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# Large-scale parallel topology optimisation of three-dimensional incompressible fluid flows in a level set, anisotropic mesh adaptation framework

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## Abstract

This paper considers the topology optimization of duct flows governed by the three-dimensional steady state Navier–Stokes equations, using anisotropic mesh adaptation to achieve a high-fidelity description of all fluid-solid interfaces. The numerical framework combines an immersed volume method solving stabilized, linear equal-order finite element formulations cast in the Variational Multiscale (VMS) framework, and level set representations of the interface, used as a posteriori anisotropic error estimator to minimize the interpolation error under the constraint of a prescribed number of nodes in the mesh. Both the resolution and remeshing steps are performed in a massively parallel framework allowing for the optimization of large-scale systems. In particular, an original parallelization strategy is used for mesh adaptation, that combines local remeshing performed sequentially and independently on each subdomain with blocked interfaces, and constrained repartitioning to optimally move the interfaces between subdomains in an optimal way, both iterated until a satisfying mesh and partition are obtained. **The proposed approach reduces the computational burden related to the call of the finite element solver, compared to classical optimization schemes working on uniform grids with similar mesh refinement. For a given number of nodes, it improves the accuracy in the geometric description of all layouts. Finally, it has the potential to alleviate the end user from most of the post-processing step aiming at extracting the final layout, due to ability of anisotropic adapted meshes to generate intrinsically smooth designs.**

Numerical results are provided for several three-dimensional problems of power dissipation minimization involving several dozen million state degrees of freedom, for which the optimal designs agree well with reference results from the literature, while providing superior accuracy over prior studies solved on isotropic meshes **(in the sense that the flow is better resolved, especially in the near-wall regions, and the layouts are more smooth)**. The potential of the method for engineering problems of practical interest is eventually exposed by optimizing the distributor section conveying the cold fluid within the plates of a plate fin heat exchanger.

**Keywords:** Topology Optimization, Fluid mechanics, Large-scale systems, Parallelization, Level Set Method, Anisotropic mesh adaptation

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## 1. Introduction

Fluid flow topology optimization aims at maximizing a measure of performance by identifying the best path for a fluid to flow in a design domain, subject to a set of design constraints, a typical example being to minimize dissipation under a constant volume of fluid constraint. The approach was initiated for mechanical design problems [1, 2], but has since spread to a variety of other physics modeled after partial differential equations, including fluids, acoustics, electromagnetics, optics and combinations thereof; see especially Ref. [3] for a recent survey dedicated to fluid flow problems. The mathematical foundation builds on iterative analysis and design update steps, often steered

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by gradient evaluations. Compared to the size and shape optimization methods it has emerged from, the main advantage of topology optimization is in the increased design freedom, that allows starting from arbitrary initial guesses and generating non-intuitive designs, even under conflicting requirements and complex correlations between design parameters and system response.

There has been a significant leap in terms of methods and approaches used for topology optimization. Those include, but are not limited to, methods of density, level set, topological derivative, phase field, and evolutionary; see Ref. [4] for a comparison and critical review of the different approaches. Leaving aside explicit boundary methods, that represent the fluid-solid interface by edges or faces of a body-fitted mesh, and have limited flexibility to handle complicated topological changes, the prevalent classes of methods for fluid flow topology optimization are the density and the level set methods. Density methods rely on Brinkman penalization to weakly enforce fluid-solid no-slip conditions in a unified domain [1, 5, 6]. They manage drastic topological changes, as the gradient (or sensitivity) information is distributed over a large part of the domain, but require a well-tuned penalization factor, small enough to ensure numerical stability of the solution and optimisation algorithms, but large enough to prevent the flow from leaking inside the solid domain. Level set methods conversely manage to capture the solid boundaries by iso-contours of a level set function [7-10]. Due to the sensitivities being located only at the solid-fluid interface, they are without a nucleation mechanism, hence the common practice to start from a design with many holes. Meanwhile, they easily handle complicated topological changes (e.g., merging or cancellation of holes), and yield well defined, crisp interface representations while avoiding the intermediate material phases (grayscale) and mesh-dependent spatial oscillations of the interface (staircasing) often encountered in density methods, unless they are combined with cut element techniques [11].

A classical topology optimization problem resorts to the discretization of a levelset function/a density field to tackle the minimization setting, along with the adoption of finite element methods to cope with the approximation of the relevant governing equations. Both discretizations generally employ identical meshes with close-to-uniform element size, small enough that all relevant physical phenomena are accurately described, but not so small that the computational cost becomes prohibitive. A recent trend in this regards has been to incorporate adaptive remeshing techniques, where one starts from a coarse base grid, then adds recursively finer and finer subgrids in the regions requiring higher resolution. This proceeds either until a maximum level of refinement is reached, or the local truncation error drops below a certain tolerance, for more sophisticated implementations endowed with error estimation routines. Within the context of fluid flow problems, particular emphasis has been put on adaptive meshing refinement schemes, using both density [12, 13] and level set methods [14, 15]; see also [16] for an application to phase field methods and [17-19] for recent efforts applying a different remeshing scheme to a combination of level set functions and adaptive body-conforming meshes. Other approaches include the one used in [20-22], where the virtual element method is used to solve topology optimization problems governed by Stokes and Navier-Stokes equations on unstructured polygonal finite element meshes (see also [23] for a comprehensive domain-agnostic survey) and the surface-capturing extended finite element method, in which cut elements are integrated using a special scheme and the interface boundary conditions are imposed using stabilised Lagrange multipliers or a stabilised Nitsche's method, although the related solutions are shown in [24] to possibly exhibit penalty- and mesh-dependent mass losses through the interface.

While fluid dynamics deals with convection dominated problems typified by the presence of strongly directional features, e.g., boundary layers where the fluid velocity exhibits steep gradients in the wall-normal direction and skin-friction plays a defining role, the adaptive algorithms applied so far to fluid flow topology optimization support almost exclusively isotropic size maps. The approach proposed in the present work consists of anisotropic mesh adaptation based on a theoretically sound tool, i.e., a recovery-based a posteriori error analysis. It enjoys several advantages. First, it substantially reduces the computational burden related to the call of the finite element solver, compared to classical optimization schemes working on uniform grids with similar mesh refinement. Second, for a given number of nodes, it improves the accuracy in the geometric description of the optimal designs while naturally conveying said accuracy to the numerical solutions, which is all perfectly in line with the recommendations made in [3] to improve upon the current state of the art. Finally, the use of anisotropic adapted meshes yields intrinsically smooth final layouts, meaning that the post-processing phase can be strongly reduced (or even skipped), and

the structure can directly move on to the production manufacturing phase, unlike most traditional algorithms, where a strong post-processing can be required to extract the final layout. Similar approaches towards free form design has been taken in [25, 26] to solve compliance minimization problems in topology optimization for structural applications. Nonetheless, our literature review did not reveal any other study combining anisotropic mesh adaptation and fluid flow topology optimization, besides the density-based optimisation of Stokes flow in Ref. [13], possibly because the notorious difficulty of finding spatial discretization schemes that meet the level of robustness required by automatic anisotropic mesh adaptation.

The scope of this article is to present and provide basic verifications of a novel level set, anisotropic mesh adaptation framework for topology optimisation of large-scale, three-dimensional (3-D) steady and laminar flow. In recent years, an increasing number of studies have dealt with efficient large-scale topology optimization, to which the reader is referred to for further information regarding the use of parallel programming using the message parsing interface (MPI) and parallel resolution of partial differential equations with scalable and high performance algorithms [27–31]. Particular emphasis is thus put here on the parallel adaptive meshing technique, whose implementation in the context of large-scale fluid flow topology optimization makes for the main novelty of this study. The latter combines local remeshing performed independently on each subdomain with fixed interfaces, and constrained repartitioning to move the interfaces between subdomains in an optimal way, both iterated until a satisfying mesh and partition are obtained. The metric map providing both the size and the stretching of mesh elements in a very condensed information data is derived from the level set. A posteriori anisotropic error estimator is then used to minimize the interpolation error under the constraint of a prescribed number of nodes in the mesh. The latter can be adjusted over the course of optimization, meaning that the base grid can be either refined or coarsened on demand: this is expected to achieve further speed-ups, as it reduces the cost of modelling the solid material away from the interface, and also to help improve manufacturability of the optimal design, which remains an issue as most classical topology optimization methods render organic designs that can be difficult to translate into computer-aided design models.

The paper organization is as follows: the governing equations for the gradient-based optimization model are formulated in Sec. 2. The stabilized finite element numerical framework and anisotropic mesh adaptation algorithm used to perform the design update step are described in Secs. 3 and 4, respectively, with additional details regarding the parallel implementation provided in Sec. 5. The implementation details of the optimization algorithm are given in Sec. 6. Finally, numerical experiments assessing relevance on a series of large-scale, three-dimensional power dissipation minimization problems (including a simplified industrial case study) are presented in section 7, with particular attention paid to highlight the improved accuracy of the obtained solutions.

## 2. Problem setting

In the following, we denote by  $\Omega$  a fixed, open bounded domain in  $\mathbb{R}^d$  (with  $d$  the space dimension), with boundary  $\partial\Omega$  oriented with inward-pointing normal vector  $\mathbf{n}$ . Throughout this study,  $\Omega = \Omega_f \cup \Omega_s$  is the disjoint reunion of two domains  $\Omega_f$  and  $\Omega_s$ . For simplicity, we refer to  $\Omega_f$  as the fluid domain, and to  $\Omega_s$  as the solid domain, although we also fill  $\Omega_s$  with a fluid for numerical convenience, as further explained in the following. The two domains are separated by an interface  $\Gamma = \Omega_f \cap \Omega_s$ , whose position we seek to optimize with respect to a certain measure of performance, here a cost function  $J$  to minimize.

### 2.1. State equations

Mathematically, the problem is characterized by a set of physical variables determined as the solutions of partial differential equations, themselves derived from modeling considerations. Here, the flow motion in the fluid domain  $\Omega_f$  is modeled after the steady incompressible Navier–Stokes equations

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega_f, \quad (1)$$

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot (2\mu \varepsilon(\mathbf{u})) \quad \text{in } \Omega_f, \quad (2)$$

where  $\mathbf{u}$  is the velocity,  $p$  is the pressure,  $\boldsymbol{\varepsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$  is the rate of deformation tensor, and we assume constant fluid density  $\rho$  and dynamic viscosity  $\mu$ . The fluid domain boundary  $\partial\Omega_f$  is split into (wall) interface  $\Gamma$ , inlet  $\Gamma_i$  (defined as the combined boundary of all surfaces where fluid enters the domain), outlet  $\Gamma_o$  (the combined boundary of all surfaces where fluid leaves the domain). Open flow boundary conditions are appended under the form of a prescribed velocity at the inlet, zero velocity at the wall

$$\mathbf{u} = \mathbf{u}_i \quad \text{on } \Gamma_i, \quad (3)$$

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma, \quad (4)$$

and a convenient outflow condition at the outlet, either a prescribed velocity

$$\mathbf{u} = \mathbf{u}_o \quad \text{on } \Gamma_o, \quad (5)$$

adjusted to ensure mass conservation, or a more natural zero pressure/zero viscous stress condition

$$p\mathbf{n} = \mu\boldsymbol{\varepsilon}(\mathbf{u}) \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \Gamma_o. \quad (6)$$

## 2.2. Adjoint-based sensitivity analysis

We assume in the following that the cost function (i) can be formulated as a surface integral over the domain boundary, rather than its interior, and (ii) does not depend on the flow quantities on the wall, which is most often true in topology optimization. It is thus expressed as integrals over all or any part of inlet and/or outlet, i.e.,

$$J_s = \int_{\Gamma_i \cup \Gamma_o} J ds. \quad (7)$$

The problem of minimizing the cost function subject to Navier–Stokes as state equations is tackled using the continuous adjoint method. The reader interested in the technicalities of the method is referred to [32]. One first forms the Lagrangian

$$\mathcal{L} = \int_{\Gamma_i \cup \Gamma_o} J ds - \int_{\Omega_f} \tilde{p} \nabla \cdot \mathbf{u} dv - \int_{\Omega_f} \tilde{\mathbf{u}} \cdot (\rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nabla \cdot (2\mu\boldsymbol{\varepsilon}(\mathbf{u}))) dv, \quad (8)$$

featuring the adjoint velocity  $\tilde{\mathbf{u}}$  as the Lagrange multiplier for the momentum equations (2) and the adjoint pressure  $\tilde{p}$  as the Lagrange multiplier for the continuity equation (1), then seeks to decompose the variation of  $\mathcal{L}$  due to a change in the interface position into individual variations with respect to the adjoint, state and design variables. The variation with respect to the adjoint variables

$$\delta_{(\tilde{\mathbf{u}}, \tilde{p})} \mathcal{L} = - \int_{\Omega_f} \delta \tilde{p} \nabla \cdot \mathbf{u} dv - \int_{\Omega_f} \delta \tilde{\mathbf{u}} \cdot (\rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nabla \cdot (2\mu\boldsymbol{\varepsilon}(\mathbf{u}))) dv, \quad (9)$$

is trivially zero as long as  $(\mathbf{u}, p)$  is solution to the above Navier–Stokes equations, in which case  $\mathcal{L} = J_s$ . After integrating by parts, the variation with respect to the state variables is

$$\begin{aligned} \delta_{(\mathbf{u}, p)} \mathcal{L} &= \int_{\Omega_f} (\nabla \cdot \tilde{\mathbf{u}}) \delta p dv + \int_{\Omega_f} (-\rho \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} + \rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}} - \nabla \tilde{p} - \nabla \cdot (2\mu\boldsymbol{\varepsilon}(\tilde{\mathbf{u}}))) \cdot \delta \mathbf{u} dv \\ &\quad + \int_{\Gamma_i \cup \Gamma_o} \partial_{\mathbf{u}} J \cdot \delta \mathbf{u} ds + \int_{\partial\Omega_f} (\tilde{p}\mathbf{n} + 2\mu\boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) \cdot \mathbf{n} + \rho(\mathbf{u} \cdot \mathbf{n})\tilde{\mathbf{u}}) \cdot \delta \mathbf{u} ds \\ &\quad - \int_{\Gamma_i \cup \Gamma_o} \partial_p J \mathbf{n} \cdot (-\delta p \mathbf{n} + 2\mu\boldsymbol{\varepsilon}(\delta \mathbf{u}) \cdot \mathbf{n}) ds - \int_{\partial\Omega_f} \tilde{\mathbf{u}} \cdot (-\delta p \mathbf{n} + 2\mu\boldsymbol{\varepsilon}(\delta \mathbf{u}) \cdot \mathbf{n}) ds, \end{aligned} \quad (10)$$

on behalf of the viscous stress being purely tangential in incompressible flows. At this stage, adjoint equations and boundary conditions are designed to ensure  $\delta_{(\mathbf{u}, p)} \mathcal{L} = 0$ , which requires the domain and boundary integrals to vanish individually in (10). Keeping in mind that we work here under the assumption of a fixed interface (since the design variable is constant), we obtain the linear, homogeneous problem

$$\nabla \cdot \tilde{\mathbf{u}} = 0 \quad \text{in } \Omega_f, \quad (11)$$

$$-\rho \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} + \rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}} = \nabla \tilde{p} + \nabla \cdot (2\mu\boldsymbol{\varepsilon}(\tilde{\mathbf{u}})) \quad \text{in } \Omega_f, \quad (12)$$

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**Algorithm 1** Simplified update scheme
 

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**Require:** Anisotropic mesh adapted to initial interface position

- 1: **loop**
  - 2:   Compute state, adjoint and cost function sensitivity
  - 3:   Set displacement in the direction of steepest slope
  - 4:   Update interface position
  - 5:   Generate anisotropic mesh adapted to new interface position
- 

driven by the non-homogeneous boundary conditions

$$\tilde{\mathbf{u}} = -\partial_p J \mathbf{n} \quad \text{on } \Gamma_i, \quad (13)$$

$$\tilde{\mathbf{u}} = \mathbf{0} \quad \text{on } \Gamma, \quad (14)$$

associated to (3)-(4), with adjoint outflow condition

$$\tilde{\mathbf{u}} = -\partial_p J \mathbf{n} \quad \text{on } \Gamma_o, \quad (15)$$

if the prescribed velocity outflow condition (5) is used, or

$$\tilde{p} \mathbf{n} + 2\mu_f \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) \cdot \mathbf{n} + \rho_f (\mathbf{u} \cdot \mathbf{n}) \tilde{\mathbf{u}} = -\partial_{\mathbf{u}} J \quad \text{on } \Gamma_o, \quad (16)$$

123 if the zero pressure/zero viscous stress outflow condition (6) is used. Expressing the interface  
124 normal deformation after [33] as

$$\delta \mathbf{u} = \beta \nabla \mathbf{u} \cdot \mathbf{n}, \quad (17)$$

125 the variation with respect to the design variable, now encompassing the domain deformation, is  
126 ultimately computed as

$$\delta_\beta J_s = \delta_\beta \mathcal{L} = \int_\Gamma \beta (\tilde{p} \mathbf{n} + 2\mu_f \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) \cdot \mathbf{n}) \cdot (\nabla \mathbf{u} \cdot \mathbf{n}) \, ds = \int_\Gamma \beta \mu_f (\nabla \tilde{\mathbf{u}} \cdot \mathbf{n}) \cdot (\nabla \mathbf{u} \cdot \mathbf{n}) \, ds, \quad (18)$$

127 where the second equality stems from the incompressibility of the state and adjoint solutions [32].  
128 This enables efficient design update schemes via first-order gradient descent methods, as the second  
129 term in the integrand is the desired sensitivity to a displacement  $\beta$  at some specific point of the  
130 interface. For instance the simplest steepest-descent algorithm implemented herein moves down  
131 the cost function, in the direction of the steepest slope using

$$\beta = -\mu (\nabla \tilde{\mathbf{u}} \cdot \mathbf{n}) \cdot (\nabla \mathbf{u} \cdot \mathbf{n}), \quad (19)$$

132 up to a positive multiplicative factor to control the step taken in the gradient direction.

