THREE PDE-CONSTRAINED OPTIMAL CONTROL PROBLEMS RELATED TO IMAGE REGISTRATION, SUPERCONDUCTIVITY, AND SPDES

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THREE OPTIMAL CONTROL PROBLEMS

- Optimal control formulation of an image registration problem
  - with Eunjung Lee
- Optimal placement of pinning sites in superconductors
  - with Haomin Lin and Janet Peterson
- An optimal control problem for stochastic partial differential equations
  - with Catalin Trenchea and Clayton Webster

AN OPTIMAL CONTROL FORMULATION OF AN IMAGE REGISTRATION PROBLEM

The image registration problem

- Given two images $\mathbf{T}(\mathbf{x})$ and $\mathbf{R}(\mathbf{x})$ defined for $\mathbf{x} \in \Omega$,

  find a mapping $\widetilde{\boldsymbol{\phi}}(\mathbf{x}) : \Omega \to \Omega$ such that $\mathbf{T}(\widetilde{\boldsymbol{\phi}}(\mathbf{x}))$
  is as "close" to $\mathbf{R}(\mathbf{x})$ as possible

  – $\Omega \subset \mathbb{R}^2$ (usually a rectangle)

  – $\mathbf{T}(\mathbf{x})$ is called the *template image*

  – $\mathbf{R}(\mathbf{x})$ is called the *reference image*

- Given $f(\mathbf{x})$ and $g(\mathbf{x})$ defined on Ω such that

$$f(\mathbf{x}) > 0 \quad \text{in } \Omega \qquad \text{and} \qquad \int_\Omega \big(f(\mathbf{x}) - 1\big) d\mathbf{x} = 0,$$

consider the problem

$$\begin{cases} \nabla \cdot \mathbf{u}(\mathbf{x}) = f(\mathbf{x}) - 1 & \text{in } \Omega \\ \nabla \times \mathbf{u}(\mathbf{x}) = g(\mathbf{x}) & \text{in } \Omega \\ \mathbf{n} \cdot \mathbf{u}(\mathbf{x}) = 0 & \text{on } \partial\Omega \\ & \\ \dfrac{\partial \boldsymbol{\phi}(t, \mathbf{x})}{\partial t} = \mathbf{u}(\boldsymbol{\phi}(t, \mathbf{x})) & \text{in } (0, 1] \times \Omega \\ \boldsymbol{\phi}(0, \mathbf{x}) = \mathbf{x} & \text{in } \Omega \end{cases} \tag{1}$$

  - it can be shown that $\boldsymbol{\phi}(1, \mathbf{x})$ is a one-to-one mapping from $\Omega \longrightarrow \Omega$ and that

$$\det \nabla \boldsymbol{\phi}(1, \cdot) = f$$

  - thus, by "adjusting" $f(\mathbf{x})$ and $g(\mathbf{x})$, one can, in principle, make $\boldsymbol{\phi}(1, \mathbf{x})$ do whatever one wants

Optimal control formulation of the image registration problem

- For the image registration problem,
  - we identify $\widetilde{\boldsymbol{\phi}}(\mathbf{x})$ with $\boldsymbol{\phi}(1,\mathbf{x})$

  and then try to

  - adjust $f(\mathbf{x})$ and $g(\mathbf{x})$ so that $\mathbf{T}(\boldsymbol{\phi}(1,\mathbf{x}))$ is as close to possible to $\mathbf{R}(\mathbf{x})$

$\Longrightarrow$ we have an optimal control problem

- Specifically, we define the functional ($\| \cdot \| = L^2(\Omega)$ norm)

$$
\begin{aligned}
\mathcal{J}(\boldsymbol{\phi}|_{t=1}, f, g) \;=\; & \|\mathbf{T}(\boldsymbol{\phi}(1,\cdot)) - \mathbf{R}\|^2 && \text{what we want to minimize} \\
& +\alpha_{f_0}\|f\|^2 + \alpha_{f_1}\|\nabla f\|^2 && \\
& \quad +\alpha_{g_0}\|g\|^2 + \alpha_{g_1}\|\nabla g\|^2 && \text{control penalization} \\
& -2\beta \int_\Omega \log f \; d\mathbf{x} && \text{enforces } f > 0 \text{ constraint}
\end{aligned}
$$

and then seek controls $f(\mathbf{x})$ and $g(\mathbf{x})$ and states $\boldsymbol{\phi}(t,\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$ such that $\mathcal{J}(\cdot,\cdot,\cdot)$ is minimized, subject to the constraints

$$\begin{cases} \nabla\cdot\mathbf{u}(\mathbf{x}) = f(\mathbf{x}) - 1 & \text{in } \Omega \\ \nabla\times\mathbf{u}(\mathbf{x}) = g(\mathbf{x}) & \text{in } \Omega \\ \mathbf{n}\cdot\mathbf{u}(\mathbf{x}) = 0 & \text{on } \partial\Omega \\ & \\ \dfrac{\partial\boldsymbol{\phi}(t,\mathbf{x})}{\partial t} = \mathbf{u}(\boldsymbol{\phi}(t,\mathbf{x})) & \text{in } (0,1]\times\Omega \\ \boldsymbol{\phi}(0,\mathbf{x}) = \mathbf{x} & \text{in } \Omega \\ & \\ \displaystyle\int_\Omega \big(f(\mathbf{x}) - 1\big)\,d\mathbf{x} = 0 & \end{cases}$$

– two interesting features:

– PDE constraint coupled to ODE constraint

– composite function $\mathbf{u}(\boldsymbol{\phi}(t,\mathbf{x}))$ of the state variables

Results

- Existence of optimal solutions
- Existence of Lagrange multipliers
- Optimality system
- Finite element approximations

- Lagrangian

$$
\begin{aligned}
&\mathcal{L}(\mathbf{u}, \boldsymbol{\phi}, f, g; \xi, \eta, \boldsymbol{\psi}, \sigma, \nu, \boldsymbol{\mu}) \\
&\quad = \mathcal{J}(\boldsymbol{\phi}|_{t=1}, f, g) - \int_\Omega (\nabla \cdot \mathbf{u} - f + 1)\xi d\mathbf{x} - \int_\Omega (\nabla \times \mathbf{u} - g)\eta d\mathbf{x} \\
&\qquad - \int_\Omega \int_0^1 \left(\frac{\partial \boldsymbol{\phi}}{\partial t} - \mathbf{u}(\boldsymbol{\phi}) \right) \cdot \boldsymbol{\psi}\; dt d\mathbf{x} - \sigma \int_\Omega (f - 1) d\mathbf{x} \\
&\qquad - \int_\Gamma (\mathbf{n} \cdot \mathbf{u})\nu d\mathbf{x} - \int_\Omega (\boldsymbol{\phi}(0, \mathbf{x}) - \mathbf{x}) \cdot \boldsymbol{\mu} d\mathbf{x}
\end{aligned}
$$

