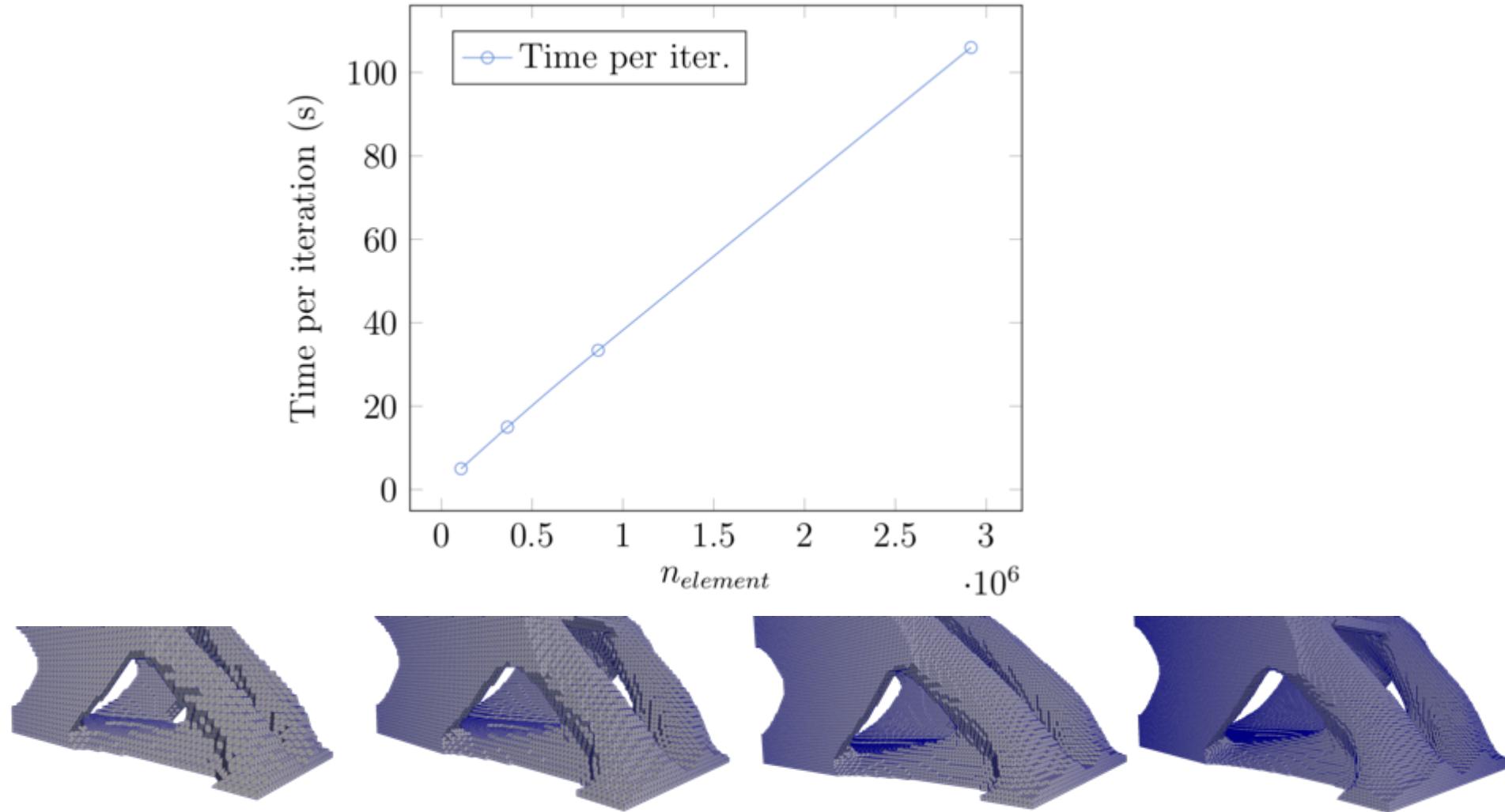
(References)

Dolean, V., Jolivet, P., & Nataf, F. (2015). An introduction to domain decomposition methods: algorithms, theory, and parallel implementation (Vol. 144). SIAM.

Moulin, J., Jolivet, P., & Marquet, O. (2019). Augmented Lagrangian preconditioner for large-scale hydrodynamic stability analysis. *Computer Methods in Applied Mechanics and Engineering*, 351, 718-743.

Numerical implementation

This ensures that this part of the TO method is scalable with respect to the number of processes and the mesh size of the models.

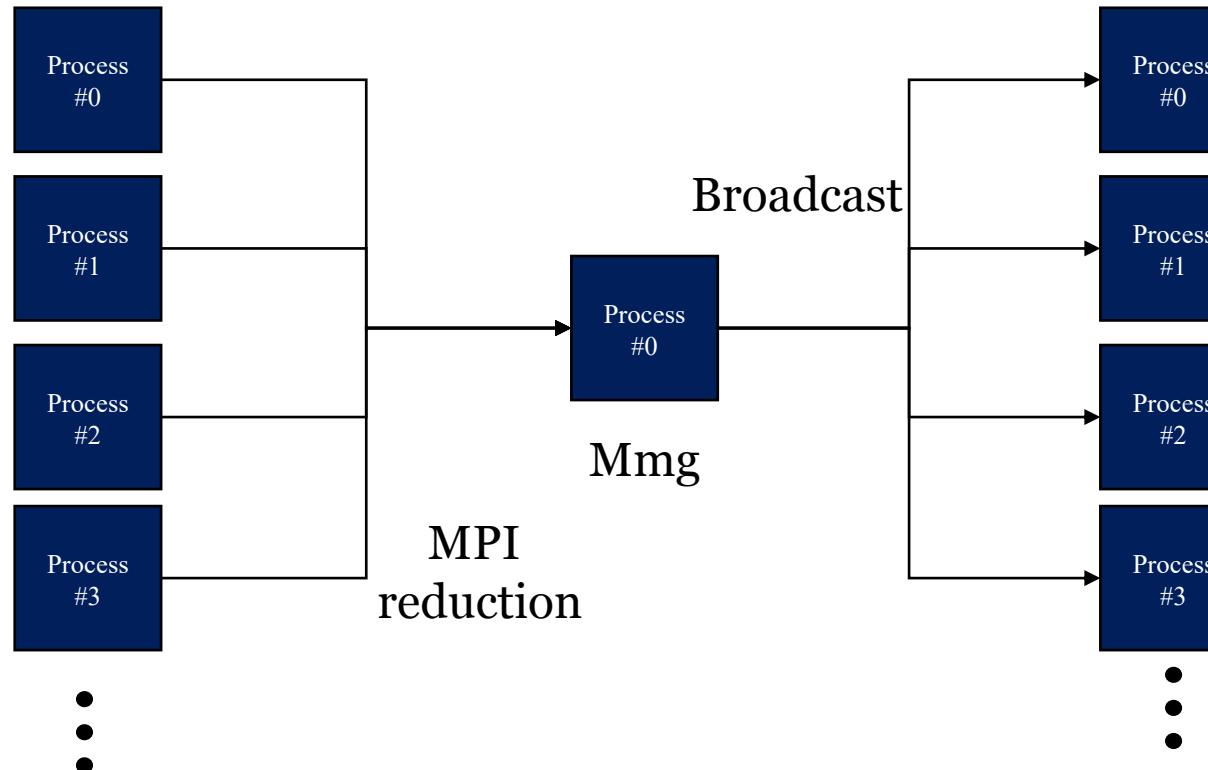


Numerical implementation

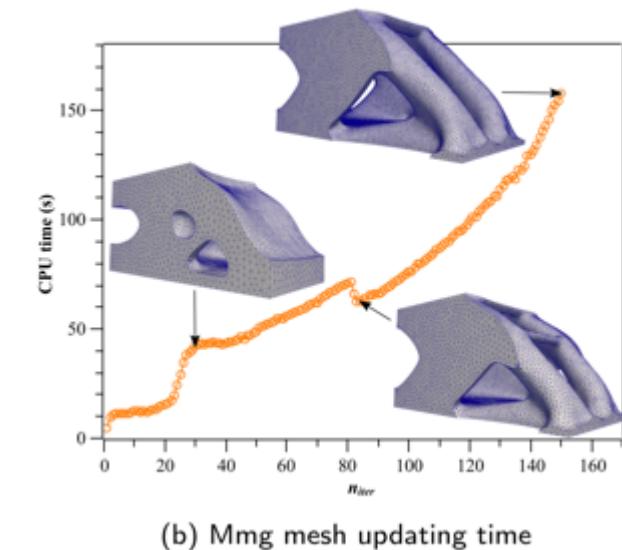
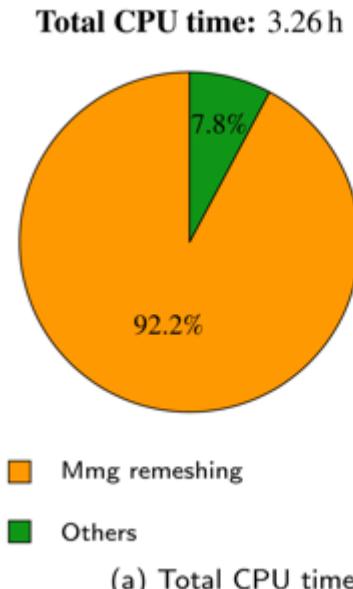
- Bottleneck (sequential Mmg)**

Mmg is performed sequentially on a single process.

We limit the problem size to less than 3 million tetrahedron elements.



