Numerical Optimization of Partial Differential Equations

Part III: applications

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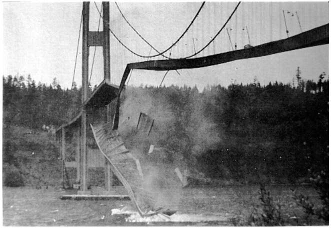
PART I
Optimal Open–Loop Control via Adjoint–Based Optimization

Motivation — Applications of Flow Control

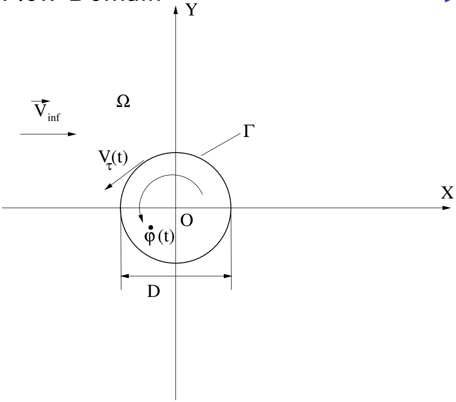
- Wake Hazard

- Fluid–Structure Interaction



Statement of the Problem (I)

- Flow Domain



- Assumptions:
  - viscous, incompressible flow
  - plane, infinite domain
  - $Re = 150$

Statement of the Problem (II)

- Find $\dot{\varphi}_{opt} = \operatorname{argmin}_{\dot{\varphi}} \mathcal{J}(\dot{\varphi})$, 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:

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

Abstract Framework (I)

- Constrained optimization problem

$$\begin{cases} \min_{(x,\varphi)} \tilde{\mathcal{J}}(x,\varphi) \\ S(x(\varphi),\varphi) = 0 \end{cases}$$

- Equivalent UNCONSTRAINED optimization problem (note that $x = x(\varphi)$)

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

- First–Order OPTIMALITY CONDITIONS ($\mathcal{U}$ - Hilbert space of controls)

$$\forall_{\varphi' \in \mathcal{U}} \quad \mathcal{J}'(\varphi;\varphi') = \left(\boldsymbol{\nabla}\mathcal{J},\varphi'\right)_{\mathcal{U}} = 0,$$

with the GÂTEAUX DIFFERENTIAL

$$\mathcal{J}'(\varphi;\varphi') = \lim_{\epsilon\to 0} \frac{1}{\epsilon}[\mathcal{J}(\varphi+\epsilon\varphi') - \mathcal{J}(\varphi)].$$

Abstract Framework (II)

- Minimization of $\mathcal{J}(\varphi)$ with a DESCENT ALGORITHM in $\mathcal{U}$ $\Longrightarrow$ solution to a STEADY STATE of the ODE in $\mathcal{U}$

$$\begin{cases} \dfrac{d\varphi}{d\tau} = -\mathcal{Q}\nabla_{\varphi}\mathcal{J}(\varphi) & \text{on } \tau \in (0,\infty) \ \text{(pseudo–time)}, \\ \varphi = \varphi_0 & \text{at } \tau = 0. \end{cases}$$

- Typically well–behaved (quadratic) cost functionals
- Typically ill–behaved constraints: THE NAVIER–STOKES SYSTEM
  - nonlinear, nonlocal, multiscale, evolutionary PDE,
- Dimensions:
  - state: 10^6 — 10^7 DoF $\times$ 10^2 — 10^3 time levels
  - control: 10^4 — 10^5 DoF $\times$ 10^2 — 10^3 time levels
- No hope of using "matrix" formulation ...
- Formulation equivalent to Lagrange Multipliers

Differential of the Cost Functional

- The cost functional:

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

- Expression for the Gâteaux differential:

$$\mathcal{J}'(\dot\varphi; h) = \frac{1}{2}\int_0^T \oint_{\Gamma_0} \Big\{ [p'(h)\mathbf{n} - \mu\mathbf{n}\cdot\mathbf{D}\,(\mathbf{v}'(h))]\cdot[\dot\varphi\,(\mathbf{e}_z\times\mathbf{r}) + \mathbf{v}_\infty] +$$
$$[p(\dot\varphi)\mathbf{n} - \mu\mathbf{n}\cdot\mathbf{D}(\mathbf{v}(\dot\varphi))]\cdot(\mathbf{e}_z\times\mathbf{r})\,h\Big\}\, d\sigma\, dt = B_1$$
$$= (\nabla\mathcal{J}(t), h)_{L_2([0,T])}$$

The fields $\{\mathbf{v}'(h), p'(h)\}$ solve the linearized perturbation system.

- How to calculate the GRADIENT $\nabla\mathcal{J}$?