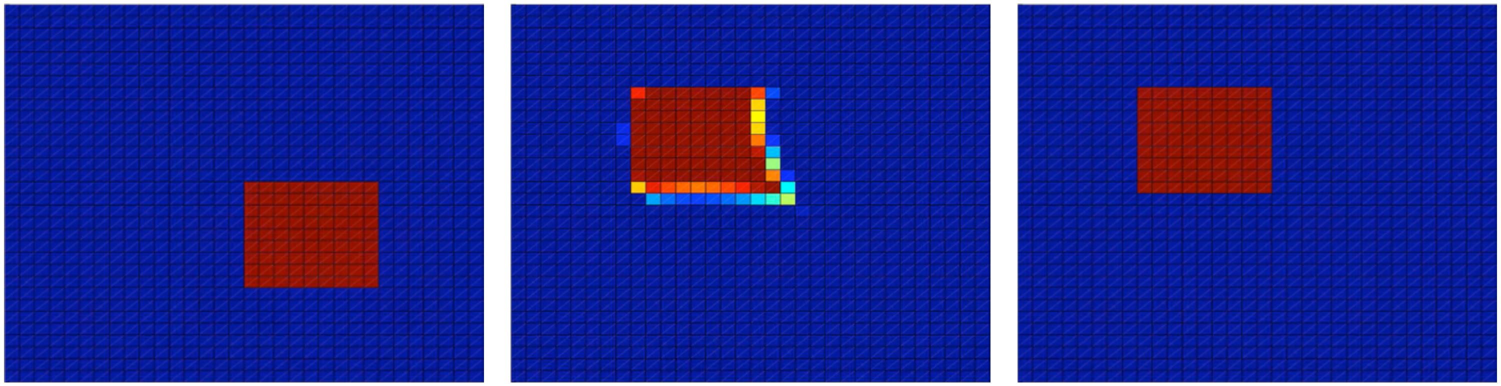
- Adjoint or co-state equations

$$
\begin{cases}
\dfrac{\partial \boldsymbol{\psi}}{\partial t} + \nabla_{\boldsymbol{\phi}} \mathbf{u}(t, \boldsymbol{\phi})\boldsymbol{\psi} = 0 & \text{in } (0,1) \times \Omega \\
\boldsymbol{\psi}(1, \mathbf{x}) = (T(\boldsymbol{\phi}(1, \mathbf{x})) - R(\mathbf{x})) \cdot \nabla_\phi T(\boldsymbol{\phi}(1, \mathbf{x})) & \text{in } \Omega \\
\nabla^\perp \eta - \nabla \xi = \displaystyle\int_0^1 |\nabla \boldsymbol{\phi}^{-1}(t, \mathbf{x})| \boldsymbol{\psi}(t, \boldsymbol{\phi}^{-1}(t, \mathbf{x})) dt & \text{in } \Omega \\
\eta = 0 & \text{on } \partial\Omega
\end{cases}
$$

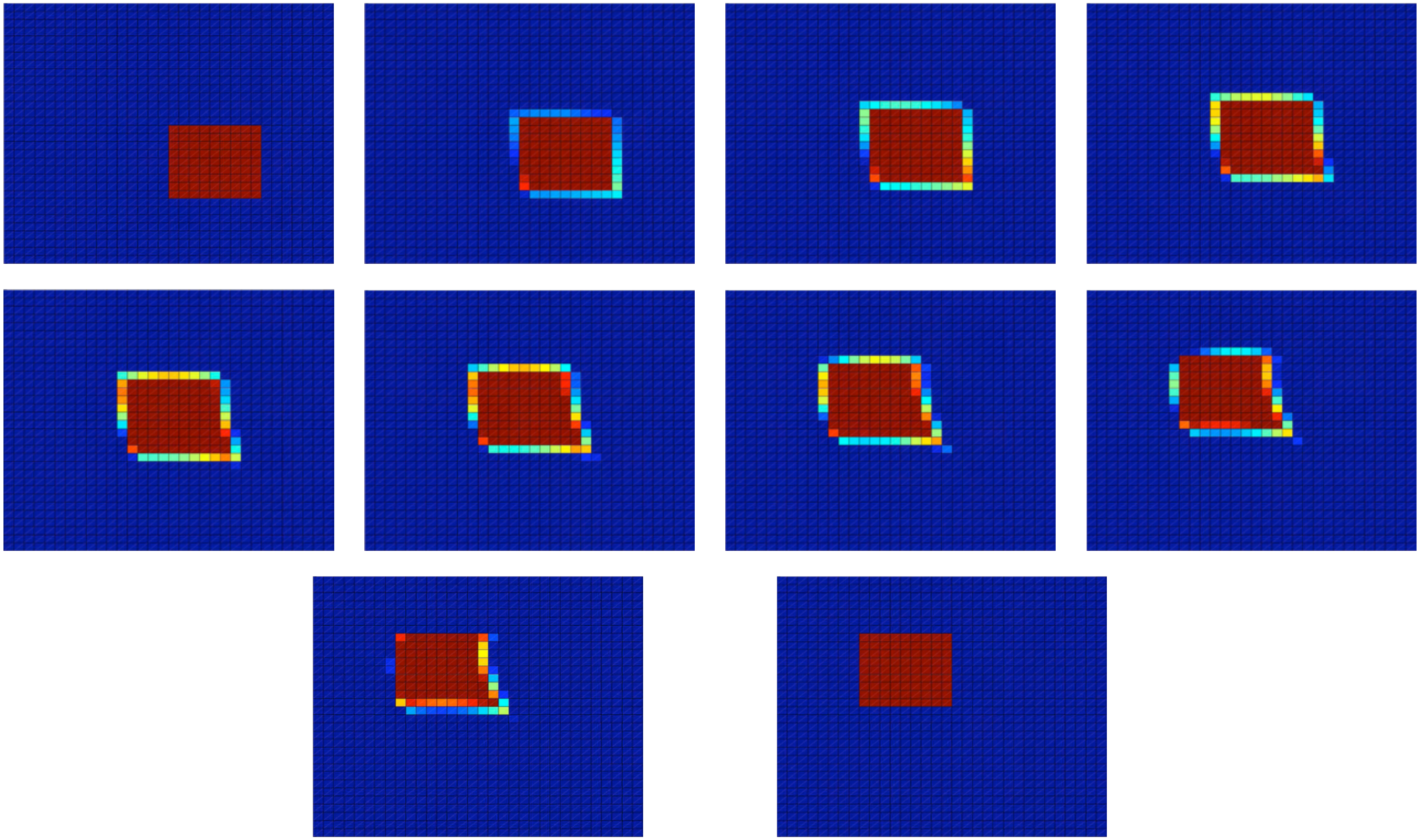
- Optimality conditions

$$\begin{cases} -\alpha_{f_1}\Delta f + \alpha_{f_0} f - \dfrac{\beta}{f} = \sigma - \xi & \text{in } \Omega \\ \mathbf{n}\cdot\nabla f = 0 & \text{on } \partial\Omega \\ -\alpha_{g_1}\Delta g + \alpha_{g_0} g = -\eta & \text{in } \Omega \\ g = 0 & \text{on } \partial\Omega \\ \sigma = \displaystyle\int_\Omega \left(\xi + \Delta f - \frac{\beta}{f}\right) dx & \end{cases}$$

