Fireshape: a shape optimization toolbox for Firedrake

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Abstract We introduce Fireshape, an open-source and automated shape optimization toolbox for the finite element software Firedrake. Fireshape is based on the moving mesh method and allows users with minimal shape optimization knowledge to tackle with ease challenging shape optimization problems constrained to partial differential equations (PDEs).

1 Introduction

One of the ultimate goals of structural optimization is the development of fully automated software that allows users to tackle challenging structural optimization problems in the automotive, naval, and aerospace industries without requiring deep knowledge of structural optimization theory. The scientific community is working actively in this direction, and recent years have seen the publication of educational material that simplifies the understanding of structural optimization algorithms and guides the development of related optimization software. These resources are based on different models, such as moving mesh methods [3,5,16,18], level-sets [4,41], phase fields [29], and SIMP [11,53,54], and are implemented in various software environments such as Matlab [53,54], FreeFem++ [1,5,18], OpenFOAM CFD [16], FEMLAB [43], and FEniCS [21,41], to mention just a few.

In this work, we introduce Fireshape: an automated shape optimization library based on the moving meshes approach that requires very limited input from the user. Shape optimization refers to the optimization of domain boundaries and plays an important role in structural design. For instance, shape optimization plays a crucial role in the design of airfoils [33,51,55] and boat hulls [1,44,46]. Shape optimization is also a useful refinement step to be employed after topology optimization [11, Ch. 1.4]. Indeed, topology optimization allows more flexibility in geometric changes and it is a powerful tool to explore a large design space. However, topology optimization usually provides slightly blurred (grey-scale) and/or staircase designs [11]. By adding a final shape optimization step, it is possible to post-process results computed with topology optimization and devise optimal designs with sharp boundaries and interfaces.

Fireshape is based on the moving meshes shape optimization approach [3, Ch. 6]. In this approach, geometries are parametrized with meshes that can be arbitrarily precise and possibly curvilinear. The mesh nodes and faces are then optimized (or “moved”) to minimize a chosen target function. The moving meshes approach is only one among several possible shape models, such as phase-fieIds [13,29], level-sets [4,12,41], and SIMP [10,11,53,54], and each model comes with advantages and disadvantages. Fireshape has been developed on the moving meshes approach because the latter has a very neat interpretation in terms of geometric transformations and is inherently compatible with standard finite element software [49]. The main drawback of the moving meshes approach is that it does not allow topological changes in a straightforward and consistent fashion. However, Fireshape has been developed
to facilitate shape optimization, and topology optimization is beyond its scope.

Fireshape couples the finite element library Firedrake \cite{31,36,37,45,50,20} with the Rapid Optimization Library (ROL) \cite{20}. Fireshape allows decoupled discretization of geometries and state constraints and it includes all necessary routines to perform shape optimization (geometry updates, regularization terms, geometric constraints, etc.). To solve a shape optimization problem in Fireshape, users must describe the objective function and the eventual constraints using the Unified Form Language (UFL) \cite{6}, a Python-based scripting language that is very similar to standard mathematical notation. Once objective functions and constraints have been implemented with UFL, users need only to provide a mesh that describes the initial design and, finally, select their favorite optimization algorithm from the optimization library ROL.

Typically the bottleneck of PDE constrained optimization code lies in the solution of the state and the adjoint equation. While Fireshape and Firedrake are both written in Python, to assemble the state and adjoint equations the Firedrake library automatically generates optimized kernels in the programming language C. The generated systems of equations are then passed to the PETSc library (also in written in C) and can be solved using any of the many linear solver and preconditioners provided by PETSc \cite{7,8,14,17,42}. This combination of Python for user facing code and C for performance critical parts is well established in scientific computing as it provides highly performant code that is straightforward to develop and use. Finally, we mention that Fireshape, just as Firedrake, PETSc and ROL, supports MPI parallelization and hence can be used to solve even large scale three dimensional shape optimization problems.

Fireshape is an open-source software licensed under the GNU Lesser General Public License v3.0. Fireshape can be downloaded at \url{https://github.com/Fireshape/Fireshape}. Its documentation contains several tutorials and is available at \url{https://fireshape.readthedocs.io/en/latest/}. To illustrate Fireshape’s capabilities and ease of use, in Section 2 we provide a tutorial and solve a three-dimensional shape optimization problem constrained to a nonlinear boundary value problem. The shape optimization knowledge required to understand this tutorial is minimal. In Section 3 we describe in detail the rich mathematical theory that underpins Fireshape. In Section 4 we describe Fireshape’s main classes and Fireshape’s extended functionality. Finally, in Section 5 we provide concluding remarks.

