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Functional Optimization of Fluidic Devices with Differentiable Stokes Flow

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Motivation



Fluidic devices are key components for a variety of products



Developing hydraulic actuators



Designing medical devices

Fabricating underwater soft robots



Motivation



However, designing fluidic devices is challenging

- The design space is large and non-trivial to parametrize
- The dynamics is computationally expensive due to the solid-fluid coupling
- Search for an optimal solution is challenging





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We propose a computational design method for fluidic devices





Fluid control







ICLR 20'

Fluid simulation



SIGGRAPH 99



SIGGRAPH 17'

Fluid system optimization



Borrvall and Petersson



Differentiable physics



ICRA 19



PMLR 18



Fluid control









ICLR 20'

Fluid simulation



SIGGRAPH 99'



SIGGRAPH 17'











Fluid control





SIGGRAPH 04'



ICLR 20'

Fluid simulation



SIGGRAPH 99'



SIGGRAPH 17'

Fluid system optimization



Borrvall and Petersson



and Maute







Fluid control





SIGGRAPH 04'

ICLR 20'

Fluid simulation



SIGGRAPH 99'



SIGGRAPH 17'

Fluid system optimization



Petersson



and Maute

Differentiable physics





ICRA 19'

PMLR 18'





Differentiable Stokes flow with a **continuous** interface

Sub-cell discretization with flexible boundary conditions

Computational design of multi-functional fluidic devices





Differentiable Stokes flow with a **continuous** interface

Sub-cell discretization with **flexible** boundary conditions

Computational design of multi-functional fluidic devices





Differentiable Stokes flow with a **continuous** interface

Sub-cell discretization with **flexible** boundary conditions

Computational design of multi-functional fluidic devices



Forward simulation



Parametric Design



Forward simulation





Forward simulation





Forward simulation





Forward simulation and backpropagation





Forward simulation, backpropagation, and optimization







Parametrizing the design space (easy)

Simulating the system with a sub-cell discretization (easy)

...and computing gradients





Parametrizing the design space (easy)

Simulating the system with a sub-cell discretization (easy)

...and computing gradients





Parametrizing the design space (nontrivial!)

Simulating the system with a sub-cell discretization (nontrivial!)

...and computing gradients (nontrivial!)



Forward simulation, backpropagation, and optimization



Optimization



We represent designs as parametric shapes





We represent designs as parametric shapes





By varying these parameters, we explore different designs



Parametric designs

Signed-distance functions



Forward simulation, backpropagation, and optimization





Forward simulation, backpropagation, and optimization





Incompressible Stokes equations

$$-\eta \Delta \boldsymbol{v}(\boldsymbol{x}) + \nabla p(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}), \qquad \boldsymbol{x} \in \boldsymbol{\Omega}$$
$$\nabla \cdot \boldsymbol{v}(\boldsymbol{x}) = 0, \qquad \boldsymbol{x} \in \boldsymbol{\Omega}$$

η: dynamic viscosity
p: pressure field
ν: velocity field
f: external force





Recap: linear elasticity

$$-\mu\Delta \boldsymbol{u}(\boldsymbol{X}) - (\mu + \lambda)\nabla[\nabla \cdot \boldsymbol{u}(\boldsymbol{X})] = \boldsymbol{f}(\boldsymbol{X})$$

μ: Lamé parameters
λ: Lamé parameters
u: displacement field
f: external force





Recap: linear elasticity

$$-\mu\Delta \boldsymbol{u}(\boldsymbol{X}) - (\mu + \lambda)\nabla[\nabla \cdot \boldsymbol{u}(\boldsymbol{X})] = \boldsymbol{f}(\boldsymbol{X})$$

Let $r(X) = -(\mu + \lambda)\nabla \cdot u(X)$ and we obtain:

$$-\mu \Delta \boldsymbol{u}(\boldsymbol{X}) + \nabla r(\boldsymbol{X}) = \boldsymbol{f}(\boldsymbol{X}), \qquad \boldsymbol{X} \in \boldsymbol{\Omega}$$
$$\nabla \cdot \boldsymbol{u}(\boldsymbol{X}) + \frac{1}{\mu + \lambda} r(\boldsymbol{X}) = 0, \qquad \boldsymbol{X} \in \boldsymbol{\Omega}$$