Sensitivities and Adjoint States

- The linearized perturbation system

$$\begin{cases} \mathcal{N}\begin{bmatrix} \mathbf{v}' \\ p' \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathbf{v}'}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{v}' + (\mathbf{v}'\cdot\boldsymbol{\nabla})\mathbf{v} - \mu\Delta\mathbf{v}' + \boldsymbol{\nabla} p' \\ -\boldsymbol{\nabla}\cdot\mathbf{v}' \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \text{in } \Omega\times(0,T), \\ \mathbf{v}' = 0 & \text{at } t = 0, \\ \mathbf{v}' = h\tau & \text{on } \Gamma\times(0,T) \end{cases}$$

- Duality pairing defining the adjoint operator

$$\left\langle \mathcal{N}\begin{bmatrix} \mathbf{v}' \\ p' \end{bmatrix}, \begin{bmatrix} \mathbf{v}^* \\ p^* \end{bmatrix} \right\rangle_{L_2(0,T;L_2(\Omega))} = \left\langle \begin{bmatrix} \mathbf{v}' \\ p' \end{bmatrix}, \mathcal{N}^*\begin{bmatrix} \mathbf{v}^* \\ p^* \end{bmatrix} \right\rangle_{L_2(0,T;L_2(\Omega))} + B_1 + B_2$$

- The adjoint system (TERMINAL VALUE PROBLEM !!)

$$\begin{cases} \mathcal{N}^*\begin{bmatrix} \mathbf{v}^* \\ p^* \end{bmatrix} = \begin{bmatrix} -\frac{\partial \mathbf{v}^*}{\partial t} - \mathbf{v}\cdot\left[\boldsymbol{\nabla}\mathbf{v}^* + (\boldsymbol{\nabla}\mathbf{v}^*)^T\right] - \mu\Delta\mathbf{v}^* + \boldsymbol{\nabla} p^* \\ -\boldsymbol{\nabla}\cdot\mathbf{v}^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \text{in } \Omega\times(0,T), \\ \mathbf{v}^* = 0 & \text{at } t = T, \\ \mathbf{v}^* = \mathbf{r}\times(\dot{\varphi}\mathbf{e}_z) + \mathbf{v}_\infty & \text{on } \Gamma\times(0,T) \end{cases}$$

Cost Functional Gradient

- The ADJOINT STATE and DUALITY PAIRING can now be used to re–express the cost functional differential as:

$$\mathcal{J}'(\dot{\varphi};h) = \frac{1}{2}\int_0^T \oint_\Gamma \{\mu R\mathbf{n}\cdot\mathbf{D}(\mathbf{v}^*)\cdot\tau + \mu\mathbf{n}\cdot\mathbf{D}(\mathbf{v}(\dot{\varphi}))\cdot(\mathbf{e}_z\times\mathbf{r})\}\; h\,d\sigma\,dt$$

- Identification of the COST FUNCTIONAL GRADIENT

$$\mathcal{J}'(\dot{\varphi};h) = (\nabla\mathcal{J}(t),h)_{L_2([0,T])} = \int_0^T \nabla\mathcal{J}(t)\,h\,dt$$

$$\boxed{\nabla\mathcal{J}(t) = \frac{1}{2}\oint_\Gamma \{\mu R\mathbf{n}\cdot\mathbf{D}(\mathbf{v}^*)\cdot\tau + \mu\mathbf{n}\cdot\mathbf{D}(\mathbf{v}(\dot{\varphi}))\cdot(\mathbf{e}_z\times\mathbf{r})\}\; d\sigma}$$

Optimality (KKT) system

- Complete optimality system for $\dot\varphi_{opt}$, $[\mathbf{v}_{opt}, p_{opt}]$, and $[\mathbf{v}^*, p^*]$

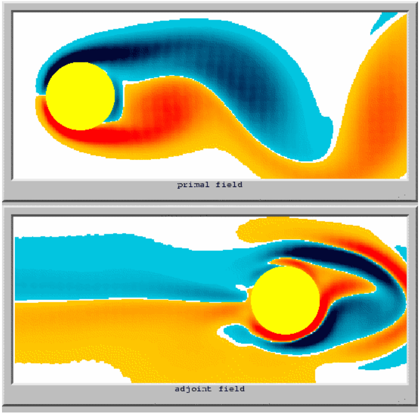
$$
\begin{cases}
\frac{1}{2}\oint_\Gamma \{\mu R \mathbf{n}\cdot\mathbf{D}(\mathbf{v}^*)\cdot\tau + \mu\mathbf{n}\cdot\mathbf{D}(\mathbf{v}(\dot\varphi_{opt}))\cdot(\mathbf{e}_z\times\mathbf{r})\}\, d\sigma = 0 \\
\begin{cases}
\begin{bmatrix} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{v} - \mu\Delta\mathbf{v} + \boldsymbol{\nabla} p \\ \boldsymbol{\nabla}\cdot\mathbf{v} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \text{in } \Omega\times(0,T), \\
\mathbf{v} = 0 & \text{at } t = 0, \\
\mathbf{v} = \dot\varphi_{opt}\tau & \text{on } \Gamma
\end{cases} \\
\begin{cases}
\mathcal{N}^*\begin{bmatrix} \mathbf{v}^* \\ p^* \end{bmatrix} = \begin{bmatrix} -\frac{\partial \mathbf{v}^*}{\partial t} - \mathbf{v}\cdot\left[\boldsymbol{\nabla}\mathbf{v}^* + (\boldsymbol{\nabla}\mathbf{v}^*)^T\right] - \mu\Delta\mathbf{v}^* + \boldsymbol{\nabla} p^* \\ -\boldsymbol{\nabla}\cdot\mathbf{v}^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \text{in } \Omega\times(0,T), \\
\mathbf{v}^* = 0 & \text{at } t = T, \\
\mathbf{v}^* = \mathbf{r}\times(\dot\varphi_{opt}\mathbf{e}_z) + \mathbf{v}_\infty & \text{on } \Gamma
\end{cases}
\end{cases}
$$

- A counterpart of the Euler–Lagrange equation
- Solved with an iterative Gradient Algorithm (e.g., Conjugate Gradients, quasi–Newton, etc.)