2 Example: Shape optimization of a pipe

For this hands-on introduction to Fireshape, we consider a viscous fluid flowing through a pipe $\Omega$ (see Figure 1) and aim to minimize the kinetic energy dissipation into heat by optimizing the design of $\Omega$. To begin with, we need to describe this optimization problem with a mathematical model.

We assume that the fluid velocity $u$ and the fluid pressure $p$ satisfy the incompressible Naver-Stokes equations \cite[Eqn. 8.1]{25}, which read

\begin{equation}
-2\nu \nabla \cdot \varepsilon u + \nabla p = 0 \quad \text{in } \Omega,
\end{equation}

\begin{equation}
\text{div } u = 0 \quad \text{in } \Omega,
\end{equation}

\begin{equation}
u u = g \quad \text{on } \partial \Omega \setminus \Gamma,
\end{equation}

\begin{equation}
p n - 2\nu \varepsilon u n = 0 \quad \text{on } \Gamma,
\end{equation}

where $\nu$ denotes the fluid viscosity, $\varepsilon u = \varepsilon(u) = \frac{1}{2} (\nabla u + \nabla u^\top)$, $\nabla u$ is the derivative (Jacobian matrix) of $u$ and $\nabla u^\top$ is the derivative transposed, $\Gamma$ denotes the outlet, and the function $g$ is a Poiseuille flow velocity \cite[p. 122]{25} at the inlet and is zero on the pipe walls. In our numerical experiment, the inlet is a disc of radius 0.5 in the $xy$-plane, and $g(x, y, z) = (0, 0, 1 - 4(x^2 + y^2))$ on the inlet.

To model the kinetic energy dissipation, we consider the diffusion term in (1a) and introduce the function

\begin{equation}
J(\Omega) = \int_{\Omega} \nu \varepsilon u : \varepsilon u \, dx,
\end{equation}

where the colon symbol : denotes the Frobenius inner product, that is, $\varepsilon u : \varepsilon u = \text{trace}(\varepsilon(u)^\top \varepsilon(u))$.

Now, we can formulate the shape optimizations problem we are considering. This reads:

Find $\Omega^*$ such that $J(\Omega^*) = \inf J(\Omega)$ subject to (1). (3)

To make this test case more interesting, we further impose a volume equality constraint on $\Omega$. Otherwise, the solution to this problem would be a pipe with arbitrarily large diameter.

In the next subsections, we explain step by step how to solve this shape optimization problem in Fireshape.

Fig. 1 Viscous fluid flows through a pipe $\Omega$ from the left to the right. A poor pipe design can lead to an excessive amount of kinetic energy being dissipated into heat.
To this end, we need to create: a mesh that approximates the initial guess Ω (Section 2.1), an object that describes the PDE-constraint (1) (Section 2.2), an object that describes the objective function (2) (Section 2.3), and, finally, a “main file” to set up and solve the optimization problem (3) (Section 2.4).

2.1 Step 1: Provide an initial guess

The first step is to provide a mesh that describes an initial guess of Ω. For this tutorial, we create this mesh using the software Gmsh [50]. The initial guess employed is sketched in Figure 1. For the geometric details, we refer to the code archived on Zenodo [58].

2.2 Step 2: Implement the PDE-constraint

The second step is to implement a finite element solver of the Navier-Stokes equations (1). To derive the weak formulation of (1a), we multiply Equation (1a) with a test (velocity) function \( v \) that vanishes on \( \partial \Omega \setminus \Gamma \), and Equation (1b) with a test (pressure) function \( q \). Then, we integrate over \( \Omega \), integrate by parts [25, Eq. 3.18], and impose the boundary condition (1d). The resulting weak formulation of equations (1) reads:

\[
\int_{\Omega} 2 \nu \varepsilon u : \varepsilon v - p \operatorname{div}(v) + v \cdot (\nabla u) u + q \operatorname{div}(u) \, dx = 0
\]

for any pair \((v, q)\).

To implement the finite element discretization of (4), we create a class `NavierStokesSolver` that inherits from the Fireshape’s class `PdeConstraint`, see Listing 1. To discretize (4), we employ P2-P1 Taylor-Hood finite elements, that is, we discretize the trial and test velocity functions \( u \) and \( v \) with piecewise quadratic Lagrangian finite elements, and the trial and test pressure functions \( p \) and \( q \) with piecewise affine Lagrangian finite elements. It is well known that this is a stable discretization of the incompressible Navier-Stokes equations [25, pp 136-137].

