Numerical Optimization of Partial Differential Equations

Part III: applications

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Optimal Open–Loop Control
   PDE–Constrained Optimization
   Determination of the Gradient $\nabla J$ via Adjoint System
   Results

Inverse Problem of Vortex Reconstruction
   Euler System & Inverse Formulation
   Solution Approach
   Results

Geometry Optimization in Heat Transfer
   Motivation & Mathematical Model
   Optimization Problem
   Results
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 \( \dot{\varphi}_{opt} = \arg\min_{\varphi} \mathcal{J}(\varphi) \), where

\[
\mathcal{J}(\varphi) = \frac{1}{2} \int_{0}^{T} \left\{ \left[ \text{power related to the drag force} \right] + \left[ \text{power needed to control the flow} \right] \right\} dt
\]

\[
= \frac{1}{2} \int_{0}^{T} \int_{\Gamma_0} \left\{ \left[ p(\dot{\varphi})n - \mu n \cdot D(v(\dot{\varphi})) \right] \cdot \left[ \dot{\varphi} (e_z \times r) + v_\infty \right] \right\} d\sigma dt
\]

Subject to:

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

- Constrained optimization problem

\[
\begin{aligned}
\min_{(x,\varphi)} \tilde{J}(x, \varphi) \\
S(x(\varphi), \varphi) = 0
\end{aligned}
\]

- Equivalent \textbf{UNCONSTRAINED} optimization problem (note that \(x = x(\varphi)\))

\[
\min_{\varphi} \tilde{J}(x(\varphi), \varphi) = \min_{\varphi} J(\varphi)
\]

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

\[
\forall \varphi' \in \mathcal{U} \quad \mathcal{J}'(\varphi; \varphi') = (\nabla \mathcal{J}, \varphi')_{\mathcal{U}} = 0,
\]

with the \textbf{Gâteaux differential}

\[
\mathcal{J}'(\varphi; \varphi') = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} [\mathcal{J}(\varphi + \varepsilon \varphi') - \mathcal{J}(\varphi)].
\]
Abstract Framework (II)

- Minimization of $J(\varphi)$ with a **descent algorithm** in $U$ \(\implies\) solution to a **steady state** of the ODE in $U$

\[
\begin{cases}
\frac{d\varphi}{d\tau} = -Q \nabla \varphi J(\varphi) & \text{on } \tau \in (0, \infty) \text{ (pseudo–time)}, \\
\varphi = \varphi_0 & \text{at } \tau = 0.
\end{cases}
\]

- 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
The cost functional:

\[ J(\dot{\varphi}) = \frac{1}{2} \int_{0}^{T} \left\{ \begin{array}{l}
\text{power related to the drag force} \\
\text{power needed to control the flow}
\end{array} \right\} dt 
\]

\[ = \frac{1}{2} \int_{0}^{T} \int_{\Gamma_0} \left\{ [p(\varphi)n - \mu n \cdot D(v(\varphi))] \cdot [\varphi(e_z \times r) + v_\infty] \right\} d\sigma dt, \]

Expression for the Gâteaux differential:

\[ J'(\dot{\varphi}; h) = \frac{1}{2} \int_{0}^{T} \int_{\Gamma_0} \left\{ [p'(h)n - \mu n \cdot D(v'(h))] \cdot [\varphi(e_z \times r) + v_\infty] + \\
[p(\varphi)n - \mu n \cdot D(v(\varphi))] \cdot (e_z \times r) h \right\} d\sigma dt = B_1 \]

\[ = (\nabla J(t), h)_{L^2([0,T])} \]

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

How to calculate the \textbf{Gradient} \( \nabla J \)?
Sensitivities and Adjoint States

- The linearized perturbation system

\[
\begin{aligned}
\mathcal{N} \begin{bmatrix} v' \\ p' \end{bmatrix} &= \begin{bmatrix} \frac{\partial v'}{\partial t} + (v \cdot \nabla) v' + (v' \cdot \nabla) v - \mu \Delta v' + \nabla p' \\ -\nabla \cdot v' \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{in } \Omega \times (0, T), \\
v' &= 0 \\
v' &= h_T 
\end{aligned}
\]