Solve RDE



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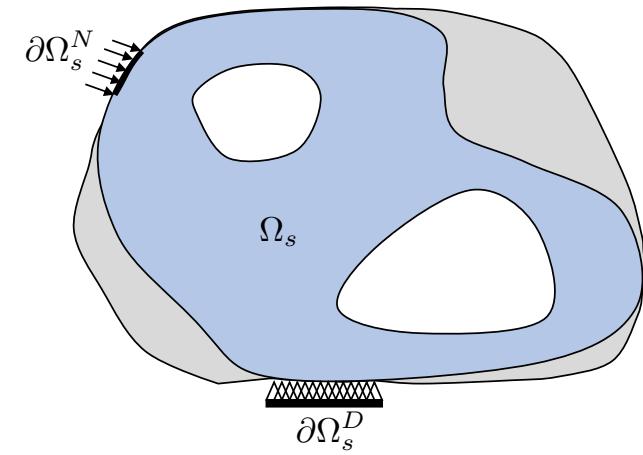
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Compliance problem

Optimization model

$$\inf_{\chi_\phi \in \mathcal{X}} J(\Omega) = \int_{\Gamma_N} \bar{g} \cdot u \, d\Gamma$$

s.t.
$$\begin{cases} R_1 = -\operatorname{div}(C : e(u)) = 0 & \text{in } \Omega \\ G_1 = \frac{\int_D \chi_\phi \, d\Omega}{\int_D \, d\Omega} - V_{max} \leq 0 \\ u = 0 & \text{on } \Gamma_D \\ (C : e(u)) \cdot n = \bar{g} & \text{on } \Gamma_N. \end{cases}$$





Compliance problem

Adjoint problem & Sensitivity

Lagrangian:

$$\mathcal{L}(\tilde{u}, \tilde{v}, \Omega) = \int_{\Gamma_N} g \cdot \tilde{u} d\Gamma - \int_{\Omega} (\operatorname{div}(C : e(\tilde{u}))) \cdot \tilde{v} d\Omega$$

Applying integration by part and divergence theorem

$$\mathcal{L}(\tilde{u}, \tilde{v}, \Omega) = \int_{\Gamma_N} g \cdot \tilde{u} d\Gamma + \int_{\Omega} (e(\tilde{u}) : C) : e(\tilde{v}) d\Omega - \int_{\Gamma_N} g \cdot \tilde{v} d\Gamma$$

According to KKT condition:

$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{u}}(u, v, \Omega), \xi \right\rangle = \int_{\Gamma_N} g \cdot \xi d\Gamma + \int_{\Omega} (e(\xi) : C) : e(\tilde{v}) d\Omega = 0$$

The following equation should be satisfied with any arbitrary ξ

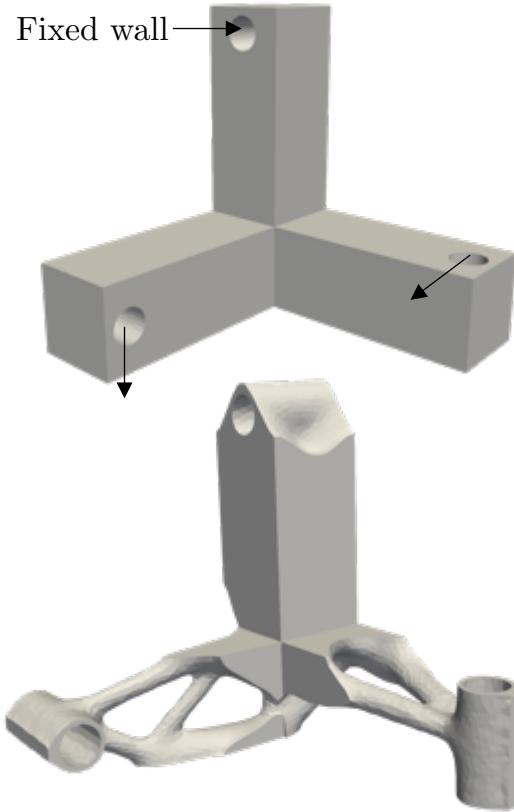
$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{u}}(u, v, \Omega), \xi \right\rangle = - \int_{\Omega} \operatorname{div}(C : e(\tilde{v})) \cdot \xi dx + \int_{\Gamma_D} ((C : e(\tilde{v}))) \cdot n \Big) \cdot \xi d\Gamma + \int_{\Gamma_N} ((C : e(\tilde{v})) \cdot n) + g \Big) \cdot \xi d\Gamma = 0$$

Adjoint problem:
$$\begin{cases} \operatorname{div}(C : e(v)) = 0 & \text{in } \Omega \\ v = 0 & \text{on } \Gamma_D \\ -\tilde{g} = \bar{g} & \text{on } \Gamma_N \end{cases}$$

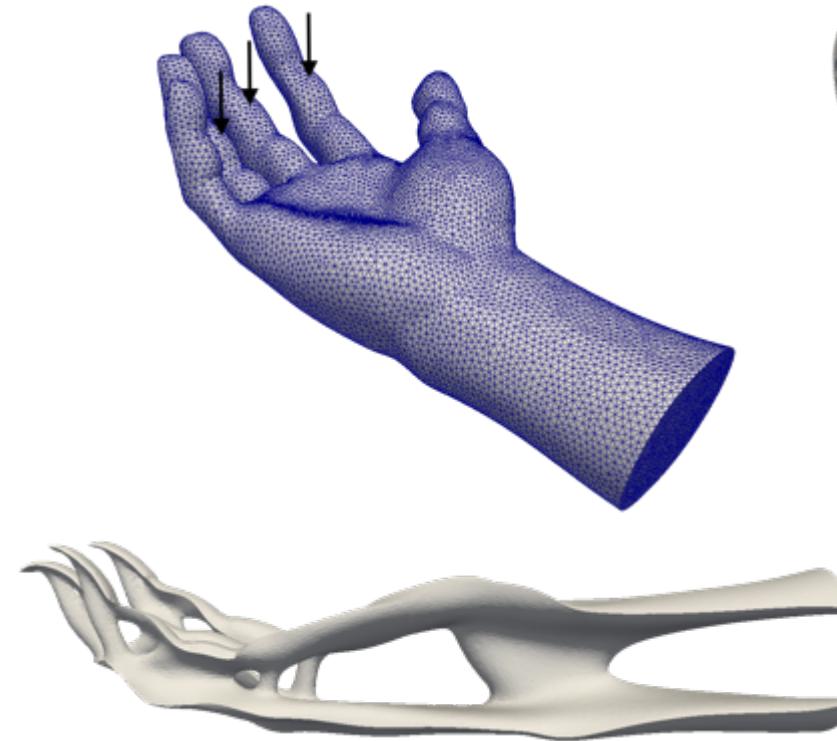
Design sensitivity:

$$\bar{F}' = -(e(v) : C) : e(u) + \lambda_1$$

Design examples



- i7 @ 2.30GHz, 4 cores
- Memory size 16 GB
- 100,000 elements
- Runtime: $\approx 30 \text{ min}$

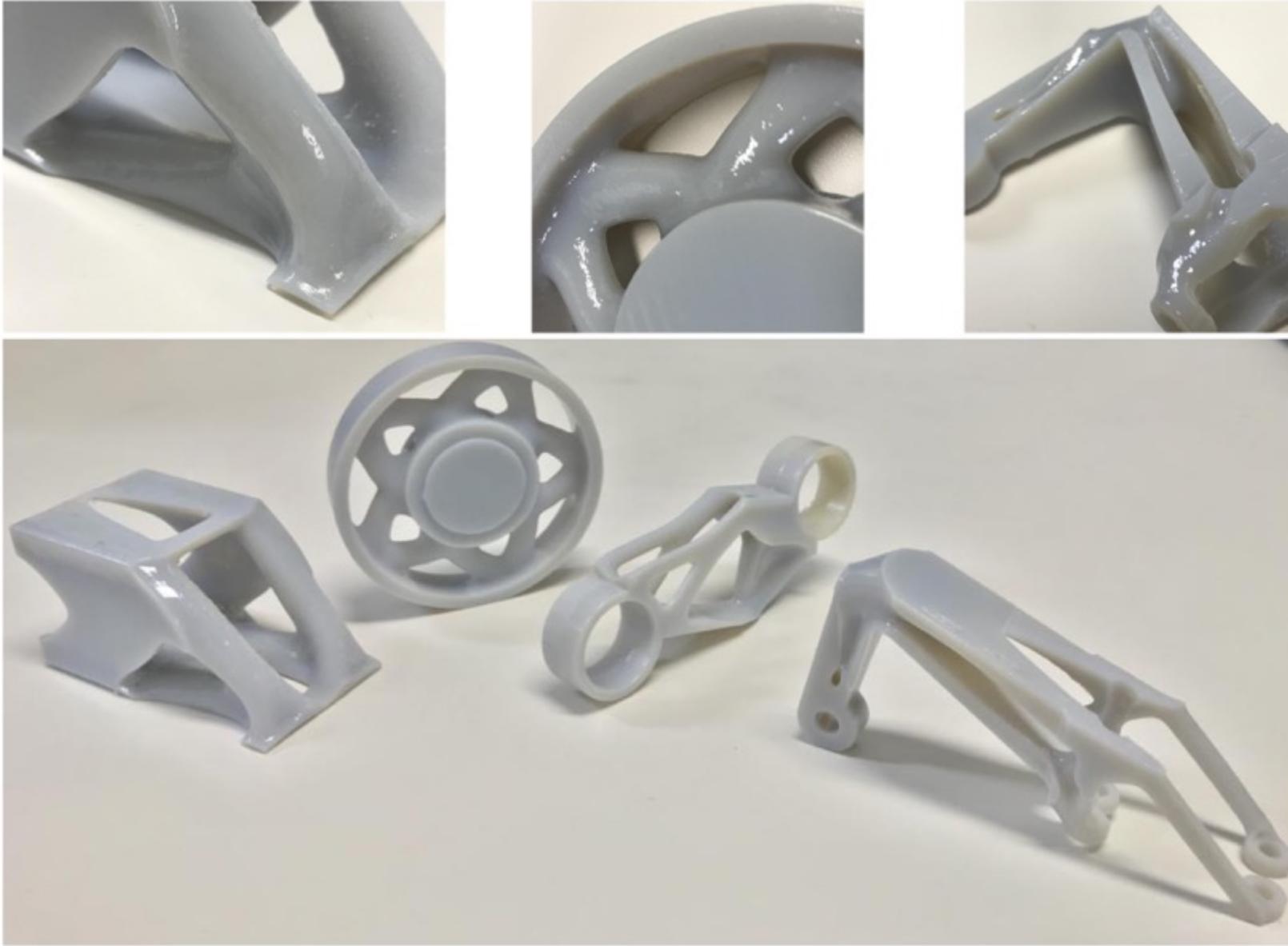


- Xeon(R) W-2155 V4 @ 3.30GHz, 10 cores
- Memory size 64 GB
- 500,000 elements
- Runtime: $\approx 90 \text{ min}$



