Optimal Reconstruction of Constitutive Relations in Complex Multiphysics Systems

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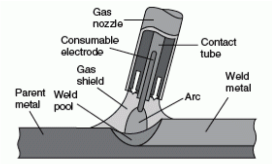
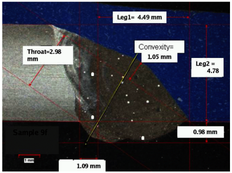
Agenda

1. Introduction
   - Motivation
   - Model Problem
   - Differentiability of Map $\mu \to T$
2. Parameter Estimation as Optimization Problem
   - Formulation
   - Adjoint Equations and Gradients
   - Algorithm
3. Computational Results
   - Set–Up
   - Validation of Gradients
   - Reconstruction Results

Modeling & Optimization of Thermo–Fluid Phenomena

- Application: Welding in Automotive Industry





- Problem: Unknown Material Properties of Alloys in Liquid Phase
  - viscosity $\mu(T)$
  - thermal conductivity $k(T)$
  - electric conductivity $\sigma(T)$
  - surface tension $\gamma(T)$

  } all functions of temperature T

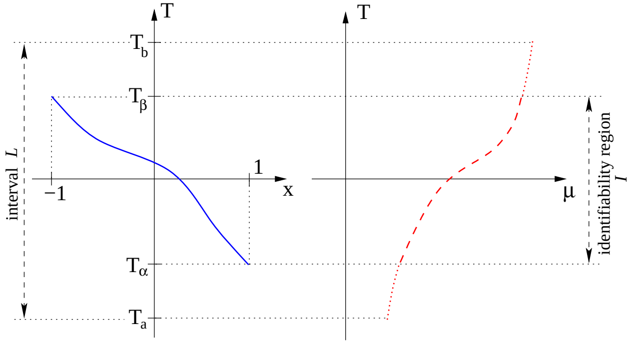
- Goal: Reconstruct $\mu(T)$, $K(T)$, $\sigma(T)$, $\gamma(T)$, etc., based on available measurements

Parameter Estimation as Optimization Problem

Two distinct formulations of an inverse problem of the parameter estimation:

a) material properties dependent on the **space** variable, i.e., the **independent** variable, and

b) material properties dependent on the **state** variable, i.e., the **dependent** variable (very few results in the literature)



Problem

Develop and validate a computational method for reconstruction of state–dependent material properties based on incomplete and noisy measurements

- **Strategy:**
  - Inverse problem formulated as **partial differential equation (PDE)–constrained optimization** problem which can be solved using an **adjoint–based gradient method**.
  - Implement an **"optimize–then–discretize"** approach where the optimality conditions and the optimization algorithm are both formulated based on the **continuous (PDE)** setting.
- **Earlier Work: Chavent & Lemonnier (1974, in French)**
  - Existence of solutions, gradients $\boldsymbol{\nabla}\mathcal{J}$ discontinuous and difficult to compute, reconstruction on the identifiability interval only
- **Our Main Contributions:**
  - Developed an efficient computational approach to evaluate cost functional gradients using adjoint variables
  - Extension of reconstruction beyond the Identifiability Region $\mathcal{I}$

Result of Chavent & Lemonnier (1974)

Posons pour cela:

$$\phi(x,t) = \sum_{i=1}^{n} \frac{\partial y}{\partial x_i}(x,t) \frac{\partial p}{\partial x_i}(x,t) \qquad \phi \in L^1(Q). \tag{80}$$

Pour tout $\zeta \in \mathbb{R}$ posons:

$$Q_\zeta = \{(x,t) \in Q \,|\, y(x,t) \geq \zeta\} \tag{81}$$

$$\gamma(\zeta) = \int_{Q_\zeta} \phi(x,t)\,dx\,dt \tag{82}$$

L'ensemble Q_ζ est défini à un ensemble de mesure nulle près, mais la fonction $\gamma(\zeta)$ est définie sans équivoque.