To address the nonlinearity in (4), we use PETSc’s Scalable Nonlinear Equations Solvers (SNES) [7-9, 14, 17, 42]. In each iteration, SNES linearizes Equation (4) and solves the resulting system with a direct solver. In general, it is possible that the SNES solver fails to converge sufficiently quickly (in our code, we allow at most 100 SENS iterations). For instance, this happens if the finite element mesh self-intersects, or if the initial guess used to solve (4) is not sufficiently good. Most often, these situations happen when the optimization algorithm takes an optimization step that is too large. In these cases, we can address SNES’ failure to solve (4) by reducing the optimization step. In practice, we deal with these situations with Python’s `try: ... except: ...` block. If the SNES solver fails with a `ConvergenceError`, we catch this error and set the boolean flag \texttt{self.failed\_to\_solve} to \texttt{True}. This flag
is used to adjust the output of the objective function J, see Section 2.3.

2.3 Step 3: Implement the objective function

The third step is to implement a code to evaluate the objective function J defined in Equation (2). For this, we create a class EnergyDissipation that inherits from Fireshape’s class ShapeObjective, see Listing 2. Of course, evaluating J requires access to the fluid velocity \( \mathbf{u} \). This access is implemented by assigning the variable self.pde_solver. This variable gives access also to the variable NavierStokesSolver.failed_to_solve, which can be used to control the output of J when the Navier-Stokes’ solver fails to converge. Here, we decide that the value of J is NaN (“not a number”) if the Navier-Stokes’ solver fails to converge.

```python
from firedrake import *
from fireshape import *
from PDEConstraint import NavierStokesSolver
import ROL
from PDEConstraint import energyDissipation
import numpy as np

class EnergyDissipation(ShapeObjective):
    """Kinetic energy dissipation."""
    def __init__(self, pde_solver: NavierStokesSolver, *args, **kwargs):
        super().__init__(*args, **kwargs)
        self.pde_solver = pde_solver

    def __call__(self):
        """Evaluate misfit functional."""
        nu = self.pde_solver.viscosity
        if self.pde_solver.failed_to_solve:
            return np.nan + dx(self.pde_solver.mesh.m)
        else:
            z = self.pde_solver.solution
            u, p = split(z)
            return nu * inner(sym(grad(u)), sym(grad(u)))
```

Lst. 2 Objective function J (2), which quantifies the kinetic energy dissipation of the fluid. Note that J returns NaN (“not a number”) if the solver of the PDE-constraint (4) fails to converge.

2.4 Final step: Set up and solve the problem

At this stage, we have all the necessary ingredients to tackle the shape optimization problem (3). The final step is to create a “main file” that loads the initial mesh, sets-up the optimization problem, and solves it with an optimization algorithm. The rest of this section contains a line-by-line description of the “main file”, which is listed in Listing 3.

```
from firedrake import *
from fireshape import *
import fireshape.zoo as fsz
import ROL
from PDEConstraint import NavierStokesSolver
from objective import energyDissipation

# setup problem
mesh = Mesh("pipe.msh")
bbox = [(-0.5, +0.5), (-0.5, +5.5), (2, 12)]
opt = [3, 3, 3]; levels = [2, 2, 4]
Q = B splineControlSpace(mesh, bbox, orders, levels,
    boundary_regularities=[0, 0, 2], fixed_dims=[0, 2])
q = ControlVector(Q, LaplaceInnerProduct(Q))

# create PDE-constrained objective functional
J = energyDissipation(e, Q, cb=cb)

# add regularization to improve mesh quality
Jq = fsz.MoYoSpectralConstraint(10, Constant(0.5), Q)
J = ReducedObjective(J, e)

# setup volume constraint
vol = fsz.VolumeFunctional(Q)
vol0 = vol.value(q, None)

# save state variable evolution in file u.pvd

# create PDE-constrained objective functional
J = ReducedObjective(J, e)

# add regularization to improve mesh quality
Jq = fsz.MoYoSpectralConstraint(10, Constant(0.5), Q)
J = ReducedObjective(J, e)

# Set up volume constraint
vol = fsz.VolumeFunctional(Q)
vol0 = vol.value(q, None)
C = EqualityConstraint([vol], target_value=[vol0])
M = ROL.StdVector(1)

# setup PDE constraint
viscosity = Constant(1/10.)
e = NavierStokesSolver(Q.mesh, viscosity)

# save state variable evolution in file u.pvd

# ROL parameters
params_dict = {
    'General': {'Secant': {'Type': 'Limited-Memory BFGS',
            'Maximum Storage': 20}},
    'Step': {'Type': 'Augmented Lagrangian',
            'Augmented Lagrangian': {
                'Subproblem Step Type': 'Trust Region',
                'Subproblem Iteration Limit': 50,
                'Penalty Parameter Growth Factor': 2}},
    'Status Test': {'Gradient Tolerance': 1e-2,
                    'Step Tolerance': 1e-2,
                    'Constraint Tolerance': 1e-2,
                    'Iteration Limit': 10}}

params = ROL.ParameterList(params_dict, "Parameters")
problem = ROL.OptimizationProblem(J, q, econ=M, emul=M)
solver = ROL.OptimizationSolver(problem, params)
solver.solve()
```

Lst. 3 Minimize the kinetic energy dissipation of a fluid using Fireshape.