Analogy between Stokes flow and linear elasticity

Stokes flow

Linear elasticity

$$-\eta \Delta \boldsymbol{v}(\boldsymbol{x}) + \nabla p(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}), \ \boldsymbol{x} \in \Omega$$
$$-\mu \Delta \boldsymbol{u}(\boldsymbol{X}) + \nabla r(\boldsymbol{X}) = \boldsymbol{f}(\boldsymbol{X}), \quad \boldsymbol{X} \in \Omega$$
$$\nabla \cdot \boldsymbol{v}(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \Omega$$
$$\nabla \cdot \boldsymbol{u}(\boldsymbol{X}) + \frac{1}{\mu + \lambda} r(\boldsymbol{X}) = 0, \quad \boldsymbol{X} \in \Omega$$

Note the duality between η , v, p and μ , u, r.

Right \rightarrow left when $\lambda \rightarrow \infty$ (strict incompressibility).



Analogy between Stokes flow and linear elasticity

Previous work: use Stokes flow techniques to solve elasticity



Analogy between Stokes flow and linear elasticity

Previous work: use Stokes flow techniques to solve elasticity

Our model: quasi-incompressible Stokes flow

We use elasticity solvers to solve Stokes flow

- More numerically robust solvers
- Fewer variables (no pressure term)
- Easier to derive gradients



A note on boundary conditions: Dirichlet

 $v(x) = \alpha(x), \qquad x \in \partial \Omega$

α : velocity profile





A note on boundary conditions: no-slip/no-separation

$v(x) = \alpha(x),$	$x \in \partial \Omega$
$\boldsymbol{v}(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x})=0$,	$x \in \partial \Omega$
$\boldsymbol{ au}_t(\boldsymbol{x}) = 0$,	$x \in \partial \Omega$
\boldsymbol{lpha} : velocity profile	
<i>n</i> : normal	
τ_t : tangent traction	





Forward simulation, backpropagation, and optimization



Optimization



Forward simulation, backpropagation, and optimization





Consider a hybrid cell





Consider a hybrid cell





Consider a hybrid cell



4 Gaussian quadrature points in each cell



Consider a hybrid cell



4 Gaussian quadrature points in each cell

Weight of each point = area of the polygon

Soundary conditions are integrated along the interface



Forward simulation, backpropagation, and optimization





Forward simulation, backpropagation, and optimization





Recap: quasi-incompressible Stokes flow (linear elasticity)

$$-\mu\Delta \boldsymbol{u}(\boldsymbol{X}) - (\mu + \lambda)\nabla[\nabla \cdot \boldsymbol{u}(\boldsymbol{X})] = \boldsymbol{f}(\boldsymbol{X})$$

s.t. Boundary conditions.



Recap: quasi-incompressible Stokes flow (linear elasticity)

 $-\mu\Delta \boldsymbol{u}(\boldsymbol{X}) - (\mu + \lambda)\nabla[\nabla \cdot \boldsymbol{u}(\boldsymbol{X})] = \boldsymbol{f}(\boldsymbol{X})$

s.t. Boundary conditions.

After discretization from the variational form (Quadratic programming)

 $\min_{\boldsymbol{u}} \boldsymbol{u}^{\mathsf{T}} \boldsymbol{K}(\boldsymbol{\theta}) \boldsymbol{u}$ s.t. $\boldsymbol{C}(\boldsymbol{\theta}) \boldsymbol{u} = \boldsymbol{d}(\boldsymbol{\theta})$



Recap: quasi-incompressible Stokes flow (linear elasticity)

$$-\mu\Delta \boldsymbol{u}(\boldsymbol{X}) - (\mu + \lambda)\nabla[\nabla \cdot \boldsymbol{u}(\boldsymbol{X})] = \boldsymbol{f}(\boldsymbol{X})$$

s.t. Boundary conditions.

After discretization from the variational form (Quadratic programming)

$$\min_{u} u^{\mathsf{T}} K(\theta) u$$

s.t. $C(\theta) u = d(\theta)$

Note that the stiffness matrix and the boundary conditions are determined by the design parameter $\boldsymbol{\theta}$.

Recap: Forward Simulation



Forward simulation, backpropagation, and optimization





Forward simulation, backpropagation, and optimization





Most of the computation requires the chain rule only

But there are two exceptions!

Exception 1: gradients w.r.t. the area of a polygon



A brute-force implementation plus autodiff leads to lots of if-else branches!