On a alors le

Théorème 8. *Avec les hypothèses et notations du théorème* 7, *plus* (80) *à* (82), *la fonction* γ *définie en* (82) *est bornée et continue sur* R. *Elle définit en particulier une distribution sur* R, *et on a*

$$\begin{cases} \forall \delta a \in \mathscr{a}: \\ J'(a)\delta a = \left\langle \dfrac{d\gamma}{d\zeta}, \delta a \right\rangle. \end{cases} \tag{83}$$

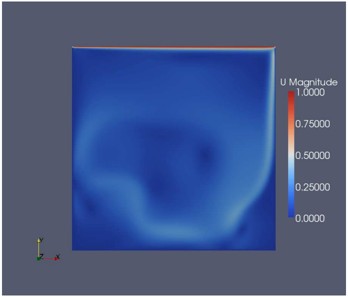
Démonstration: Pour tout $\zeta \in R$ on a: $|\gamma(\zeta)| \leq \|\phi\|_{L^1(Q)}$, donc γ est bornée sur $\mathbb{R}$. Posons:

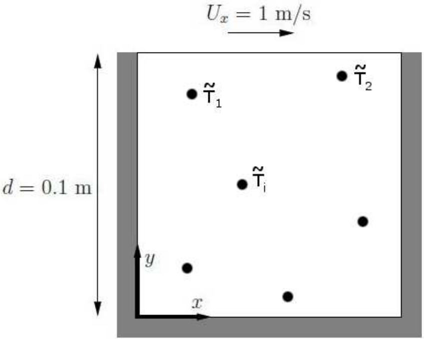
$$Y(\zeta) = \begin{cases} 1 \;\; si \;\; \zeta \geq 0 \\ 0 \;\; si \;\; \zeta < 0 \end{cases} \qquad \forall \zeta \in \mathbb{R}.$$

Alors en notant y *un* représentant de la classe de fonctions y, (82) se réécrit:

$$\gamma(\zeta) = \int_Q Y(y(x,t) - \zeta)\phi(x,t)\,dx\,dt. \tag{84}$$

- **Model System:** Unsteady Mass, Momentum & Energy Transfer
- **Geometry:** 2D Lid–Driven Cavity Problem with Heat Transfer





- **Measurements:** (pointwise) temperature measurements $\{\tilde{T}_i\}_{i=1}^{M}$ at a number of points $\{\mathbf{x}_i\}_{i=1}^{M}$ in the domain Ω

- **Governing System:**
  - Navier–Stokes equation with temperature–dependent viscosity
  - Energy equation

$$
\begin{aligned}
\partial_t \mathbf{u} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla} p - \boldsymbol{\nabla}\cdot\left[\mu(T)[\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T]\right] &= 0 && \text{in } \Omega,\\
\boldsymbol{\nabla}\cdot\mathbf{u} &= 0 && \text{in } \Omega,\\
\partial_t T + \mathbf{u}\cdot\boldsymbol{\nabla} T + \boldsymbol{\nabla}\cdot[k\boldsymbol{\nabla} T] &= 0 && \text{in } \Omega.
\end{aligned}
$$

subject to

$$
\begin{aligned}
\mathbf{u} &= 0 && \text{on } \partial\Omega,\\
T &= T_b && \text{on } \partial\Omega,\\
\mathbf{u}(0) &= \mathbf{u}_0, && T(0) = T_0.
\end{aligned}
$$

- **Goal:** Reconstruct $\mu(T)$ based on temperature measurements $\{\tilde{T}_i\}_{i=1}^M$ inside the domain Ω
- **Remark:** $\mu(T) > 0$ required for well–posedness ($\Rightarrow$ second principle of thermodynamics)

Differentiability of Map $\mu \rightarrow T$

Simplified Model: solving parameter estimation problem for

$$\begin{aligned} -\boldsymbol{\nabla} \cdot [\mu(T)\, \boldsymbol{\nabla} T] &= g \quad \text{in } \Omega, \\ T &= T_0 \quad \text{on } \partial\Omega. \end{aligned} \tag{1}$$

is equivalent in a suitably–defined variational (weak) setting to finding the solution to the operator equation

$$\mathcal{F}(\mu) = T, \tag{2}$$

where $\mathcal{F} : \mathcal{K} \rightarrow L_2(\Omega)$ and $\mathcal{K}$ is the set of constitutive relations

$$\mathcal{K} = \{\mu(T) \text{ piecewise } C^1 \text{ on } \mathcal{L};\ 0 < m_k < \mu(T) < M_k,\ \forall\, T \in \mathcal{L}\}.$$