- Duality pairing defining the adjoint operator

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

- The adjoint system (TERMINAL VALUE PROBLEM!!)

\[
\begin{aligned}
\mathcal{N}^* \begin{bmatrix} v^* \\ p^* \end{bmatrix} &= \begin{bmatrix} -\frac{\partial v^*}{\partial t} - v \cdot [\nabla v^* + (\nabla v^*)^T] - \mu \Delta v^* + \nabla p^* \\ -\nabla \cdot v^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{in } \Omega \times (0, T), \\
v^* &= 0 \\
v^* &= r \times (\dot{\varphi} e_z) + v_\infty \quad \text{on } \Gamma \times (0, T)
\end{aligned}
\]
Cost Functional Gradient

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

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

Identification of the COST FUNCTIONAL GRADIENT

\[ \mathcal{J}'(\dot{\varphi}; h) = (\nabla \mathcal{J}(t), h)_{L^2([0,T])} = \int_0^T \nabla \mathcal{J}(t) \, h \, dt \]

\[ \nabla \mathcal{J}(t) = \frac{1}{2} \int_\Gamma \left\{ \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{v}^*) \cdot \mathbf{\tau} + \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{v}(\varphi)) \cdot (\mathbf{e}_z \times \mathbf{r}) \right\} \, d\sigma \]
Optimality (KKT) system

- Complete optimality system for \( \dot{\phi}_{opt}, [v_{opt}, p_{opt}] \), and \([v^*, p^*]\)

\[
\frac{1}{2} \int_{\Gamma} \left\{ \mu R n \cdot D(v^*) \cdot \tau + \mu n \cdot D(v(\dot{\phi}_{opt})) \cdot (e_z \times r) \right\} \, d\sigma = 0
\]

\[
\begin{cases}
\frac{\partial v}{\partial t} + (v \cdot \nabla)v - \mu \Delta v + \nabla p = 0 & \text{in } \Omega \times (0, T), \\
v = 0 & \text{at } t = 0, \\
v = \dot{\phi}_{opt} \tau & \text{on } \Gamma \\
N^* \left[ \begin{array}{c} v^* \\ p^* \end{array} \right] = \left[ -\frac{\partial v^*}{\partial t} - v \cdot [\nabla v^* + (\nabla v^*)^T] - \mu \Delta v^* + \nabla p^* \right] = 0 & \text{in } \Omega \times (0, T), \\
v^* = 0 & \text{at } t = T, \\
v^* = r \times (\dot{\phi}_{opt} e_z) + v_\infty & \text{on } \Gamma
\end{cases}
\]

- 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 $\dot{\phi}^0$
1. Solve for $\{\mathbf{v}(\dot{\phi}^i); p(\dot{\phi}^i)\}$ on $[0, T]$
2. Solve for $\{\mathbf{v}^*(\dot{\phi}^i); p^*(\dot{\phi}^i)\}$ on $[0, T]$
3. Use $\{\mathbf{v}(\dot{\phi}^i); p(\dot{\phi}^i)\}$ and $\{\mathbf{v}^*(\dot{\phi}^i); p^*(\dot{\phi}^i)\}$ to compute $\nabla \mathcal{J}^i(t)$ on $[0, T]$
4. update control according to $\dot{\phi}^{i+1}(t) = \dot{\phi}^i(t) - \alpha_i \gamma_i (\nabla \mathcal{J}(t))$
5. iterate 1. through 4. until convergence, i.e. until $\nabla \mathcal{J}^i(t) \simeq 0$
Primal and Adjoint Simulations for Cylinder Rotation as Control
Results

- No Control

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

- Optimal Control $\dot{\phi}_{opt}$, drag coefficient $c_D$, transverse velocity $v$
PART II
Inverse Problem of Vortex Reconstruction

joint work Ionut Danaila (Université de Rouen)
Ubiquitous Vortex Rings

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

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

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

3D Axisymmetric Euler System

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

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

Special solutions:

- \( f(\psi) = C \text{ in } \Omega_b \implies \text{Hill’s vortex} \)
- \( f(\psi) = C \text{ for all } \psi > k \) and \( f(\psi) = 0 \text{ for all } \psi \leq k \implies \text{Norbury-Fraenkel’s vortex} \)
**Key Idea:** determine vorticity function $f(\psi)$ to match some observation data $\implies$ Inverse Problem