### 133 3. Computational methods

134 A primitive pseudo-code of the procedure for solving the above topology optimization problem is  
135 provided in Alg. 1 to repeat until a maximum number of iterations or a convergence threshold has  
136 been reached. In a nutshell, this is done here using a finite element immersed numerical framework  
137 combining implicit representation of the different domains, level set description of the interface,  
138 and anisotropic remeshing capabilities. For the sake of readability, the mesh adaptation algorithm  
139 and parallel computational framework, whose implementation in the context of fluid flow topology  
140 optimization makes for the main novelty of this study, are presented in the following as stand-alone  
141 sections. In the remainder of this section, we walk through each of the other steps and review the  
142 various problems involved and the numerical methods for solving them.

### 3.1. Level set representation of the interface

The level set method is used here to localize and capture the interface between the fluid and solid domains from the zero iso-value of a smooth level set function, classically the signed distance function defined as

$$\varphi(\mathbf{x}) = \begin{cases} -\text{dist}(\mathbf{x}, \Gamma) & \text{if } \mathbf{x} \in \Omega_f, \\ 0 & \text{if } \mathbf{x} \in \Gamma, \\ \text{dist}(\mathbf{x}, \Gamma) & \text{if } \mathbf{x} \in \Omega_s, \end{cases} \quad (20)$$

with the convention that  $\varphi < 0$  in the fluid domain. Once the sensitivity analysis has output a displacement  $\beta$  in the direction of the steepest slope, the position of the level set is updated solving a transport equation with normal velocity  $\beta \mathbf{n} / \Delta\tau$ , where  $\Delta\tau$  is a pseudo-time step to convert from displacement to velocity, that has no physical relevance since we are not concerned by the absolute displacement of a given point on the interface, only by its relative displacement with respect to its neighbors. This equation is posed in the whole domain  $\Omega$ , which is because the normal vector recovered at the interface as  $\mathbf{n} = \nabla\varphi / \|\nabla\varphi\|$  is easily extended to  $\Omega$  using (20). The main problem with this approach is that the level set after transport is generally no longer a distance function, which is especially problematic when a specific remeshing strategy depending on the distance property is used at the interface (as is the case in this study). As a result, the distance function needs to be reinitialized, which is done here using a coupled convection-reinitialization method wherein the level set function is automatically reinitialized during the resolution of the transport equation. In practice, the signed distance function is cut off using a hyperbolic tangent filter, as defined by

$$\phi = E \tanh\left(\frac{\varphi}{E}\right), \quad (21)$$

with  $E$  the cut-off thickness, so the metric property is asymptotically satisfied in the vicinity of the zero iso-value. This filtered level set is then evolved solving the auto-reinitialization equation

$$\partial_\tau \phi + \mathbf{a}_\tau \cdot \nabla \phi = S, \quad (22)$$

where we note

$$\mathbf{a}_\tau = \frac{\beta}{\Delta\tau} \mathbf{n} + \frac{\lambda}{\Delta\tau} \text{sgn}(\phi) \frac{\nabla \phi}{\|\nabla \phi\|}, \quad S = \frac{\lambda}{\Delta\tau} \text{sgn}(\phi) \left(1 - \left(\frac{\phi}{E}\right)^2\right), \quad (23)$$

and  $\lambda$  is a parameter homogeneous to a length, set to the mesh size  $h_\perp$  in the direction normal to the interface. Such an approach is shown in [34–36] to reduce the computational cost and to ensure a better mass conservation compared to the classical Hamilton–Jacobi method in which both steps are performed in succession). Moreover, since the filtered level set defined in (21) is bounded, Dirichlet boundary conditions  $\phi = \pm E$  are easily appended to Eq. (22) to explicitly design fluid and solid sub-regions of  $\partial\Omega$ . In practice, we impose here fluid at the inlet and outlet, and solid everywhere else.

### 3.2. Immersed volume method

The immersed volume method (IVM) [37–38] is used to combine the fluid and solid phases of the problem into a single fluid with variable material properties (density and viscosity). Simply put, this amounts to solving the state and adjoint equations identical to (1)–(2) and (11)–(12), but formulated on a unique mesh of the domain  $\Omega$  in which the fluid and solid domains  $\Omega_f$  and  $\Omega_s$  are immersed, and featuring phase-dependent density and viscosity adequately interpolated over a small layer around the interface and otherwise equal to their fluid and solid values. One particularity is that the thickness of the interpolation layer is user-defined and thus, it does not increase in size during the optimization, unlike the homogenization method or any other generalized material method. Using the level set function (20) as criterion for anisotropic mesh adaptation (more details provided in Sec. 3) ensures that individual material properties can be distributed accurately and smoothly as possible over the smallest possible thickness around the interface. This



is classically done using the arithmetic mean of the solid and fluid values, using a smooth Heaviside function computed from the level set to avoid discontinuities by creating an interface transition with a thickness of a few elements. Such an approach is especially relevant to thermal coupling problems, as having composite conductivity and specific heat means that the amount of heat exchanged at the interface then proceeds solely from the individual material properties on either side of it, and removes the need for a heat transfer coefficient. For the pure flow problems tackled here, though, it suffices to use constant density and viscosity equal to the fluid values, and to set the velocity to zero at all grid nodes located inside the solid domain  $\Omega_s$ . Compared to using a very high solid to fluid viscosity ratio to ensure that the velocity is zero in the solid domain, this can be seen as a hard penalty preventing the fluid from leaking across the immersed interface. The latter holds numerically because anisotropic mesh adaptation ensures that the interface does not intersect arbitrarily the mesh elements (as it precisely aims at aligning the mesh element edges along the interface), which may otherwise compromise the accuracy of the finite element approach.

### 3.3. Variational multiscale modeling

The convective terms in the incompressible Navier–Stokes and level set transport equations may cause spurious node-to-node velocity oscillations. Furthermore, the equal order linear/linear approximations used for the velocity and pressure variables may give rise to spurious pressure oscillations, albeit very desirable due to its simplicity of implementation and affordable computing cost, especially for 3-D applications. To prevent these numerical instabilities, we solve here stabilized formulations cast in the Variational Multiscale (VMS) framework, that enhance the stability of the Galerkin method via a series of additional integrals over element interior. The basic idea is to split all quantities into coarse and fine scale components, corresponding to different levels of resolution, with a coarse scale resolved by the finite element mesh and the effect of the fine scale onto the large scale approximated via consistently derived residual based terms. For the sake of simplicity in the notations, and as long as it does not lead to ambiguity, we omit in what follows the distinction between all continuous variables (e.g., domains, solutions, operators) and their discrete finite element counterparts, as well as the dependency of all variables on the iteration of the optimization process.

#### 3.3.1. Navier–Stokes equations

In practice, the state solution is computed by time-stepping the unsteady Navier–Stokes equations with large time steps to accelerate convergence towards a steady state. The stopping criterion is here for two consecutive time steps to differ by less than  $10^{-6}$  in  $L^\infty$  norm. In order to deal with the time-dependency and non-linearity of the momentum equation, the transport time of the time scale is assumed much smaller than that of the coarse scale. In return, the fine scale contribution to the transport velocity is neglected, and the fine scale is not tracked in time, although it is driven by the coarse-scale, time-dependent residuals and therefore does vary in time in a quasi-static manner. In-depth technical and mathematical details together with extensive discussions regarding the relevance of the approximations can be found in [39]. Ultimately, the coarse scale variational problem is formulated as

$$\begin{aligned} & \int_{\Omega} (\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u}) \cdot \mathbf{w} \, dv + \int_{\Omega} 2\mu \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{w}) \, dv - \int_{\Omega} p(\nabla \cdot \mathbf{w}) \, dv + \int_{\Omega} (\nabla \cdot \mathbf{u}) q \, dv \\ & - \sum_{k=1}^{N_e} \int_{\Omega_k} \tau_1 \mathbf{r}_1 \cdot (\rho \mathbf{u} \cdot \nabla \mathbf{w}) \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tau_1 \mathbf{r}_1 \cdot \nabla q \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tau_2 r_2 (\nabla \cdot \mathbf{w}) \, dv = 0, \end{aligned} \quad (24)$$

where we have considered a discretization of  $\Omega$  into  $N_e$  non-overlapping elements (triangles or tetrahedrons),  $\Omega_k$  is the domain occupied by the  $k$ th element, and  $\mathbf{r}_1$  and  $r_2$  are the momentum and continuity residuals

$$-\mathbf{r}_1 = \rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p, \quad -r_2 = \nabla \cdot \mathbf{u}, \quad (25)$$

whose second derivatives vanish since we use linear interpolation functions. Finally,  $\tau_1$  and  $\tau_2$  are ad-hoc stabilization coefficients, computed on each element after [38, 40] as

$$\tau_1 = \frac{1}{\rho (\tau_t^2(u) + \tau_d^2)^{1/2}}, \quad \tau_2 = \frac{h^2}{\tau_1}, \quad (26)$$



with convection (transport) and diffusion-dominated limits defined as

$$\tau_t(u) = c_t \frac{u}{h}, \quad \tau_d = c_d \frac{\mu}{\rho h^2}. \quad (27)$$

Here,  $u$  is a characteristic norm of the velocity on the element, computed as the average  $L^2$  norm of the nodal element velocities,  $h$  is the element size, computed as its diameter in the direction of the velocity to support using anisotropic meshes with highly stretched elements [41], and  $c_{t,d}$  are algorithmic constants taken as  $c_t = 2$  and  $c_d = 4$  for linear elements [40]. Equation (24) is discretized with a first-order-accurate time-integration scheme combining semi-implicit treatment of the convection term, implicit treatment of the viscous, pressure and divergence terms, and explicit treatment of the stabilization coefficients.

### 3.3.2. Adjoint Navier–Stokes equations

If the prescribed velocity condition (5) is used, application of the stabilized formulation, as described above, to the adjoint Navier–Stokes equations yields the following coarse scale variational problem

$$\begin{aligned} & \int_{\Omega} (-\rho \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} + \rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}}) \cdot \mathbf{w} \, dv + \int_{\Omega} 2\mu \varepsilon(\tilde{\mathbf{u}}) : \varepsilon(\mathbf{w}) \, dv + \int_{\Omega} \tilde{p}(\nabla \cdot \mathbf{w}) \, dv + \int_{\Omega} (\nabla \cdot \tilde{\mathbf{u}}) q \, dv \\ & - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_1 \tilde{\mathbf{r}}_1 \cdot (-\rho \mathbf{u} \cdot \nabla \mathbf{w}) \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_1 \tilde{\mathbf{r}}_1 \cdot \nabla q \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_2 \tilde{r}_2 (\nabla \cdot \mathbf{w}) \, dv = 0. \end{aligned} \quad (28)$$

The associated momentum and continuity residuals read

$$-\tilde{\mathbf{r}}_1 = -\rho \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} + \rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}} - \nabla \tilde{p}, \quad -\tilde{r}_2 = \nabla \cdot \tilde{\mathbf{u}}. \quad (29)$$

The stabilization coefficients are computed on each element after [42] as

$$\tilde{\tau}_1 = \frac{1}{(\tau_t^2(u) + \tau_d^2 + \tau_r^2)^{1/2}}, \quad \tilde{\tau}_2 = \tau_2, \quad (30)$$

with additional reaction-dominated limit, due to the  $\rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}}$  term associated with the production of adjoint perturbations, defined as

$$\tau_r = \rho \nabla u, \quad (31)$$

where  $\nabla u$  is a characteristic norm of  $\nabla \mathbf{u}$  on the element, computed as the average  $L^2$  norm of the nodal velocity gradients. It is important to note that the adjoint stabilization coefficients depend solely on  $\mathbf{u}$ , not  $\tilde{\mathbf{u}}$ , which is because the adjoint flow field is transported at (minus) the state velocity.

If the zero pressure/zero viscous stress condition (6) is used, then the adjoint coarse scale variational problem becomes

$$\begin{aligned} & \int_{\Omega} (-\rho \mathbf{u} \cdot \nabla \tilde{\mathbf{u}} + \rho \nabla \mathbf{u}^T \cdot \tilde{\mathbf{u}}) \cdot \mathbf{w} \, dv + \int_{\Omega} 2\mu \varepsilon(\tilde{\mathbf{u}}) : \varepsilon(\mathbf{w}) \, dv + \int_{\Omega} \tilde{p}(\nabla \cdot \mathbf{w}) \, dv + \int_{\Omega} (\nabla \cdot \tilde{\mathbf{u}}) q \, dv \\ & - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_1 \tilde{\mathbf{r}}_1 \cdot (-\rho \mathbf{u} \cdot \nabla \mathbf{w}) \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_1 \tilde{\mathbf{r}}_1 \cdot \nabla q \, dv - \sum_{k=1}^{N_e} \int_{\Omega_k} \tilde{\tau}_2 \tilde{r}_2 (\nabla \cdot \mathbf{w}) \, dv \\ & - \int_{\Gamma_o} \rho(\mathbf{u} \cdot \mathbf{n})(\tilde{\mathbf{u}} \cdot \mathbf{w}) \, ds = \int_{\Gamma_o} \partial_{\mathbf{u}} J \cdot \mathbf{w} \, ds, \end{aligned} \quad (32)$$

because the integration by part of the pressure and viscous terms unveils a boundary term

$$\int_{\partial\Omega} (\tilde{p} \mathbf{n} + 2\mu \varepsilon(\tilde{\mathbf{u}}) \cdot \mathbf{n}) \cdot \mathbf{w} \, ds = - \int_{\Gamma_o} (\rho(\mathbf{u} \cdot \mathbf{n}) \tilde{\mathbf{u}} + \partial_{\mathbf{u}} J) \cdot \mathbf{w} \, ds, \quad (33)$$

evaluated at the outlet due to the adjoint boundary condition (16).

Both problems are fully implicitly integrated, except the outflow boundary term in (32) that needs be treated explicitly for implementation convenience. Even though the last computed adjoint solution (hence pertaining to the previous design) is used to evaluate the boundary term, this simple scheme has been found to converge to identical shapes and cost function minimum, compared to solving iteratively with relaxed sub-iterations. Due to the linearity of Eqs. (11)-(12), this in turn cuts down the numerical effort, as only one single linear system needs be solved at each update step, regardless of the state outflow condition.

### 3.3.3. Interface update scheme using the convective level set method

The auto-reinitialization level set problem (22) is solved with an SUPG method, whose stabilization proceeds from that of the ubiquitous convection-diffusion-reaction equation (43, 44). The associated variational problem is formulated as

$$\int_{\Omega} (\partial_{\tau} \phi + \mathbf{a}_{\tau} \cdot \nabla \phi) \xi \, dv - \int_{\Omega_k} \tau_3 r_3 \mathbf{a}_{\tau} \cdot \nabla \xi \, dv = \int_{\Omega} S \xi \, dv, \quad (34)$$

with residual

$$-r_3 = \partial_{\tau} \phi + \mathbf{a}_{\tau} \cdot \nabla \phi - S, \quad (35)$$

and stabilization coefficient

$$\tau_3 = \frac{1}{\tau_t(a_{\tau})}. \quad (36)$$

It is easily checked that all terms scale as  $1/\Delta\tau$ , so we can set  $\Delta\tau = 1$  without any loss of generality because the solution is ultimately independent on the pseudo-time step value. Equation (34) is solved with semi-implicit treatment of the convection term (as the convection velocity  $\mathbf{a}_{\tau}$  depends on main unknown  $\phi$ ) and explicit treatment of the source term and stabilization coefficients.