Theorem

Assume that m_k is sufficiently large and solutions of (1) satisfy $\|\boldsymbol{\nabla} T\|_{L^\infty(\Omega)} < \infty$. Then the map $\mu \rightarrow T(\cdot; k)$ from $\mathcal{K}$ to $L_2(\Omega)$ is Fréchet–differentiable in the norm $H^1(\mathcal{I})$.
[Proof: see Bukshtynov, Volkov & Protas (2011)]

Reformulation as Minimization Problem:

- Define cost functional $\mathcal{J} : \mathcal{X} \to \mathbb{R}$ as

$$\mathcal{J}(\mu) \triangleq \frac{1}{2} \int_0^{t_f} \sum_{i=1}^{M} \left[T(\mathbf{x}_i; \mu) - \tilde{T}_i \right]^2$$

- Optimal reconstruction $\hat{\mu}$ obtained as an unconstrained minimizer of cost functional $\mathcal{J}$

$$\hat{\mu} = \underset{\mu \in \mathcal{X}}{\operatorname{argmin}} \, \mathcal{J}(\mu)$$

  [positivity condition $\mu(T) > 0$ not taken into account yet]

- Minimizer $\hat{\mu}$ computed with the gradient descent algorithm as $\hat{\mu} = \lim_{n\to\infty} \mu^{(n)}$, where

$$\begin{cases} \mu^{(n+1)} & = \mu^{(n)} - \tau^{(n)} \nabla_{\mu} \mathcal{J}(\mu^{(n)}), \qquad n = 1, \dots \\ \mu^{(1)} & = \mu_0 \end{cases}$$

Computation of cost functional gradient $\nabla_\mu \mathcal{J}(\mu)$:

1. Direct problem

$$\begin{aligned} \partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p - \nabla\cdot\left[\mu(T)[\nabla\mathbf{u} + (\nabla\mathbf{u})^T]\right] &= 0 && \text{in } \Omega,\\ \nabla\cdot\mathbf{u} &= 0 && \text{in } \Omega,\\ \partial_t T + \mathbf{u}\cdot\nabla T - \nabla\cdot[k\nabla T] &= 0 && \text{in } \Omega. \end{aligned}$$

2. Adjoint problem

$$\begin{aligned} -\partial_t \mathbf{u}^* - \mathbf{u}\cdot\nabla\mathbf{u}^* - \nabla\cdot\sigma^* + \mathbf{u}^*\cdot(\nabla\mathbf{u})^T + T^*\nabla T &= 0 && \text{in } \Omega,\\ \nabla\cdot\mathbf{u}^* &= 0 && \text{in } \Omega, \end{aligned}$$

$$-\partial_t T^* - \mathbf{u}\cdot\nabla T^* - \nabla\cdot[k\nabla T^*] + \frac{d\bar{\mu}}{dT}(T)[\nabla\mathbf{u}^* + (\nabla\mathbf{u}^*)^T] : \nabla\mathbf{u} =$$

$$= \sum_{i=1}^{M}[T(\mathbf{x}_i;\mu) - \tilde{T}_i]\delta(\mathbf{x} - \mathbf{x}_i) \quad \text{in } \Omega.$$

3. Cost functional (integration over level sets $T(\mathbf{x}) = s$)

$$\nabla_\mu^{L_2}\mathcal{J}(s) = -\int_0^{t_f}\int_\Omega \delta(T(\mathbf{x}) - s)[\nabla\mathbf{u}^* + (\nabla\mathbf{u}^*)^T] : \nabla\mathbf{u}\; d\mathbf{x}\, d\tau.$$

Ensuring Smoothness of Reconstructed Constitutive Relations:

1. Since constitutive relations must possess some smoothness, i.e.,

$$\mathcal{K} = \{\mu(T) \text{ piecewise } C^1 \text{ on } \mathcal{L};\; 0 < m_k < \mu(T) < M_k,\; \forall\, T \in \mathcal{L}\},$$

   the "classical" L_2 gradients may (and in fact do!) lead to discontinuities in $\mu(T)$

2. From mathematical analysis: $\mu \in H^1(\mathcal{L})$ (Sobolev space)

3. By Riesz Representation Theorem, Sobolev gradient $\nabla_\mu^{H^1}\mathcal{J}$ obtained form $\nabla_\mu^{L_2}\mathcal{J}$ through an elliptic boundary–value problem (with T an independent variable)