Measurements of the tangential velocity component

\[ m := v \cdot n_\perp = \frac{1}{r} \frac{\partial \psi}{\partial n} \]
on boundary segments $\gamma_z$ and $\gamma_b$

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:

\[ \hat{f} := \arg \min_{f \in H^1(\mathcal{I})} \mathcal{J}(f) \]

nonnegativity constraint $f(\psi) \geq 0 \ \forall \psi$
Inverse problem with unusual structure — reconstruction of a nonlinear source term $f(\psi)$

**Assumptions**

1. **domain:** $f : \mathcal{I} \to \mathbb{R}, \mathcal{I} := [0, \psi_{\text{max}}]$ — identifiability interval
2. **smoothness:** $f \in H^1(\mathcal{I})$ (square-integrable derivatives)

**Optimality condition:** $\forall f' \in H^1(\mathcal{I}) \quad J'(\hat{f}; f') = 0$

**Gradient iterations**

$$\hat{f} = \lim_{k \to \infty} f^{(k)}$$

$$f^{(k+1)} = f^{(k)} - \tau_k \nabla J(f^{(k)}), \quad k = 1, 2, \ldots$$

$$f^{(1)} = f_0,$$

$f_0$ — initial guess, $\tau_k$ — step size at $k$-th iteration

**Positivity enforcement via transformation**

$$f_+ = (1/2)g^2, \quad J_g(g) := J((1/2)g^2)$$
Gradient Expression — sensitivity of cost functional $\mathcal{J}(f)$ with respect to perturbations of the vorticity function $f(\psi)$

$$\nabla^2_{L^2} \mathcal{J}(s) = - \int_{\gamma_s} \psi^* r \left( \frac{\partial \psi}{\partial n} \right)^{-1} d\sigma, \quad s \in [0, \psi_{\text{max}}].$$

$$\gamma_s := \{ x \in \Omega : \psi(x) = s \}$$ — streamfunction level sets
ψ* — solution of adjoint system

\[
\nabla \cdot \left( \frac{1}{r} \nabla \psi^* \right) + r f_\psi(\psi) \psi^* = 0 \quad \text{in } \Omega,
\]

\[
\psi^* = \alpha_b \left( \frac{1}{r} \frac{\partial \psi}{\partial n} \bigg|_{\gamma_b} - m \right) \quad \text{on } \gamma_b,
\]

\[
\psi^* = \alpha_z \left( \frac{1}{r} \frac{\partial \psi}{\partial n} \bigg|_{\gamma_z} - m \right) \quad \text{on } \gamma_z,
\]

Smoothness ensured via Sobolev gradients:

\[
\mathcal{J}'(f; f') = \left\langle \nabla^{L_2} \mathcal{J}(f), f' \right\rangle_{L_2(\mathcal{I})} = \left\langle \nabla^{H^1} \mathcal{J}(f), f' \right\rangle_{H^1(\mathcal{I})} \quad \Rightarrow \quad \left( I - \varphi^2 \frac{d^2}{ds^2} \right) \nabla^{H^1} \mathcal{J} = \nabla^{L_2} \mathcal{J} \quad \text{in } \mathcal{I},
\]

\[
\nabla^{H^1} \mathcal{J} = 0 \quad \text{at } s = 0,
\]

\[
\frac{d}{ds} \nabla^{H^1} \mathcal{J} = 0 \quad \text{at } s = \psi_{\max},
\]

Algorithm easily implemented in FreeFEM++
Reconstruction of Hill’s Vortex

\[ \frac{J(f(k))}{J(f(0))} \]

\[ \frac{\Gamma(f(k))}{\Gamma_{\text{Hill}}^{-1}} , \frac{I(f(k))}{I_{\text{Hill}}^{-1}}, \frac{E(f(k))}{E_{\text{Hill}}^{-1}} \]

\[ \psi(\rho) \]

\[ f(\rho) \]

\[ f_0 \]

\[ \frac{f(\psi)}{f_{\text{Hill}}} \]

\[ \frac{\psi_{\max}}{\psi_{\text{Hill}}} \]

\[ f(\psi) \]

\[ f(\rho) \]
Reconstruction of Vortex Rings from DNS Data ($Re = 17,000$)