An Iterative Optimization Procedure

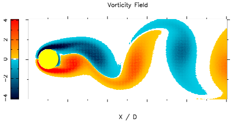
0. provide initial guess $\dot{\varphi}^0$
1. Solve for $\left\{\mathbf{v}(\dot{\varphi}^i); p(\dot{\varphi}^i)\right\}$ on $[0, T]$
2. Solve for $\left\{\mathbf{v}^*(\dot{\varphi}^i); p^*(\dot{\varphi}^i)\right\}$ on $[0, T]$
3. Use $\left\{\mathbf{v}(\dot{\varphi}^i); p(\dot{\varphi}^i)\right\}$ and $\left\{\mathbf{v}^*(\dot{\varphi}^i); p^*(\dot{\varphi}^i)\right\}$ to compute $\nabla\mathcal{J}^i(t)$ on $[0, T]$
4. update control according to $\dot{\varphi}^{i+1}(t) = \dot{\varphi}^i(t) - \alpha_i\gamma_i\left(\nabla\mathcal{J}(t)\right)$
5. iterate 1. through 4. until convergence, i.e. until $\boldsymbol{\nabla} J^i\,(t) \simeq 0$

Primal and Adjoint Simulations for Cylinder Rotation as Control

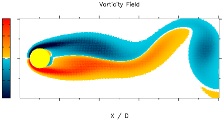


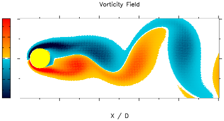
Results

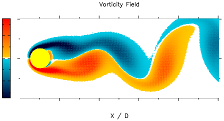
- No Control



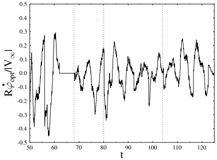
- Flow Pattern Modifications due to Control ($T = 6$)

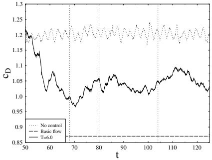


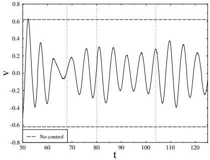




- Optimal Control $\dot{\varphi}_{opt}$, drag coefficient c_D, transverse velocity v



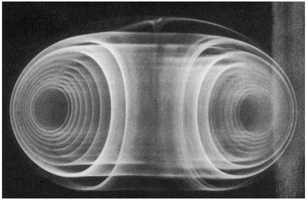




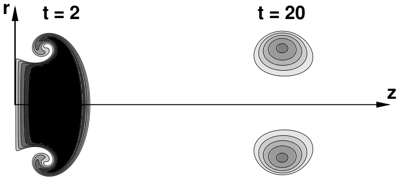
PART II
Inverse Problem of Vortex Reconstruction

joint work Ionut Danaila (Université de Rouen)

- Ubiquitous Vortex Rings



Lim & Nickels, 1995



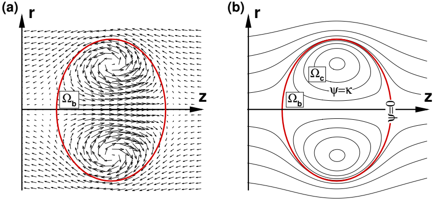
Danaila & Heiles, 2008

- Models of Vortex Rings:
  - based on linearized equations (Kaplanski & Rudi, 1999, 2005)
  - obtained with perturbation techniques (Fukumoto, 2010)
  - inviscid models: Hill's and Norbury-Fraenkel's vortices

- Present Approach:

  OPTIMAL VORTEX RINGS VIA INVERSE FORMULATION

- Inviscid vortex ring in a moving frame of reference



$$\frac{\omega}{r} = \begin{cases} f(\psi) & \text{in} \quad \Omega_b, \\ 0 & \text{elsewhere}, \end{cases}$$

$f(\psi)$ — Vorticity Function (unspecified)

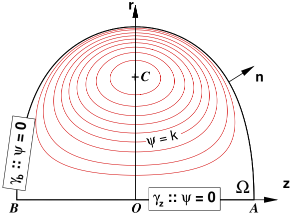
- 3D Axisymmetric Euler System

$$\mathcal{L}\psi = -r\,f(\psi) \quad \text{in } \Omega,$$
$$\psi = 0 \quad \text{on } \gamma.$$

where $\mathcal{L} := \frac{\partial}{\partial z}\left(\frac{1}{r}\frac{\partial}{\partial z}\right) + \frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}\right) = \boldsymbol{\nabla}\cdot\left(\frac{1}{r}\boldsymbol{\nabla}\right)$ and $\boldsymbol{\nabla} := \left[\frac{\partial}{\partial z}, \frac{\partial}{\partial r}\right]^T$.

- Special solutions:
  - $f(\psi) = C$ in Ω_b $\implies$ Hill's vortex
  - $f(\psi) = C\ \forall\psi > k$ and $f(\psi) = 0\ \forall\psi \le k$ $\implies$ Norbury-Fraenkel's vortex

- KEY IDEA: determine vorticity function $f(\psi)$ to match some observation data $\Longrightarrow$ Inverse Problem
- Measurements of the tangential velocity component



$$m := \mathbf{v} \cdot \mathbf{n}^{\perp} = \frac{1}{r}\frac{\partial \psi}{\partial n}$$

on boundary segments γ_z and γ_b

- Cost Functional

$$\mathcal{J}(f) := \frac{\alpha_b}{2}\int_{\gamma_b}\left(\frac{1}{r}\frac{\partial \psi}{\partial n}\bigg|_{\gamma_b} - m\right)^2 d\sigma + \frac{\alpha_z}{2}\int_{\gamma_z}\left(\frac{1}{r}\frac{\partial \psi}{\partial n}\bigg|_{\gamma_z} - m\right)^2 d\sigma,$$