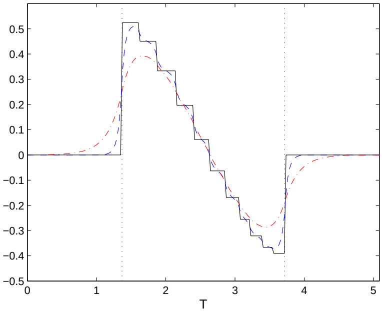
Variant 1

$$\begin{aligned} \nabla_k^{H^1}\mathcal{J} - l^2\frac{d^2}{ds^2}\nabla_k^{H^1}\mathcal{J} &= \nabla_k^{L_2}\mathcal{J} && \text{on } (T_a, T_b), \\ \frac{d}{ds}\nabla_k^{H^1}\mathcal{J} &= 0 && \text{for } s = T_a, T_b \end{aligned}$$

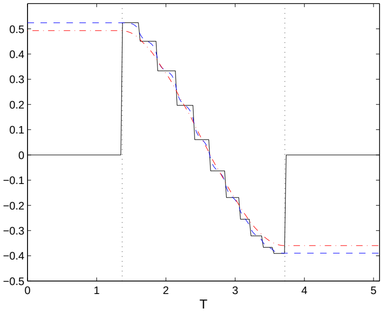
Variant 2

$$\begin{aligned} \nabla_k^{H^1}\mathcal{J} - l^2\frac{d^2}{ds^2}\nabla_k^{H^1}\mathcal{J} &= \nabla_k^{L_2}\mathcal{J} && \text{on } (T_\alpha, T_\beta), \\ \frac{d}{ds}\nabla_k^{H^1}\mathcal{J} &= 0 && \text{for } s = T_\alpha, T_\beta, \\ \nabla_k^{H^1}\mathcal{J}(s) &= \nabla_k^{H^1}\mathcal{J}(T_\alpha) && \text{for } s \in [T_a, T_\alpha], \\ \nabla_k^{H^1}\mathcal{J}(s) &= \nabla_k^{H^1}\mathcal{J}(T_\beta) && \text{for } s \in [T_\beta, T_b] \end{aligned}$$

L_2 vs. H^1 Gradients as Functions of T



Variant 1



Variant 2

(blue) $l = 0.05$, (red) $l = 0.2$

Computational Algorithm:

0. provide initial guess $\mu^{(0)}(s)$
1. Solve governing system for $\{\mathbf{u}, T\}$
2. Solve adjoint system for $\{\mathbf{u}^*, T^*\}$
3. Use $\mathbf{u}$ and $\mathbf{u}^*$ to compute $\boldsymbol{\nabla}_\mu^{H^1}\mathcal{J}$
4. update the constitutive relation according to
$$\mu^{(n+1)} = \mu^{(n)} - \tau^{(n)}\boldsymbol{\nabla}_\mu\mathcal{J}(\mu^{(n)})$$
5. iterate 1. through 4. until convergence, i.e. until $\boldsymbol{\nabla}_\mu^{H^1}\mathcal{J} \simeq 0$

Set up for Numerical Simulations

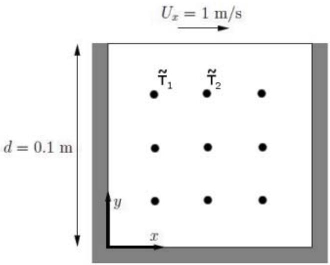
- algebraic expressions for **viscosity** $\mu(T)$

$$\mu(T) = C_1 e^{C_2/(C_3+T)} \quad (Arrhenius)$$
$$\mu(T) = C_1 e^{C_2/T} \quad (Andrade)$$

  with $C_1 = \frac{U_{max}}{Re}$ and $C_2 = 10^{-3} \div 10^3$

- for simplicity, **thermal conductivity** $k = 0.002 = const$
- $Re = 100$
- **geometry:** 2D lid–driven cavity flow
- **boundary conditions**
  top boundary: $u_x = U = 1,\ u_y = 0,$
  $T = 500$
  other boundaries: : $u_x = u_y = 0,\ T = 300$

- **"synthetic" temperature measurements:** 9 thermal sensors uniformly distributed inside the cavity to capture the temperature corresponding to unknown $\mu(T)$



Direct and Adjoint Fields: Vorticity

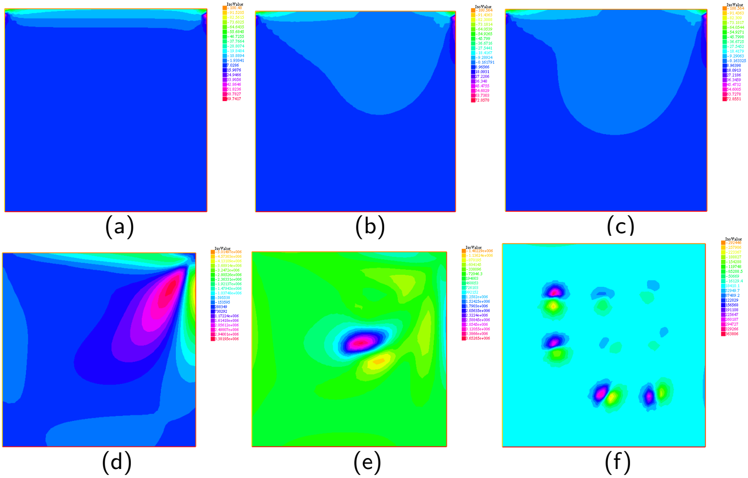


Figure: ω (a,b,c), ω^* (d,e,f) for $t = 0.2$ (a,d), $t = 3.0$ (b,e), $t = 5.8$ (c,f)

Direct and Adjoint Fields: Temperature

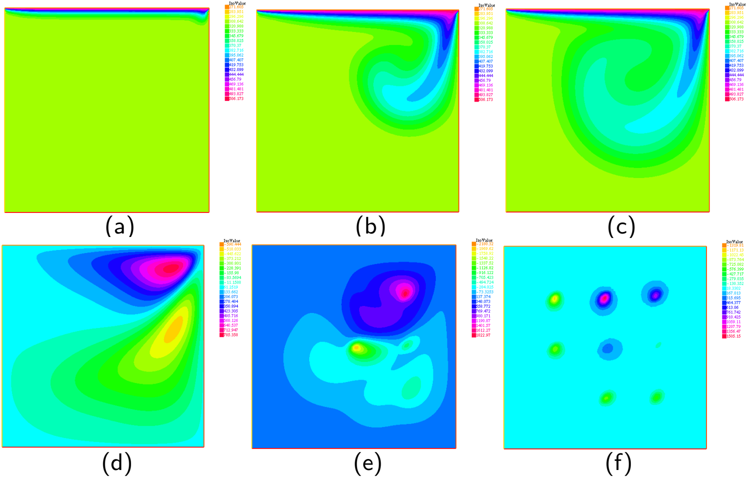
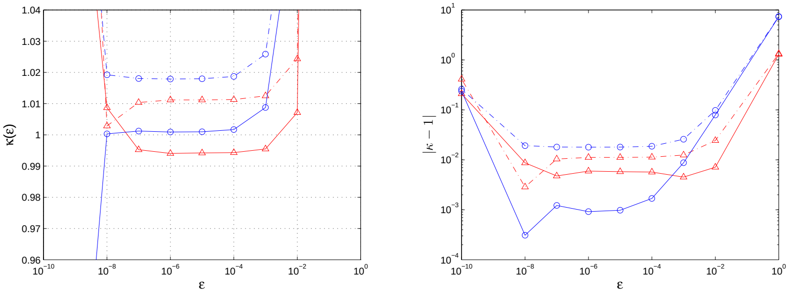


Figure: T (a,b,c), T^* (d,e,f) for $t = 0.2$ (a,d), $t = 3.0$ (b,e), $t = 5.8$ (c,f)

Validation of Gradients



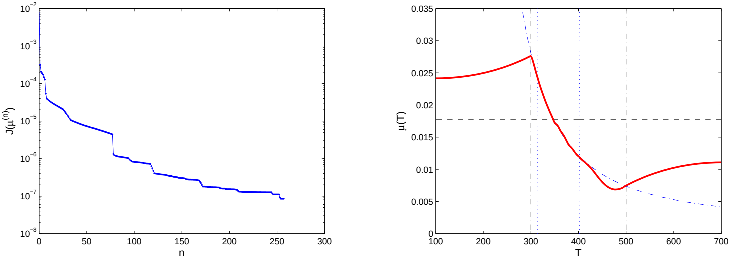
- Directional differential $\mathcal{J}'(\mu;\mu')$ obtained in two ways: finite–difference approximation and using adjoint field, ratio

$$\kappa(\epsilon) \triangleq \frac{\epsilon^{-1}\left[\mathcal{J}(\mu+\epsilon\mu')-\mathcal{J}(\mu)\right]}{\int_{-\infty}^{+\infty}\boldsymbol{\nabla}_{\mu}\mathcal{J}(s)\,\mu'(s)\,ds}$$