- Xeon(R) E5-2698 V4 @ 2.20GHz, 40 cores
- Memory size 256 GB
- 2.9 million elements
- Runtime: $\approx 25\text{hr}$

3D printed prototypes



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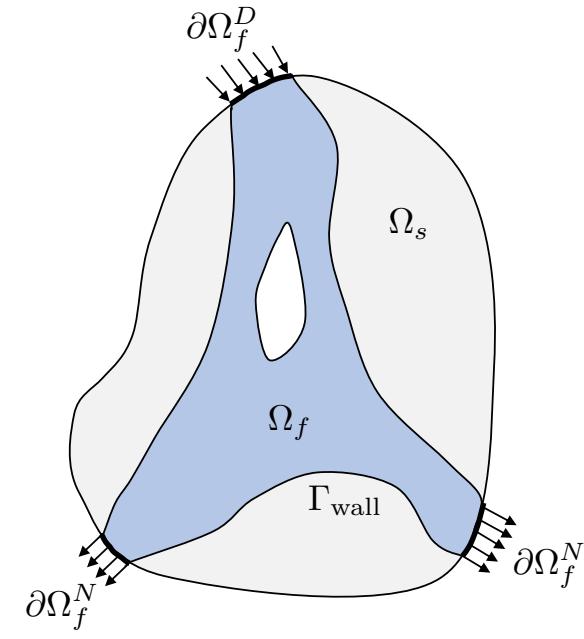
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Power dissipation problem

Optimization model

$$\inf_{\chi_\phi \in \chi} J = \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \left(p + \frac{1}{2} |\mathbf{u}|^2 \right) (-\mathbf{u} \cdot \mathbf{n}) d\Gamma.$$

$$s.t. \begin{cases} R_1 = (\mathbf{u} \cdot \nabla) \mathbf{u} - \frac{1}{Re} \nabla \cdot (\nabla \mathbf{u}) + \nabla p + \alpha \mathbf{u} = 0 \\ R_2 = -\nabla \cdot \mathbf{u} = 0. \\ G_1 = \frac{\int_D \chi_\phi d\Omega}{\int_D d\Omega} - V_{max} \leq 0 \\ \mathbf{u} = 0 \quad \text{on } \Gamma_{\text{wall}} \\ \mathbf{u} = \mathbf{u}_{\text{in}} \quad \text{on } \Gamma_{\text{in}} \\ \left(-p \mathbf{I} + \frac{1}{Re} \nabla \cdot (\nabla \mathbf{u}) \right) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{\text{out}}. \end{cases}$$



$$\chi_\phi = 0, \alpha \rightarrow \infty, F \rightarrow \infty \quad \mathbf{u} = 0$$

$$\chi_\phi = 1, \alpha \rightarrow 0, F \rightarrow 0 \quad \text{N-S equation}$$

$$\alpha = \alpha_{\max} \frac{q(1 - \chi_\phi)}{q + \chi_\phi} \quad \alpha_{\max} = \left(1 - \frac{1}{Re}\right) \frac{1}{Da}$$

Power dissipation problem

Adjoint problem & Design sensitivity

Adjoint equations

$$\begin{cases} -\mathbf{u} \cdot \nabla \mathbf{u}_A + \mathbf{u}_A \cdot \nabla \mathbf{u}^T - \frac{1}{Re} \nabla \cdot (\nabla \mathbf{u}_A) + \alpha \mathbf{u}_A + \nabla p_A = 0 \\ -\nabla \cdot \mathbf{u}_A = 0 \end{cases}$$

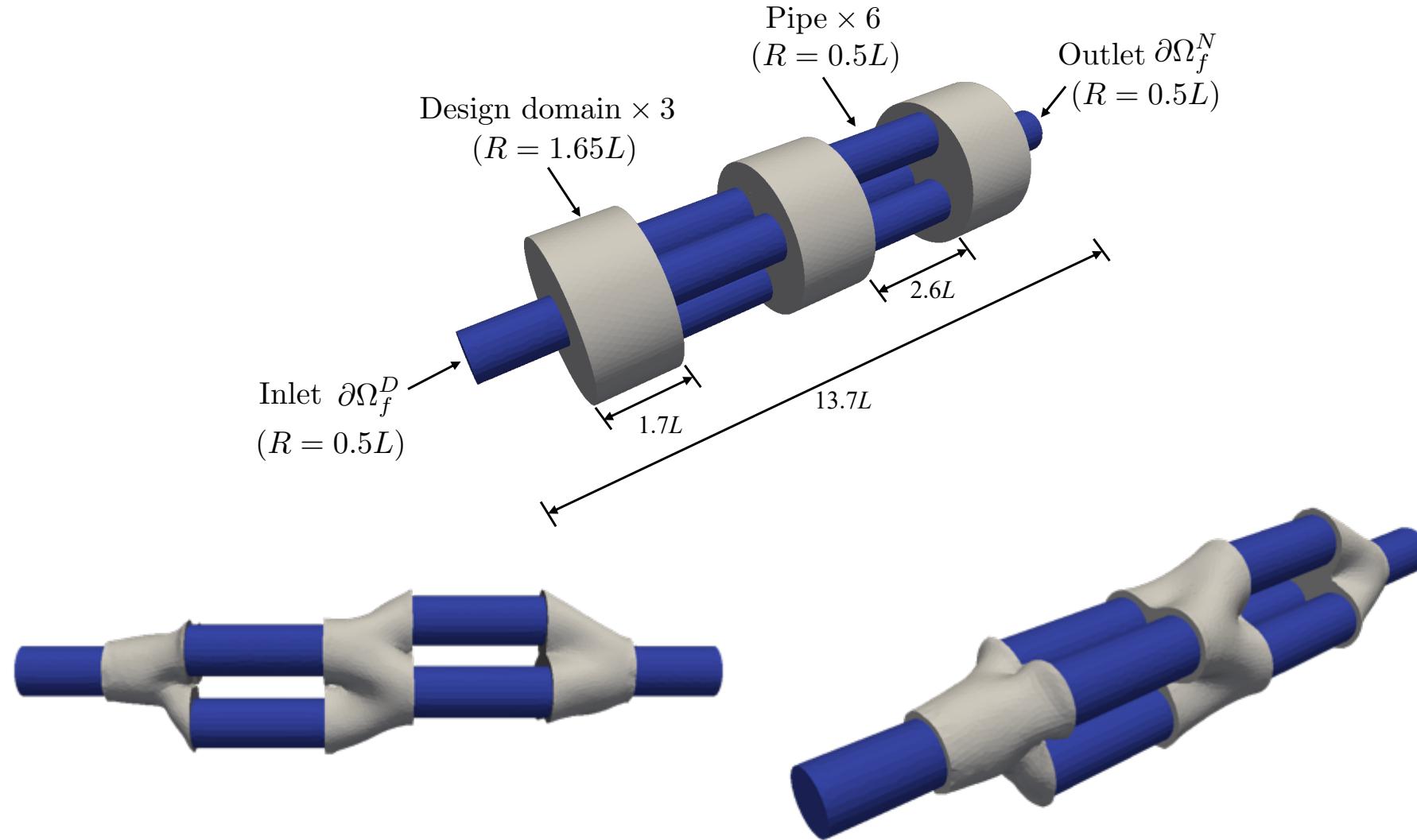
Adjoint B.C.

$$\begin{cases} -\left(\frac{1}{2}(\mathbf{u} \cdot \mathbf{u}) + p\right) \mathbf{n} - \mathbf{u}(\mathbf{u} \cdot \mathbf{n}) + \mathbf{u}_A(\mathbf{u} \cdot \mathbf{n}) + \frac{1}{Re} (\nabla \mathbf{u}_A) \cdot \mathbf{n} - p_A \mathbf{n} = 0 & \text{on } \Gamma_{\text{out}} \\ \mathbf{u}_A = \mathbf{u} & \text{on } \Gamma_{\text{in}} \\ \mathbf{u}_A = 0 & \text{on } \Gamma_{\text{wall}} \end{cases}$$

Design sensitivity

$$F' = - \int_{\Omega} \frac{q\alpha_{\max}(q+1)}{(q+\chi_{\phi})^2} \mathbf{u} \cdot \mathbf{u}_A + \lambda_1$$