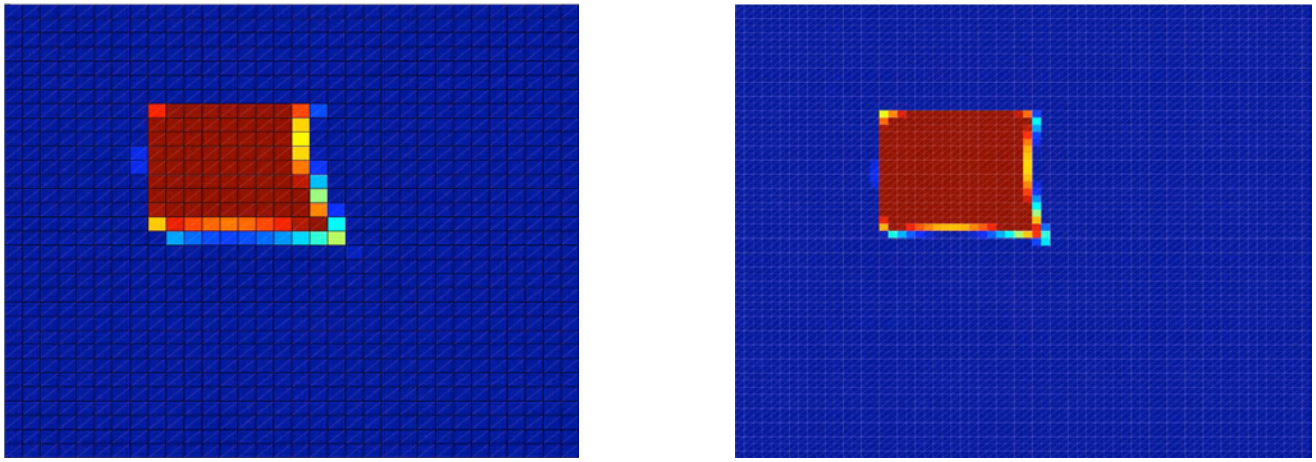
Computational results



$\mathbf{T}(\mathbf{x})$ $\mathbf{T}(\boldsymbol{\phi}(1, \mathbf{x}))$ $\mathbf{R}(\mathbf{x})$



$\mathbf{T}(\boldsymbol{\phi}(t, \mathbf{x}))$ for $0 \leq t \leq 1$ and $\mathbf{R}(\mathbf{x})$



$\mathbf{T}(\boldsymbol{\phi}(1,\mathbf{x}))$ on coarser and finer grid

OPTIMAL PLACEMENT OF PINNING SITES IN SUPERCONDUCTORS

Pinning in superconductors

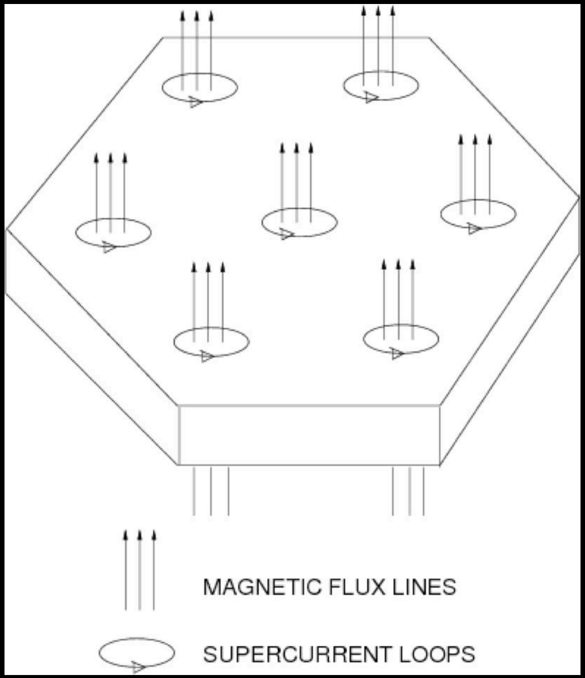
- An useful thing to do is to transmit (resistenceless) currents through superconducting samples, e.g., wires

- An important technological problem is to arrange things so that one transmits the largest possible resistenceless current

- Unfortunately, if one has a very pure sample (i.e., one free of defects) of a superconducting material, transmiting even a miniscule current can cause resistance

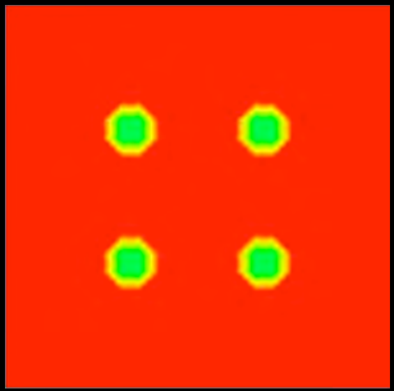
  – let's see why this is so

- In conductors of current practical interest (e.g., high-temperature superconductors), magnetic fields penetrate a sample in the form of (magnetic) flux tubes (called vortices)

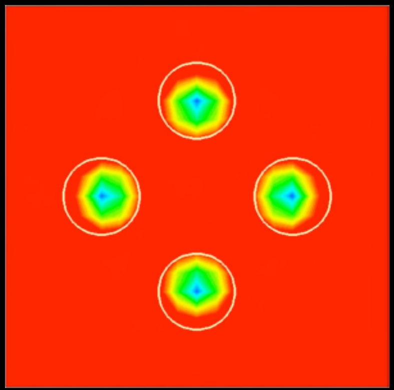


- If a current is applied and the sample is pure, then the magnetic flux lines will move, resulting in resistance (Lorentz force)

- The game is then to somehow make the sample "impure" so that the vortices are pinned, i.e., so that they do not move, when a current is applied
  - many mechanisms are known to pin vortices, e.g.,
    - grain and twin boundaries, thinner regions in the sample, impurities



vortex configuration in a pure superconductor with no applied current; any applied current will cause the vortices to move