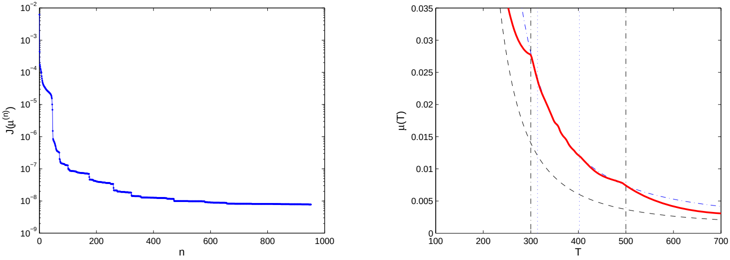
red and blue denote different perturbations μ'

- Note that $\kappa \to 1$ as $\Delta t \to 0$

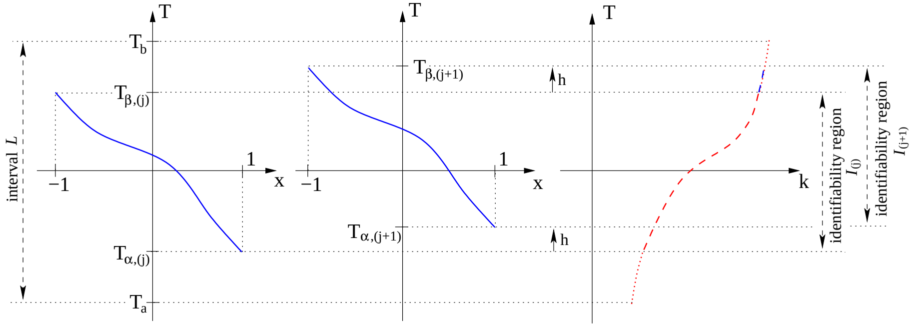
- constant initial guess $\mu^{(0)}$



- variable initial guess $\mu^{(0)}$

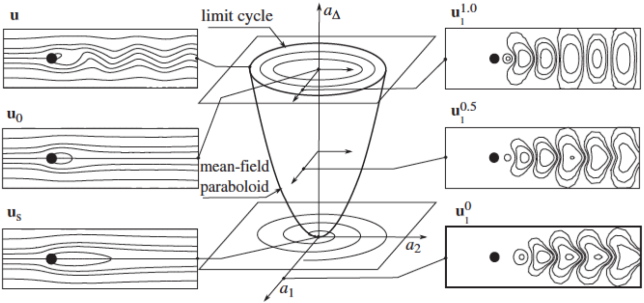


Shifting Identifiability Interval



Extensions (with B. Noack, Université de Poitiers)

- Optimal reconstruction of inertial manifolds in reduced-order models



Tadmor et al. (2011)

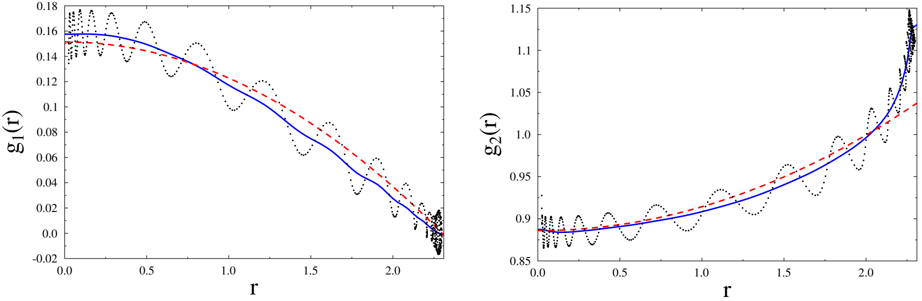
- From ∞-dim to dim $= 3$ (using POD modes as basis)