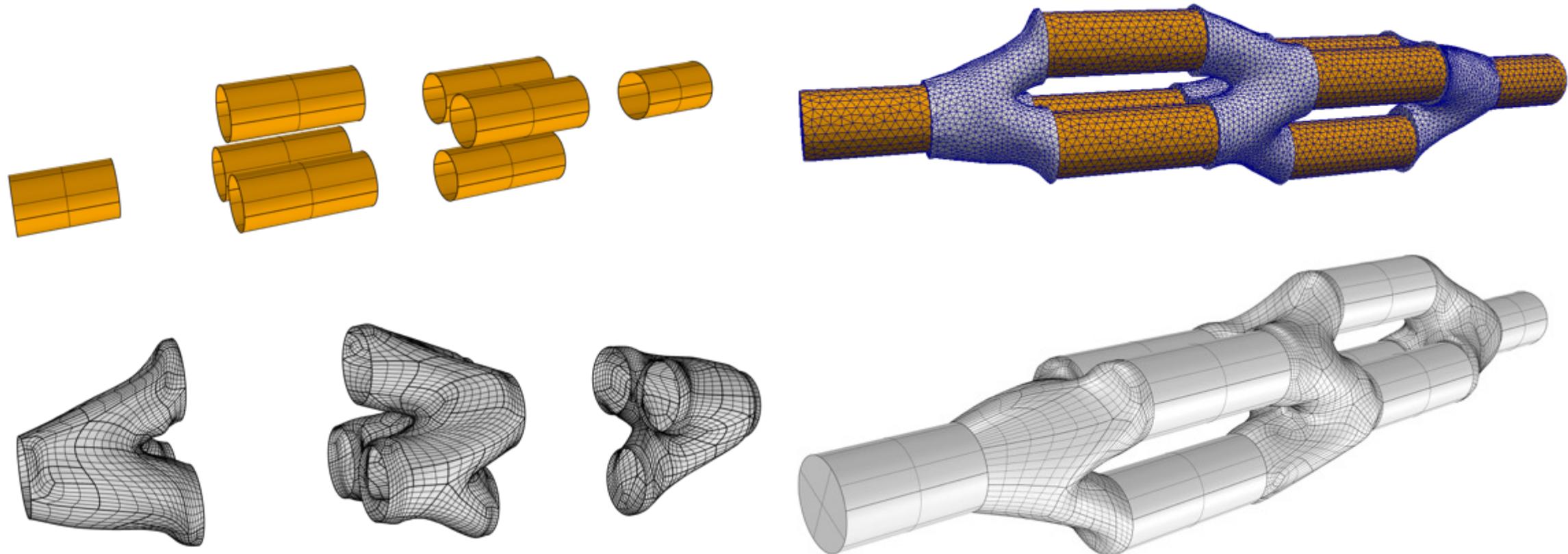
Design examples (Diesel oxidation catalyst)



$Re=300$

Design examples (Diesel oxidation catalyst)

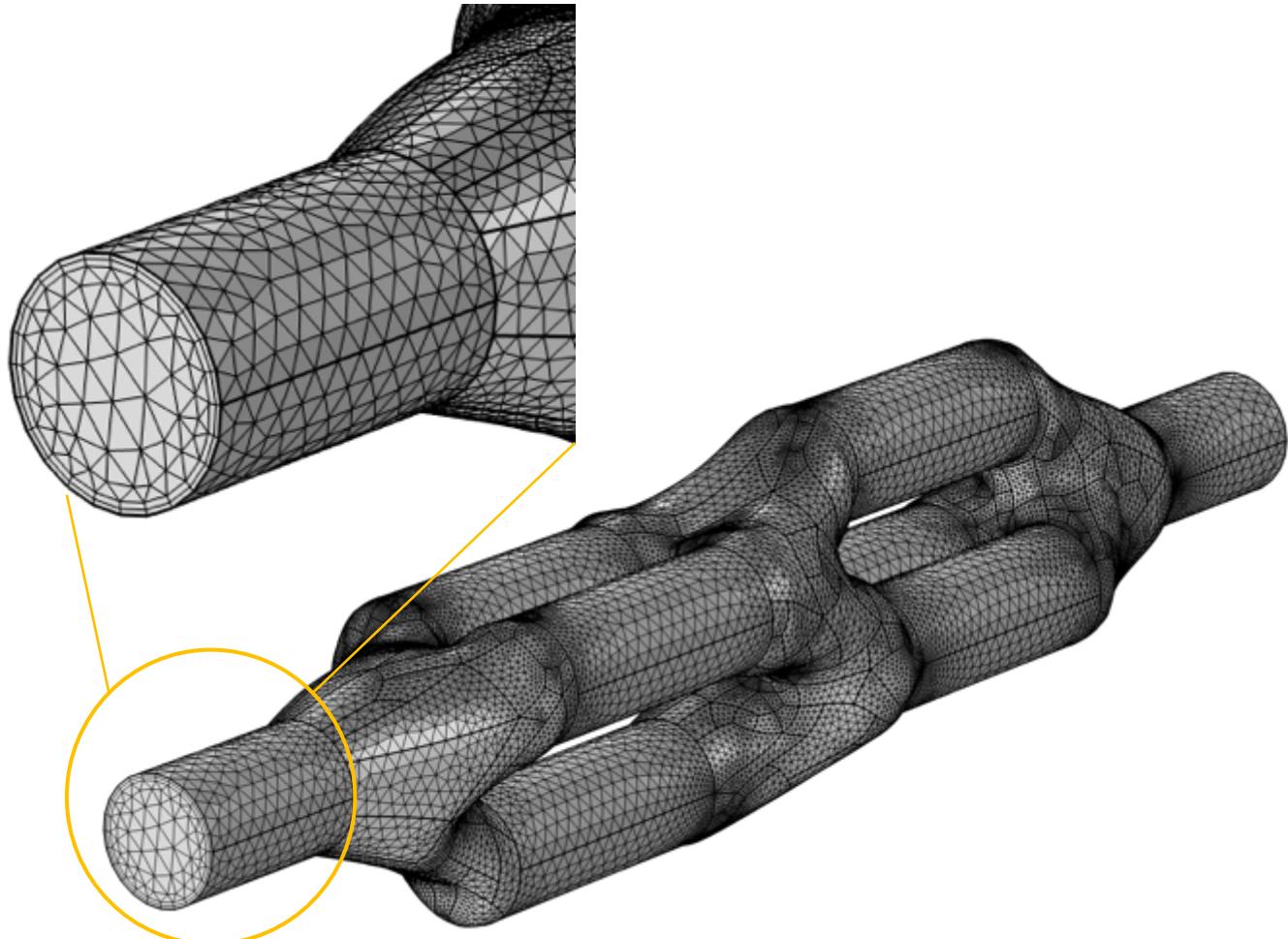
B-Reps conversion (Mesh → CAD)



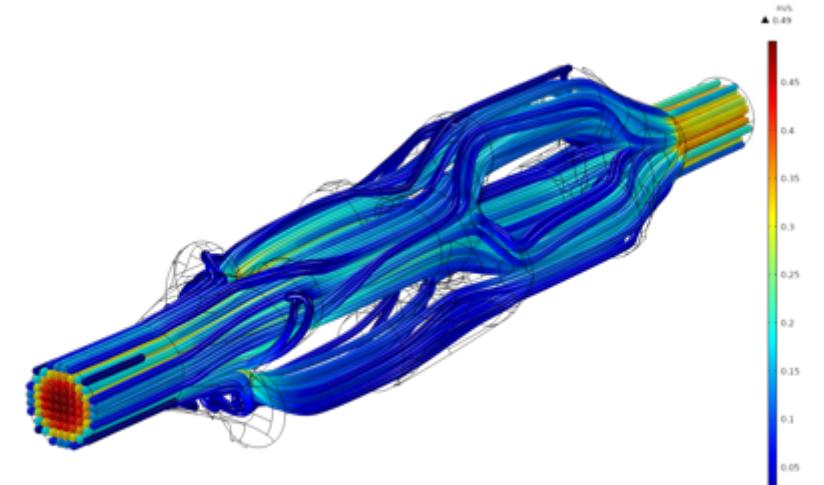
(Contributed by Kousei Wano)

Design examples (Diesel oxidation catalyst)

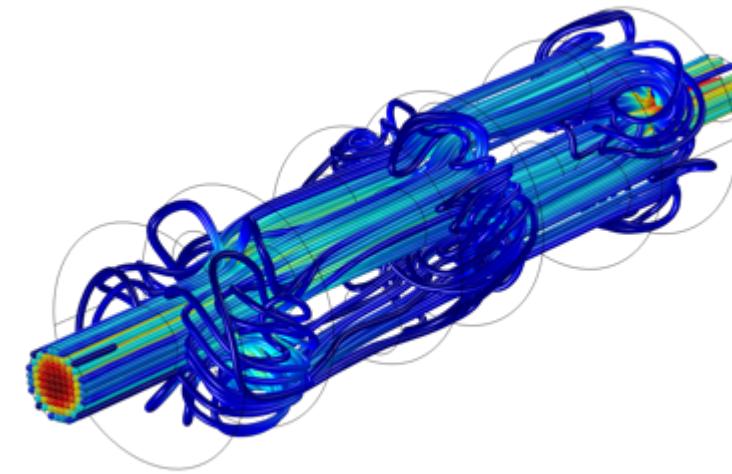
Numerical experiment



Boundary layer mesh



Optimized design



Initial design

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Fluid-structure-interaction problem

Optimization model

$$\inf_{\chi_\phi \in \mathcal{X}} J(\Omega) = \int_{\Gamma_{s,f}} \mathbf{g} \cdot \mathbf{u} d\Gamma$$