## 4. Anisotropic mesh adaptation

### 4.1. Construction of an anisotropic mesh

The main idea of anisotropic, metric-based mesh adaptation is to generate a uniform mesh (with unit length edges and regular elements) in a prescribed Riemannian metric space, but anisotropic and well adapted (with highly stretched elements) in the Euclidean space. Assuming that, in the context of metric-based adaptation methods, controlling the interpolation error suffices to master the global approximation error, the objective can be formulated as finding the mesh, made up of at most  $N_n$  nodes, that minimizes the linear interpolation error in the  $L^1$  norm. Following the lines of (45, 46), an edge-based error estimator combined to a gradient recovery procedure is used to compute, for each node, a metric tensor that prescribes a set of anisotropic directions and stretching factors along these directions, without any direct information from the elements, nor any underlying interpolation. The optimal stretching factor field is obtained by solving an optimization problem using the equi-distribution principle under the constraint of a fixed number of nodes in the mesh, after which a new mesh is generated using the parallel procedure described in Sec. 5.

### 4.2. Edge error estimate

Given a mesh  $\Omega_h$  of the domain  $\Omega$ , we denote by  $\mathbf{x}^{ij}$  the edge connecting a given node  $\mathbf{x}^i$  to  $\mathbf{x}^j \in \Sigma(i)$ , where  $\Sigma(i)$  is the set of nodes connected to  $\mathbf{x}^i$ , and the number of such nodes is noted as  $|\Sigma(i)|$ . Also, given a regular analytical scalar function  $\psi$  defined on  $\Omega$ , and its P1 finite element approximation  $\psi_h$  computed on  $\Omega_h$ , we follow (45) and estimate the interpolation error along the edge  $\mathbf{x}^{ij}$  as the projection along the edge of the second derivative of  $\psi$ . This is obtained projecting along the edge a Taylor expansion of the gradient of  $\psi$  at  $\mathbf{x}^j$  to give

$$\varepsilon_{ij} = |\mathbf{g}^{ij} \cdot \mathbf{x}^{ij}|, \quad (37)$$

where the  $i$  and  $j$  superscripts indicate nodal values at nodes  $\mathbf{x}^i$  and  $\mathbf{x}^j$ , respectively,  $\mathbf{g}^i = \nabla \psi(\mathbf{x}^i)$  is the exact value of the gradient at  $\mathbf{x}^i$ , and  $\mathbf{g}^{ij} = \mathbf{g}^j - \mathbf{g}^i$  is the variation of the gradient along the edge. Although Eq. (37) involves only values of the gradient at the edge extremities and can thus be evaluated without resorting to resource expensive Hessian reconstruction methods, this however requires the gradient of  $\psi$  to be known and continuous at the nodes, which in turn requires full knowledge of  $\psi$ . Meanwhile, only the linear interpolate  $\psi_h$  is known in practice, whose gradient is piecewise constant and discontinuous from element to element, although its projection along the edges is continuous since it depends only on the nodal values of the field.

297 A recovery procedure is thus used to build a continuous gradient estimator defined directly at  
 298 the nodes. It is shown in [45] that a suitable error estimate preserving second-order accuracy is  
 299 obtained substituting the reconstructed gradient for the exact gradient in (37), to give

$$\varepsilon_{ij} = |\bar{\mathbf{g}}^{ij} \cdot \mathbf{x}^{ij}|, \quad (38)$$

300 where  $\bar{\mathbf{g}}^{ij} = \bar{\mathbf{g}}^j - \bar{\mathbf{g}}^i$  and we denote by  $\bar{\mathbf{g}}^i$  the recovered gradient of  $\psi_h$  at node  $\mathbf{x}^i$ . The latter is  
 301 defined in a least-square sense as

$$\bar{\mathbf{g}}^i = \operatorname{argmin}_{\mathbf{g} \in \mathbb{R}^d} \sum_{j \in \Sigma(i)} |(\mathbf{g} - \nabla \psi_h) \cdot \mathbf{x}^{ij}|^2, \quad (39)$$

302 for which an approximate solution using the nodal values as sole input is shown in [45] to be

$$\bar{\mathbf{g}}^i = (\mathbf{X}^i)^{-1} \cdot \sum_{j \in \Sigma(i)} (\psi_h(\mathbf{x}^j) - \psi_h(\mathbf{x}^i)) \mathbf{x}^{ij}, \quad (40)$$

303 where  $\mathbf{X}^i$  is the length distribution tensor defined as

$$\mathbf{X}^i = \frac{1}{|\Sigma(i)|} \sum_{j \in \Sigma(i)} \mathbf{x}^{ij} \otimes \mathbf{x}^{ij}, \quad (41)$$

304 that gives an average representation of the distribution of the edges sharing an extremity.

#### 305 4.3. Metric construction

306 In order to relate the error indicator  $\varepsilon_{ij}$  defined in (38) to a metric suitable for mesh adaptation  
 307 purposes, we introduce the stretching factor  $s_{ij}$  as the ratio between the length of the edge  $\mathbf{x}^{ij}$   
 308 after and before the adaptation. The metric at node  $\mathbf{x}^i$  is sought to generate unit stretched edge  
 309 length in the metric space, that is,

$$(s_{ij} \mathbf{x}^{ij})^T \cdot \mathbf{M}^i \cdot (s_{ij} \mathbf{x}^{ij}) = 1, \quad \forall j \in \Sigma(i), \quad (42)$$

310 for which an approximate least-square solution is shown in [45] to be

$$\mathbf{M}^i = \left( \frac{d}{|\Sigma(i)|} \sum_{j \in \Sigma(i)} s_{ij}^2 \mathbf{x}^{ij} \otimes \mathbf{x}^{ij} \right)^{-1}, \quad (43)$$

311 provided the nodes in  $\Sigma(i)$  form at least  $d$  non co-linear edges with  $\mathbf{x}^i$ , which holds if the mesh is  
 312 valid. The metric solution of (43) is ultimately computed setting a target total number of nodes  
 313  $N_n$ . Assuming a total error equi-distributed among all edges, the stretching factor is shown in [46]  
 314 to be

$$s_{ij} = \left( \frac{\sum_i N_i(1)}{N_n} \right)^{\frac{2}{d}} \varepsilon_{ij}^{-1/2}, \quad (44)$$

315 where  $N_i(1)$  is the number of nodes generated in the vicinity of node  $\mathbf{x}^i$  for a unit error, given by

$$N_i(1) = \left( \det \left( \frac{d}{|\Sigma(i)|} \sum_{j \in \Sigma(i)} \varepsilon_{ij}^{1/2} \frac{\mathbf{x}^{ij}}{|\mathbf{x}^{ij}|} \otimes \frac{\mathbf{x}^{ij}}{|\mathbf{x}^{ij}|} \right) \right)^{-1/2}. \quad (45)$$

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**Algorithm 2** Anisotropic mesh adaptation algorithm

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**Require:** Anisotropic adapted mesh

- 1: Set number of nodes  $N_n$
  - 2: Compute  $\psi_h$  on current mesh
  - 3: **for** each node  $\mathbf{x}^i$  **do**
  - 4:   Compute length distribution tensor  $\mathbf{X}^i$  using (41)
  - 5:   Compute nodal recovered gradient  $\bar{\mathbf{g}}^i$  using (40)
  - 6:   **for** all edges  $\mathbf{x}^{ij}$  **do**
  - 7:     Compute edge recovered gradient  $\bar{\mathbf{g}}^{ij}$
  - 8:     Compute edge-based error  $\varepsilon_{ij}$  using (38)
  - 9:     Compute stretching factor  $s_{ij}$  using (44)
  - 10:   Compute metric  $\mathbf{M}^i$  using (43)
  - 11: Generate new mesh by local improvement in the neighborhood of the nodes and edges [47]
  - 12: Interpolate  $\psi_h$  on new mesh using classical linear interpolation
- 

#### 4.4. Level set-based adaptation criteria

In order to simplify and clarify the presentation, the main steps needed for metric construction at the nodes is summarized in algorithm 2. In practice, the sole variable used for error estimation purpose is the filtered level set defined in (21), as it satisfies the metric property in a thin layer around the interface (in particular it preserves the zero iso-value of  $\varphi$ , which is the only relevant information for mesh adaptation purposes), but avoids unnecessary adaption of the mesh further away from the interface, where the interpolation error is close-to-zero, due to  $\|\nabla\phi\| \sim 0$ . This means that the criterion for mesh adaptation is purely geometric, i.e., the same mesh is pre-adapted around the fluid-solid interface, then used to compute all quantities needed to perform the next design update step. Nonetheless, it is worth mentioning that the approach also supports more complex adaptation criteria featuring physical quantities, thus providing the ability to dynamically adapt the mesh during the simulations. The common method to adapt a mesh to several variables is to combine the metrics corresponding to each individual variable using metric intersection algorithms, which is known to incur a relatively high computational cost and to have potentially non-unique, suboptimal outcome. Conversely, the present approach allows building directly a unique metric from a multi-component error vector combining level set and any relevant flow quantity of interest, as definition (38) is easily extended to account for several sources of error [48]. Indeed, if we consider  $\boldsymbol{\psi} = (\psi_1, \psi_2, \dots, \psi_p)$  a vector consisting of  $p$  scalar variables, it comes out straightforwardly that the error is now a vector  $\boldsymbol{\varepsilon}_{ij} = (\varepsilon_{ij,1}, \varepsilon_{ij,2}, \dots, \varepsilon_{ij,p})$ , whose  $L^2$  norm can serve as simple error value for the edge from which to compute the stretching factor (44) and ultimately, the metric solution of (43). For instance, the  $2d + 3$  sized nodal vector field defined as

$$\boldsymbol{\psi}_h(\mathbf{x}^i) = \left( \frac{\phi_h^i}{\max_{j \in \Sigma(i)} \phi_h^j}, \frac{u_{h_{k \in \{1 \dots d\}}}^i}{\|\mathbf{u}_h^i\|}, \frac{\|\mathbf{u}_h^i\|}{\max_{j \in \Sigma(i)} \|\mathbf{u}_h^j\|}, \frac{\tilde{u}_{h_{k \in \{1 \dots d\}}}^i}{\|\tilde{\mathbf{u}}_h^i\|}, \frac{\|\tilde{\mathbf{u}}_h^i\|}{\max_{j \in \Sigma(i)} \|\tilde{\mathbf{u}}_h^j\|} \right), \quad (46)$$

can be used to combine adaptivity with respect to the norm and direction of the state and adjoint velocity vectors, in addition to the level set. Because all fields are normalized by their respective global maximum, a field much larger in magnitude cannot dominate the error estimator, meaning that the variations of all variables are fairly taken into account. This benefits problems involving more complex physics, e.g., turbulence, heat transfer, fluid-structure interaction, multiple phases, possibly in interaction with one another, all the more so in the context of topology optimization, as the difference in the spatial supports of the state and adjoint quantities (that stems from the non-normality of the linearized evolution operator [49]) may otherwise yield conflicting requirements in terms of the regions of the computational domain most in need of refinement.

## 5. Parallel computational framework

The numerical resolution framework relies on the in-house, parallel, finite element library Cim-LIB.CFD [48], whose organization relies on fundamental choices allowing an efficient implementa-

tion of high-level parallel algorithms. We discuss below the efficient tools to generate and adapt the meshes, and to solve the large-scale linear systems arising from the finite element discretization, steps where most computational time is spent. Another key aspect of the method is the ability of the stabilized finite element formulations to support using anisotropic adapted meshes in both the fluid and solid domains, regardless of the problem dimensionality. On the one hand, using linear approximations for all variables drastically reduces the size of the systems that need be solved. To give a taste, the meshes used herein are made up of about 5 million elements yielding a total of 3.5 million degrees of freedom, but 20 million degrees of freedom using quadratic approximations for the velocities, hence a reduction by nearly 80%. On the other hand, using anisotropic meshes decreases the cost of improving the numerical precision, as the number of nodes needs be increased only in the direction of interest. This makes a huge difference in 3-D calculations, as the accuracy can be improved by a factor of 2 (in the best case scenario) using only 2 times as many nodes, instead of 8.

### 5.1. Parallel resolution

Computing the numerical solutions to the governing **Navier-Stokes, adjoint Navier-Stokes and level-set advection equations** considered herein requires solving large-scale linear systems (or non-linear systems that may lead to the resolution of several linear systems if an implicit discretization scheme is used). To this end, the resolution step makes a clear distinction between those large-scale systems that need be stored and solved, and their local contributions at the element levels. Namely, all finite element formulations are only implemented sequentially at the element level, then assembled and solved in parallel using the PETSc library [50], that offers a wide range of parallel data structures (linear and non-linear solvers as well as preconditioners) and can be run on large computing clusters. Here, only semi-implicit and explicit discretization schemes are used, and the associated linear systems are sufficiently well conditioned to be solved by iterative methods. We thus use the Generalized Minimal Residual algorithm with block Jacobi incomplete LU preconditioning, and consider the solutions to be converged if the absolute residuals are less than  $10^{-6}$ .

### 5.2. Parallel adaptive remeshing

Although most numerical solvers have embraced parallel computing as a way to continue to improve performance, it is less common to see massively parallel computation using anisotropic adapted unstructured meshes, let alone if the mesh is dynamically adapted to track the interface deformations. An original parallelization strategy is used here for the mesh adaptation step, based on an independent subdomain remeshing under the constraint of blocked interfaces. **An initial mesh is partitioned into several submeshes using a parallel graph/mesh partitioning/repartitioning algorithm that allows to balance well the number of mesh entities (vertices or elements) per processor [51-53].** Remeshing operations are then performed with a sequential mesh adaptator on each subdomain with an extra treatment of the interfaces, using the procedure described in [47], based on a topological representation of the computational domain. In practice, a level-set based error estimate is computed for each subdomain. An iterative approach is used, in which remeshing is performed concurrently on each processor while the interfaces between sub-domains are locked to avoid any communication between processors. Then, to obtain a satisfactory final mesh regarding the quality function, a repartitioning step is performed to move the interface inside the domain in order to enable re-meshing in a next phase. As illustrated in Figure 1, the algorithm iterates until all items have been re-meshed. Finally, the new mesh is repartitioned over the allocated CPUs to take into account for the changes of mesh topology in the computational loads distribution. Note, the constraint on the number of mesh elements could be considered as local to each subdomain. In this case, solving the error estimate problem is straightforward, as all computations are local and there is no need to exchange data between the processors. The local constraint on the number of elements implies the generation of a new mesh with the same number of elements per processor. This allows avoiding heavy load balancing cost after each mesh adaptation, but tends towards an overestimate of the mesh density on subdomains where flow activity is almost neglected. From a scaling point of view, such an approach leads to a weak scalability model for which the problem size grows linearly with respect to the number of processors. To derive a hard scalability model with

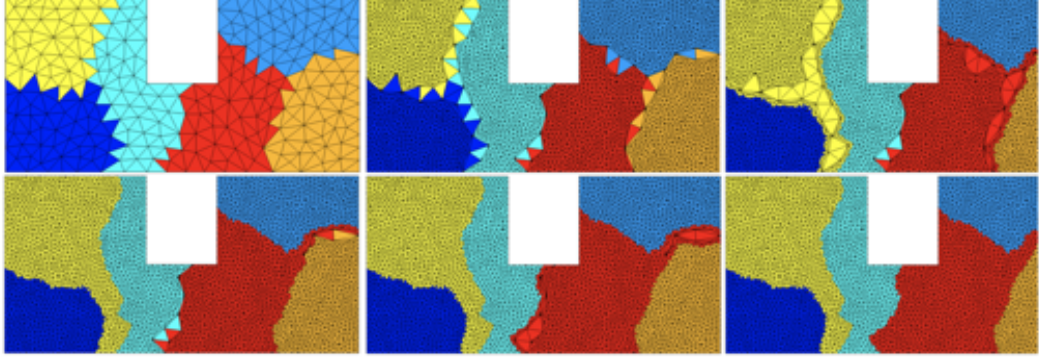


Figure 1: Illustration of the iterative parallel remeshing steps on a model 2-D distributed mesh.

good parallel performances, the constraint on the number of elements for the new generated mesh is thus handled globally, with the global number of elements over the entire domain distributed with respect to the mesh density prescribed by the error estimator. In doing so, the parallel behavior of the mesh adaptation is very close to the serial one and the error analysis is still the same, although load rebalancing is required after each mesh adaptation stage.

Because the parallel remesher is made of nested iterations between remeshing and repartitioning, the metric map providing both the size and the stretching of mesh elements needs to be transported after each repartitioning step. Indeed, it is given as a nodal field, hence one scalar value per node, and must be updated after each migration or renumbering. The parallel adaptive remeshing is thus the combination of three iteratively nested steps: (i) independent adaptive remeshing per subdomain, (ii) constrained repartitioning and (iii) updating the metric map. Depending on the problem dimensionality, three to five iterations of remeshing and repartitioning are typically needed to build the optimal mesh, but the time spent per iteration decreases drastically as fewer and fewer elements and nodes need to be moved and migrated across processors, as we only need to move bad quality zones inside the domain in order to remesh them. For several test cases in two and three dimensions, this simple approach is shown in [54] to yield close-to-optimal parallel remeshing speed-up up to 32 cores.