- Variational Minimization Problem: $\boxed{\hat{f} := \operatorname{argmin}_{f \in H^1(\mathcal{I})} \ \mathcal{J}(f)}$
  - nonnegativity constraint $f(\psi) \geq 0 \ \forall \psi$

- Inverse problem with unusual structure — reconstruction of a nonlinear source term $f(\psi)$
- Assumptions
  1. domain: $f : \mathcal{I} \rightarrow \mathbb{R}$, $\mathcal{I} := [0, \psi_{\max}]$ — identifiability interval
  2. smoothness: $f \in H^1(\mathcal{I})$ (square-integrable derivatives)
- Optimality condition: $\forall_{f' \in H^1(\mathcal{I})} \quad \mathcal{J}'(\hat{f}; f') = 0$
- Gradient iterations $\hat{f} = \lim_{k\to\infty} f^{(k)}$

$$
\begin{aligned}
f^{(k+1)} &= f^{(k)} - \tau_k \nabla \mathcal{J}(f^{(k)}), \quad k = 1, 2, \dots \\
f^{(1)} &= f_0,
\end{aligned}
$$

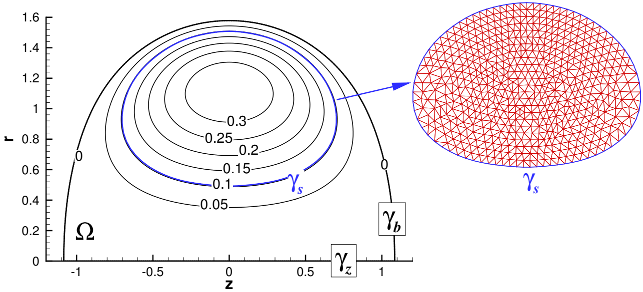
  f_0 — initial guess, τ_k — step seize at k-th iteration
- Positivity enforcement via transformation

$$
f_+ = (1/2)g^2, \qquad \mathcal{J}_g(g) := \mathcal{J}((1/2)g^2)
$$

- Gradient Expression — sensitivity of cost functional $\mathcal{J}(f)$ with respect to perturbations of the vorticity function $f(\psi)$

$$\nabla^{L_2}\mathcal{J}(s) = -\int_{\gamma_s} \psi^* \, r \left(\frac{\partial \psi}{\partial n}\right)^{-1} d\sigma, \quad s \in [0, \psi_{\max}].$$

$\gamma_s := \{\mathbf{x} \in \Omega \, : \, \psi(\mathbf{x}) = s\}$ — streamfunction level sets



- ψ^* — solution of adjoint system

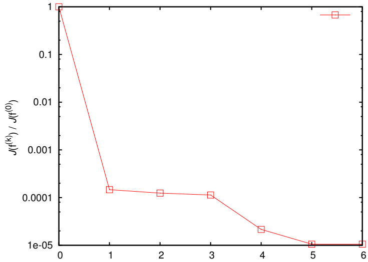
$$\nabla \cdot \left(\frac{1}{r}\nabla\psi^*\right) + rf_\psi(\psi)\,\psi^* = 0 \qquad \text{in } \Omega,$$
$$\psi^* = \alpha_b\left(\frac{1}{r}\frac{\partial\psi}{\partial n}\Big|_{\gamma_b} - m\right) \qquad \text{on } \gamma_b,$$
$$\psi^* = \alpha_z\left(\frac{1}{r}\frac{\partial\psi}{\partial n}\Big|_{\gamma_z} - m\right) \qquad \text{on } \gamma_z,$$

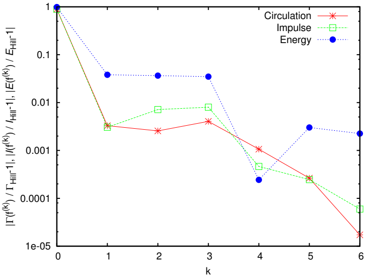
- Smoothness ensured via Sobolev gradients:

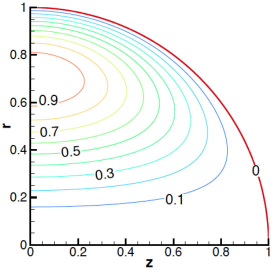
$$\mathcal{J}'(f;f') = \left\langle \nabla^{L_2}\mathcal{J}(f), f'\right\rangle_{L_2(\mathcal{I})} = \left\langle \nabla^{H^1}\mathcal{J}(f), f'\right\rangle_{H^1(\mathcal{I})} \quad \Longrightarrow \quad \begin{aligned} \left(I - \ell^2\frac{d^2}{ds^2}\right)\nabla^{H^1}\mathcal{J} &= \nabla^{L_2}\mathcal{J} && \text{in } \mathcal{I}, \\ \nabla^{H^1}\mathcal{J} &= 0 && \text{at } s = 0, \\ \frac{d}{ds}\nabla^{H^1}\mathcal{J} &= 0 && \text{at } s = \psi_{\max}, \end{aligned}$$

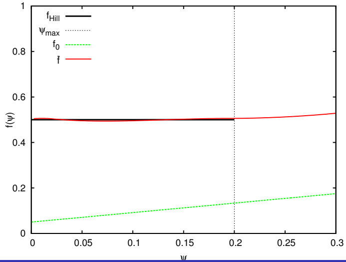
- Algorithm easily implemented in `FreeFEM++`