Navier-Stokes:

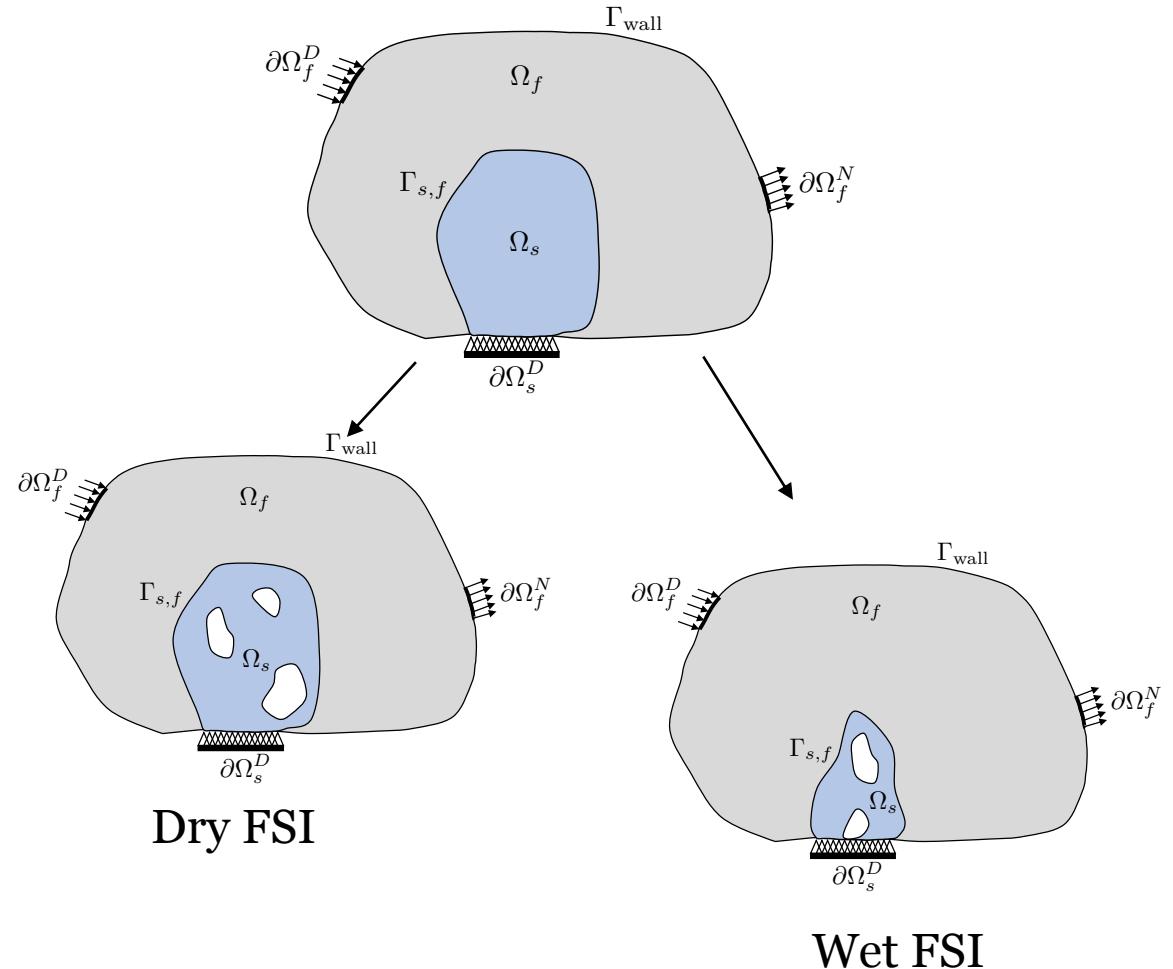
$$\begin{cases} -\operatorname{div}(\sigma_f(\mathbf{v}, p)) + \nabla \mathbf{v} \cdot \mathbf{v} = \mathbf{f}_f & \text{in } \Omega_f \\ \operatorname{div}(\mathbf{v}) = 0 & \text{in } \Omega_f \\ \mathbf{v} = \mathbf{v}_0 & \text{on } \partial\Omega_f^D \\ \sigma_f(\mathbf{v}, p)\mathbf{n} = 0 & \text{on } \partial\Omega_f^N \\ v = 0 & \text{on } \Gamma \end{cases}$$

Elasticity:

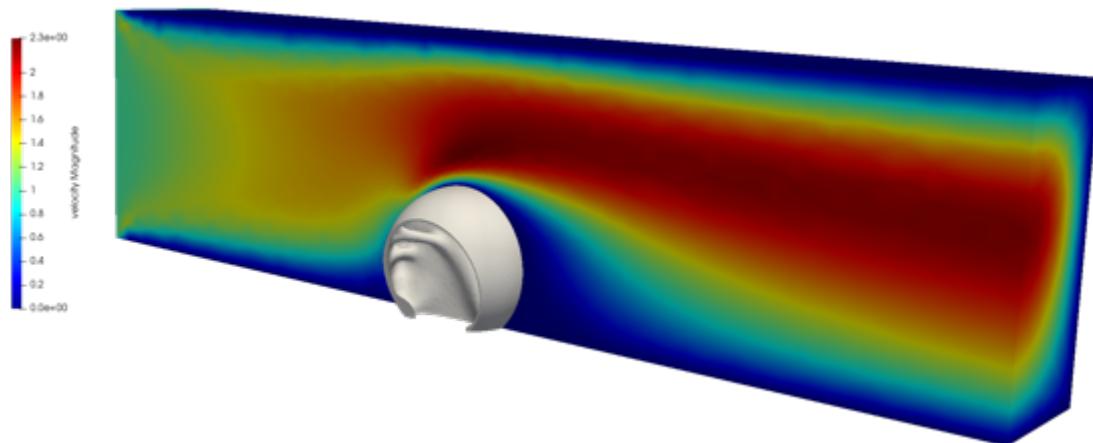
$$\begin{cases} -\operatorname{div} \sigma_s(\mathbf{u}) = 0 & \text{in } \Omega_s \\ \mathbf{u} = 0 & \text{on } \partial\Omega_s^D \\ \sigma_s(\mathbf{u}) \cdot \mathbf{n}_s = \sigma_f(\mathbf{v}) \cdot \mathbf{n}_f & \text{on } \Gamma_{s,f}. \end{cases}$$

Weakly coupled condition:

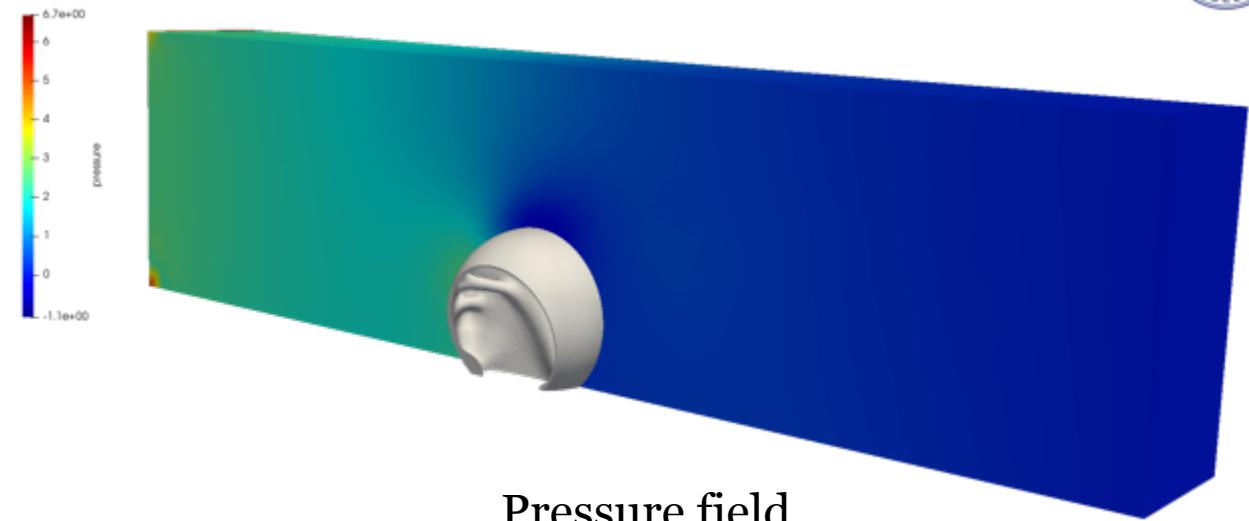
$$\sigma_f(\mathbf{v}, p)\mathbf{n} = \sigma_s(\mathbf{u}, T_S)\mathbf{n}$$



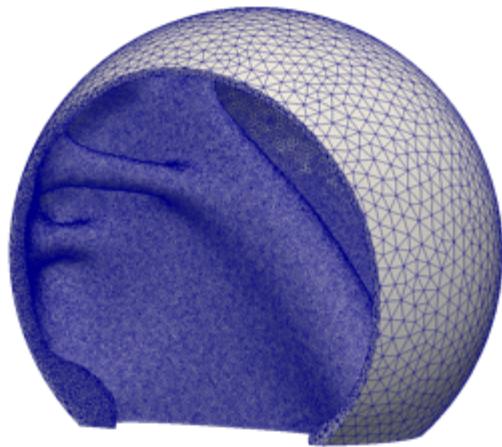
Design examples (Dry-FSI)