### 5.3. Dynamic load balancing

In this work, we follow the same load balancing strategy than in Ref. [51], to which the interested reader is referred for technical details. A cost function is defined and takes into account the theoretical computation and communication time of the allocated resources. Then, the load balancing process is realized using two major steps: (i) forming disjoint pairs of processors that are susceptible to minimize the cost function, and (ii) optimizing the cartography on each pair. This optimization is done by transferring mesh nodes or mesh cells from a processor to the other using the notion of strip migration. These two steps are repeated as long as the global cost of the partition can be optimized. The results from [103] show that the use of this method on various system architectures allows accelerating the mesh partitioning process. In terms of scalability, a linear behavior is observed. An example of load balancing is given in Fig. 2 for the same example than in Fig. 1 after the parallel remeshing procedure. One notices that the partition in Fig. 2(a) is not optimal, as the size of the interfaces is too large, which could have a damaging impact on the communication costs. The cost function is thus optimized using the previously described load balancing procedure by transferring nodes from one processor to the other, in order to obtain the final optimal partition presented on the right side of Fig. 2(b).

## 6. Numerical implementation

### 6.1. Geometrical constraints

Fluid flow topology optimization is generally performed under geometrical constraints, typically, constant or upper bounded surfaces and/or volumes to avoid the two extreme cases of the



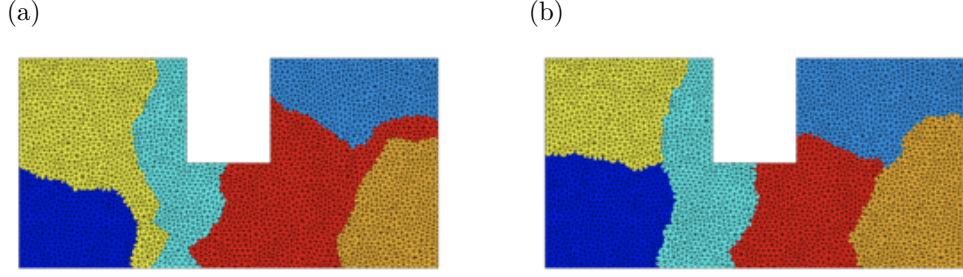


Figure 2: (a) Before and (b) after load balancing for the same model 2-D distributed mesh as in Fig. 1

solid domain clogging the entire design domain or disappearing altogether, as in pressure drop minimization and drag minimization problems, respectively. This is usually done adding penalty terms to the Lagrangian, each of which consists of an empirical penalty parameter multiplied by a measure of violation of the constraint, whose variations with respect to the state and design variables snowballs into the derivation of the adjoint problem and of the cost function sensitivity. Here, the constraint of a constant volume of fluid  $V_{target}$  is applied a posteriori, i.e., we solve the unconstrained problem presented in Sec. 2 with no penalty term added to the Lagrangian (although the optimization remains subject to Navier–Stokes as state equations). Once the convective level set method presented in Sec. 3.3.3 has updated the interface position, a first pass of anisotropic mesh adaptation is performed, after which the volume of the fluid domain is computed as

$$V_\varphi = \int_{\Omega} H_\epsilon(\varphi) \, dv, \quad (47)$$

where  $H_\epsilon$  is the smoothed Heaviside function on the fluid domain defined as

$$H_\epsilon(\varphi) = \begin{cases} 1 & \text{if } \varphi < -\epsilon, \\ \frac{1}{2} \left( 1 - \frac{\varphi}{\epsilon} - \frac{1}{\pi} \sin \left( \pi \frac{\varphi}{\epsilon} \right) \right) & \text{if } |\varphi| \leq \epsilon, \\ 0 & \text{if } \varphi > \epsilon, \end{cases} \quad (48)$$

and  $\epsilon$  is a regularization parameter set to  $2h_\perp$ . A simple dichotomy approach is then used to optimize a constant deformation  $\delta\varphi$  meant to enlarge ( $\delta\varphi < 0$ ) or shrink ( $\delta\varphi > 0$ ) the fluid domain, until the difference  $|V_{\varphi+\delta\varphi} - V_{target}|$  between the actual and target volumes drops below a certain tolerance, at which point we cut off  $\varphi + \delta\varphi$  and perform a second pass of mesh adaptation. Two points are worth mentioning: first, because each offset changes the min-max values of the truncation, the above procedure requires knowledge of the level set  $\varphi$ , not just the filtered level set  $\phi$ . A brute force algorithm therefore performs beforehand a complete reconstruction of the distance function from the zero iso-value of  $\phi$ , as only the filtered level set (not the level set) is evolved during the convection-reinitialization step. Second, only small deformations are considered so that no intermediate mesh adaptation passes are required. By doing so, the total cost is essentially that of performing the second pass of mesh adaptation, as further discussed in the following.

## 6.2. Steepest descent update rule

In practice, the displacement used to perform the update step is defined as

$$\beta = -\theta \frac{\mu(\nabla \tilde{\mathbf{u}} \cdot \mathbf{n}) \cdot (\nabla \mathbf{u} \cdot \mathbf{n}) \chi_\Gamma(\mathbf{x})}{\max_{\Omega} \mu(\nabla \tilde{\mathbf{u}} \cdot \mathbf{n}) \cdot (\nabla \mathbf{u} \cdot \mathbf{n}) \chi_\Gamma(\mathbf{x}) \prod_l \zeta(\|\mathbf{x} - \mathbf{X}_s^l\|)}, \quad (49)$$

where  $\theta > 0$  is a descent factor controlling the step taken in the gradient direction, and  $\chi_\Gamma$  and  $\zeta$  are activation functions between 0 and 1 ensuring that the design is fittingly updated only in relevant regions of the computational domain. More details are as follows:

- $\chi_\Gamma$  is a binary filter returning a value of 1 only at nodes within a distance  $E$  of the interface. This is because the normal vector in a level set framework is recovered as  $\mathbf{n} = \nabla \phi / \|\nabla \phi\|$ , so



the displacement is non-zero in the whole fluid domain, even far from the interface where  $\mathbf{n}$  has unit norm because  $\|\nabla\phi\|$  only tends asymptotically to zero. In return, the update step can break down numerically at nodes nearly equidistant from two subparts of the interfaces, which can occur for instance at the centerline of a channel.

- $\zeta$  is a smooth filter assigning 0 value to some subset  $\mathbf{X}_s^l \in \partial\Omega$  that can be either a point or a curve, and  $\|\mathbf{x} - \mathbf{X}_s^l\|$  is the shortest-path distance to  $\mathbf{X}_s^l$ . Such subsets are singled out prior to optimization, because the flow there may be driven to a singularity, and ill-defined velocity gradients may cause large, unphysical displacements. Such singularities can be dealt with numerically by appending fluid/solid Dirichlet boundary conditions to the level set convection-reinitialization problem. Nonetheless, they must not be included in the normalization step to avoid forcing excessively small displacements along the remaining part of the interface, and thereby considerably slowing down the convergence rate of the iterative optimization process. We use here hyperbolic tangent filters

$$\zeta(r) = \frac{1}{2} + \frac{1}{2} \tanh\left(\alpha_s \tan\left(-\frac{\pi}{2} + \frac{\pi}{2} \frac{r}{r_s + \epsilon_{s1}} + \epsilon_{s2}\right)\right), \quad (50)$$

increasing from 0 to 1 within a distance of  $2r_s$  from the singularity, with  $r_s$  a transition radius such that

$$4r_s < \min_{l,m} \|\mathbf{X}_s^l - \mathbf{X}_s^m\|, \quad (51)$$

to prevent overlaps,  $\alpha_s$  a steepness parameter controlling the sharpness of the transition, and  $\epsilon_{s1,2}$  small regularization parameters to avoid local discontinuities.

Ultimately, the above filtering and normalization steps ensure that the level set is updated using a displacement that is non-zero only in a thin layer of thickness  $E$  about the interface, minus a certain number of singular subsets.

### 6.3. Descent factor

It follows from Eq. (49) that the descent factor  $\theta$  physically represents the maximum displacement amplitude over the update region of interest. In practice, though, the actual numerical displacement, estimated from the difference between zero iso-value of the filtered level set before and after transport, has been found to be well below its theoretical value. This is because the state and adjoint velocities are forced to zero on the solid domain. The displacement, being driven by the velocity gradients, is thus also zero everywhere in the solid, except in a very narrow region about the interface, typically a couple of elements thick. As a result, it is not possible to explicitly control the displacement achieved numerically at each iteration. A simple scheme to do so would have been to repeatedly evolve the interface with a small descent factor until the difference between the cumulated and target displacement drops below a certain tolerance. However, the interface can be evolved only once per update step, as the gradient information is lost if the displacement happens to be in the direction of the solid, for the same reason mentioned above. We thus tune the descent factor manually on a case by case basis, for the achieved displacement to be slightly smaller than the cut-off thickness. This has been found to be a satisfactory trade-off between accuracy and numerical effort, as the number of iterations required for convergence remains affordable, and the position of the evolved interface is accurately tracked. Displacements larger than the cut off thickness conversely move the level set into regions of the computational domain lacking the proper mesh refinement, which has been found to ultimately affect the accuracy of the interface representation.

### 6.4. General algorithm

Figure 3 shows the flowchart of the implemented topology optimization algorithm, in which anisotropic mesh adaptation is key to capture the interface with the highest precision possible. The necessary algorithmic parameters common to all examples documented in the following are given in Tab. 1. Note, as a consequence of the level set-based technique used to enforce the volume

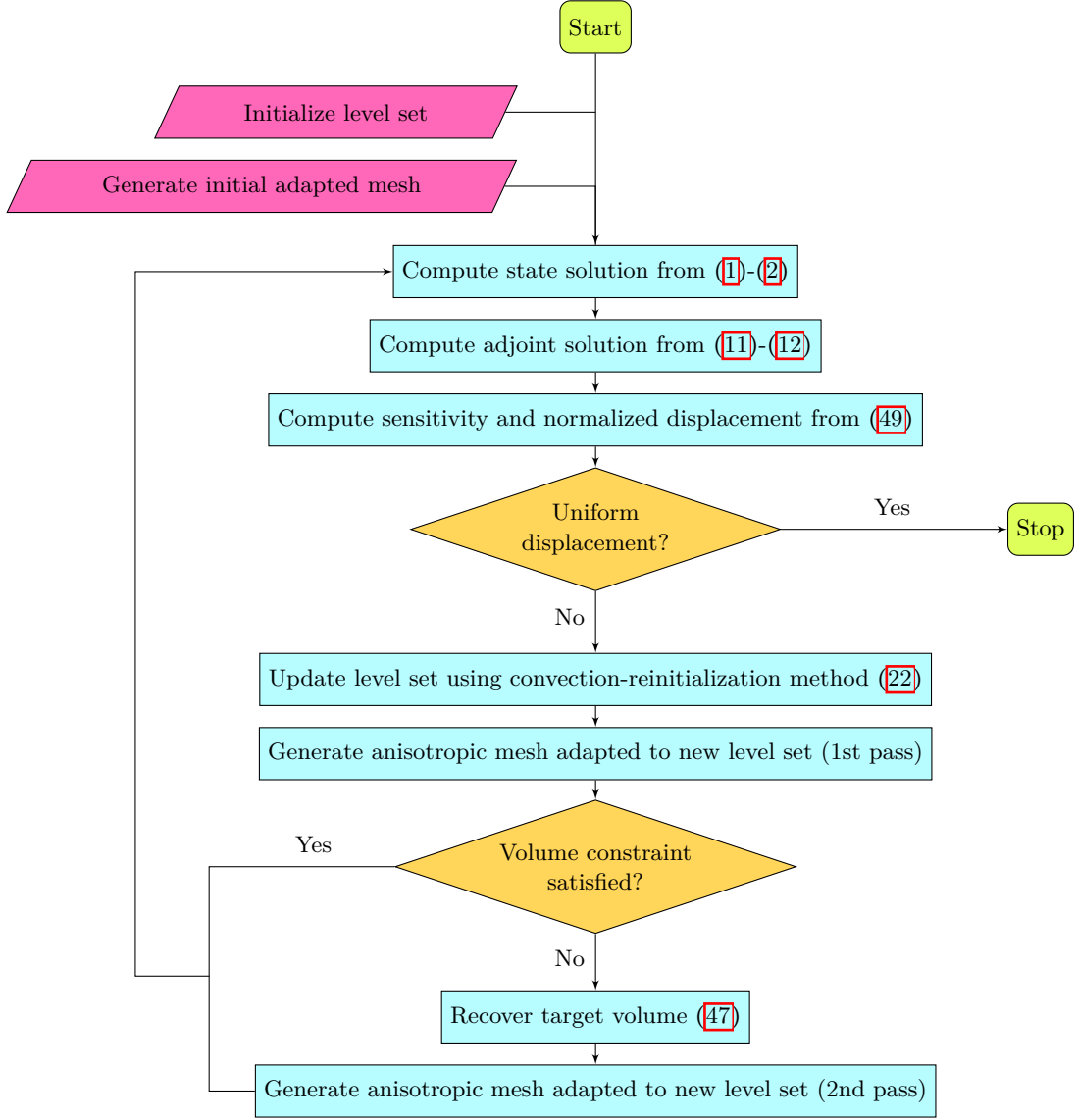


Figure 3: Flowchart of performance topology optimization procedure.

of fluid constraint, convergence is achieved not when the displacement is identically zero, as would be the case using a penalized Lagrangian approach, but when the displacement is uniform along the interface. This is not easily done on the fly, though, so we rather iterate until a maximum number of iterations has been reached and estimate convergence a posteriori.

## 7. Numerical benchmarks

This section assesses the accuracy and efficiency of the numerical framework through a series of topology optimization problems, for which the novelty lies not necessarily in the associated optimal designs themselves, but in the accuracy to which the optimal interfaces are captured in the simulation model. Each problem is tackled on 64 cores of a cluster of AMD Rome EPYC 7502 bi-processors. The cost function to minimize is the net inward flux of total pressure through the boundaries, taken as a measure of the total power dissipated by a fluid dynamic device. Since the orientation of the normal  $\mathbf{n}$  yields  $\mathbf{u} \cdot \mathbf{n}|_{\Gamma_i} > 0$  and  $\mathbf{u} \cdot \mathbf{n}|_{\Gamma_o} < 0$ , this can be expressed in the form

$h_{\perp} = 0.0001$	Min. interface normal mesh size
$\Delta t = 0.1$	CFD Numerical time step
$E = 0.005$	Level set cut off thickness
$ \delta\varphi  = 0.0005$	Initial volume recovery offset
$r_s = 0.0125$	Transition radius
$\alpha_s = 2.1$	Sharpness parameter
$(\epsilon_{s1}, \epsilon_{s2}) = (0.0005, 0.005)$	Regularization parameters

Table 1: Algorithmic parameters.

of (7) using

$$J = p_{tot}(\mathbf{u} \cdot \mathbf{n}) = (p + \frac{1}{2}\rho(\mathbf{u} \cdot \mathbf{u}))(\mathbf{u} \cdot \mathbf{n}). \quad (52)$$

All examples aim at finding the best path for a fluid to flow in a reference design domains under the form of cubic or cuboid (parallelepipedic) cavities, with either a single or multiple identical inlets, all cylindrical, and a single or multiple identical outlets, either cylindrical or rectangular. For each case, the sole control parameter is the Reynolds number, built here on inlet diameter and maximum inlet velocity (the same for all inlets).

The remainder of the practical implementation details are as follows:

- All design domains are initialized with solid inclusions coming in various shapes and sizes. **No new holes are created over the course of optimization, in the absence of a dedicated mechanism for seeding solid occlusions, but** from experience, all problems tackled in the following are essentially insensitive to the initial design provided a sufficiently large number of inclusions is used.
- The admissible error on the target volume is set to 1% in two dimensions, and 5% in three dimensions.
- The fluid is systematically conveyed into and out of the design domain using leads of length  $l_i$  (the same at all inlets) and  $l_o$  (the same at all outlets) appended normal to the boundary. This is for numerical consistency, as the exact problem formulation in the literature may vary depending on the case, and it is not always clear whether such leads should be included in the design domain. **This is the case here,** although the leads are not considered in the volume constraint, neither in definition of the target volume nor in the computation of the volume of fluid.
- The singular subsets excluded from the displacement normalization step are the sharp intersections between the leads and the boundary of the cavities, hence each smooth filter  $\zeta$  transitions from 0 to 1 over either a torus of minor radius  $2r_s$  (for all inlets and cylindrical outlets) or a set of intersecting cylinders of radius  $2r_s$  (for all rectangular outlets). Note, this is not a consequence of explicitly representing the leads, as the exact same procedure has been found suitable without such appendage.
- The leads are excluded from the displacement normalization step, for which we simply add to the max argument of (49) a binary filter returning a value of 0 at all nodes located inside the pipes. This is again to avoid slowing down the convergence rate of the iterative optimization process, as the maximum displacement is otherwise located in the leads, because the easiest way to minimize the dissipated power is to suppress the flow by having the solid entirely clogging the leads.
- Without seeking to optimize the performance, all optimization runs have been found to converge within a few hundreds iterations, which is essentially the number of steps used to fulfill the fluid volume constraint while ensuring that the displacement achieved at each iteration remains below the level set cut-off thickness (more details in the following).