Reconstruction of Hill's Vortex

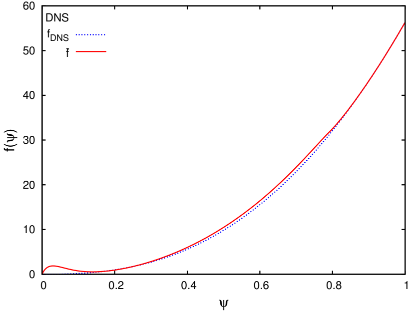


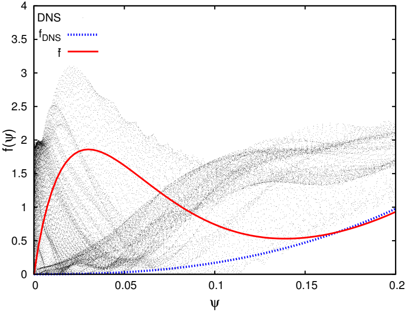






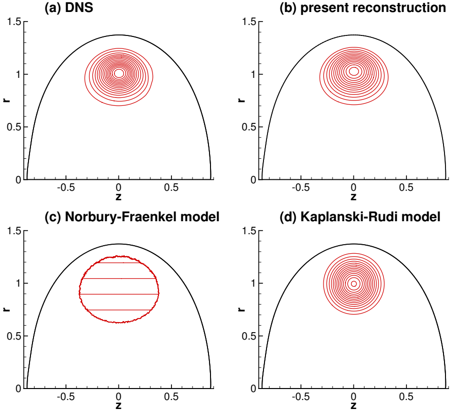
Reconstruction of Vortex Rings from DNS Data ($Re = 17,000$)





$\cdots$ DNS data — $- - -$ empirical fit f_{DNS} — optimal reconstruction $\hat{f}$

Reconstruction of Vortex Rings from DNS Data ($Re = 17,000$)

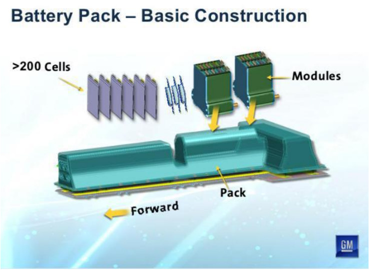


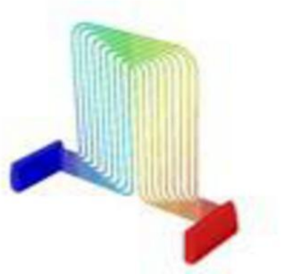
Vorticity distribution in space

PART III
Geometry Optimization in Heat Transfer

joint work Xiaohui Peng and Katya Niakhai
(former Master's students at McMaster)

- PROBLEM: Efficient cooling of a battery system





- GOAL: determine optimal shape of cooling channels for a prescribed heat distribution

- Few mathematically precise results in literature
  $\Longrightarrow$ need to develop new tools

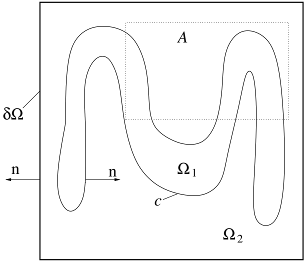
- 2D thermally isolated domain
- time–independent
- heat conduction only
- cooling channel — line heat sink modelled with Newton's law of cooling

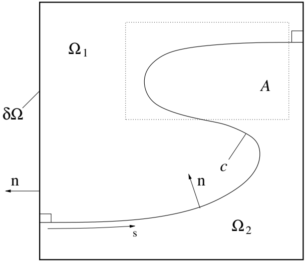
$$S = \gamma(u - u_0)$$

u_0 — temperature of the coolant fluid in the channel modelled by the coil $\mathcal{C}$,

$$u_0(s) = T_a + \frac{T_b - T_a}{L} s, \quad s \in [0, L],$$

- want to maintain prescribed temperature $\overline{u}$ in the subdomain $\mathcal{A}$ (revised optimization objective)





- Governing System

$$
\begin{aligned}
-k\Delta u_1 &= q && \text{in } \Omega_1, \\
-k\Delta u_2 &= q && \text{in } \Omega_2, \\
u_1 &= u_2 && \text{on } \mathcal{C} \\
\frac{\partial u_2}{\partial n} - \frac{\partial u_1}{\partial n} &= \gamma\,(u_1 - u_0) && \text{on } \mathcal{C} \\
\frac{\partial u_2}{\partial n} &= 0 && \text{on } \partial\Omega,
\end{aligned}
$$

where

- Ω_1 — the *interior* of the curve $\mathcal{C}$,
- Ω_2 — the *exterior* of the curve $\mathcal{C}$,
- $u_i(\mathbf{x})$ is the temperature distribution u restricted in the domain Ω_i, for $i = 1, 2$,
- k is the heat conductivity coefficient (a known material property),
- q is the distribution of heat sources (battery heating),
- $\mathbf{n}$ are the unit outer normal on $\mathcal{C}$ and $\partial\,\Omega$

- Assuming:
  - a given distribution of heat sources $q(\mathbf{x})$,
  - heat transfer described by governing equation,
  - a fixed length $L = \oint_{\mathcal{C}} ds$ of the cooling channel $\mathcal{C}$,

  find the *shape* of the curve $\mathcal{C}$ which ensures that over the subdomain $\mathcal{A}$ the actual temperature $u(x, y)$ is as close as possible to the prescribed temperature $\overline{u}$
- Define

$$\mathcal{J}(\mathcal{C}) = \int_A (u - \overline{u})^2 \, d\Omega$$

- Formal statement of optimization problem

$$\boxed{\begin{aligned} &\max_{\mathcal{C}} \ \mathcal{J}(\mathcal{C}), \\ &\text{subject to:} \quad \text{Governing System}, \\ &\qquad\qquad\qquad \oint_{\mathcal{C}} ds = L \end{aligned}}$$

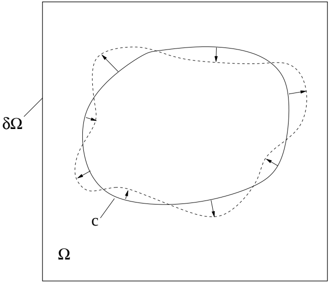
- Optimal shape $\tilde{\mathcal{C}}$ characterized by the condition

$$\mathcal{J}'(\tilde{\mathcal{C}}, \mathbf{Z}) = 0 \quad \text{for all shape perturbations } \mathbf{Z}$$

- Gradient descent algorithm

$$\mathbf{x}_{\mathcal{C}}^{(n+1)} = \mathbf{x}_{\mathcal{C}}^{(n)} - \tau_n \, \mathbf{n} \, \boldsymbol{\nabla} \mathcal{J}(\mathcal{C}^{(n)}), \quad n = 1, 2, \dots,$$
$$\mathbf{x}_{\mathcal{C}}^{(0)} = \mathbf{x}_{\mathcal{C}_0},$$

where $\boldsymbol{\nabla}\mathcal{J}(\mathcal{C}^{(n)})$ is the gradient of the cost functional



- Problem of SHAPE OPTIMIZATION (contour geometry),
- SHAPE CALCULUS: parametrization of geometry

$$\mathbf{x}(t,\mathbf{Z}) = \mathbf{x} + t\mathbf{Z} \qquad \text{for } \mathbf{x} \in \Gamma_{SL}(0),$$

  where $\mathbf{Z} : \Omega_{SL} \to \mathbb{R}^2$ is the perturbation "velocity" field.
- Gâteaux Shape Differential

$$\mathcal{J}'(\Gamma_{SL}(0);\mathbf{Z}) \triangleq \lim_{t\to 0} \frac{\mathcal{J}(\Gamma_{SL}(t,\mathbf{Z})) - \mathcal{J}(\Gamma_{SL}(0))}{t}.$$

- Main Theorem [shape–differentiation of integrals w.r.t. the shape of the domain]:

$$\left(\int_{\Omega(t,\mathbf{Z})} f\, d\Omega + \int_{\partial\Omega(t,\mathbf{Z})} g\, ds \right)' = \int_{\Omega(0)} f'\, d\Omega + \int_{\partial\Omega(0)} g'\, ds + \\ + \int_{\partial\Omega(0)} \left(f + \varkappa g + \frac{\partial g}{\partial n} \right) \mathbf{Z}\cdot\mathbf{n}\, ds,$$

- How to compute the gradient $\nabla\mathcal{J}$?

- L_2 Gradient $\nabla^{L_2}\mathcal{J}(\mathcal{C}^{(n)})$ computed as follows

$$\nabla^{L_2}\mathcal{J}(\mathcal{C}^{(n)}) = \frac{\gamma}{k}(u_1 - u_0)\left(\frac{\partial u_1^*}{\partial n} - \kappa\, u_1^*\right) - \frac{\gamma}{k}\frac{\partial u_2}{\partial n}\, u_1^* - \lambda\,\kappa \quad \text{on } \mathcal{C}^{(n)}$$

where u_1^* and u_2^* are solutions of the following ADJOINT SYSTEM

$$\begin{aligned}
k\Delta u_1^* &= (u - \overline{u})\,\chi_{A_1} && \text{in } \Omega_1,\\
k\Delta u_2^* &= (u - \overline{u})\,\chi_{A_2} && \text{in } \Omega_2,\\
u_1^* - u_2^* &= 0 && \text{on } \mathcal{C}^{(n)},\\
k\left(\frac{\partial u_2^*}{\partial n} - \frac{\partial u_1^*}{\partial n}\right) &= -\gamma\, u_1^* && \text{on } \mathcal{C}^{(n)},\\
\frac{\partial u_2^*}{\partial n} &= 0 && \text{on } \partial\Omega_2
\end{aligned}$$

- Optimal step size τ_n computed via line–minimization (using Brent's method)

$$\tau_n = \operatorname{argmin}_{\tau>0}\{\mathcal{J}(\mathcal{C}^{(n)} - \tau\,\nabla\mathcal{J}(\mathcal{C}^{(n)}))\}$$

- Incorporation of the Length Constraint

$$\boxed{\oint_{\mathcal{C}} ds = L_0}$$

- Modified (augmented) cost functional:

$$\mathcal{J}_\alpha(\mathcal{C}) := \mathcal{J}(\mathcal{C}) + \frac{\alpha}{2}\left(\oint_{\mathcal{C}} ds - L_0\right)^2,$$

where $\alpha \in \mathbb{R}$ is a parameter

- After shape–differentiating the constraint, modified gradient

$$\nabla^{L_2}\mathcal{J}_\alpha(\mathcal{C}) = \nabla^{L_2}\mathcal{J}(\mathcal{C}) + \alpha\left(\oint_{\mathcal{C}^{(m)}} ds - L_0\right)\kappa$$

- Gradients obtained using Riesz Representation Theorem

$$\mathcal{J}'(\mathcal{C};\zeta\mathbf{n}) = \left\langle \nabla^{\mathcal{X}}\mathcal{J}, \zeta \right\rangle_{\mathcal{X}(\mathcal{C})}$$

$\mathcal{X}$ — selected Hilbert space

- What is the required regularity of the gradients $\nabla\mathcal{J}$?
  - $\mathbf{x}_{\mathcal{C}}(s)$ must be (at least) continuous
  - L_2 gradients $\nabla^{L_2}\mathcal{J}(\mathcal{C})$ $[\mathcal{X} = L_2(\mathcal{C})]$ may be discontinuous ...

- Need Sobolev Gradients $[\mathcal{X} = H^1(\mathcal{C})]$

$$\left\langle \nabla^{H^1}\mathcal{J}, \zeta \right\rangle_{H^1(\mathcal{C})} = \int_0^L \nabla^{H^1}\mathcal{J}\zeta + \ell^2 \frac{\partial \nabla^{H^1}\mathcal{J}}{\partial s}\frac{\partial \zeta}{\partial s}\, ds, \quad \forall_{\zeta\in H^1(\mathcal{C})}$$

$$\Longrightarrow \begin{cases} \left(1 - \ell^2 \dfrac{\partial^2}{\partial s^2}\right) \nabla^{H^1}\mathcal{J} = \nabla^{L_2}\mathcal{J} & \text{on } (0, L), \\ \text{Periodic boundary conditions} & \text{(P1)}, \\ \dfrac{\partial}{\partial s}\nabla^{H^1}\mathcal{J}\Big|_{s=0,L} = 0 & \text{(P2)}. \end{cases}$$

- Reformulation of the Governing System:

$$u = u_p + u_h \quad \text{in } \Omega,$$

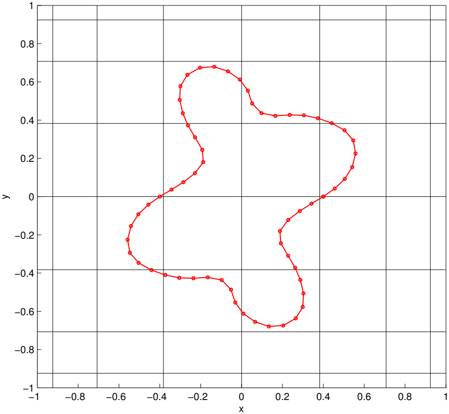
where $\forall_{\mathbf{x}\in\Omega\backslash\mathcal{C}} \quad u_h(\mathbf{x}) = -\frac{1}{2\pi}\oint_{\mathcal{C}} \ln|\mathbf{x}-\mathbf{x}_{\mathcal{C}}|\,\mu(\mathbf{x}_{\mathcal{C}})\,d\sigma.$

- The new dependent variables $\{u_p(\mathbf{x}),\, \mathbf{x}\in\Omega; \mu(\mathbf{x}), \mathbf{x}\in\mathcal{C}\}$ satisfy

$$\begin{aligned} -k\,\Delta\, u_p &= q && \text{in } \Omega, \\ \mu(\mathbf{x}) + \frac{\gamma}{2\pi\, k}\oint_{\mathcal{C}} \ln|\mathbf{x}-\mathbf{x}_{\mathcal{C}}|\,\mu(\mathbf{x}_{\mathcal{C}})\,d\sigma &= \frac{\gamma}{k}(u_p + u_h - u_0) && \text{on } \mathcal{C}, \\ \frac{\partial u_p}{\partial n} &= -\frac{\partial u_h}{\partial n} && \text{on } \partial\Omega. \end{aligned}$$

- Analogously for the Adjoint System with $\{u_p^*(\mathbf{x}),\, \mathbf{x}\in\Omega; \mu^*(\mathbf{x}), \mathbf{x}\in\mathcal{C}\}$

- Two coupled subproblems:
  - Poisson equation for u_p (resp., u_p^*)
  - Singular Boundary Integral Equation for μ (resp., μ^*)



- Optimal discretization for each subproblem:
  - spectral Chebyshev method for u_p (resp., u_p^*) in Ω

$$\mathbf{\Delta}^N \mathbf{U} = \mathbf{f} + \mathbf{q},$$

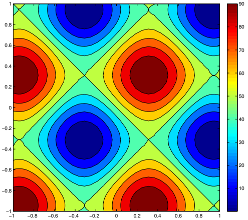
  - spectral boundary-integral method with an analytic treatment of the singular kernel for μ (resp., μ^*) on $\mathcal{C}$

$$\left(\mathbf{I} + \frac{\gamma}{k}\mathbf{K}_1 + \frac{\gamma}{k}\mathbf{K}_2\right)\mathbf{m} + \frac{\gamma}{k}\mathbf{P}\mathbf{U} = \frac{\gamma}{k}\, u_0 \mathbf{1},$$