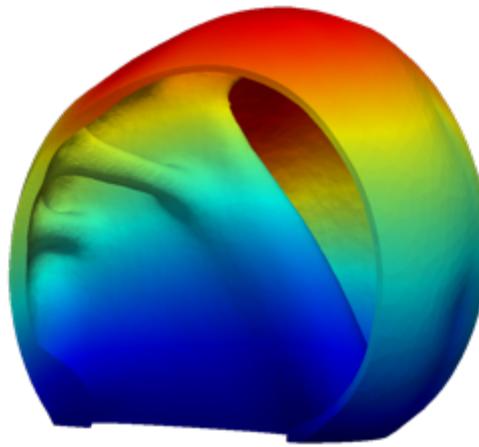
Velocity field



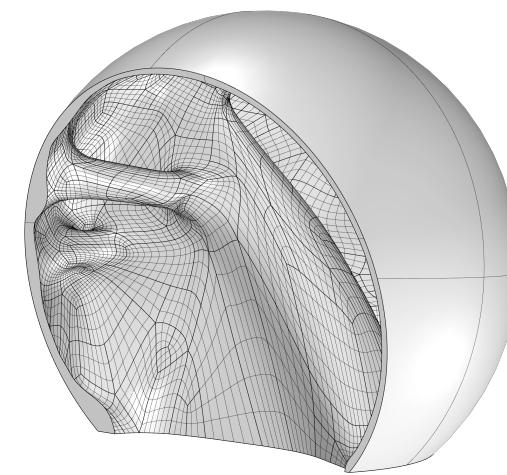
Pressure field



Optimal solution

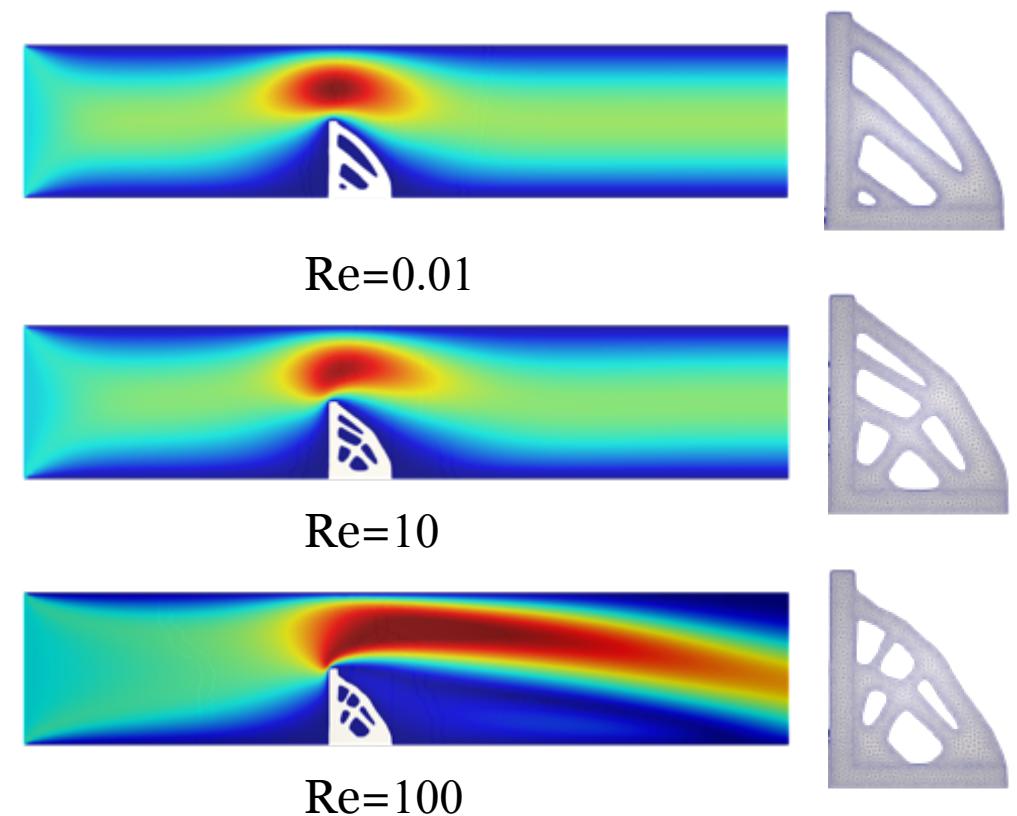
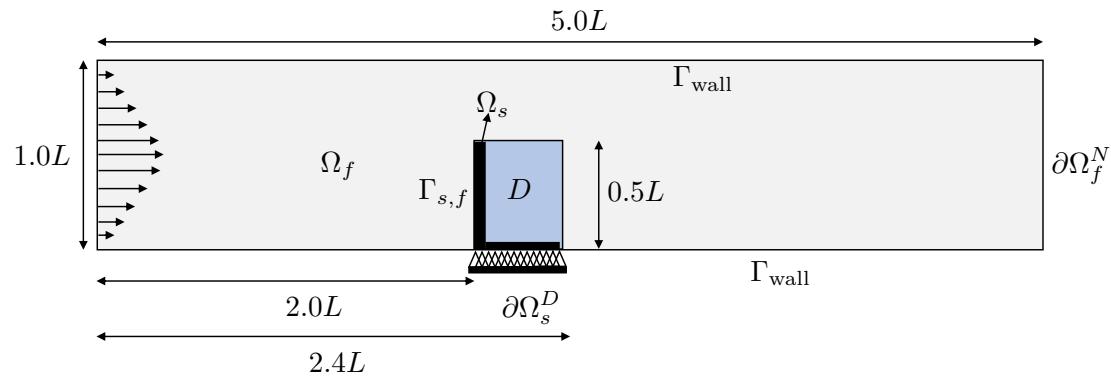


Deformation (amplified)



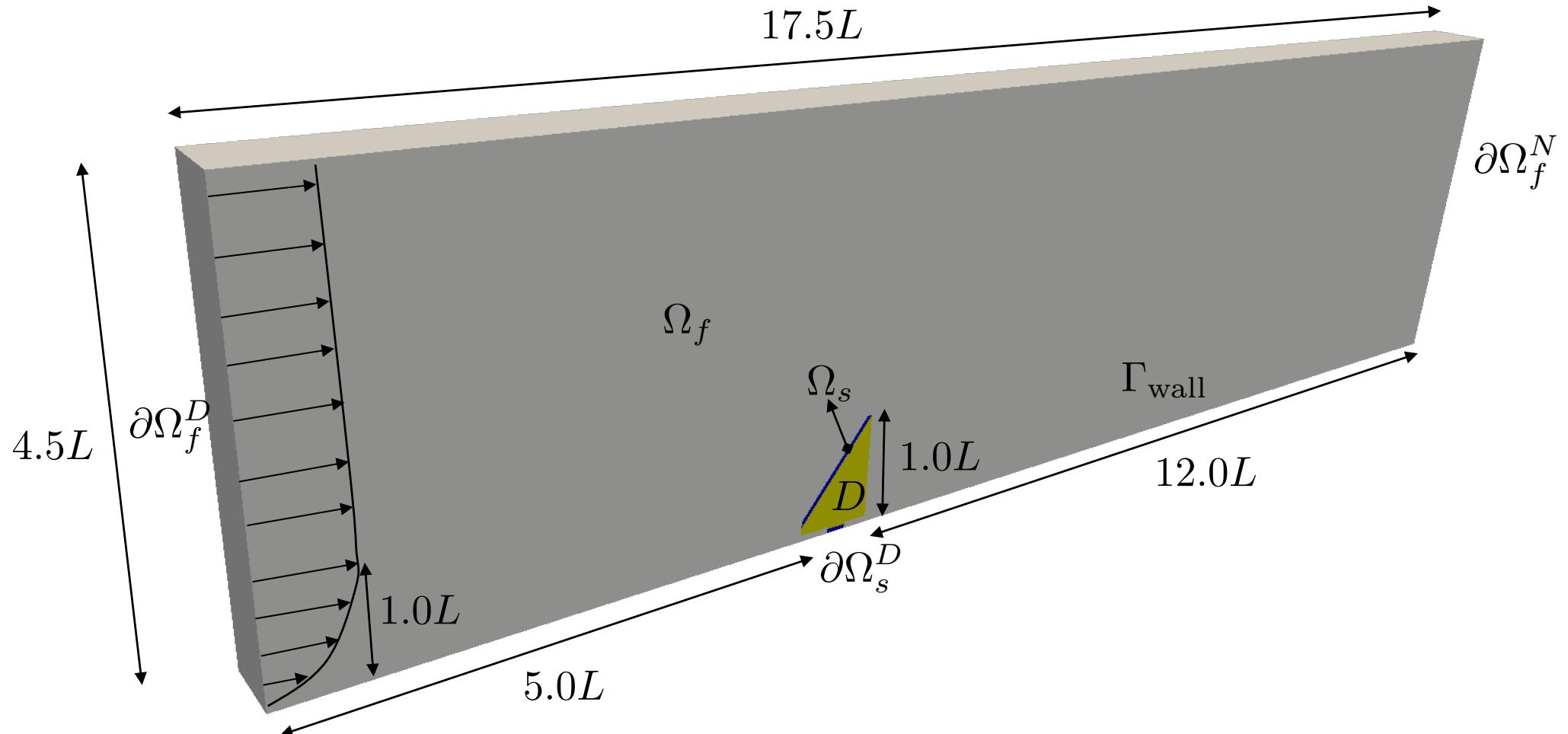
B-Reps conversion

Design examples (Wet-FSI)