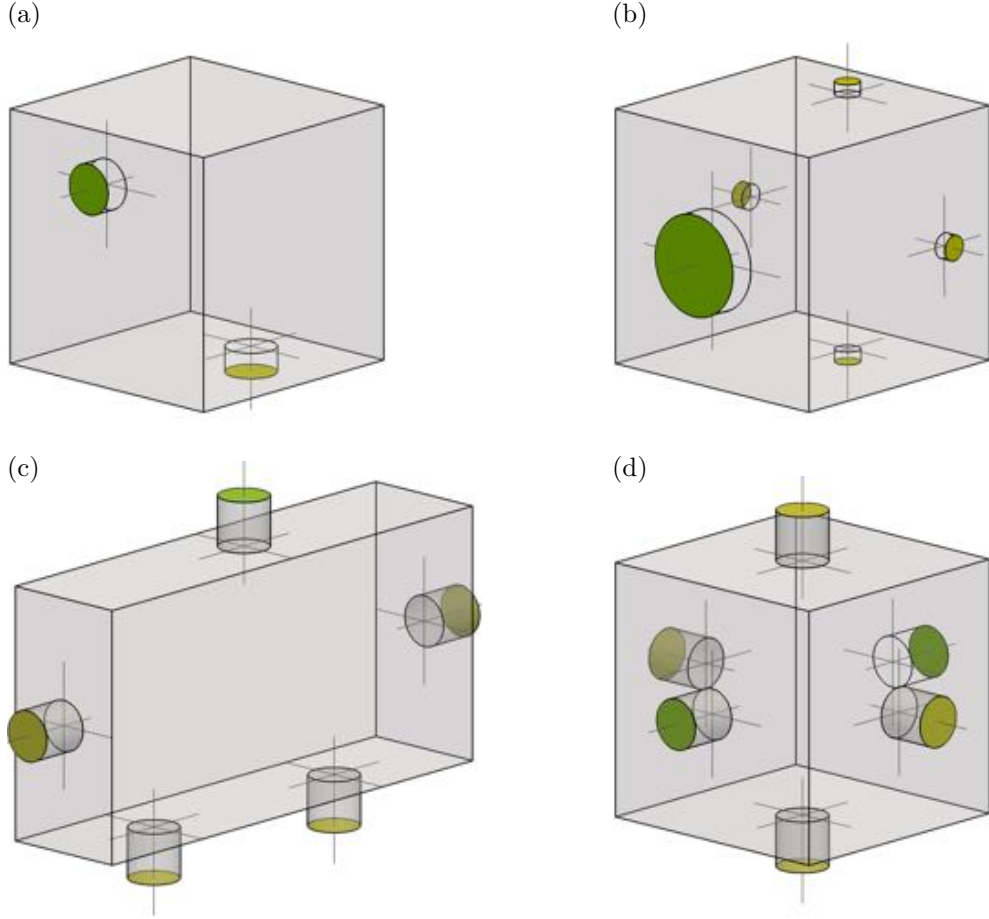


Figure 4: Problem set-up for the (a) single inlet/single outlet (b-c) single inlet/multiple outlets and (d) multiple inlets/multiple outlets examples.

- All 3-D meshes have been checked to have an element-to-node ratio close to 5, as should be for dens meshes made up of tetrahedral elements. In order to ease the comparison with the available literature, the mesh information is thus documented in the following in terms of its equivalent number of elements, defined as  $N_{el} = 5N_n$ .

Finally, all systems considered in the following have from 1 up to 3 reflectional symmetries. Nonetheless, we do not reduce the computational cost by modeling only a half (or a quarter/eighth) of the domain together with symmetry boundary conditions, which is feasible [24] but would somehow contradict the objective of assessing the method in the context of large-scale CFD systems. The entire domain is thus discretized, and we let symmetry arise as a result of the optimization process, even though this likely increases the number of iterations needed to achieve convergence.

### 7.1. Single inlet/single outlet duct flow

We optimize first the single inlet / single outlet duct flow whose setup is shown in Fig. 4(a). The design domain is a cubic cavity of unit length, that has one circular inlet on the left side, one circular outlet at the bottom, and reflectional symmetry with respect to the inlet/outlet plane. The aim is to determine the optimal design of the pipe bend that connects the inlet to the outlet and minimizes the dissipated power subject to the constraint that the fluid must occupy a given fraction of the total volume. The boundary conditions for this case consist of a normal to the boundary, parabolic inlet velocity profile and a zero pressure/zero viscous stress condition. This is a classical benchmark for 2-D topology optimization in fluid dynamics [12, 15, 55-58], hence the line of thought here is to provide first a verification and characterization of the method in two dimensions, then extend the analysis in three dimensions, for which the amount of available literature is much more scarce [24, 58].

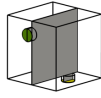
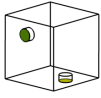
		
$\Omega = [0; 1] \times [0; 1]$	$[0; 1] \times [0; 1] \times [0; 1]$	Design domain
$d = 2$	3	Problem dimensionality
$V_{target} = 0.25$	0.039	Target volume of fluid
$V_{\varphi,0} = 0.25$	0.76	Initial volume of fluid
$Re = 2$	$\gg$	Reynolds number
$\mathbf{x}_i = (-0.1, 0.8)$	$(-0.1, 0.8, 0.5)$	Inlet center coordinates
$u_i = 0.2$	$\gg$	Inlet centerline velocity
$e_i = 0.2$	$\gg$	Inlet diameter
$l_i = 0.1$	$\gg$	Inlet leads length
$\mathbf{x}_o = (0.8, -0.1)$	$(0.8, 0.5, -0.1)$	Outlet center coordinates
$e_o = 0.2$	$\gg$	Outlet diameter
$l_o = 0.1$	$\gg$	Outlet leads length
$N_n = 20000$	1M	Nb. mesh nodes
$N_{el} = 40000$	5M	Nb. mesh elements

Table 2: Numerical parameters for the single inlet/single outlet duct flow problem.

#### 7.1.1. Two-dimensional case

The 2-D analysis is carried out in the symmetry plane slicing the 3-D domain through the inlet/outlet centerlines; see Tab. 2 for provision of all relevant numerical parameters. The design domain reduces to a square cavity of unit length, with one inlet on the left side and one outlet at the bottom, discretized here with 40000 elements<sup>1</sup>. The fluid is set to occupy 25% of the cavity, which is the same volume<sup>2</sup> as the quarter annulus fitting exactly to the inlet and outlet. The initial design shown in Fig. 5 consists of spherical occlusions arranged for the initial fluid to match the target within the desired tolerance, meaning that the volume constraint is satisfied right away. The optimization run is illustrated in Fig. 5 by the anisotropic adapted mesh and zero level set of a selected sample. It can be seen that the method easily handles the topological changes occurring over the course of optimization, e.g., merging or cancellation of holes. Also, all adapted meshes exhibit the expected orientation and deformation of the mesh elements, whose longest edges are parallel to the solid boundaries. The elements are naturally and automatically coarsened in smooth regions where the filtered level set is constant, all the more so in the solid domain where only a few ten elements are used. Meanwhile, they are extremely refined near the interface for the velocity to smoothly transition to zero across the boundary layer. In return, the interfaces are sharply captured, not only at optimality but during all stages of the optimization. This represents a major improvement in accuracy of the geometric representation with respect to the available recent literature, as even traditional (isotropic) adaptive mesh refinement techniques have been shown to yield quality issues (staircase effects) in smoothly curved regions. Ultimately, we obtain an almost straight channel nearly identical to that documented in [55], which is because most energy is dissipated by shear at low Reynolds numbers, so an optimal flow pipe is preferably as short and wide as possible.

#### 7.1.2. Three-dimensional case

The problem is now tackled in three dimensions, with the entire cubic cavity discretized into 5000000 (5M) mesh elements. The fluid is now set to occupy 3.9% of the cavity, which is the same as the quarter torus fitting exactly to the inlet and outlet. All other numerical parameters

<sup>1</sup>The mesh information is documented in terms of the equivalent number of elements  $N_{el} = 2N_n$  if  $d = 2$ , as the meshes then have an element-to-node ratio close to 2, as should be for dense meshes made up of triangular elements.

<sup>2</sup>Actually cross-sectional area or volume per unit length in the third dimension, in which case we choose to keep the volume terminology for the sake of generality.

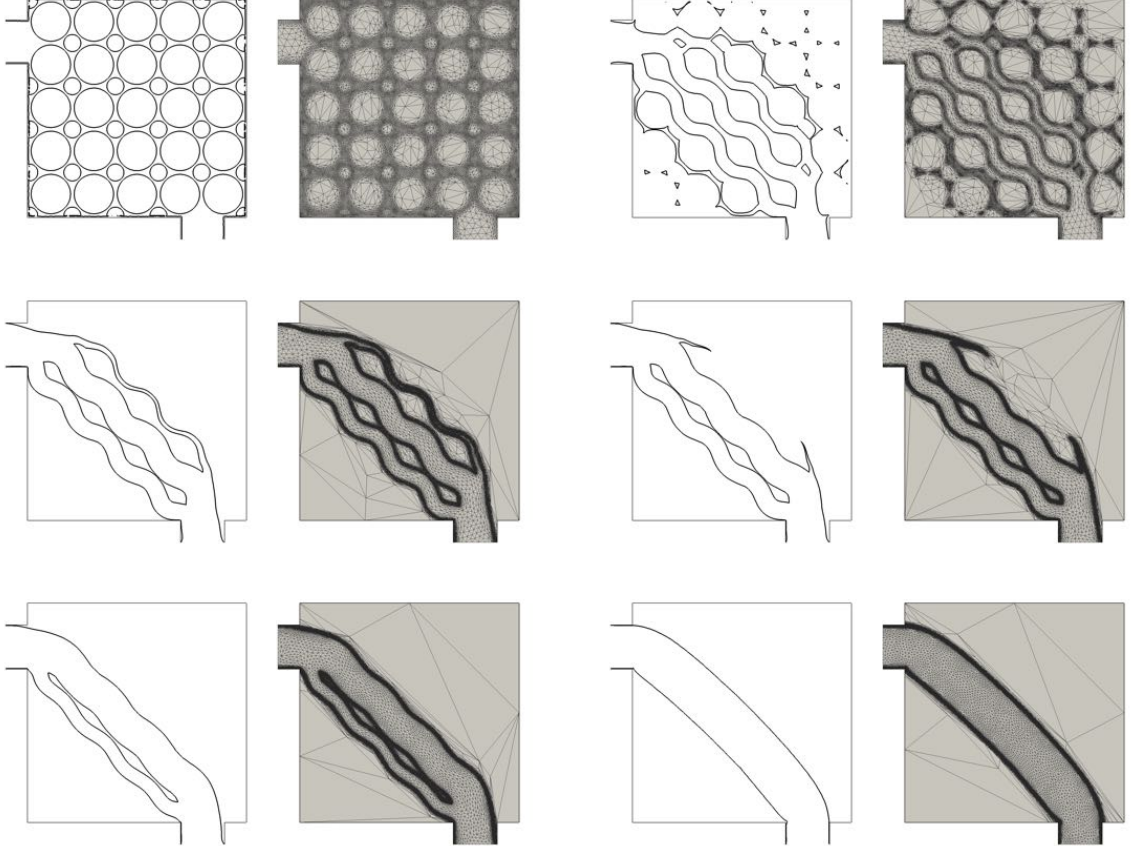


Figure 5: Two-dimensional optimization of the single inlet/single duct flow presented in Fig. 4(a). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled over the course of optimization using the parameters given in Tab. 2. The associated volume of fluid of all samples matches the target (25%) within the desired tolerance.

are documented in Tab. 2. The initial design in Fig. 6 consists of spherical occlusions occupying about 24% of the cavity. The volume of fluid therefore initially fills about 76% of the cavity, in violation of the volume constraint. This is because many more smaller inclusions are needed to recover the proper volume, which in turn would either dramatically increase the surface of the interfaces that needs be captured (and thus the number of mesh elements needed to maintain the numerical accuracy), or risk clogging the fluid path due to insufficient mesh refinement. As shown in the convergence history presented in Fig. 7, there is thus an initial transient during which the cost function, albeit low, has little physical meaning, as the constraint value is decreased up to the point where it reaches the target within the desired tolerance. Once the constraint is satisfied, the cost function adjusts until a feasible minimum is found, that corresponds to the almost straight pipe shown in Fig. 6, that closely resembles that in [58], but with vastly superior accuracy. To give a taste, the element size is about  $6 \times 10^{-4}$  at the interface and 0.01 in the fluid domain, with up to 40-50 elements distributed across a pipe diameter. In comparison, the problem in the aforementioned reference is tackled with a uniform grid made up of 162000 tetrahedral elements, hence an element size of about 0.0375, which is insufficient to claim accuracy of the numerical solutions since only 5-6 grid points can be distributed across a pipe diameter. Again, the method handles well the various topological changes occurring over the course of optimization, and all adapted meshes exhibit extremely stretched elements regardless of the interface complexity, that allow sharply representing the fluid and solid domains and accurately computing the fluid solutions during all stages of optimization.



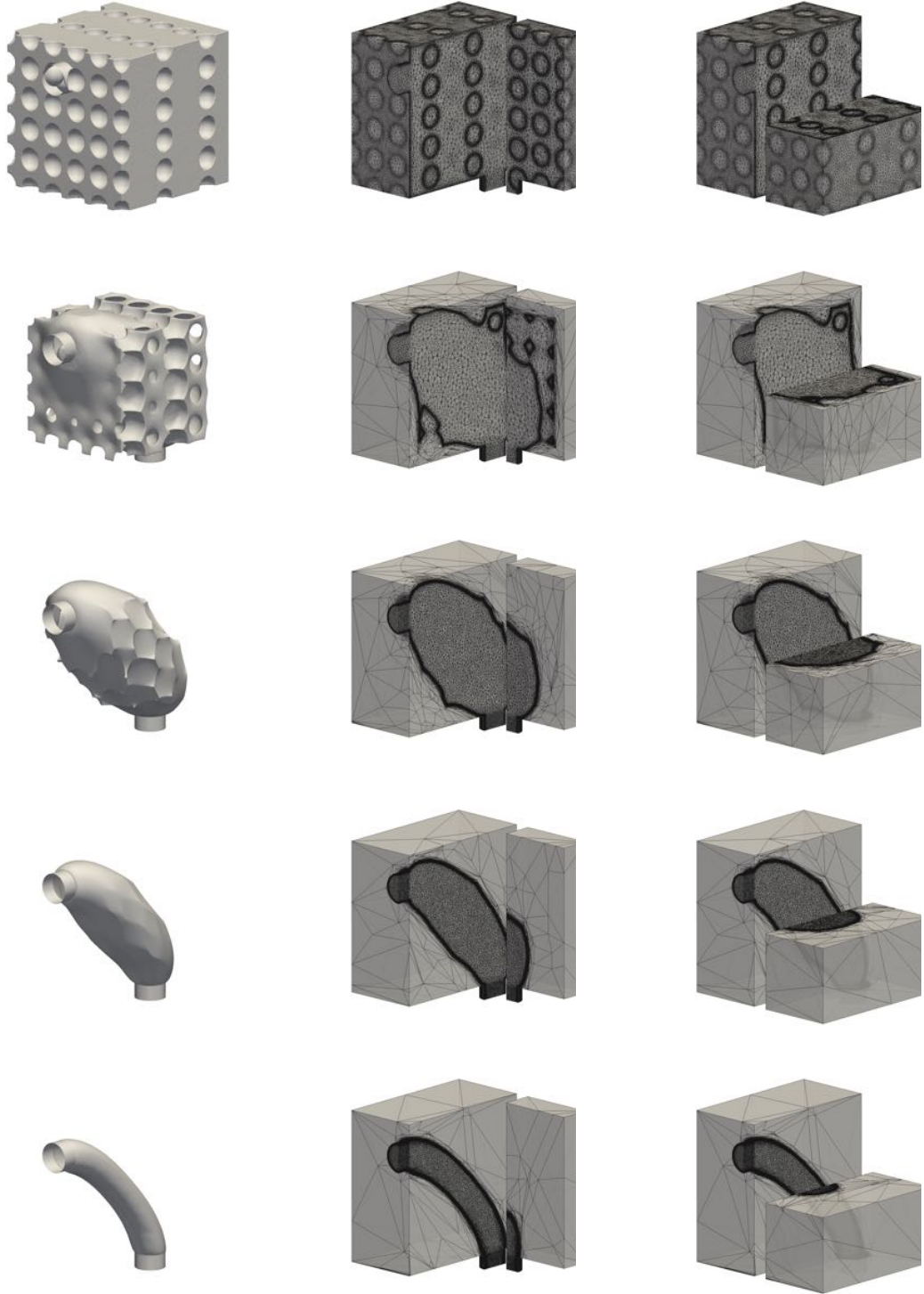


Figure 6: Optimization of the single inlet/single outlet duct flow presented in Fig. 4(a). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 1, 402, 548, 700 and 900 (from top to bottom) using the parameters given in Tab. 2. The associated volumes of fluid are 77.0%, 40.8%, 27.5%, 13.7% and 3.94%, respectively.