$$\left.\begin{aligned} \partial_t \mathbf{u} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla} p - \nu \boldsymbol{\Delta}\mathbf{u} &= 0 \quad \text{in } \Omega, \\ \boldsymbol{\nabla}\cdot\mathbf{u} &= 0 \quad \text{in } \Omega, \end{aligned}\right\} \quad \Longrightarrow \quad \left\{\begin{aligned} \dot{r} &= g_1(r)\, r, \\ \dot{\theta} &= g_2(r), \\ a_3 &= g_3(r), \end{aligned}\right.$$

where $r := \sqrt{a_1^2 + a_2^2}$ and $\theta := \arctan(a_2/a_1)$

Reconstructions

$g_1(r)$ in $\dot{r} = g_1(r)\, r$ $\qquad$ $g_2(r)$ in $\dot{\theta} = g_2(r)$



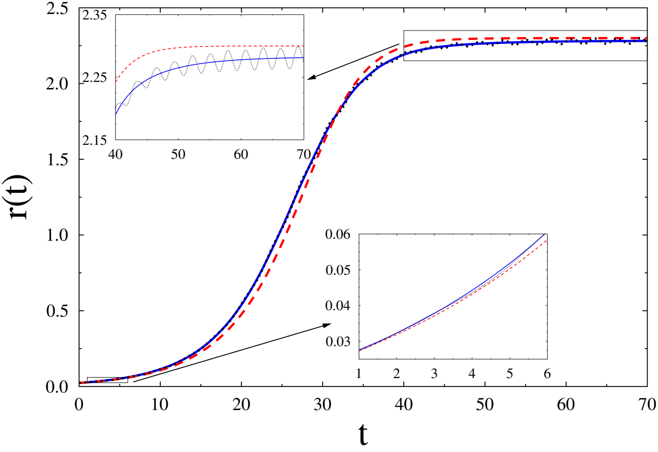
- - - Initial Guess (Mean-Field Model)

$$\dot{r}(t) = \left[\sigma_1 - \beta_\Delta\, \alpha_\Delta^M\, r^2(t)\right] r(t), \qquad \dot{\theta}(t) = \omega_1 + \gamma_\Delta \alpha_\Delta^M\, r^2(t)$$

—— Optimal Reconstruction

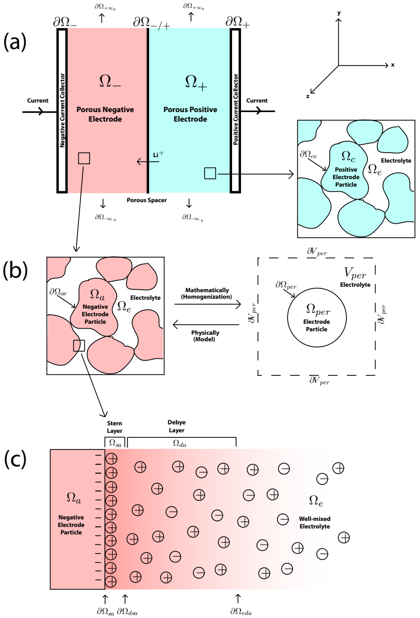
$\cdots$ $\frac{1}{r}\frac{dr}{dt}(r(t_i))$, $\frac{d\theta}{dt}(r(t_i))$, $i = 1, \ldots, N_T$

Comparison of Output (state magnitude r)



- - - Initial Guess (Mean-Field Model), —— Optimal Reconstruction,
··· Measurement Data

Emerging Application: Multiscale Problems in Non-Equilibrium Thermodynamics (Electrochemistry in Li-Ion Batteries)



Conclusions

- Optimization–based approach to reconstruction of state–dependent constitutive relations
- Smoothness of reconstructed relations ensured by Sobolev gradients
- A systematic procedure to extend the identifiability region
- extension (reduction) to finite dimension straightforward
- Follow–up work — generalize to more complicated problems, e.g.,
  - reconstruct the surface tension $\gamma(T)$ in problems with phase change
  - "positivity" condition $k(T) > 0$ replaced by the Clausius–Duhem inequality
  - Optimal closure models in RANS and LES

$$\rho\langle \mathbf{u}'\mathbf{u}'\rangle = \nu_T \left[\boldsymbol{\nabla}\tilde{\mathbf{u}} + (\boldsymbol{\nabla}\tilde{\mathbf{u}})\right]^T$$

Optimal reconstruction of eddy viscosity: $\nu_T = f(\boldsymbol{\nabla}\tilde{\mathbf{u}})$

References

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