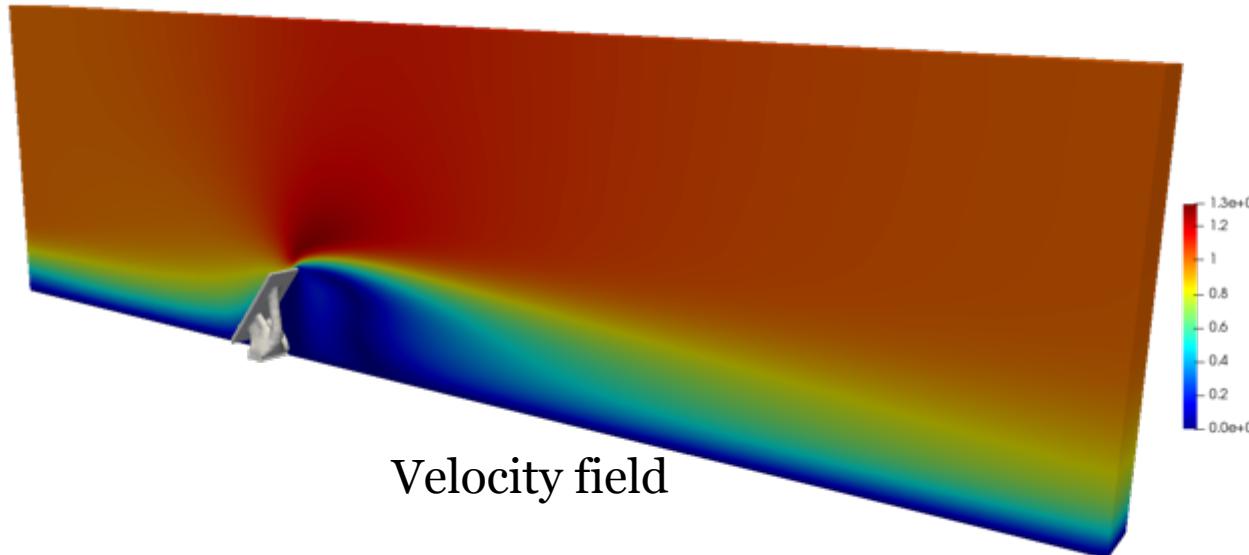
Design examples (Wet-FSI)

Solar-plate support design

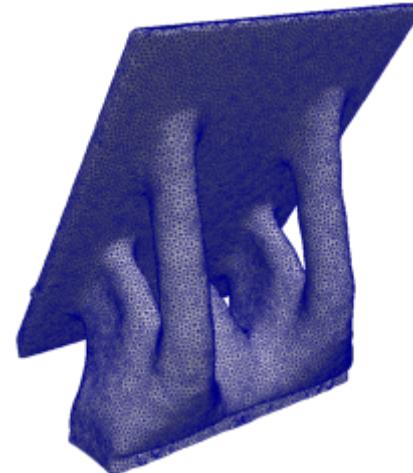


Design examples (Wet-FSI)

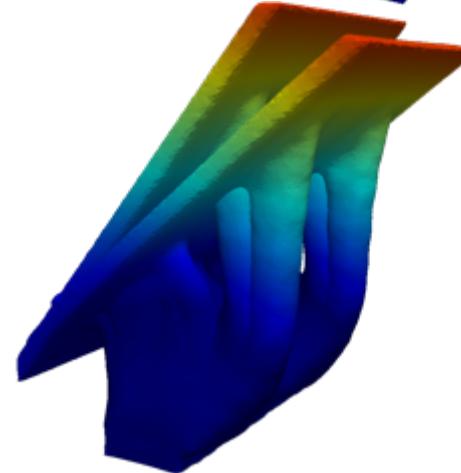
Solar-plate support design



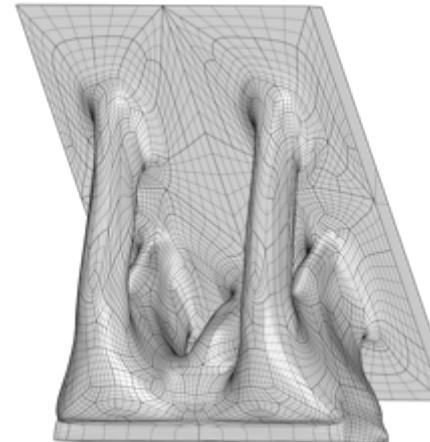
Velocity field



Optimal solution



Deformation (amplified)

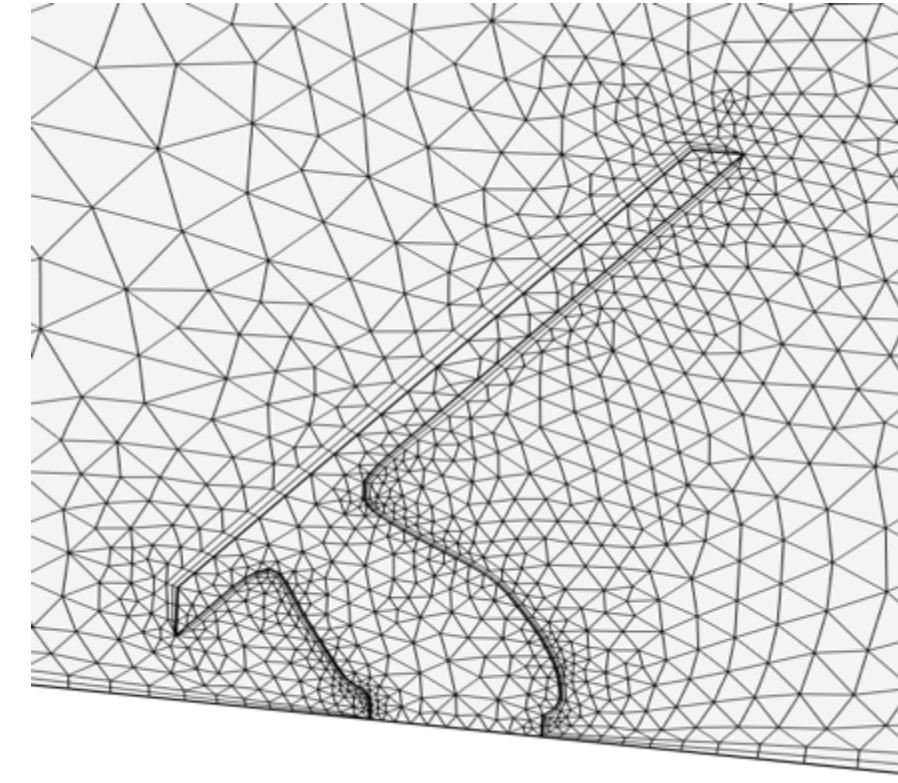
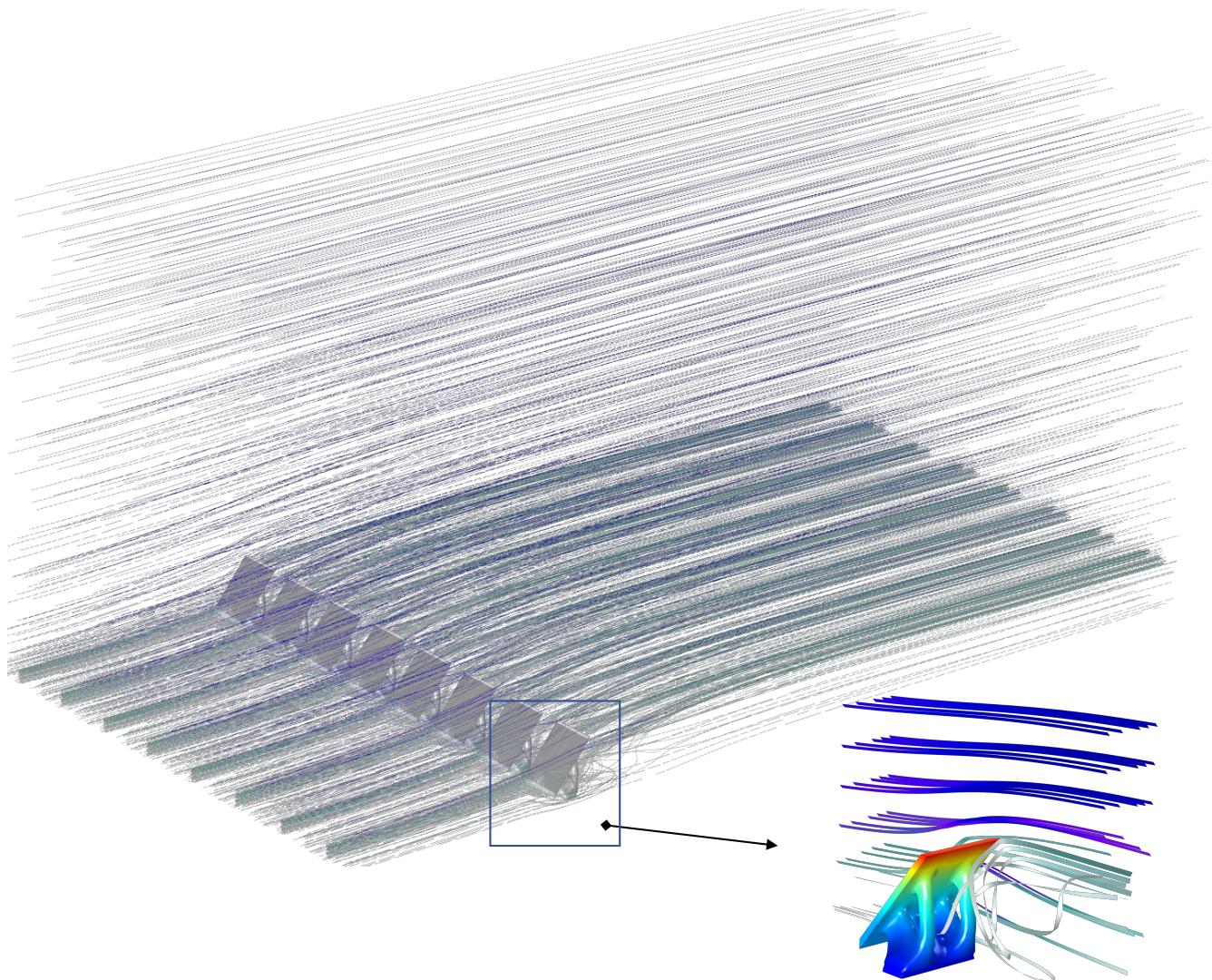