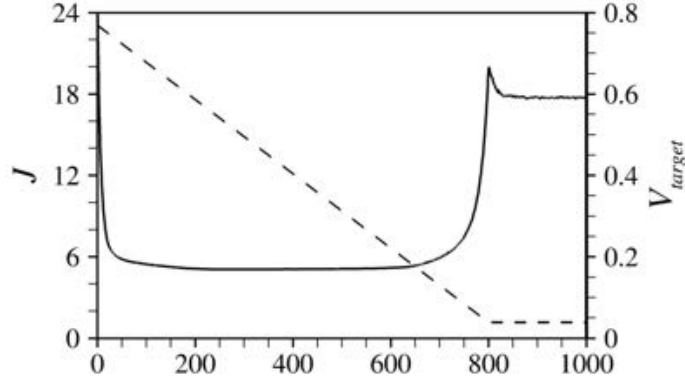


Figure 7: Convergence history for the 3-D bend pipe problem with 5M elements. All cost function values made non dimensional using the inlet diameter and maximum inlet velocity (equivalently, using  $\rho v_i^3 e_i^2$  as reference cost functional value). The dashed line shows the decrease in the target volume.

### 7.1.3. Discussion

The parallel remeshing strategy for the 3-D case is illustrated in Fig. 8 showing for the same iterations already sampled in Fig. 6 the 64 submeshes generated by the graph/mesh partitioning/repartitioning algorithm, each shown by a different color and handled sequentially by a different processor. The various submeshes are initially uniformly distributed in the whole domain, due to the presence of the multiple solid occlusions. Nonetheless, they quickly reorganize to cover the vicinity of the interface, where the mesh refinement is maximum, with only a handful of submeshes needed to handle the coarse solid domains, meaning that the load is well balanced between the processors.

It is worth noticing that the large number of nodes used here is mostly useful during the early stage of optimization. This is because the surface of the interfaces (perimeter in two dimensions) that needs be captured is initially dramatically large to the many solid inclusions, then decreases substantially after the first dozens of iterations, as has been found computing the surface area

$$S_\varphi = \int_{\Omega} \delta_\epsilon(\varphi) dv, \quad (53)$$

where  $\delta_\epsilon$  is the Dirac function

$$\delta_\epsilon(\varphi) = \begin{cases} \frac{1}{2\epsilon} \left( 1 + \cos\left(\pi \frac{\varphi}{\epsilon}\right) \right) & \text{if } |\varphi| \leq \epsilon, \\ 0 & \text{if } |\varphi| > \epsilon, \end{cases} \quad (54)$$

smoothed with the same regularization parameter  $\epsilon$  as the Heaviside function (48). Also, the anisotropic mesh adaptation algorithm refines the mesh in hierarchical importance of the level set gradient. If new geometrical features associated with high gradients appear in the solution, the mesh is automatically coarsened in regions with lower gradient and refined near the newly emerging features. If the number of nodes is large, as has been the case so far, the decrease in the interface surface area allows resolving finer, more complex patterns without degrading the accuracy in other parts of the design domain, because the coarsened regions are actually over-resolved. This shows through the progressive mesh refinement in the fluid domain in Figs. 5 and 6 as more and more elements become available to improve the mesh in other regions of the domain.

### 7.2. Single inlet/multiple outlets duct flow

This section is devoted to a series of more complex duct flow problems with one inlet and multiple outlets. All cases are tackled with boundary normal, parabolic velocity profiles prescribed at the inlets and the outlets, with outlet centerline velocities adjusted for the the total amount of mass flow exiting through the outlets to match exactly that entering through the inlet. The objective for doing so is twofold: first, it forces the inlet to connect to all the outlets, and thereby

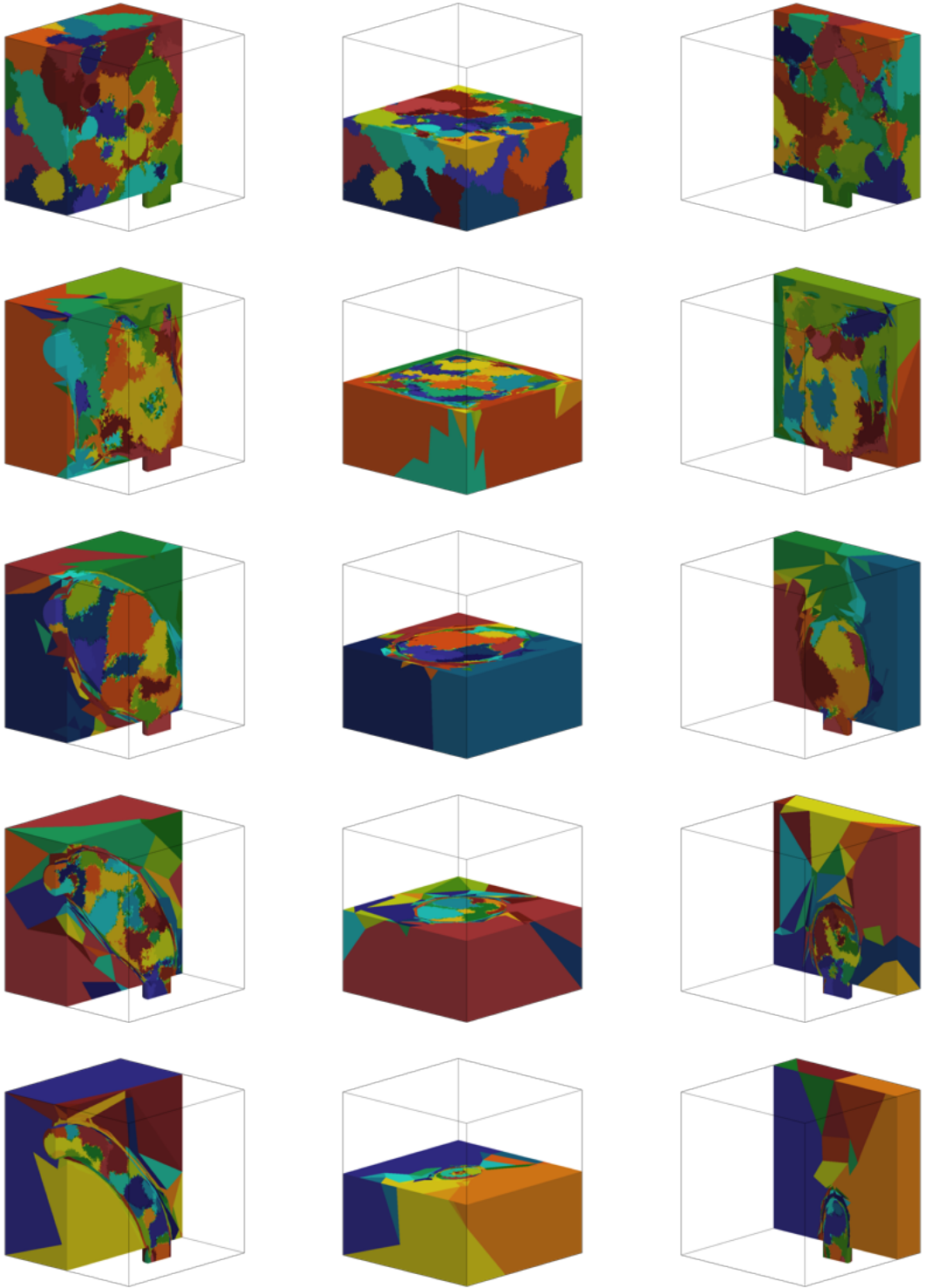


Figure 8: Illustration of mesh partitioning for the three dimensional, single inlet/single outlet duct flow. The colors in these plots represent the 64 subdomains generated by the graph/mesh partitioning/repartitioning for the same iterations sampled in Fig. 6.

660 emphasizes the ability of the numerical framework to engineer complex designs, as a more natural  
 661 zero pressure/viscous stress condition may allow the flow to exit via a single outlet to save the  
 662 cost of pipe splitting. Second, it reduces the computational cost, as the possibility of having


		
$\Omega = [0; 1] \times [0; 1] \times [0; 1]$	$[0; 2] \times [0; 1] \times [0; 0.5]$	Design domain
$d = 3$	3	Problem dimensionality
$V_{target} = 0.15$	0.10	Target volume of fluid
$V_{\varphi,0} = 0.76$	0.37	Initial volume of fluid
$Re = 2$	2	Reynolds number
$u_i = 0.2$	0.2	Inlet centerline velocity
$e_i = 0.4$	0.2	Inlet diameter
$l_i = 0.1$	0.2	Inlet leads length
$\mathbf{x}_i = (-0.1, 0.5, 0.5)$	$(1, 1.2, 0.25)$	Inlet center coordinates
$u_{o1} = 0.8$	0.6667	Outlet 1 centerline velocity
$u_{o2} = 0.8$	0.6667	Outlet 2 centerline velocity
$u_{o3} = 0.8$	0.3333	Outlet 3 centerline velocity
$u_{o4} = 0.8$	0.3333	Outlet 4 centerline velocity
$e_o = 0.1$	0.2	Outlet diameter
$l_o = 0.05$	0.2	Outlet leads length
$\mathbf{x}_{o1} = (0.75, 0.5, -0.05)$	$(-0.2, 0.5, 0.25)$	Outlet 1 center coordinates
$\mathbf{x}_{o2} = (0.75, 0.5, 1.05)$	$(2.2, 0.5, 0.25)$	Outlet 2 center coordinates
$\mathbf{x}_{o3} = (0.75, -0.05, 0.5)$	$(0.5, -0.2, 0.25)$	Outlet 3 center coordinates
$\mathbf{x}_{o4} = (0.75, 1.05, 0.5)$	$(1.5, -0.2, 0.25)$	Outlet 4 center coordinates
$N_n = 1M$	$\gg$	Nb. mesh nodes
$N_{el} = 5M$	$\gg$	Nb. mesh elements

Table 3: Numerical parameters for the single inlet/multiple outlets duct flow problems.

different number of pipes connect to an outlet may give existence to multiple local minimizers, whose basin of attraction can slow down the convergence; see for instance Ref. [59] for an example of competition between the single and double-ended wrench minimizers to the 2-D double pipe problem. In practice, our literature review did not reveal any study tackling multiple outlets 3-D topology optimization problems with zero pressure/viscous stress or zero stress conditions, except for a few cases in Ref. [24] adding mass flow rate constraints to the Lagrangian to similarly force the flow to exit via all outlets.

For the first example whose setup is shown in Fig. 4(b), the design domain is a cubic cavity of unit length, that has one inlet on the left side and four identical outlets at the top/bottom and on the front/back sides, each having 1/4 of the fluid flow entering through the inlet. For the second example whose setup is presented in Fig. 4(c), the design domain is a cuboid cavity of unit height and aspect ratio 2:1:0.5, that has one inlet at the top, and four identical outlets: two on the left and right sides, each having 1/3 of the fluid flow entering through the inlet, and two at the bottom, each having 1/6 of the inflow. Both domains have two reflectional symmetries with respect to the two inlet/outlet planes, but are discretized in their entirety using 5M mesh elements. For the first case, the initial design in Fig. 9 is made up of spherical solid occlusions occupying about 24% of the cavity. For the second case, we take advantage of the fact that all inlet and outlets are in the same plane and initialize the design with cylindrical solid occlusions filling about 63% of the cavity. The volume of fluid in each case is thus initially about 76% (first case) and 37% (second case), and decreases over the course of optimization until it reaches the target within the desired tolerance. The latter is set low to 15% in the first case, and 10% in the second case, to avoid trivial solutions and promote the formation of separate fluid channels.

For both cases, the optimization goes through several complex stages all accurately represented on anisotropic adapted meshes, as evidenced by the selected samples shown in Figs. 9-10. Similarly to what could be observed in the bend case, all mesh elements are coarse and regular away from the interface but fine and elongated on either side of the interface, to allow accurately representing

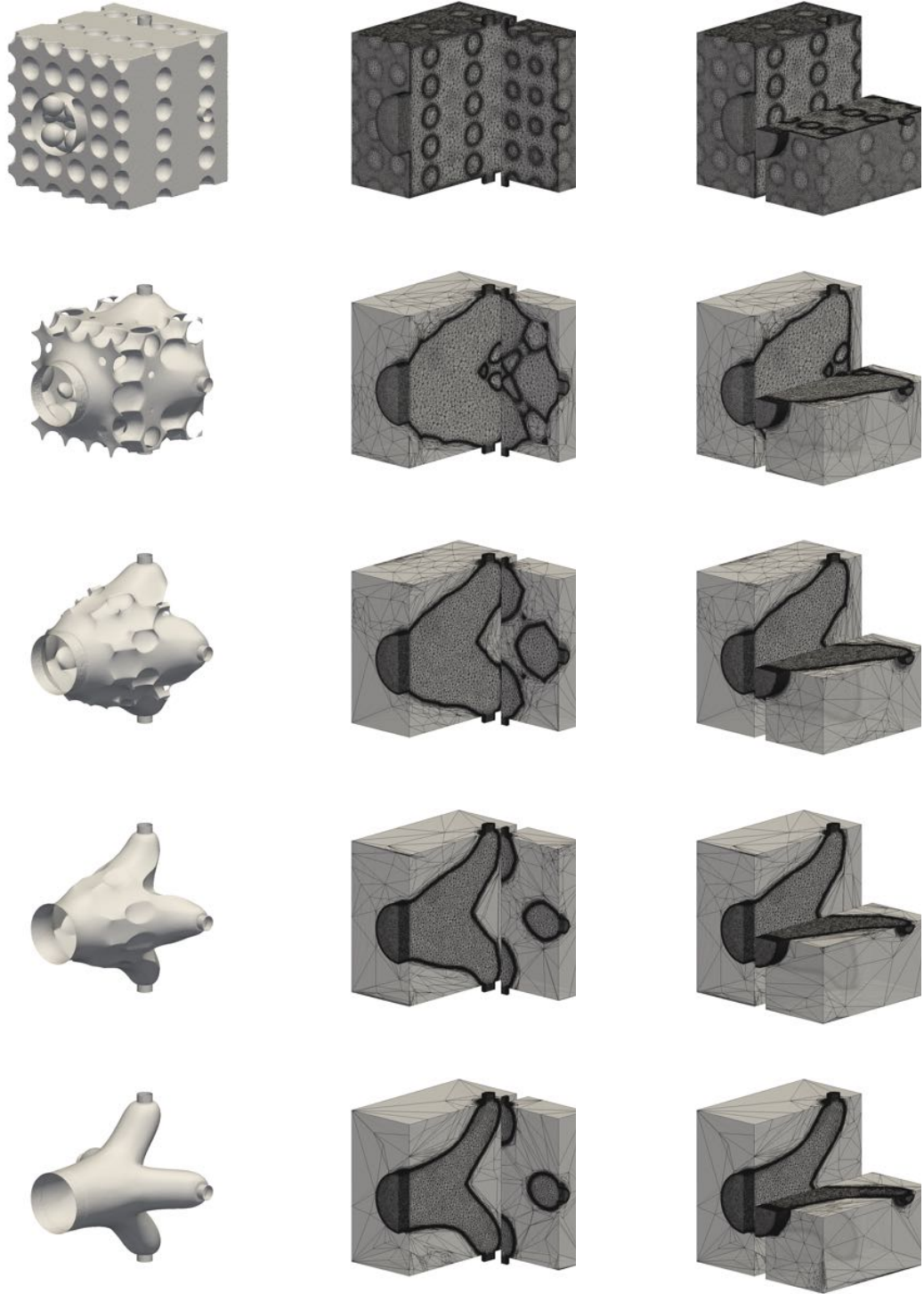


Figure 9: Optimization of the single inlet/multiple outlet duct flow presented in Fig. 4(b). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 1, 505, 624, 750 and 1050 (from top to bottom) using the parameters given in Tab. 3. The associated volumes of fluid are 75.6%, 37.8%, 28.9%, 19.5% and 15.0%, respectively.

the boundary layers regardless of topology complexity, even in the leads. The optimal duct for the first case is a wide pipe splitting at mid length into four identical, thinner pipes, each connecting to an outlet. This layout stands as the better trade-off between transporting fluid the shortest

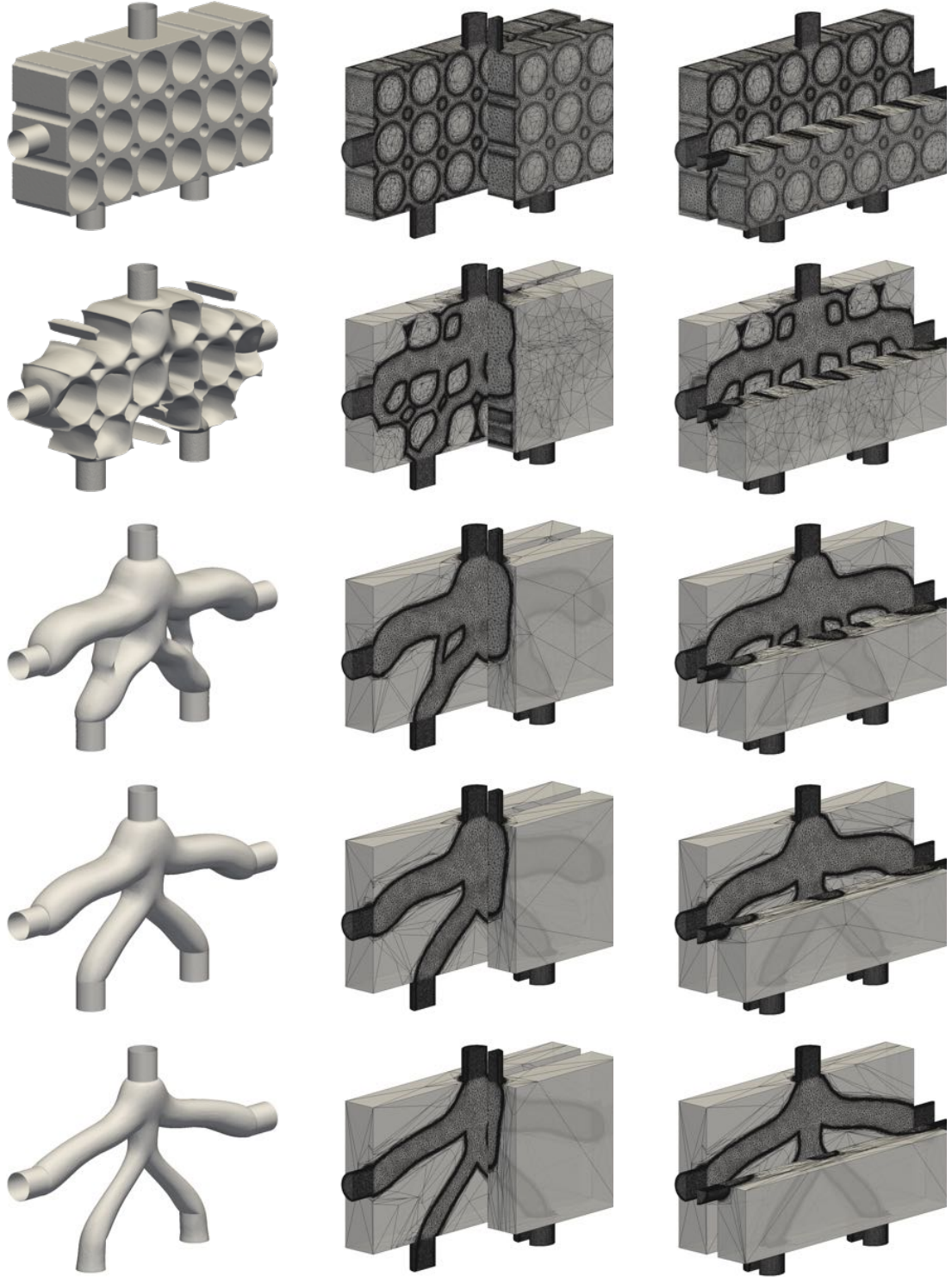
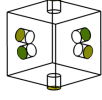


Figure 10: Optimization of the single inlet/multiple outlet duct flow presented in Fig. 4(c). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 1, 60, 110, 180 and 300 (from top to bottom) using the parameters given in Tab. 3. The associated volumes of fluid are 36.2%, 30.0%, 24.8%, 17.5% and 9.9%, respectively.

way, and transporting it in the widest possible pipe, and is consistent with the results documented in [58], although the optimal shapes therein exhibit quality issues (staircase effects) and anisotropic





$\Omega = [0; 1] \times [0; 1] \times [0; 1]$	Design domain
$d = 3$	Problem dimensionality
$V_{target} = 0.05$	Target volume of fluid
$V_{\varphi,0} = 0.73$	Initial volume of fluid
$Re = 2$	Reynolds number
$u_{i1} = 0.2$	Inlet 1 centerline velocity
$u_{i2} = 0.2$	Inlet 2 centerline velocity
$e_i = 0.2$	Inlet diameter
$l_i = 0.2$	Inlet leads length
$\mathbf{x}_{i1} = (-0.2, 0.5, 0.5)$	Inlet 1 center coordinates
$\mathbf{x}_{i2} = (1.2, 0.5, 0.5)$	Inlet 2 center coordinates
$u_{o1} = 0.1$	Outlet 1 centerline velocity
$u_{o2} = 0.1$	Outlet 2 centerline velocity
$u_{o3} = 0.1$	Outlet 3 centerline velocity
$u_{o4} = 0.1$	Outlet 4 centerline velocity
$e_o = 0.2$	Outlet diameter
$l_o = 0.2$	Outlet leads length
$\mathbf{x}_{o1} = (0.5, 0.5, -0.2)$	Outlet 1 center coordinates
$\mathbf{x}_{o2} = (0.5, 0.5, 1.2)$	Outlet 2 center coordinates
$\mathbf{x}_{o3} = (0.5, -0.2, 0.5)$	Outlet 3 center coordinates
$\mathbf{x}_{o4} = (0.5, 1.2, 0.5)$	Outlet 4 center coordinates
$N_n = \textcolor{red}{1M}$	Nb. mesh nodes
$N_{el} = \textcolor{red}{5M}$	Nb. mesh elements

Table 4: Numerical parameters for the multiple inlet/multiple outlets duct flow problem.

mesh adaptation represents a tremendous improvement in this regards. For the second case, the optimal duct comprises a wide pipe immediately splitting into three pipes: two symmetrical pipes connecting to the lateral outlets, and a central pipe quickly splitting into two symmetrical pipes connecting to the bottom outlets. All pipes are reasonably straight, and the lateral pipes are wider than their bottom counterparts. This is because most of the flow exits through the left/right outlets and optimal pipes at low Reynolds numbers are preferably short and wide, as splitting the fluid stream further away from the inlet **would** require complex bending patterns to connect the outlets, which in turn **would** increase the transport distance and **would thus be** detrimental in terms of cost function.

### 7.3. Multiple inlets/multiple outlets duct flow

In this example, the focus is on a duct flow problem with multiple inlet and outlets, whose setup is shown in Fig. 4(d). The design domain has two identical inlets on the left and right sides, and four identical outlets on all other sides, hence three reflectional symmetries with respect to the outlet and the two inlet/outlet planes. Parabolic inflow/outflow conditions are formulated in the same way as above, with outflow velocities adjusted for each outlet to have 1/4 of the fluid flow entering through the inlets. The entire cavity is discretized using **5M** mesh elements. The initial design in Fig. 11 consists of spherical occlusions occupying about 27% of the cavity, after which the volume of fluid is progressively decreased, starting at 73% of the cavity, **down** until it reaches a 5% target within the desired tolerance. The optimization documented in Fig. 11 occurs within two different steps, all involving **crisp** interfaces represented on extremely stretched mesh elements: first, the design looks to be converging to a series of 8 straight pipes connecting each inlet to all four outlets, a duct arrangement that has the same reflectional symmetries as the design domain. This agrees well with the optimal documented in [24] while resembling conceptually the 2-D results

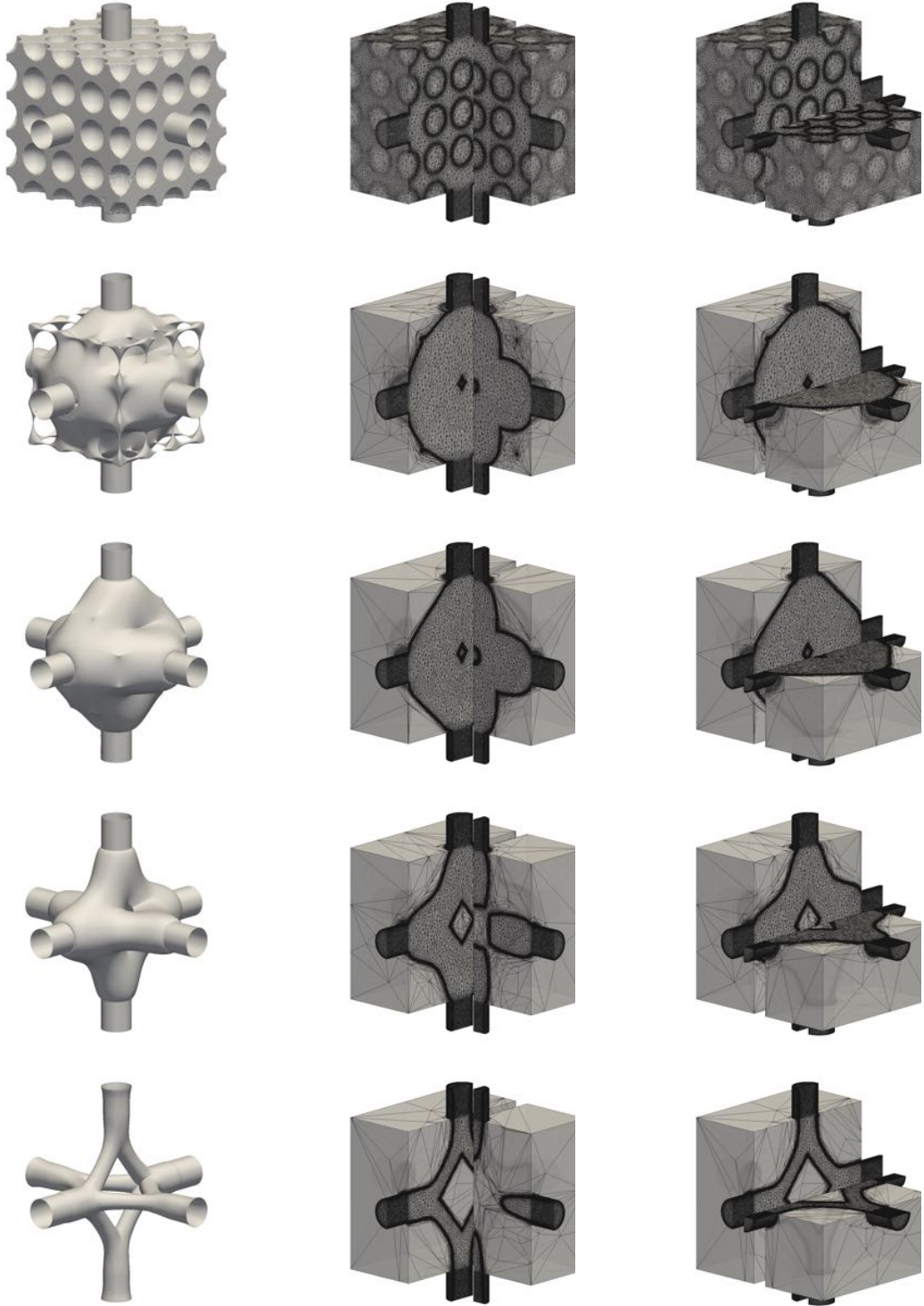


Figure 11: Optimization of the multiple inlet/multiple outlet duct flow presented in Fig. 4(d). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 1, 201, 283, 400 and 550 (from top to bottom) using the parameters given in Tab. 2. The associated volumes of fluid are 72.8%, 45.9%, 34.8%, 18.9% and 4.9%, respectively.

from [60]. Nonetheless, this turns to be only a local minimizer, as we show in Fig. 12 that the optimization carries on under constant volume of fluid, and progressively wipes off 4 out of the 8 pipes, for the optimal duct to ultimately consist of 4 straight but wider pipes connecting each inlet



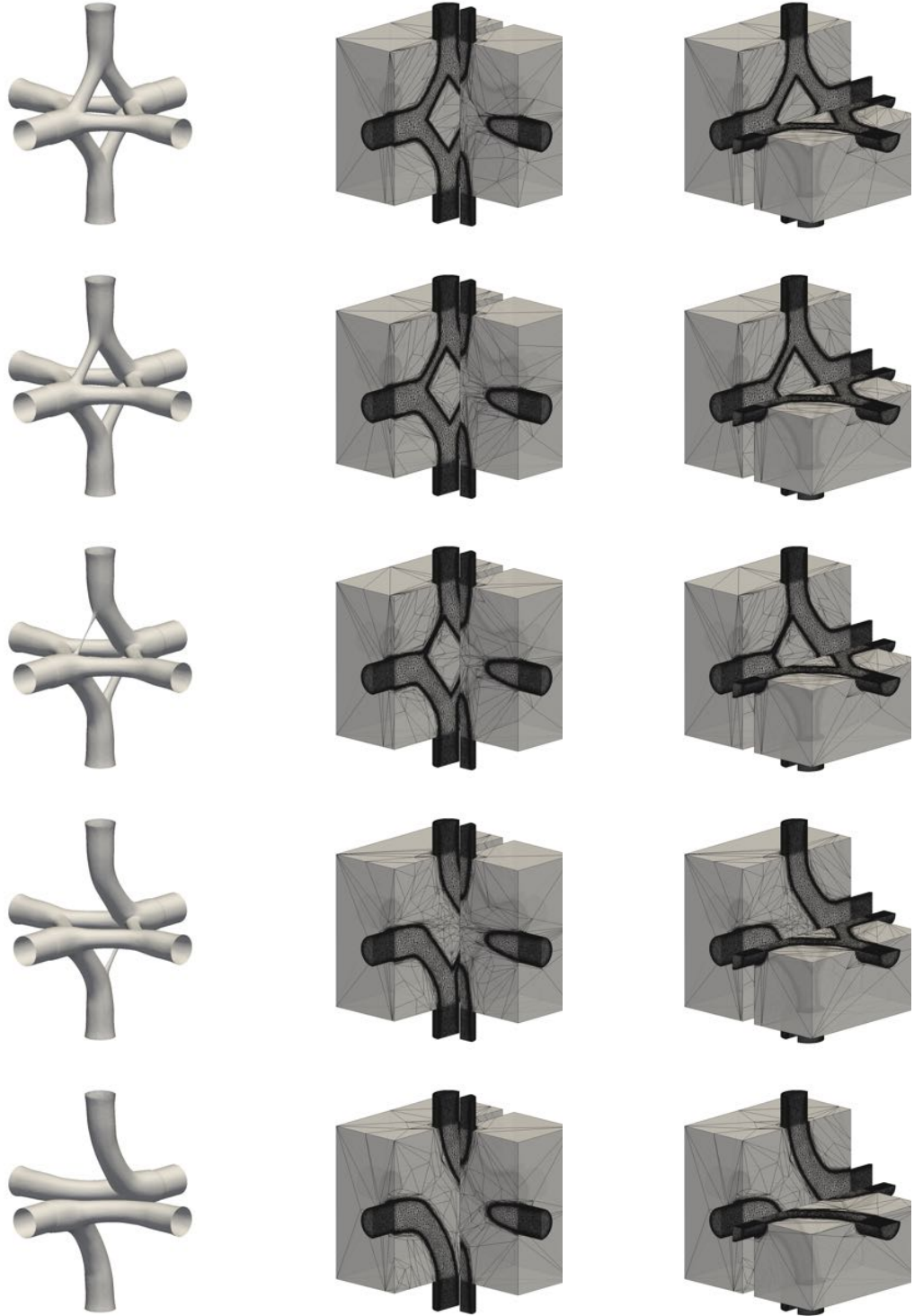


Figure 12: Optimization of the multiple inlet/multiple outlet duct flow presented in Fig. 4(d). The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 700, 800, 830, 850 and 1000 (from top to bottom) using the parameters given in Tab. 2. The associated volume of fluid of all samples matches the target (5%) within the desired tolerance.

720 to two outlets two-by-two perpendicular to one another (the whole arrangement being symmetric  
 721 with respect to one of the bisector planes). This stresses the importance of performing full-scale  
 722 optimization, as the cost function of the asymmetric design is noticeably lower (by almost 30%),

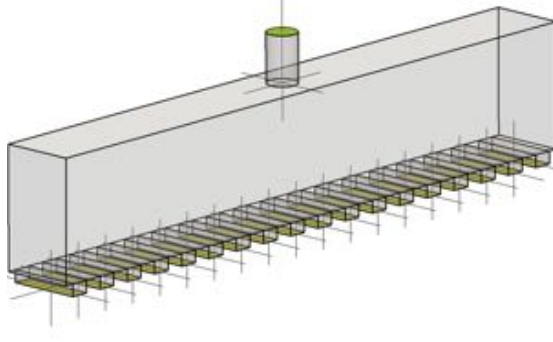
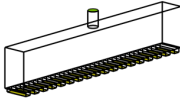


Figure 13: Problem set-up for the simplified plate fin heat exchangers (PFHE) case study.



$\Omega = [0; 2.7] \times [0; 0.7] \times [0; 0.3]$	Design domain
$d = 3$	Problem dimensionality
$V_{target} = 0.10$	Target volume of fluid
$V_{\varphi,0} = 0.20$	Initial volume of fluid
$Re = 4$	Reynolds number
$u_{i1} = 0.4$	Inlet centerline velocity
$e_i = 0.12$	Inlet diameter
$l_i = 0.2$	Inlet leads length
$\mathbf{x}_{i1} = (1.35, 0.7, 0.15)$	Inlet center coordinates
$u_{ok} = 0.00591$	Outlet $k$ centerline velocity
$e_o = (0.075; 0.3)$	Outlet width
$l_o = 0.05$	Outlet leads length
$\mathbf{x}_{ok} = (0.075 + 0.15k, 0.35, 0.15)$	Outlet $k$ center coordinates
$N_n = 1M$	Nb. mesh nodes
$N_{el} = 5M$	Nb. mesh elements

Table 5: Numerical parameters for the plate fin heat exchanger distributor problem.

and relying on simple problem symmetries to reduce the cost can thus yield suboptimal results; see [24] where only 1/8 of the cavity is simulated.

#### 7.4. Application to a simplified industrial case study

In this section, we consider application of the numerical framework to an engineering problem of practical interest. The focus is on plate fin heat exchangers (PFHE), a specific type of compact, lightweight heat exchangers widely used in air conditioning and petro-chemical industries (also in railway engines and motor cars). Most PFHEs consist of layers of plates with the space between two adjacent plates forming the channel in which the hot fluid flows through. Fins are placed between the flat plates to both hold the plates together, and form a secondary surface for heat transfer. We leave aside here the question of heat transfer, and assess the ability of our numerical framework to minimize the total pressure drop in a design domain representative of the refrigerant distributor of a heat exchanger comprising multiple outlet orifices. Only the distributor section is modeled numerically. The design domain is the cuboid of height 0.5 and aspect ratio 2.7:0.5:0.3 shown in Fig. 13, that has one cylindrical inlet at the top, and 18 rectangular outlets at the bottom, each of which is the entry section into one of the 18 plates and has 1/18 of the fluid flow entering through the inlet. In return, there is no need to model either the fins or the hot fluid, since the latter flows orthogonally between the plates. Parabolic velocity profiles are prescribed



Figure 14: Optimization of the plate fin heat exchanger distributor presented in Fig. 13. The zero iso-value of the level set function and associated anisotropic adapted meshes are sampled at intermediate iterations 1, 80, 120, 200 and 400 (from top to bottom) using the parameters given in Tab. 2. The associated volumes of fluid are 50%, 39.2%, 34.6%, 25.4% and 24.9%, respectively.

740 at the inlets and the outlets, with the outflow distribution in each outlet section defined as the  
741 Cartesian product of parabolic variations along the two lines of symmetry, which stands as a  
742 first approximation of the series-based, theoretical velocity profile of flow through a channel of

rectangular cross-section [61]. The entire domain is meshed with 5M elements, with the remaining parameters given in Table 5. Due to the cavity low aspect ratio in the third dimension, the initial design is initialized with cylindrical solid occlusions occupying about 65% of the cavity, and the volume of fluid is progressively decreased until it reaches the target within the desired tolerance. This yields the optimal duct shown in Fig. 14, that delivers most of the fluid in the center area of the cavity before distributing it to the plates via the comb-like structure at the bottom, and showcases the potential of the method for smooth, lightweight heat exchanger solutions.

### 7.5. Discussion

This last section is dedicated to discussing the numerical cost of the presented approach. Figure 15(a) presents detailed timing results obtained by averaging (and normalizing to achieve unit average time per iteration) dedicated update steps performed on 64 cores (150 steps in 2-D, 50 steps in 3-D). In 2-D, the cost of an iteration is dominated by that of computing the state solution (about 10 Navier–Stokes iterations representing 50% of the total cost, which can be scaled down substantially in the context of steady-state problems using an iterative Newton-like method), and otherwise by that of adapting the mesh (about 30% of the total cost). Using the same number of processors, the cost of a 3-D iteration is larger than its 2-D counterpart by roughly three orders of magnitude, the cost of which is essentially that of the two passes of mesh adaptation (about a cumulative 75% of the total cost, although the cost of the first pass is twice as large as that of the second pass, since (i) the volume constraint is not applied at each design step, only when the difference between the actual and target volumes exceeds the 5% tolerance, and (ii) less elements and nodes need to be moved and migrated across processors. Meanwhile, the cost of both geometrically reinitializing the signed distance function level set and of optimizing the volume constraint offset is very affordable, as it represents less than 4% in total, with 4-5 dichotomy iterations needed to reach the desired accuracy. The timing results reported in Figs. 15(c-f) show that the same conclusions carry over when applying the method to the other multiple inlet/outlet duct flows tackled herein, including the more complicated, practical PFHE case in Sec. 7.4. The only difference is in the cost of the volume constraint step, as the frequency at which consecutive corrections are applied indirectly depends on the number of design steps taken to reach the target volume. This gives hope that the observed trends may carry over to any other problem of same dimensionality, tackled with comparable parameters.

The associated absolute run times per iteration shown in Fig 16 are seen to be very consistent, in the sense that they change little from case to case. In return, the total run times reported in Tab. 6 are entirely driven by the number of design steps needed to converge. Here, the reported cost is essentially that of recovering the proper volume of fluid, as fulfilling the proper volume constraint from the outset requires a larger number of smaller solid inclusions, which would either dramatically increase the surface of the interfaces that needs be captured (and thus the number of mesh elements needed to maintain the numerical accuracy), or risk clogging the fluid path due to insufficient mesh refinement. Because the single inlet/multiple outlet duct flow presented in Fig. 4(d) and the plate fin heat exchanger distributor presented in Fig. 13 all rely on cylindrical, not spherical inclusions, their run time benefits from a lower initial volume of fluid (in the range between 35 and 50%, while all other case start above 75%), which speeds up the process of meeting the desired target volume. Once this has been done, all cases converge within about 200 iterations (about 60h of resolution time, a similar run time being achieved when initializing the single inlet/single outlet test case with a quarter torus fitting exactly to the inlet and outlet). The only exception is the multiple inlet/multiple outlet duct flow presented in Fig. 4(d), as an extra 300 iterations are needed to bypass the basin of attraction of the symmetric local minimizer and reach the asymmetric global minimizer. The reported run times, while large in a vacuum, are actually much lower than those that required to converge on a fixed uniform grid with similar mesh refinement. To give a taste, discretizing the single inlet/single outlet case with a uniform element size of  $5 \times 10^{-3}$  would require about 70M elements, even though the interface value achieved here is one order of magnitude smaller. It is also worth emphasizing in this regards that we did not seek to optimize efficiency, neither by adjusting the initial design (we actually used numerous inclusions on purpose to showcase the ability of the method to support complex topological changes), nor by fine tuning the descent factor (the only requirement being that the displacement achieved at each step must be below the cut-off thickness of the level set for the evolved interface to remain accurately tracked).

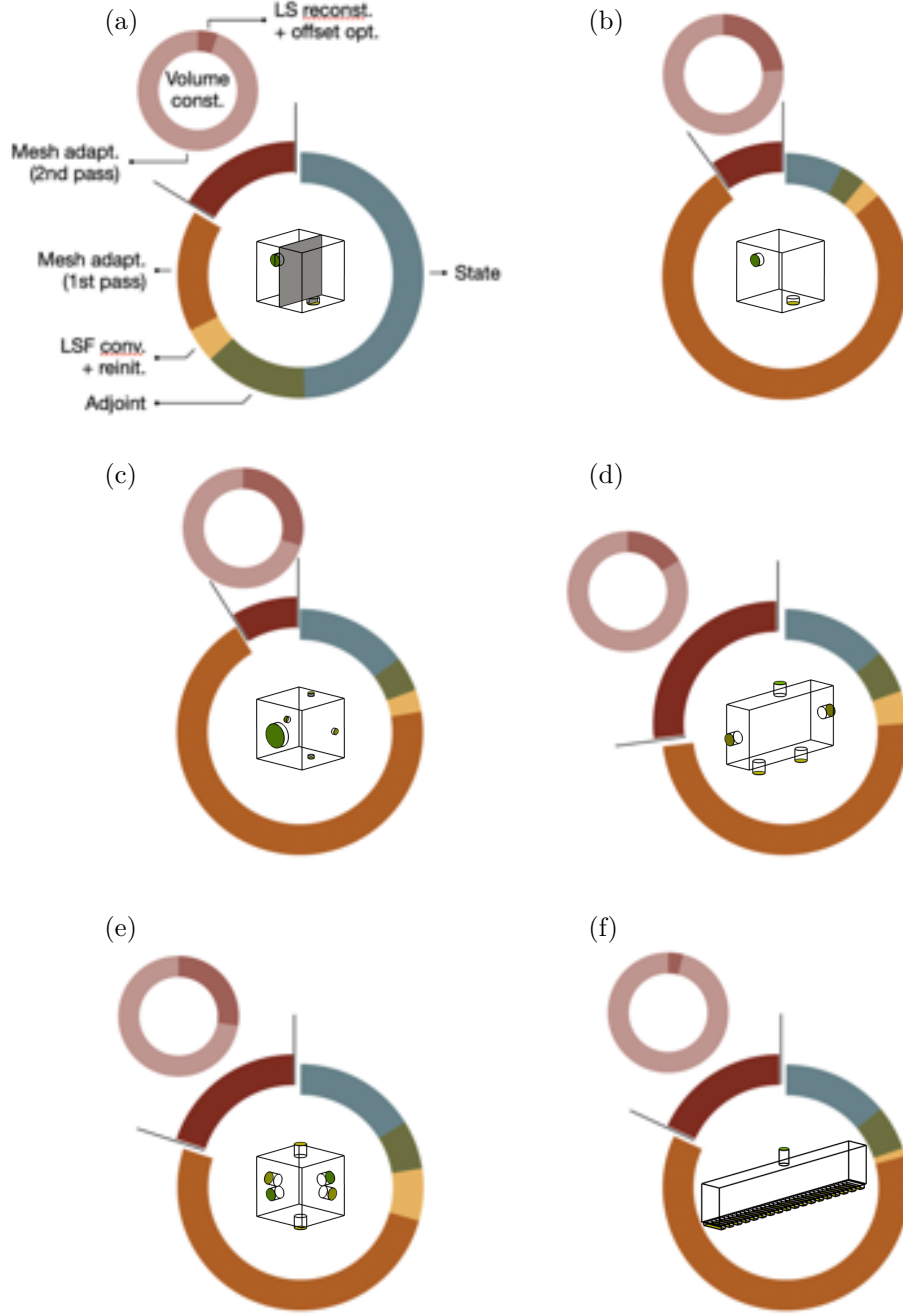


Figure 15: (a) Computational cost of the implemented algorithm, as obtained averaging 150 update steps of the 2-D single inlet/single duct flow presented in Fig. 4(a). (b) Same as (a) for 50 update steps of the 3-D single inlet/single duct flow presented in Fig. 4(a). (c-f) Same as (b) for the (c) single inlet/multiple outlet duct flow presented in Fig. 4(b), (d) single inlet/multiple outlet duct flow presented in Fig. 4(c), (e) multiple inlet/multiple outlet duct flow presented in Fig. 4(d), and (f) plate fin heat exchanger distributor presented in Fig. 13. All simulation parameters are those provided in Tabs. 15. The LS and LSF labels stand for level set (LS) and filtered level set (LSF), respectively.

## 8. Conclusion

The present study performs topology optimization of large-scale, three-dimensional Navier–Stokes flows using anisotropic meshes adapted under the constraint of a fixed number of nodes. The proposed approach combines a level set method to represent the boundary of the fluid domain by the zero iso-value of a signed distance function, and stabilized formulations of the state, adjoint, and level set transport equations cast in the Variational Multiscale (VMS) framework. The method

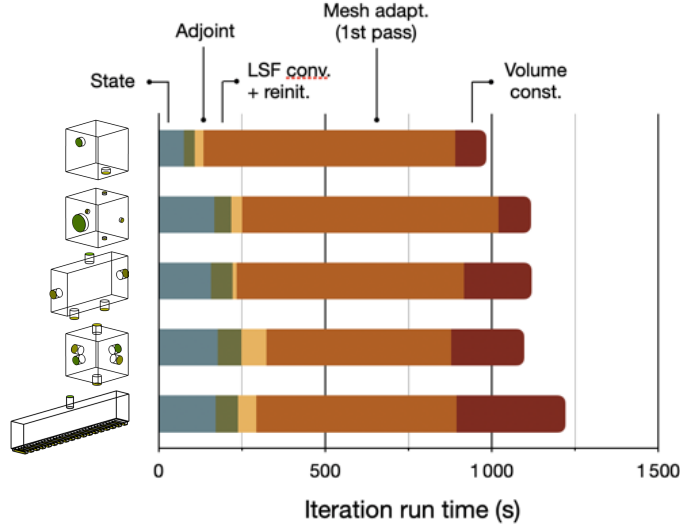


Figure 16: Average run time per iteration for the various cases documented in Fig. 15

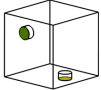

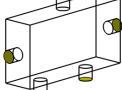
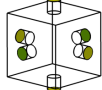
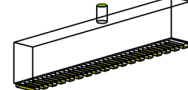
					
64	»	»	»	»	Nb. cores
290h	340h	150h	330h	170h	Run time
1000	1000	500	1000	400	Nb. design steps
800	800	200	500	250	Nb. steps to target volume

Table 6: Run times for the various cases documented in Fig. 15

has been shown to allow for drastic topology changes during the optimization process. Nonetheless, the main advantage over existing methods is the ability to capture all interfaces to a very high degree of accuracy using adapted meshes whose anisotropy matches that of the numerical solutions. Also, the retained approach considerably decreases the cost of improving the numerical precision, as the number of nodes needs be increased only in the anisotropy direction, hence only 2 times as many nodes are required to improve the resolution by a factor of 2, while 8 times as many nodes are required in classical isotropic 3-D calculations. This gives hope that the method can ease the transition to manufacturable CAD models that closely resemble the optimal topology.

The method has been tested on several large-scale examples of power dissipation minimization involving several dozen million state degrees of freedom. The obtained optimal designs agree well with the existing literature, which assesses the relevance of the present implementation for designing complex fluidic devices. This is further illustrated by a simplified (in terms of flow regime) industrial case aimed at optimizing the distributor section of a fin plate heat exchanger. All cases considered converge within a few hundred iterations, with detailed computational efficiency data showing that the computational time in large-scale 3-D problems is dominated by the meshing/remeshing steps. It is worth emphasizing in this regards that we did not seek to optimize efficiency, neither by adjusting the initial design, nor by fine tuning the descent factor, the only requirement being that the displacement achieved at each step must be below the cut-off thickness of the level set for the evolved interface to remain accurately tracked. Here, the reported cost is essentially that of recovering the proper volume of fluid, as fulfilling the proper volume constraint from the outset requires a larger number of smaller solid inclusions, which would either dramatically increase the surface of the interfaces that needs be captured (and thus the number of mesh elements needed to maintain the numerical accuracy), or risk clogging the fluid path due to insufficient mesh refinement. Future work should include application to real life, multiphysics problems (e.g., heat transfer of



multiphase flows), as well as the extension to transient and turbulent problems. Evaluating multi-component adaptation criteria taking into account the difference in the spatial supports of the state and adjoint solutions is also of primary interest to further improve the accuracy of the gradient evaluations.

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