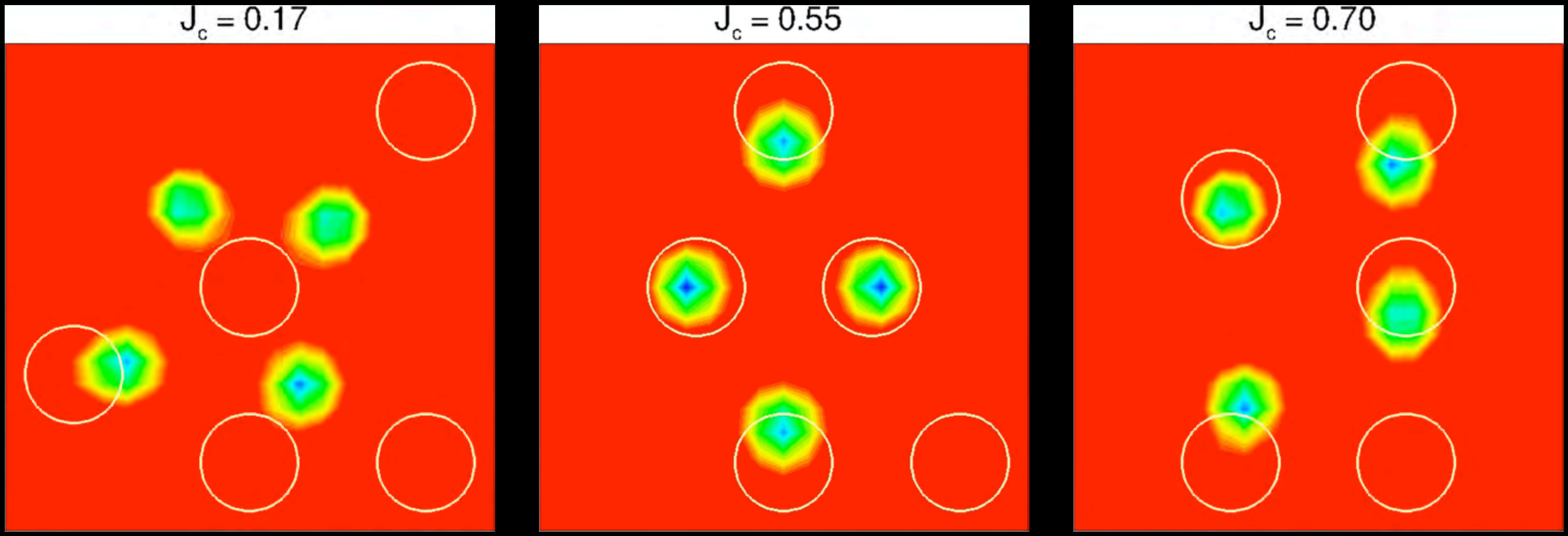
vortex configuration in a superconductor with impurities (the circles) and no applied current; a finite but not too large current may be applied without causing the vortices to move

– however, for any pinning mechanisms,

  – if the applied current is large enough,
    the vortices will become de-pinned and resistance will result

- The largest current that can be applied without causing vortex movement (and therefore resistance) is called the critical current and is of huge interest

- The location of the impurities can have a big effect on the critical current J_c



- Naturally, one asks the question:
  - can one systematically determine the placement of the impurities so that the critical current is maximized?
- If one could do this, it is technologically feasible to construct samples having the optimal impurities distribution

An optimal placement problem

- We assume that
  - all the impurities are of the same size and shape, i.e., they are all circular with the same radius
  - the number M of impurities is fixed
- As a result, the control parameters are given by the
  - the coordinates $\{x_i, y_i\}_{i=1}^{M}$ of the centers of the M circles
  - the applied current J
- the state variables are
  - the complex-valued order parameter ψ
  - the vector-valued magnetic potential $\mathbf{A}$

- The constraint equations are the time-dependent Ginzburg-Landau equations, modified to include the effects of impurities and applied currents
  - the TDGL equations have the form

$$\frac{\partial \psi}{\partial t} = F\big(\psi, \mathbf{A}; J, \{x_i, y_i\}_{i=1}^{M}\big)$$
$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{G}\big(\psi, \mathbf{A}; J, \{x_i, y_i\}_{i=1}^{M}\big)$$

- It remains to define an objective functional to be minimized that

$$\left.\begin{array}{c}\text{doesn't like vortices to move}\\ \text{and}\\ \text{likes big applied currents}\end{array}\right\} \Longrightarrow \quad \mathcal{J}(\psi, J) = \int_{t_1}^{t_2}\int_{\Omega}\left(\frac{\partial|\psi|}{\partial t}\right)^2 d\mathbf{x}dt - \alpha J$$

Results

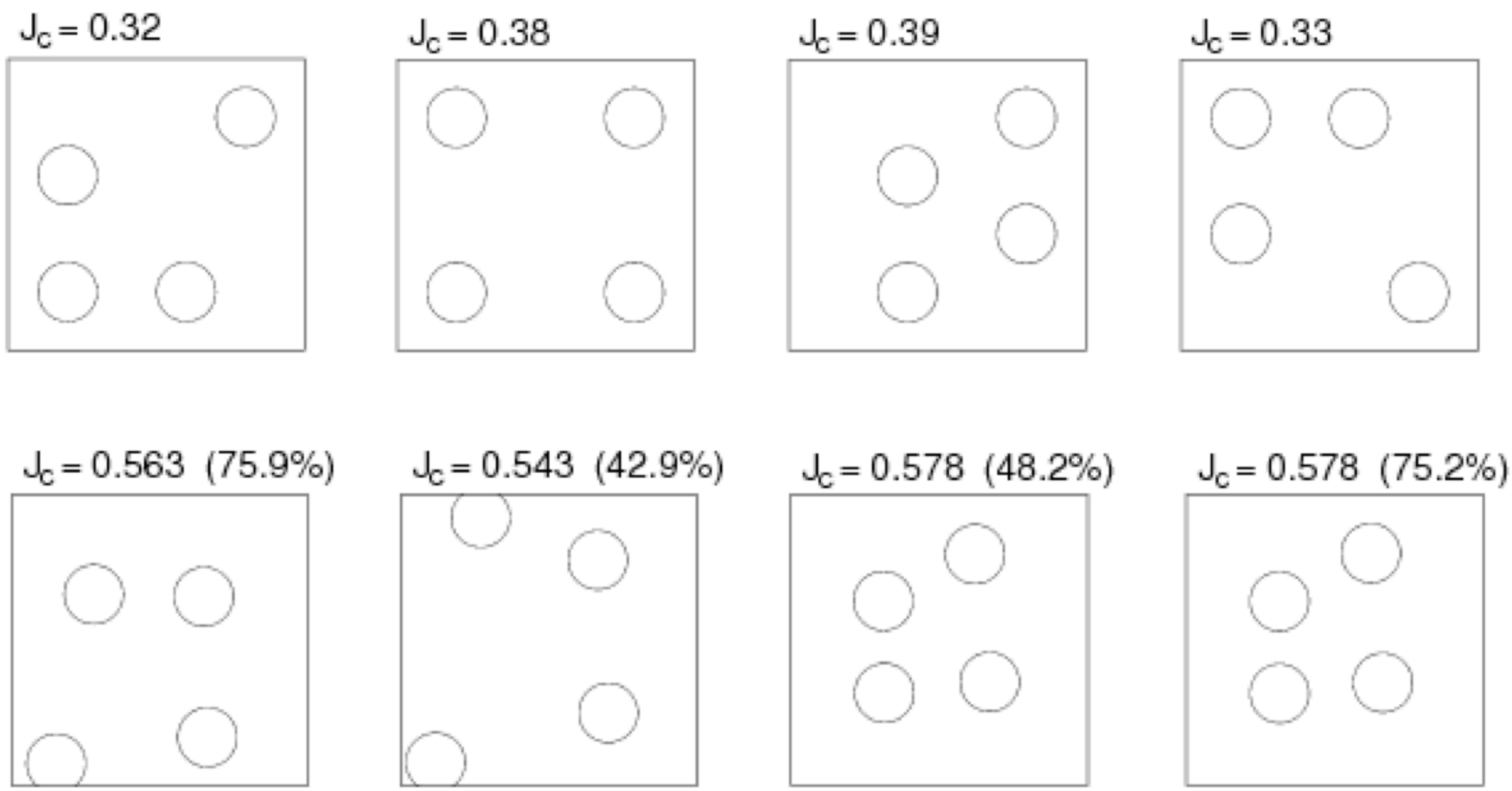
- Existence of optimal solutions
- Derivation of sensitivity equations
- Effective optimization algorithm
- Development and analysis of finite element approximations

Computational results

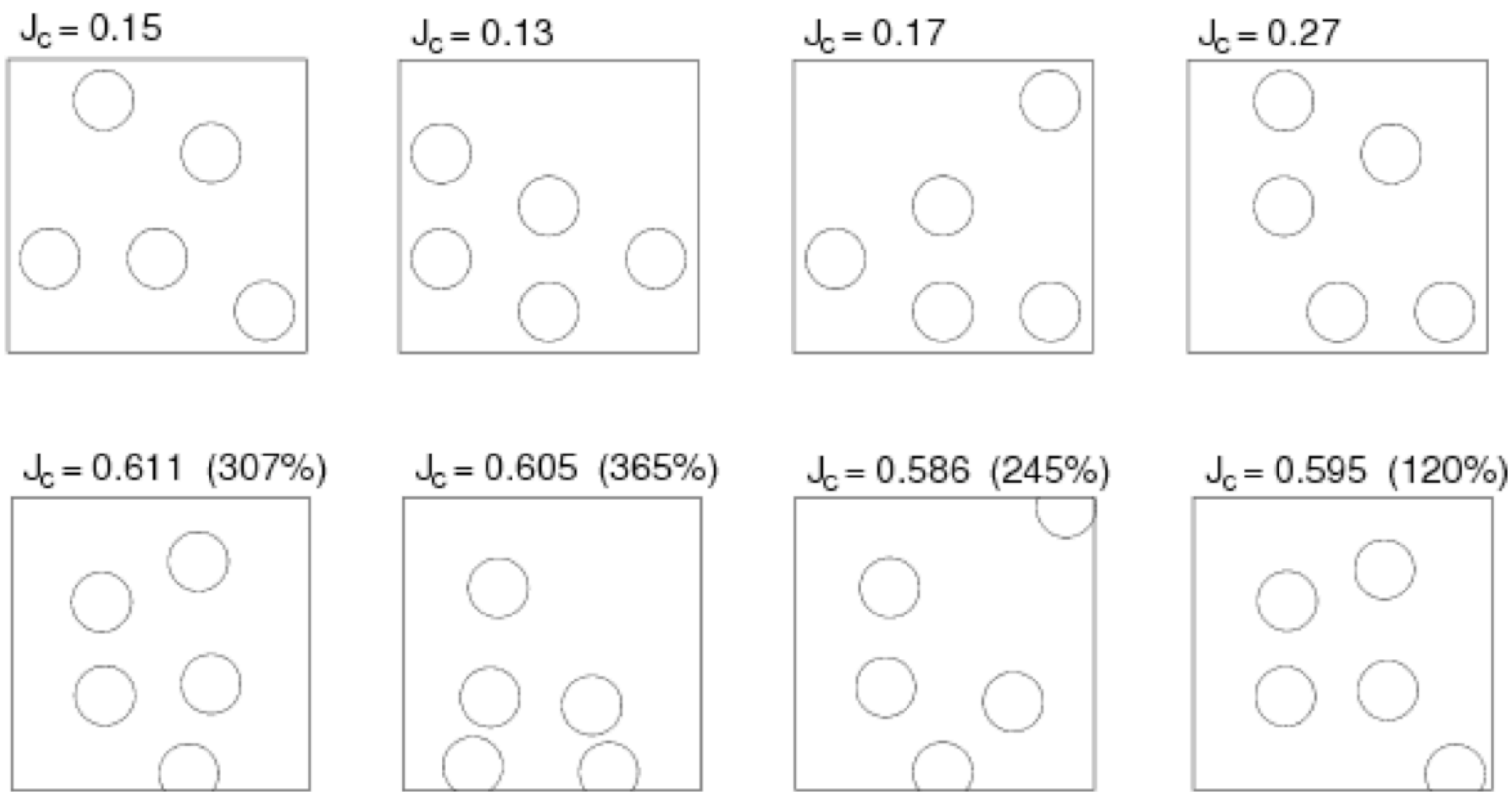
- Our functional has multiple local minima, so that one obtains different "optimal" solution for different initial placement of the impurities

- However, in every case, we obtain a significant improvement in the critical current

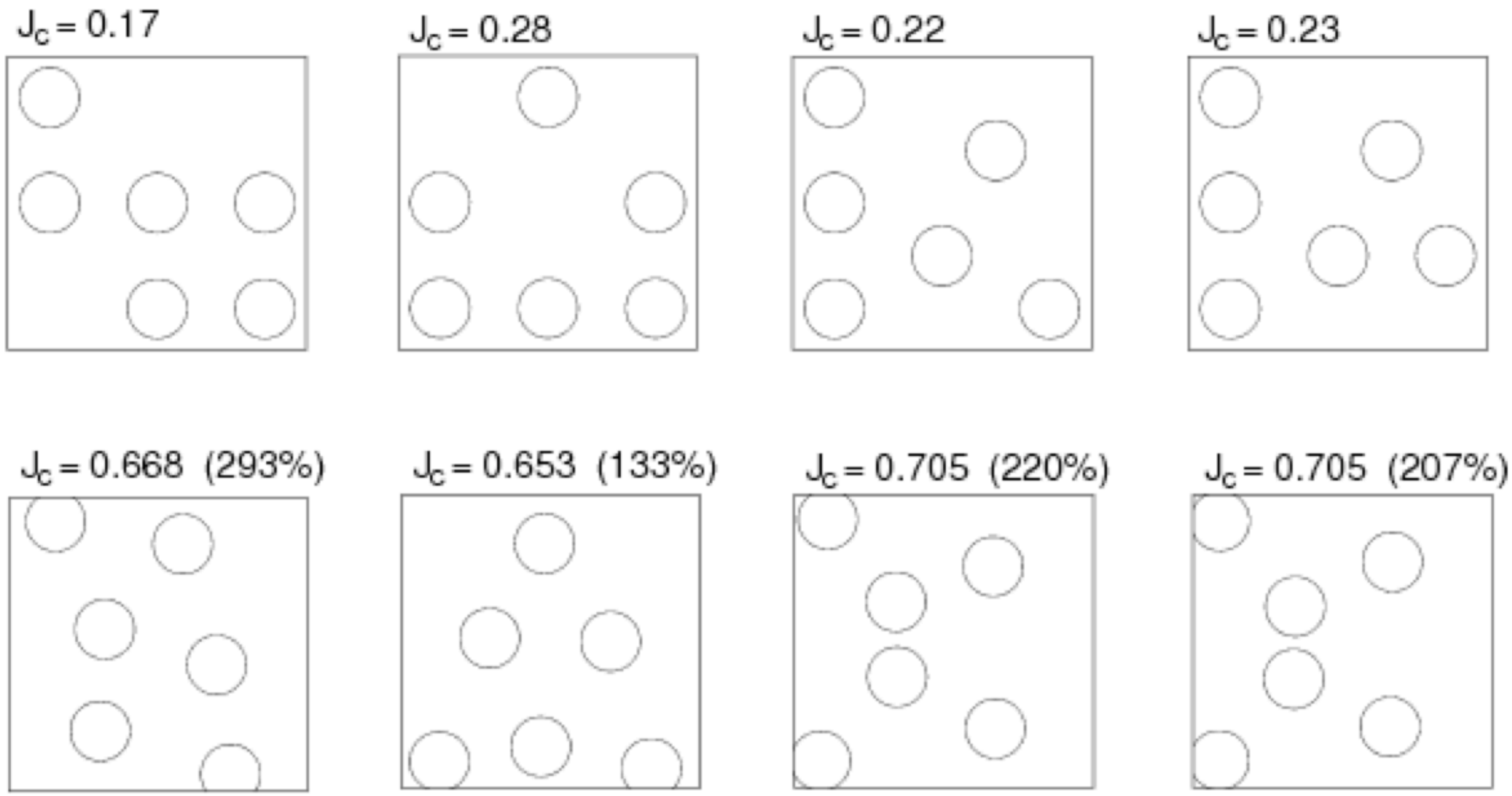
- In addition, the optimal values of the critical currents obtained for different initial placement are not too different



Initial (top) and resulting optimal (bottom) impurity placement and the corresponding critical currents for $M = 4$



Initial (top) and resulting optimal (bottom) impurity placement and the corresponding critical currents for $M = 5$



Initial (top) and resulting optimal (bottom) impurity placement and the corresponding critical currents for $M = 6$

AN OPTIMAL CONTROL PROBLEM FOR STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS

Optimization problems

- The state system

$$-\nabla \cdot \big(\kappa(\omega, \mathbf{x}) \nabla u(\omega, \mathbf{x})\big) = f(\omega, \mathbf{x}) \quad \text{in } \Omega \times D$$

$$u(\omega, \mathbf{x}) = 0 \quad \text{on } \Omega \times \partial D$$

  - ω is an elementary event in a probability space Ω
  - $\mathbf{x}$ is a point in the spatial domain D
  - $\kappa(\omega, \mathbf{x})$ and $f(\omega, \mathbf{x})$ are correlated random fields
  - the solution $u(\omega, \mathbf{x})$ is also a random field

- Optimal control problem
  - $\kappa(\omega, \mathbf{x})$ is given
  - $f(\omega, \mathbf{x})$ to be determined
  - given target function $\widehat{u}(\omega, \mathbf{x})$ may be deterministic or may be a random field
  - cost functional ($\mathsf{E}(\cdot)$ denotes the expected value)

$$\mathcal{F}(u, f; \widehat{u}) = \mathsf{E}\Big(\|u(\omega, \cdot) - \widehat{u}(\omega, \cdot)\|^2_{L^2(D)} + \alpha \|f(\omega, \cdot)\|^2_{L^2(D)} \Big)$$

$\Longrightarrow$

find a state u and a control f such that $\mathcal{F}(u, f; \widehat{u})$ is minimized subject to the state system being satisfied

- Parameter identification problem
  - $f(\omega, \mathbf{x})$ is given
  - $\kappa(\omega, \mathbf{x})$ to be determined
  - given target function $\widehat{u}(\omega, \mathbf{x})$ may be deterministic or may be a random field
  - cost functional

$$\mathcal{K}(u, \kappa; \widehat{u}) = \mathsf{E}\Big(\|u(\omega, \cdot) - \widehat{u}(\omega, \cdot)\|^2_{L^2(D)} + \beta \|\nabla \kappa(\omega, \cdot)\|^2_{L^2(D)} \Big)$$

$\Longrightarrow$

find a state u and a coefficient function κ such that $\mathcal{K}(u, \kappa; \widehat{u})$ is minimized subject to the state system being satisfied

Results

- Existence of optimal solutions

- Existence of Lagrange multipliers

- Derivation of optimality system

  – the adjoint or co-state system

$$-\nabla \cdot \Big(\kappa(\omega,\mathbf{x})\nabla\xi(\omega,\mathbf{x})\Big) \;=\; -\Big(u(\omega,\mathbf{x}) - \widehat{u}(\omega,\mathbf{x})\Big) \qquad \text{in } \Omega \times D$$

$$\xi(\omega,\mathbf{x}) \;=\; 0 \qquad \text{on } \Omega \times \partial D$$

  – optimality condition

$$\mathsf{E}\Big(-\beta\Delta\kappa + \nabla u \cdot \nabla \xi \Big) = 0$$

- Discretization of noise so that κ, f, $\widehat{u}$, and u depend on a parameter vector $\vec{y}(\omega) = (y_1(\omega), \ldots, y_N(\omega))^T$
  - these parameters may be "knobs" in an experiment
  - alternately, they could result from an approximation, e.g., a truncated Karhunen-Loevy expansion, of a correlated random field
- finite element analyses of stochastic collocation method (in progress)
  - isotropic and anisotropic Smolyak sparse grids are used as collocation points
- development of gradient method to effect optimization

Computational results

- choose target $\widehat{u} = x(1 - x^2) + \sum_{i=1}^{N} \sin\big(\frac{n\pi x}{L}\big) y_n(\omega)$

- choose optimal $\kappa = (1 + x^3) + \sum_{i=1}^{N} \cos\big(\frac{n\pi x}{L}\big) y_n(\omega)$

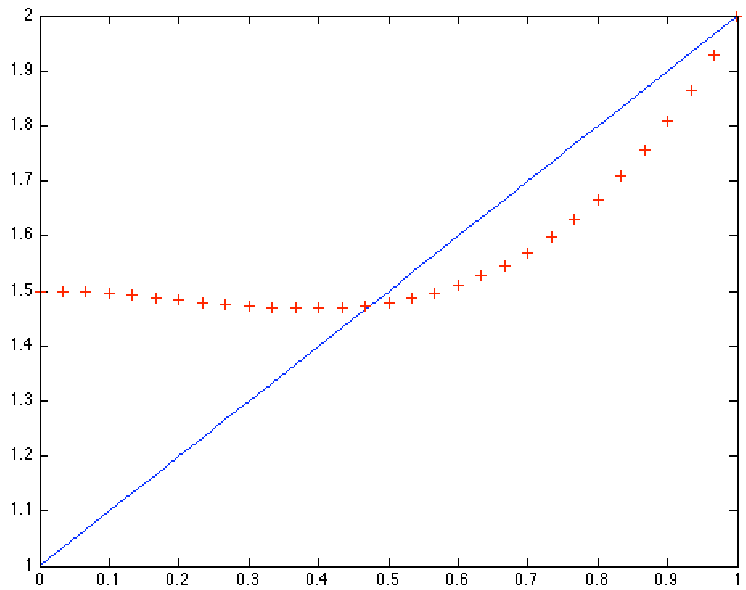
- set $f = -\nabla \cdot \big(\kappa \nabla \widehat{u}\big)$

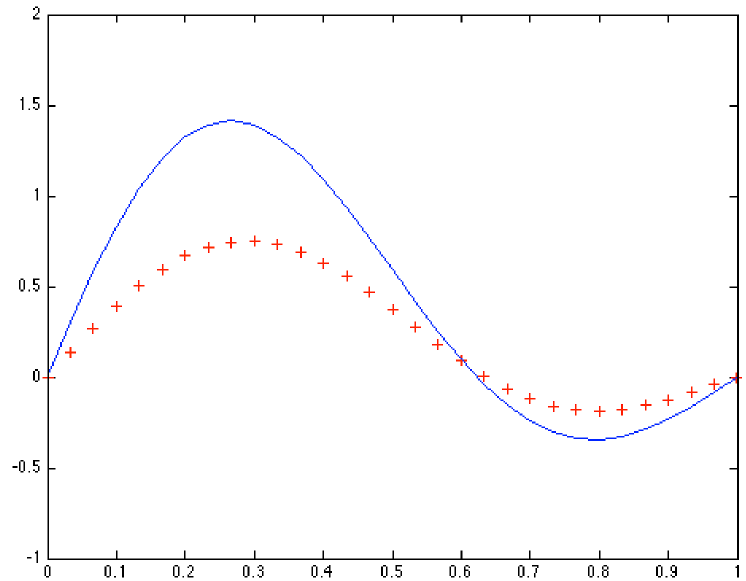
- choose initial $\kappa = 1 + x$

- assume y_i uniform on $[-1, 1]$ with $\mathsf{E}(y_i) = 0$ and $\mathsf{E}(y_i y_j) = \delta_{ij}$

$\Longrightarrow$

given random f and $\widehat{u}$, identify the expectation of both the control $\mathsf{E}(\kappa)$ and the state $\mathsf{E}(u)$ and compare with the exact statistical quantities