- In lines 1-6, we import all necessary Python libraries and modules.
- In lines 8-13, we load the mesh of the initial design and we specify how to discretize the domain \( \Omega \) (see Sections 4.1 and 4.2 for more details about the Fireshape classes ControlSpace and InnerProduct).
- In lines 15-16, we initiate the Navier-Stokes’ finite element solver.
2.5 Results

Running the code contained in Listing 3 optimizes the pipe design when the fluid viscosity $\nu$ is 0.1, which corresponds to Reynolds-number $Re = 1/\nu = 10$. Of course, the resulting shape depends on the fluid viscosity. A natural question is how the optimized shape depends on this parameter. To answer this question, we can simply run Listing 3 for different Reynold-numbers (by modifying line 13 with the desired value) and inspect the results. Here we perform this comparison for $Re \in \{1, 250, 500, 750, 1000\}$.

In Figure 2, we show the initial design and plot the magnitude of the fluid velocity on a cross section of the pipe for different Reynold-numbers. In Figure 3, we show the resulting optimized shapes, and in Figure 4 the corresponding magnitudes of the fluid velocity. Qualitatively, we observe that, as the Reynolds-number increase, we obtain increasingly S-shaped designs that avoid high curvature at the two fixed ends. Finally, we remark that the objective is reduced by approximately 6.9\%, 9.5\%, 10.8\%, 11.7\% and 12.1\%, respectively.

3 Shape optimization via diffeomorphisms

In this section, we describe the theory that underpins Fireshape. We begin with a brief introduction to PDE-fails to converge. This modification is necessary to solve (4) at high Reynolds-numbers. The code used to obtain these results can be found at [58].
3.1 Optimization with PDE-constraints

The basic ingredients to formulate a PDE-constrained optimization problems are: a control variable $q$ that lives in a control space $Q$, a state variable $u$ that lives in a state space $U$, and that solves a (possibly nonlinear) state equation $A(q, u) = 0$, and a real function $J : Q \times U \to \mathbb{R}$ to be minimized.

**Example:** Equation (3) is a PDE-constrained optimization problem. The control variable $q$ corresponds to the domain $\Omega$, the state variable $u$ represents the pair velocity-pressure $(u, p)$, the nonlinear constraint $A$ represents the Navier-Stokes equations [1], and $J$ is a PDE-constrained objective function [2]. The state space $U$ corresponds to the space of pairs $(a, b)$ with weakly differentiable velocities $a$ that satisfy $a = g$ on $\partial \Omega \setminus \Gamma$ and that solves a state equation $A(q, u) = 0$.

Most numerical methods for PDE-constrained optimization attempt to construct a sequence of controls $\{q^{(k)}\}_{k \in \mathbb{N}}$ and corresponding states $\{u^{(k)}\}_{k \in \mathbb{N}}$ that minimizes $J(q^{(k)}, u^{(k)}) = \inf_{q, u} \{ J(q, u) : A(q, u) = 0 \}$.

Often, the sequence $\{q^{(k)}\}_{k \in \mathbb{N}}$ is constructed using derivatives of the function $J$ and of the constraint $A$. Common approaches are steepest descent algorithms and Newton methods (in their quasi, Krylov, or semi-smooth versions) [31, 40]. These algorithms ensure that the sequence $\{J(q^{(k)}, u^{(k)})\}_{k \in \mathbb{N}}$ decreases. In special cases, it is even possible to show that the sequence $\{q^{(k)}\}_{k \in \mathbb{N}}$ converges [34]. Although it may be difficult to ensure these assumptions are met in industrial applications, these optimization algorithms are still powerful tools to improve state-of-the-art designs and are widely used to perform shape optimization.

3.2 Shape optimization and shape calculus

Shape optimization with PDE constraints is a particular branch of PDE-constrained optimization where the control space $Q$ is a set of domain shapes. The space of shapes is notoriously difficult to characterize uniquely. For instance, one could describe shapes through their boundary regularity, or as level-sets, or as local epigraphs [19, ch. 2]. The choice of the shapes’ space characterization plays an important role in the concrete implementation of a shape optimization algorithm, and it can also affect formulas that result by differentiating $J$ with respect to perturbations of the shape $q$. To be more precise, different methods generally lead to the same first order shape derivative formula, but differ on shape derivatives of higher order [19, ch. 9].