... DNS data  \[\text{---} \text{ empirical fit } f_{DNS}\] \[\text{---} \text{ optimal reconstruction } \hat{f}\]
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 \(\Rightarrow\) 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

\[ S = \gamma (u - u_0) \]

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

want to maintain prescribed temperature \( \bar{u} \) in the subdomain \( \Omega \) (revised optimization objective)
Governing System

\[-k \Delta u_1 = q \quad \text{in } \Omega_1,
\]
\[-k \Delta u_2 = q \quad \text{in } \Omega_2,
\]
\[u_1 = u_2 \quad \text{on } C
\]
\[\frac{\partial u_2}{\partial n} - \frac{\partial u_1}{\partial n} = \gamma (u_1 - u_0) \quad \text{on } C
\]
\[\frac{\partial u_2}{\partial n} = 0 \quad \text{on } \partial \Omega,
\]

where

- $\Omega_1$ — the *interior* of the curve $C$,
- $\Omega_2$ — the *exterior* of the curve $C$,
- $u_i(x)$ is the temperature distribution $u$ restricted in the domain $\Omega_i$, for $i = 1, 2$,
- $k$ is the heat conductivity coefficient (a known material property),
- $q$ is the distribution of heat sources (battery heating),
- $n$ are the unit outer normal on $C$ and $\partial \Omega$.
Assuming:
- a given distribution of heat sources \( q(x) \),
- heat transfer described by governing equation,
- a fixed length \( L = \oint_C ds \) of the cooling channel \( C \),

find the shape of the curve \( C \) which ensures that over the subdomain \( A \) the actual temperature \( u(x, y) \) is as close as possible to the prescribed temperature \( \bar{u} \).

Define
\[
\mathcal{J}(C) = \int_A (u - \bar{u})^2 \, d\Omega
\]

Formal statement of optimization problem
\[
\max_C \mathcal{J}(C),
\]
subject to: Governing System,
\[
\oint_C ds = L
\]
Optimal shape $\tilde{C}$ characterized by the condition

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

Gradient descent algorithm

$$x_C^{(n+1)} = x_C^{(n)} - \tau_n \mathbf{n} \nabla J(C^{(n)}), \quad n = 1, 2, \ldots,$$

$$x_C^{(0)} = x_{C_0},$$

where $\nabla J(C^{(n)})$ is the gradient of the cost functional.
Problem of **SHAPE OPTIMIZATION** (contour geometry),

**SHAPE CALCULUS**: parametrization of geometry

\[ x(t, \mathbf{Z}) = x + t\mathbf{Z} \quad \text{for} \quad x \in \Gamma_{SL}(0), \]

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]:

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

How to compute the gradient \( \nabla \mathcal{J} \) ?
L₂ Gradient \( \nabla^{L₂} J(C^{(n)}) \) computed as follows

\[
\nabla^{L₂} J(C^{(n)}) = \frac{\gamma}{k}(u₁ - u₀) \left( \frac{\partial u₁^*}{\partial n} - \kappa u₁^* \right) - \frac{\gamma}{k} \frac{\partial u₂}{\partial n} u₁^* - \lambda \kappa \quad \text{on } C^{(n)}
\]

where \( u₁^* \) and \( u₂^* \) are solutions of the following ADJOINT SYSTEM

\[
\begin{align*}
kΔu₁^* &= (u - \overline{u}) \chi_{A_1} \quad \text{in } Ω₁, \\
kΔu₂^* &= (u - \overline{u}) \chi_{A_2} \quad \text{in } Ω₂, \\
u₁^* - u₂^* &= 0 \quad \text{on } C^{(n)}, \\
k \left( \frac{\partial u₂^*}{\partial n} - \frac{\partial u₁^*}{\partial n} \right) &= -\gamma u₁^* \quad \text{on } C^{(n)}, \\
\frac{\partial u₂^*}{\partial n} &= 0 \quad \text{on } ∂Ω₂
\end{align*}
\]