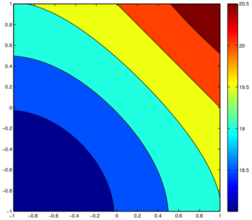
  - spectral interpolation $\mathbf{P}$ to couple u_p and μ (resp., u_p^* and μ^*)

$$\begin{bmatrix} -\mathbf{\Delta}^N & \mathbf{B} \\ \frac{\gamma}{k}\mathbf{P} & \mathbf{I} + \frac{\gamma}{k}\mathbf{K}_1 + \frac{\gamma}{k}\mathbf{K}_2 \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{m} \end{bmatrix} = \frac{1}{k} \begin{bmatrix} \mathbf{q} \\ \gamma\, u_0\, \mathbf{1} \end{bmatrix}.$$

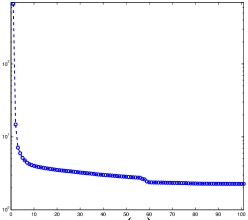
CASE I: $\alpha = 0$



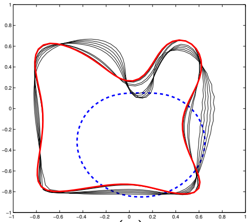
$q(x, y)$



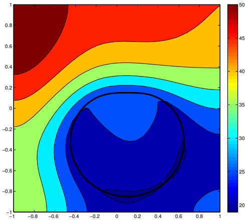
$\overline{u}$



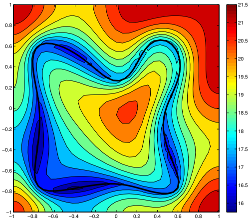
$\mathcal{J}(\mathcal{C}^{(m)})$



$\mathcal{C}^{(m)}$

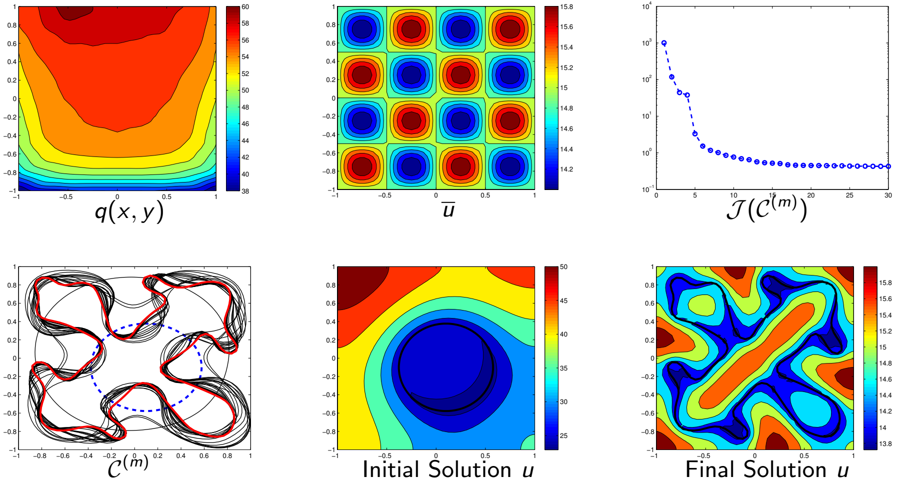


Initial Solution u

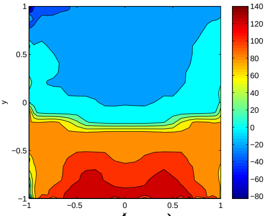


Final Solution u

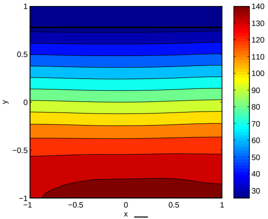
CASE II: $\alpha = 0$



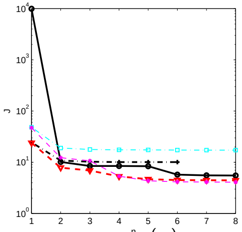
CASE III: $\alpha = 0, 1, 10, 10^2, 10^3$; $L_0 = 2.3$



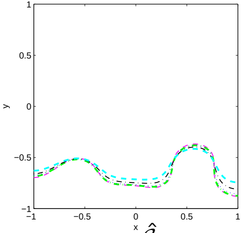
$q(x, y)$



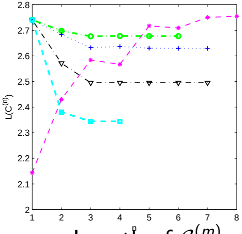
$\overline{u}$



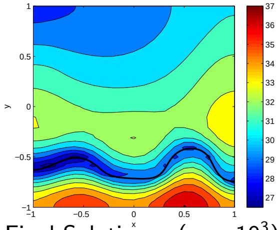
$\mathcal{J}(\mathcal{C}^{(m)})$



$\hat{\mathcal{C}}$



Length of $\mathcal{C}^{(m)}$



Final Solution u ($\alpha = 10^3$)

Conclusions

- Formulation of PDE control and estimation problems as constrained optimization
  - PDE–constrained gradients via Adjoint Equations
  - Vorticity form of the adjoint equations
  - Optimization of free boundary problems via shape–differential calculus
- Inverse Problem of Vortex Reconstruction
  - Nonintuitive insights revealed by reconstruction from DNS data
  - Big Question: what are the fundamental accuracy limits for representation of real flows in terms of inviscid models?
- Shape-optimization approach for a model of 2D steady heat transfer
  - Shape calculus
  - Spectrally-accurate solution of the governing and adjoint PDE systems

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- References Part III — Shape Optimization:
  - X. Peng, K. Niakhai and B. Protas, "A Method for Geometry Optimization in a Simple Model of Two-Dimensional Heat Transfer", *SIAM Journal on Scientific Computing* **35**, B1105–B1131, 2013.