In this work, we model the control space $Q$ as the images of bi-Lipschitz geometric transformations $T$ applied to an initial set $\Omega \subset \mathbb{R}^d$ [19, ch. 3], that is,

$$Q := \{ q = T(\Omega) : \Omega \subset \mathbb{R}^d \to \mathbb{R}^d \text{ is bi-Lipschitz} \}, \quad (5)$$

see Figure 5. We choose this model of $Q$ because it provides an explicit description of the domain boundaries via $\partial (T(\Omega)) = T(\partial \Omega)$, and because it is compatible with higher-order finite elements [49], as explained in detail in the Section 3.3. Henceforth, we use the term differomorphism to indicate that a geometric transformation $T$ is bi-Lipschitz.

![Fig. 5](image_url) To construct the control space $Q$, we select an initial set $\Omega$ and a set of diffeomorphisms $\{T\}$ (black arrows), and collect every image $T(\Omega)$.
In this setting, the shape derivative of \( J \) corresponds to the classical Gâteaux derivative in the Sobolev space \( W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \). To see this, let us momentarily remove the PDE-constraint, and only consider a shape functional of the form \( \Omega \rightarrow J(\Omega) \). The shape derivative of \( J \) at \( \Omega \) is the linear and continuous operator \( dJ(\Omega, \cdot) : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \rightarrow \mathbb{R} \) defined by

\[
dJ(\Omega, V) := \lim_{t \searrow 0} \frac{J(\Omega + tV) - J(\Omega)}{t},
\]

where \( \Omega \) is the set \( \Omega = \{ x + tV(x) : x \in \Omega \} \). By replacing \( \Omega \) with \( q \), where \( \Omega \) denotes the identity transformation defined by \( I(x) = x \) for any \( x \in \mathbb{R}^d \), Equation (6) can be equivalently rewritten as

\[
dJ(q, V) := \lim_{t \searrow 0} \frac{J(q + tV) - J(q)}{t}.
\]

We highlight that this interpretation immediately generalizes to any \( q \in Q \) and can be used to define higher order shape derivatives.

The same definition of shape derivative holds in the presence of PDE-constraints: the shape derivative at \( q \) of the function \( J : Q \times U \rightarrow \mathbb{R} \) subject to \( A(q, u) = 0 \) is the linear and continuous operator defined by

\[
dJ(q, u, V) := \lim_{t \searrow 0} \frac{J(q + tV, u_t) - J(q, u)}{t},
\]

where \( u_t \) is the solution to \( A(q + tV, u_t) = 0 \). Computing shape derivative formulas using (7) may present the difficulty of computing the shape derivative of \( u \), which intuitively arises by the “chain rule” formula. The shape derivative of \( u \), which is sometimes called “material derivative” of \( u \), can be eliminated with the help of adjoint equations (34, Sec. 1.6.2). This process can be automated by introducing the Lagrange functional (34, Sec. 1.6.3)

\[
L(q, u, p) := J(q, u) + \langle A(q, u), p \rangle.
\]

The term \( \langle A(q, u), p \rangle \) stems from testing the equation \( A(q, u) = 0 \) with a test function \( p \) in the same way it is usually done when writing a PDE in its weak form.

**Example:** If \( A \) denotes the Navier-Stokes equations (1), then \( \langle A(q, u), p \rangle \) corresponds to the weak formulation (4).

The advantage of introducing the Lagrangian (8) is that, by choosing \( p \) as the solution to the adjoint equation

\[
\langle \partial_u A(q, u), p \rangle = -\partial_q J(q, u) \quad \text{for all } u \in U,
\]

where \( \partial_u \) denotes the partial differentiation with respect to the variable \( u \), the shape derivative of \( J \) can be computed as

\[
dJ(q, u, V) = \partial_q L(q, u, p, V),
\]

where \( \partial_q \) denotes partial differentiation with respect to the variable \( q \). This is advantageous because partial differentiation does not require computing the shape derivative of \( u \).

The Lagrangian approach to compute derivatives of PDE-constrained functionals is well established (39), and its steps can be replicated by symbolic computation software. Probably, the biggest success in this direction is the dolfin-adjoint project (20,17), which derives “the adjoint and tangent-linear equations and solves them using the existing solver methods in Fi niCS/Firedrake” (17). Thanks to the shape differentiation capabilities of UFL introduced in (32), dolfin-adjoint is also capable of shape differentiating PDE-constrained functionals (22).