Optimal step size \( τ_n \) computed via line–minimization (using Brent’s method)

\[
τ_n = \arg\min_{τ > 0} \{ J(C^{(n)}) - τ \nabla J(C^{(n)}) \} 
\]
Incorporation of the Length Constraint

\[ \oint_{C} ds = L_0 \]

Modified (augmented) cost functional:

\[ J_\alpha(C) := J(C) + \frac{\alpha}{2} \left( \oint_{C} ds - L_0 \right)^2, \]

where \( \alpha \in \mathbb{R} \) is a parameter

After shape–differentiating the constraint, modified gradient

\[ \nabla^{L^2} J_\alpha(C) = \nabla^{L^2} J(C) + \alpha \left( \oint_{C^{(m)}} ds - L_0 \right) \kappa \]
Gradients obtained using Riesz Representation Theorem

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

\( \mathcal{X} \) — selected Hilbert space

What is the required regularity of the gradients \( \nabla \mathcal{J} \)?

- \( x_C(s) \) must be (at least) continuous
- \( L_2 \) gradients \( \nabla^{L_2} \mathcal{J}(C) \) \( [\mathcal{X} = L_2(C)] \) may be discontinuous ...

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

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

\[
\begin{cases}
\left(1 - \ell^2 \frac{\partial^2}{\partial s^2}\right) \nabla^{H^1} \mathcal{J} = \nabla^{L_2} \mathcal{J} & \text{on } (0, L), \\
\text{Periodic boundary conditions } (P1), \\
\left. \frac{\partial}{\partial s} \nabla^{H^1} \mathcal{J} \right|_{s=0,L} = 0 & (P2).
\end{cases}
\]
Reformulation of the Governing System:

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

where \( \forall x \in \Omega \backslash C \quad u_h(x) = -\frac{1}{2\pi} \oint_C \ln |x - x_C| \mu(x_C) \, d\sigma. \)

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

\[ -k \Delta u_p = q \quad \text{in} \ \Omega, \]

\[ \mu(x) + \frac{\gamma}{2\pi k} \oint_C \ln |x - x_C| \mu(x_C) \, d\sigma = \frac{\gamma}{k} (u_p + u_h - u_0) \quad \text{on} \ C, \]

\[ \frac{\partial u_p}{\partial n} = -\frac{\partial u_h}{\partial n} \quad \text{on} \ \partial\Omega. \]

Analogously for the Adjoint System with \( \{u_p^*(x), x \in \Omega; \mu^*(x), x \in C\} \)
Two coupled subproblems:

- Poisson equation for \( u_p \) (resp., \( u_p^* \))
- Singular Boundary Integral Equation for \( \mu \) (resp., \( \mu^* \))
Optimal discretization for each subproblem:

- spectral Chebyshev method for \( u_p \) (resp., \( u_p^* \)) in \( \Omega \)

\[
\Delta^N U = f + q,
\]

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

\[
\left( I + \frac{\gamma}{k} K_1 + \frac{\gamma}{k} K_2 \right) m + \frac{\gamma}{k} P U = \frac{\gamma}{k} u_0 1,
\]

- spectral interpolation \( P \) to couple \( u_p \) and \( \mu \) (resp., \( u_p^* \) and \( \mu^* \))

\[
\begin{bmatrix}
-\Delta^N & B \\
\frac{\gamma}{k} P & I + \frac{\gamma}{k} K_1 + \frac{\gamma}{k} K_2
\end{bmatrix}
\begin{bmatrix}
U \\
m
\end{bmatrix} = \frac{1}{k}
\begin{bmatrix}
q \\
\gamma u_0 1
\end{bmatrix}.
\]
CASE I: $\alpha = 0$

- $q(x, y)$
- $\overline{u}$
- $\mathcal{J}(C^{(m)})$
- $C^{(m)}$
- Initial Solution $u$
- Final Solution $u$
CASE II: $\alpha = 0$

- $q(x, y)$
- $\bar{u}$
- $J(C^{(m)})$
- $C^{(m)}$
- Initial Solution $u$
- Final Solution $u$
CASE III: $\alpha = 0, 1, 10, 10^2, 10^3; L_0 = 2.3$
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
References Part I — Open–Loop Control:

References Part II — Inverse Problem of Vortex Reconstruction:

References Part III — Shape Optimization: