Numerical Optimization of Partial Differential Equations

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- Pritpal 'Pip' Matharu
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Goal ("key learning outcome"):

introduction to state-of-the-art computational approaches to solution of PDE optimization problems, including actual computer implementation

Key Challenge:

dealing with the PDE constraint

Applications of PDE Optimization

- Open-loop optimal control of distributed systems
  - flow control problems in fluid mechanics (e.g., optimization of lift and/or drag, mixing, etc.)
  - structural optimization is solid mechanics
  - process optimization in chemical engineering
  - portfolio optimization in investing
- State and parameter estimation for distributed systems
  - inverse problems for PDEs (e.g., medical imaging)
  - data assimilation in Numerical Weather Prediction ("4D VAR")

General Framework (I)

- Equation-constrained optimization problem

$$(\star) \qquad \begin{cases} \min\limits_{(x,\varphi)} \tilde{\mathcal{J}}(x,\varphi) \\ \text{subject to:} \quad S(x,\varphi) = 0 \end{cases}$$

where:

- $x \in \mathcal{X}$ — the state variable ($\mathcal{X}$ is a suitable function (Hilbert) space)
- $\varphi \in \mathcal{U}$ — the control (decision) variable
- $\tilde{\mathcal{J}} \; : \; \mathcal{X} \times \mathcal{U} \rightarrow \mathbb{R}$ — objective functional
- $S \; : \; \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X}^*$ — constraint (PDE)

General Framework (II)

- The constraint $S(x,\varphi)=0$ be handled by introducing the *Lagrange multiplier* $\lambda \in \mathcal{X}$, such that we can define the Lagrangian

$$\mathcal{L}(x,\varphi,\lambda) = \tilde{\mathcal{J}}(x,\varphi) - \langle \lambda, S(x,\varphi)\rangle_{\mathcal{X}\times\mathcal{X}^*}$$

- The constrained minimizers are then found by solving

$$\min_{(x,\varphi,\lambda)\in\mathcal{X}\times\mathcal{U}\times\mathcal{X}} \mathcal{L}(x,\varphi,\lambda)$$

General Framework (III)

- If the constraint equation $S(x,\varphi) = 0$ can be solved for x (cf. implicit function theorem), then $x = x(\varphi)$ and one can define the *reduced* objective functional

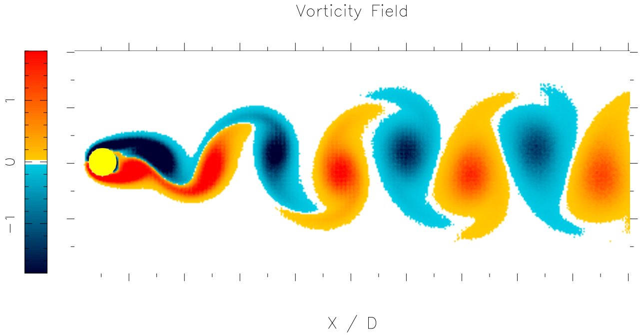
$$\mathcal{J}(\varphi) := \tilde{\mathcal{J}}(x(\varphi), \varphi)$$

- Constrained optimization problem $(\star)$ can then replaced with the following equivalent unconstrained problem

$$\min_{\varphi \in \mathcal{U}} \mathcal{J}(\varphi)$$

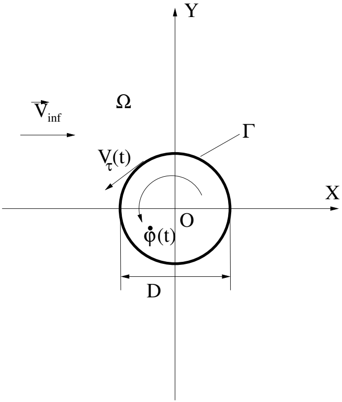
- *Inequality* constraints are more difficult to handle, especially in the context of PDE optimization, and will not be considered here

Vorticity fields on the flow past an obstacle



A Classical Flow Control Problem in Fluid Mechanics

- Flow Domain



- Assumptions:
  - viscous, incompressible flow
  - plane, infinite domain
  - $Re = 150$
- State variables:
  - velocity: $\mathbf{v} \ : \ \Omega \to \mathbb{R}^d$
  - pressure: $p \ : \ \Omega \to \mathbb{R}$
- Control variables:
  - rate of rotation:

$$\dot{\varphi} \ : \ [0, T] \to \mathbb{R}$$

Statement of the Problem (II)

- Find $\dot{\varphi}_{opt} = \operatorname{argmin}_{\dot{\varphi} \in L^2(0,T)} \mathcal{J}(\dot{\varphi})$, where

$$\mathcal{J}(\dot{\varphi}) = \frac{1}{2}\int_0^T \left\{ \left[\begin{array}{c} \text{power related to} \\ \text{the drag force} \end{array} \right] + \left[\begin{array}{c} \text{power needed to} \\ \text{control the flow} \end{array} \right] \right\} dt$$
$$= \frac{1}{2}\int_0^T \oint_{\Gamma_0} \{[p(\dot{\varphi})\mathbf{n} - \mu\mathbf{n}\cdot\mathbf{D}(\mathbf{v}(\dot{\varphi}))]\cdot[\dot{\varphi}\,(\mathbf{e}_z \times \mathbf{r}) + \mathbf{v}_\infty]\}\, d\sigma\, dt$$

- Subject to:

$$\begin{cases} \left[\begin{array}{c} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{v} - \mu\Delta\mathbf{v} + \boldsymbol{\nabla} p \\ \boldsymbol{\nabla}\cdot\mathbf{v} \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \end{array} \right] & \text{in } \Omega \times (0,T), \\ \mathbf{v} = 0 & \text{at } t = 0, \\ \mathbf{v} = \dot{\varphi}_{opt}\tau & \text{on } \Gamma \end{cases}$$

Optimization vs. Discretization

- Optimize-then-Discretize: optimality conditions and gradient expressions derived at the continuous (PDE) level and only then discretized $\Longleftarrow$ will focus on this approach
  - formulation independent of discretization
  - allows one to exploit the analytic structure of the problem (e.g., regularity, etc.)
  - works well with mesh refinement in the numerical solution of PDEs
- Discretize-then-Optimize: the PDE problem is discretized first and then treated as optimization problem in finite dimension
  - PDE discretization errors do not affect the optimization procedure
  - can take advantage of Automatic Differentiation (AD) tools
  - may be more suitable for very large problems

- Part I: basic optimization concepts in $\mathbb{R}^n$
  - gradients and gradient flows
  - fixed and optimal step sizes
  - linear and nonlinear conjugate gradients
  - constraints, projections and Lagrange multipliers
- Part II: optimization with PDE constraints
  - Riesz theorem and gradient extraction
  - adjoint calculus
  - preconditioning and Sobolev gradients
- Part III: applications
  - flow control
  - shape optimization
- All presentations available at
  http://www.math.mcmaster.ca/bprotas/lecture_notes.shtml