**Remark 1** Optimization algorithms are usually based on steepest descent directions to update the control variable \( q \). A steepest descent direction is a direction \( V^* \) that minimizes the derivative \( dJ \). Since \( dJ \) is linear, it is necessary to introduce a norm \( ||\cdot|| \) on the space of possible perturbations \( \{V\} \) (the tangent space of \( Q \) at \( q \)), and to restrict the search of a steepest descent direction to directions \( V \) of length \( ||V|| = 1 \). A natural choice would be to select the \( W^{1,\infty} \)-norm \( \|
\) with respect to which a minimizer has been shown to exists for most functionals (49, Prop. 3.1). However, in practice it is more convenient to employ a norm that is induced by an inner product, so that the steepest descent direction corresponds to the Riesz representative of \( dJ \) with respect to the inner product (34, p. 98).

### 3.3 Geometric transformations, moving meshes, and parametric finite elements

To solve a PDE-constrained optimization problem iteratively, it is necessary to employ a numerical method that is capable of solving the constraint \( A(q, u) = 0 \) for any feasible control \( q \). In shape optimization, this translates into the requirement of a numerical scheme that can solve a PDE on a domain that changes at each iteration of the optimization algorithm. There are several competing approaches to construct a numerical scheme with this feature, such as the level-set method (10) or the phase field approach (11), among others.

In Fireshape, we employ the approach sometimes know as “moving mesh” method (3,10). In its simplest version (see Figure 8), this method replaces (or approximates) the initial domain \( \Omega \) with a polygonal mesh \( \Omega_h \), On this mesh, the state and adjoint equations are solved

\[4\] The norm \( ||V||_{1,\infty} \) is the maximum between the essential supremum of \( V \) and of its derivative \( DV \).
with a standard finite element method, whose construction on polygonal meshes is immediate. For instance, depending on the nature of the state constraint, one may solve the state and adjoint equations using linear Lagrangian or P2-P1 Taylor-Hood finite elements (see Section 2.2). With the state and adjoint solutions at hand, one employs shape derivatives (see Remark 4 and Section 1.2) to update the coordinates of mesh nodes while retaining the mesh connectivity of $\Omega$. This leads to a new mesh that represents an improved design. This update process is repeated until some prescribed convergence criteria are met.

Fig. 6 Simplest approach to PDE-constrained shape optimization. An initial mesh (left) is used to compute state and adjoint variables. This information, together with shape derivatives, is used to devise an update of the nodes' coordinates (center). A new and improved initial guess is obtained by updating the nodes' coordinates and retaining the initial mesh connectivity (right). This process is repeated until convergence.

The moving mesh method we just described is a simple and yet powerful method. However, in its current formulation, it requires polyhedral meshes, which limits the search space $Q$ to polyhedra. In the remaining part of this section, we describe an equivalent interpretation of the moving mesh method that generalizes to curved domains. Additionally, this alternative interpretation allows approximating state and adjoint variables with arbitrarily high-order finite elements without suffering from reduction of convergence order due to poor approximation of domain boundaries [15, Ch. 4.4].

We begin by recalling the standard construction of parametric finite elements. For more details, we refer to [15] Sect. 2.3 and 4.3]. To construct a parametric finite element space, one begins by partitioning the domain $\Omega$ into simpler geometric elements $\{K_i\}$ (usually triangles or tetrahedra, as depicted in the first row of Figure 7). Then, one introduces a reference element $\hat{K}$ and a collection of diffeomorphisms $\{F_i\}$ that map the reference element $\hat{K}$ to the various $K_i$ in the triangulation (second row).

Fig. 7 To construct finite element basis functions, one usually begins by triangulating a domain Omega (first row) and then introducing diffeomorphisms $F_i$ that map the reference element $\hat{K}$ to the various $K_i$ in the triangulation (second row).

Keeping this knowledge about parametric finite elements in mind, we can revisit the moving mesh method (see Figure 6). There, the main idea was to update only nodes' coordinates and keep the mesh connectivity unchanged, so that constructing finite elements on the new mesh is straightforward. In [49], it has been shown that the new finite element space can also be obtained by modifying the parametric construction of finite elements on the original domain $\Omega$. In the next paragraphs, we give an extended explanation (with adapted notation) of the demonstration given in [49].

Let $T$ denote the transformation employed to modify the mesh $\Omega_b$ on the left in Figure 6 into the new and perturbed mesh $T(\Omega_b)$ on the right in Figure 6. Additionally, let $\{T(K_i)\}$ denote the simple geometric elements that constitute the latter. Using the parametric approach, we can construct finite elements on the new mesh by introducing a collection of diffeomorphisms $\{F_i\}$ that map the reference element $\hat{K}$ to the

\[ F_i(x) = \sum_m \mu_m^i \beta_m(x) \quad \text{for every } x \in \hat{K}. \] (9)

Finite elements constructed following this procedure are usually called parametric, because they rely on the parametrization $\{F_i\}$. Note that the most common finite elements families, such as Lagrangian, Raviart–Thomas, or Nedelec finite elements, are indeed parametric.

For linear Lagrangian finite elements, the two set of reference local basis functions $\{b_j\}$ and $\{\beta_m\}$ coincide.
various $T(K_i)$s, that is, $\hat{F}_i(\hat{K}) = T(K_i)$ for every value of the index $i$; see Figure 8.

The behavior of the transformation $T$ in Figure 6 is prescribed only the mesh nodes. Since its behavior on the interior of the mesh triangles can be chosen arbitrarily, we can decide that $T$ is piecewise affine on each triangle. This convenient choice implies that $T$ can be written as a linear combination of piecewise affine Lagrangian finite elements defined on the first mesh, that is, $T(x) = \sum_i \nu_i B_i(x)$ for every $x$ in $\Omega$, where $\{\nu_i\}$ are some coefficient vectors and $\{B_i\}$ are global basis functions of the space of piecewise affine Lagrangian finite elements defined on the partition $\{K_i\}$. Since Lagrangian finite elements are constructed via pullbacks to the reference element, for every element $K_i$ there are coefficient vectors $\{\nu_{i,m}\}$ so that the restriction $T|_{K_i}$ of $T$ on $K_i$ can be rewritten as $T|_{K_i}(x) = \sum_i \nu_i B_i|_{K_i}(x) = \sum_m \nu_{i,m} \hat{B}_m(F_i^{-1}(x))$.

Therefore, the composition $T|_{K_i} \circ F_i$ is of the form $T|_{K_i} \circ F_i(x) = \sum_m \nu_{i,m} \hat{B}_m(x)$ for every $x \in \hat{K}$, (10)

that is, of the same form of Equation 9. This implies that, to construct finite elements on the perturbed geometry $T(\Omega_0)$, we only need to replace the original coefficients $\{\mu_{i,m}\}$ in Equation 9 with the new coefficients $\{\nu_{i,m}\}$ from Equation 10.

This alternative and equivalent viewpoint on the moving mesh method generalizes naturally to higher-order finite element approximations. Indeed, one of the key steps to ensure that higher-order finite elements achieve higher-order convergence on curved domains is to employ sufficiently accurate polynomial interpolation of domain boundaries [15, Ch. 4.4]. This boundary interpolation can be encoded in the diiffeomorphisms $\{F_i\}$ by using higher-order Lagrangian local basis functions. Therefore, simply employing higher-order Lagrangianularity requirements are met. In Fireshape, the class

finite element transformations $T$ leads to a natural extension of moving mesh method to higher-order finite elements.

This alternative and equivalent viewpoint generalizes further to allow the use of any arbitrary discretization of the transformation $T$ (for instance, using B-splines [35], harmonic polynomials, or radial basis functions [57]). The only requirement to be fulfilled to ensure the desired order of convergence $p$ is that the maps $T \circ F_i : x \mapsto T(F_i(x))$ satisfy the asymptotic algebraic estimates

$$\|D^\alpha(T \circ F_i)\| = O(h^\alpha) \quad \text{for } 0 \leq \alpha \leq p,$$

where $D^\alpha(T \circ F_i)$ denotes the $\alpha$th derivative of $T \circ F_i$. Using a different discretization of the transformation $T$ can give several advantages, like increasing the smoothness $T$ (because finite elements are generally only Lipschitz continuous) or varying how shape updates are computed during the optimization process [24].

Remark 2 An issue that can arise with the moving mesh method is that it can lead to poor quality (or even tangled) meshes. In terms of geometric transformations, a mesh with poor quality corresponds to a transformation $T$ for which the value $\max_{\alpha} \|D^\alpha T\|$ is large (and a tangled mesh to a transformation $T$ that is not a diffeomorphism). To a certain extent, it is possible to enforce moderate derivatives by employing suitable metrics to extract descent directions from shape derivatives (for instance, by using linear elasticity based inner products with a Cauchy-Riemann augmentation [38]) and/or by adding penalty terms to the functional $J$ (as in Section 2.4).

4 Anatomy of Fireshape

In this section, we give more details about Fireshape’s implementation and features. Fireshape is organized in a few core Python classes (and associated subclasses) that implement the control space $Q$, the metric to be employed by the optimization algorithm, and the (possibly PDE-constrained) objective function $J$. The following subsections describe these classes.

4.1 The class ControlSpace

Fireshape models the control space $Q$ of admissible domains using geometric transformations $T$ as in Equation 5 (see also Figure 5). From a theoretical perspective, the transformations $T$ can be discretized in numerous different ways as long as certain minimal reg-
\textbf{ControlSpace} allows the following options: (i) Lagrangian finite elements defined on the same mesh employed to solve the state equation, (ii) Lagrangian finite elements defined on a mesh coarser than the mesh employed to solve the state equation, and (iii) tensorized B-splines defined on a separate Cartesian grid (not to be confused with a spline or Bézier parametrization of the domain boundary, see Figure 9).

If discretization (i) can be considered to be the default option, discretization (ii) allows introducing a regularization by discretizing the geometry more coarsely (so-called “regularization by discretization”), whereas B-splines allow constructing transformation with higher regularity (Lagrangian finite elements are only Lipschitz continuous, whereas B-splines can be continuously differentiable and more).

The class \textbf{ControlSpace} can be easily extended to include additional discretization options, such as radial basis functions and harmonic polynomials.

4.2 The class \textbf{InnerProduct}

To formulate a continuous optimization algorithm, we need to specify how to compute lengths of vectors (and, possibly, how to compute the angle between two vectors). The class \textbf{InnerProduct} addresses this requirement and allows selecting an inner product \((\cdot,\cdot)_{H}\) to endow the control space \(Q\) with\(^6\).

The choice of the inner product affects how steepest-descent directions are computed. Indeed, a steepest-descent direction is a direction \(V\) of length \(\|V\|_{H} = 1\) such that \(dJ(q,V)\) is minimal. Let \(\alpha := \|dJ(q,\cdot)\|_{*}\) denote the length of the operator \(\|dJ(q,\cdot)\|\) measured with respect to the dual norm. Then \(^{34}\) p. 103, the steepest descent direction \(V\) satisfies the equation
\[
\alpha(V, W)_{H} = -dJ(q, W) \quad \text{for all } W \text{ in } H,
\]
which clearly depends on the inner product \((\cdot,\cdot)_{H}\).

The control space \(Q\) can be endowed with different inner products. In Fireshape, the class \textbf{InnerProduct} allows the following options: (i) an \(H^{1}(\Omega)\) inner product based on standard Galerkin stiffness and mass matrices, (ii) a Laplace inner product based on the Galerkin stiffness matrix, and (iii) an elasticity inner product based on the linear elasticity mechanical model. These options can be complemented with additional homogeneous Dirichlet boundary conditions to specify parts of the boundary \(\partial\Omega\) that are not to be modified during the shape optimization procedure.

Although all three options are equivalent from a theoretical perspective, in practice it has been observed that option (iii) generally leads to geometry updates that result in meshes of higher equality compared to options (i) and (ii). A thorough comparison is available in \(^{38}\), where the authors also suggest to consider complementing these inner products with terms stemming from Cauchy-Riemann equations to further increase mesh quality. This additional option is readily available in Fireshape.

4.3 The classes \textbf{Objective} and \textbf{PdeConstraint}

In the vast majority of cases, users who aim to solve a PDE-constrained shape optimization problem are only required to instantiate the two classes \textbf{Objective} and \textbf{PdeConstraint}, where they can specify the formula of the function \(J\) to be minimized and the weak formulation of its PDE-constraint \(A(\Omega, u) = 0\) (see Sections 2.2 and 2.3, for instance). Since Fireshape is built on top of the finite element library Firedrake, these formulas must be written using the Unified Form Language (UFL). We refer to the tutorials on the website \(^{27}\) for more details about Firedrake and UFL.

4.4 Supplementary classes

Fireshape also includes a few extra classes to specify additional constraints, such as volume or perimeter constraints on the domain \(\Omega\), or spectral constraints to control the singular values of the transformation \(T\). For more details about these extra options, we refer to Fireshape’s documentation and tutorials \(^{28}\).

5 Conclusions

We have introduced Fireshape: an open-source and automated shape optimization toolbox for the finite element software Firedrake. Fireshape is based on the
moving mesh method and allows user with minimal shape optimization knowledge to tackle challenging shape optimization problems constrained to PDEs. In particular, Fireshape computes adjoint equations and shape derivatives in an automated fashion, allows decoupled discretizations of control and state variables, and gives full access to Firedrake’s and PETSc’s discretization and solver capabilities as well as to the extensive optimization library ROL.

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Contributions Alberto Paganini and Florian Wechsung have contributed equally to the development of the software Fireshape and to this manuscript.

Conflict of interest statement On behalf of all authors, the corresponding author states that there is no conflict of interest.

Replication of results For reproducibility, we cite archives of the exact software versions used to produce the results in this paper. All major Firedrake components have been archived on Zenodo [58]. An installation of Firedrake with components matching those used to produce the results in this paper can be obtained following the instructions at https://www.firedrakeproject.org/download.html. The exact version of the Fireshape library used for these results has also been archived at [59]. The latest version of the Fireshape library can be found at https://github.com/Fireshape/Fireshape

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