B-Reps conversion

- Xeon(R) E5-2698 V4 @ 2.20GHz, 40 cores
- Memory size 256 GB
- Fluid: 528,676 elements, \approx 6.3 million DOFs
- Solid: 244,727 elements
- Runtime: \approx 9.3hr

Design examples (Wet-FSI)

Numerical experiment in **COMSOL Multiphysics**



Boundary layer mesh



Paper submitted & under preparation

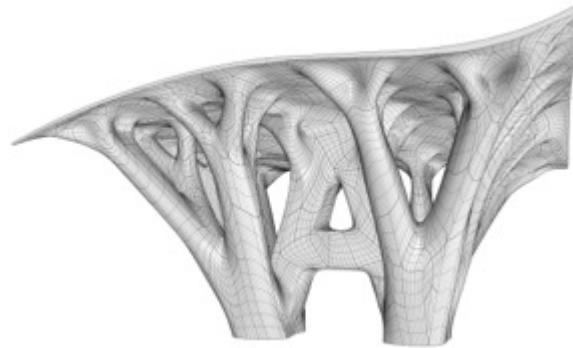
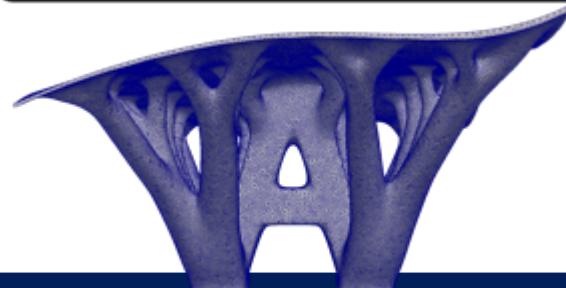
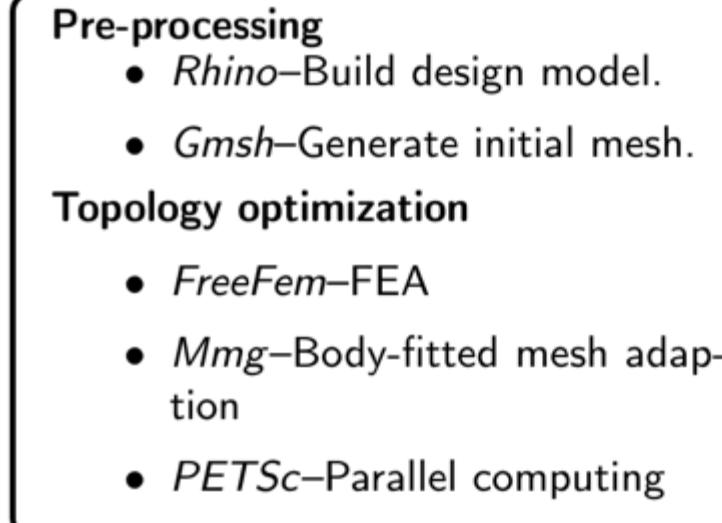
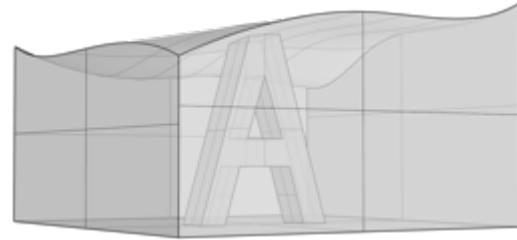
References

1. Li, H.*, Yamada, T., Jolivet, P., Furuta, K., Kondoh, T., Izui, K., & Nishiwaki S*. "Full-scale 3D structural topology optimization using adaptive mesh refinement based on level-set method." [under review].
2. Li, H.*, Yamada, T., Jolivet, P., Wano, K., Kondoh, T., Furuta, K., Izui, K., & Nishiwaki S*. "Three-dimensional topology optimization of fluid-structure system using body-fitted mesh adaption based on the level-set method." [under preparation].

Content Page

1. Intro. to structural topology optimization
2. RDE based LSM
3. Body-fitted mesh adaption
4. Numerical implementation
5. Design examples
6. Conclusion & Future works

Conclusion



Post-processing

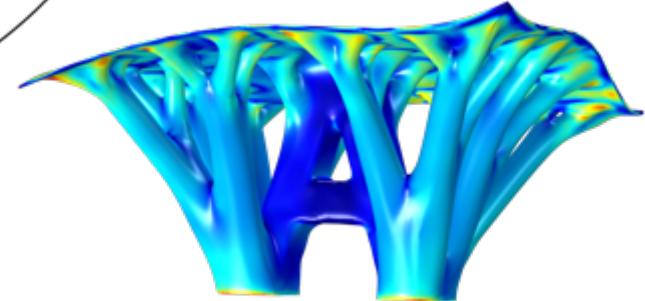
- *Blender*—Repair mesh.
- *S-generator*—B-Rep conversion.

Numerical test

- *COMSOL*—simulation.

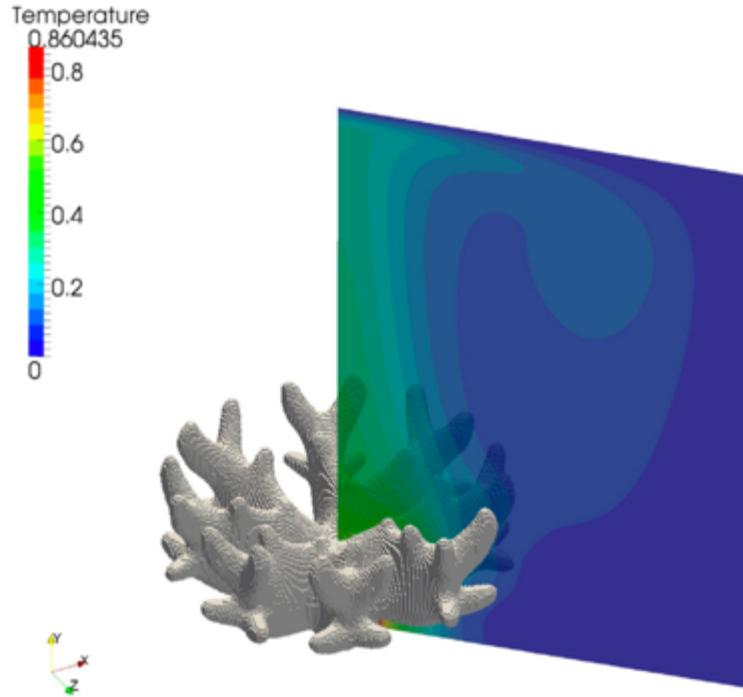
Manufacturing

3D-printing/CNC machining



Complete product development workflow

Future works – Passive heat sink design



(Alexandersen et al., 2016)

$$\begin{aligned} \text{minimise}_{\gamma \in \mathcal{D}} : \quad & f(\gamma, T) = \int_{\omega} s(\mathbf{x}) T dV \\ \text{subject to} : \quad & g(\gamma) = \int_{\Omega_d} 1 - \gamma dV \leq v_f \int_{\Omega_d} dV \\ & \mathcal{R}(\gamma, \mathbf{u}, p, T) = 0 \\ & 0 \leq \gamma(\mathbf{x}) \leq 1 \forall \mathbf{x} \in \Omega_d \end{aligned}$$

Steady-state incompressible Navier–Stokes equations coupled to the thermal convection–diffusion equation through the Boussinesq approximation and body force is expressed through the Brinkman model.

$$\begin{aligned} u_j \frac{\partial u_i}{\partial x_j} - \text{Pr} \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{\partial p}{\partial x_i} &= -\alpha(\mathbf{x}) u_i - \text{Gr} \text{Pr}^2 e_i^g T \\ \frac{\partial u_j}{\partial x_j} &= 0 \\ u_j \frac{\partial T}{\partial x_j} - \frac{\partial}{\partial x_j} \left(K(\mathbf{x}) \frac{\partial T}{\partial x_j} \right) &= s(\mathbf{x}) \end{aligned}$$

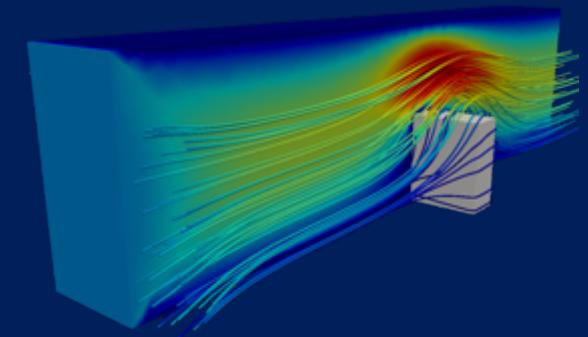


FREEFEM DAYS
12th EDITION - PARIS

Thank you for your attention!

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Appendix

- Thermo-fluid example
- Authors

Authors



Hao LI*



Prof. T. Yamada



Dr. P. Jolivet



Prof. K. Izui



Prof. S. Nishiwaki



Dr. T. Kondoh