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Exception 1: gradients w.r.t. the area of a polygon



A brute-force implementation plus autodiff leads to lots of if-else branches!

Our solution: deriving gradients from a closed-form solution [Barrow 79']



Most of the computation requires the chain rule only

But there are two exceptions!

Exception 2: gradients through the QP problem

$$\min_{\boldsymbol{u}} \boldsymbol{u}^{\mathsf{T}} \boldsymbol{K}(\boldsymbol{\theta}) \boldsymbol{u}$$

s.t. $\boldsymbol{C}(\boldsymbol{\theta}) \boldsymbol{u} = \boldsymbol{d}(\boldsymbol{\theta})$



Most of the computation requires the chain rule only

But there are two exceptions!

Exception 2: gradients through the QP problem

$$\min_{\boldsymbol{u}} \boldsymbol{u}^{\mathsf{T}} \boldsymbol{K}(\boldsymbol{\theta}) \boldsymbol{u}$$

s.t. $\boldsymbol{C}(\boldsymbol{\theta}) \boldsymbol{u} = \boldsymbol{d}(\boldsymbol{\theta})$

$$\Rightarrow \begin{pmatrix} K(\theta) & C^{\top}(\theta) \\ C(\theta) & 0 \end{pmatrix} \begin{pmatrix} \widetilde{u} \\ \widetilde{\lambda} \end{pmatrix} = \begin{pmatrix} 0 \\ d(\theta) \end{pmatrix}$$

KKT conditions



Most of the computation requires the chain rule only

But there are two exceptions!

Exception 2: gradients through the QP problem (matrix reused)

$$\begin{split} \min_{u} u^{\mathsf{T}} K(\theta) u \\ s. t. \mathcal{C}(\theta) u = d(\theta) \end{split} & \longleftrightarrow \begin{pmatrix} K(\theta) & \mathcal{C}^{\mathsf{T}}(\theta) \\ \mathcal{C}(\theta) & \mathbf{0} \end{pmatrix} \begin{pmatrix} \widetilde{u} \\ \widetilde{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ d(\theta) \end{pmatrix} \\ & \mathsf{KKT \ conditions} \end{aligned} \\ \begin{pmatrix} K(\theta) & \mathcal{C}^{\mathsf{T}}(\theta) \\ \mathcal{C}(\theta) & \mathbf{0} \end{pmatrix} \begin{pmatrix} \delta \widetilde{u} \\ \delta \widetilde{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \delta d(\theta) \end{pmatrix} - \begin{pmatrix} \delta K(\theta) & \delta \mathcal{C}^{\mathsf{T}}(\theta) \\ \delta \mathcal{C}(\theta) & \mathbf{0} \end{pmatrix} \begin{pmatrix} \widetilde{u} \\ \widetilde{\lambda} \end{pmatrix} \\ & \mathsf{Sensitivity \ analysis} \end{split}$$



Forward simulation, backpropagation, and optimization



Optimization



Forward simulation, backpropagation, and optimization





Sample a few random designs





Pick the best one to initialize the optimization



Best initial guess

L-BFGS optimization



Pick the best one to initialize the optimization



Results: Fluidic Twister



Flexible handling of boundary conditions matters



Initial guess

Optimized design (no-separation) Optimized design (no-slip)

Results: Fluidic Twister



Flexible handling of boundary conditions matters



Initial guess

Optimized design (no-separation) Optimized design (no-slip)

Results: Fluidic Switch



Optimization with multiple configurations



Switch is off

Results: Fluidic Switch



Optimization with multiple configurations





Switch is off

Switch is on

Results: Fluidic Switch



Optimization with multiple configurations



More Results



Fluid gates





Results: Convergence Study



Simulating under refinement







Enforcing incompressibility



Ablation Study: Global Search



Comparisons between w/ and w/o sampling initial guesses







Differentiable simulation ⊃ applying the chain rule

Discretization and boundary conditions need careful treatment

Gradients speed up the process of finding optimal designs ...and they are more effective when combined with global search





Differentiable simulation ⊃ applying the chain rule

Discretization and boundary conditions need careful treatment

Gradients speed up the process of finding optimal designs

...and they are more effective when combined with global search

Thank You for Watching



Code is available

GitHub link:

https://github.com/mitgfx/diff_stokes_flow

or scan