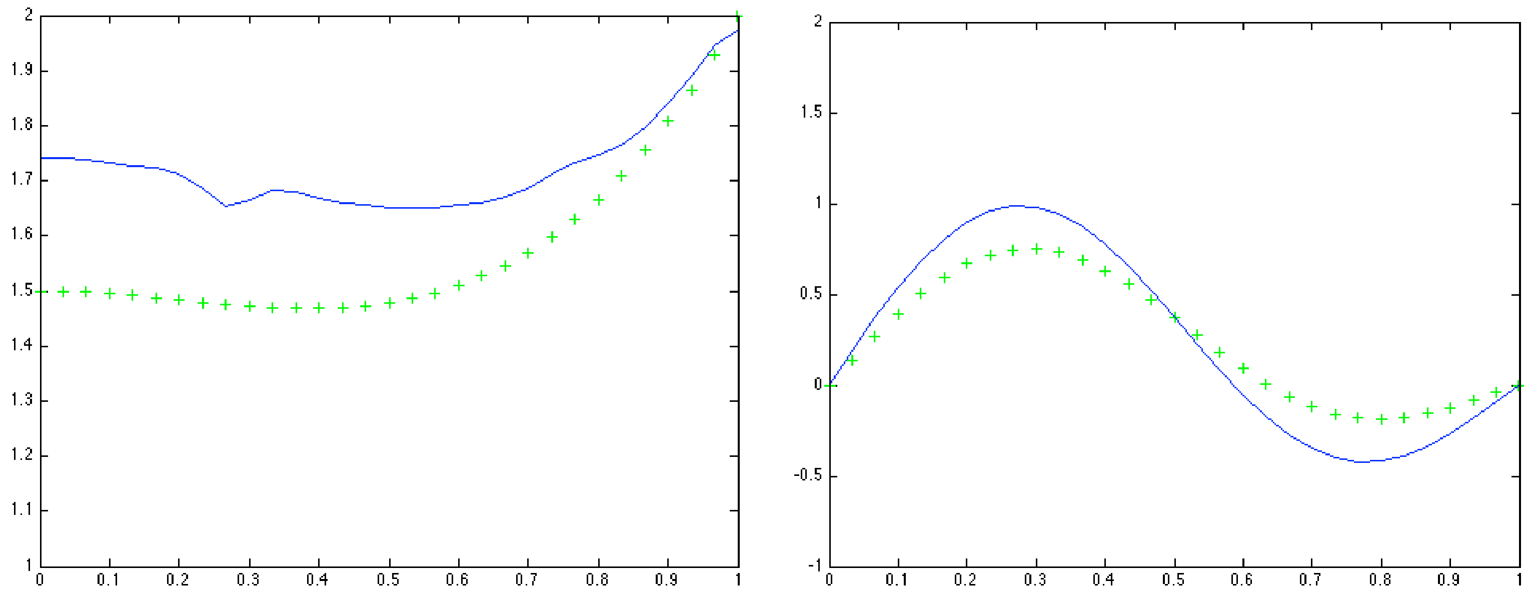




Left: expected value of initial (blue) and target (red) coefficient κ

Right: expected value of initial and target solution u

Number of random variables $= N = 1$

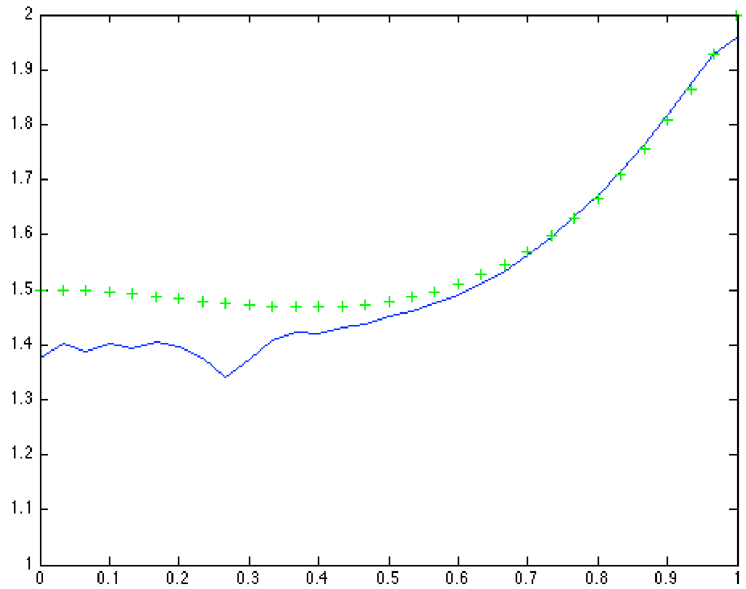


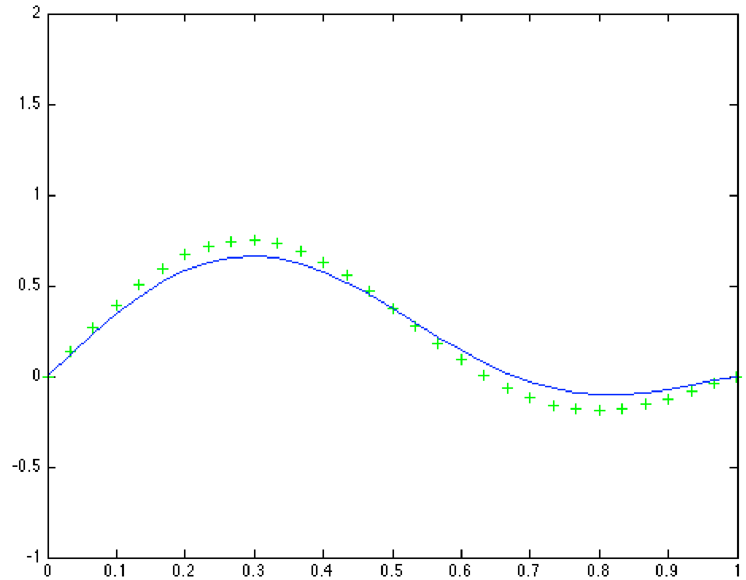
Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 1$

Number of Monte Carlo samples $= M = 1$



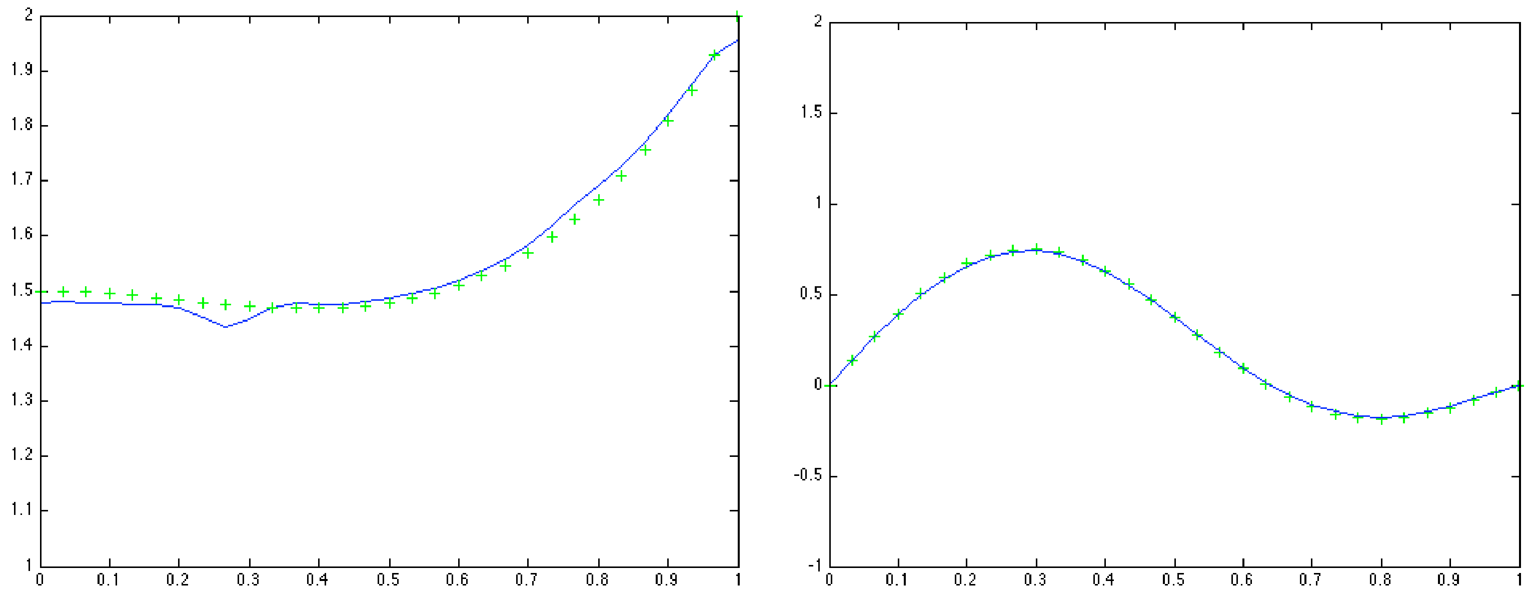


Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 1$

Number of Monte Carlo samples $= M = 10$

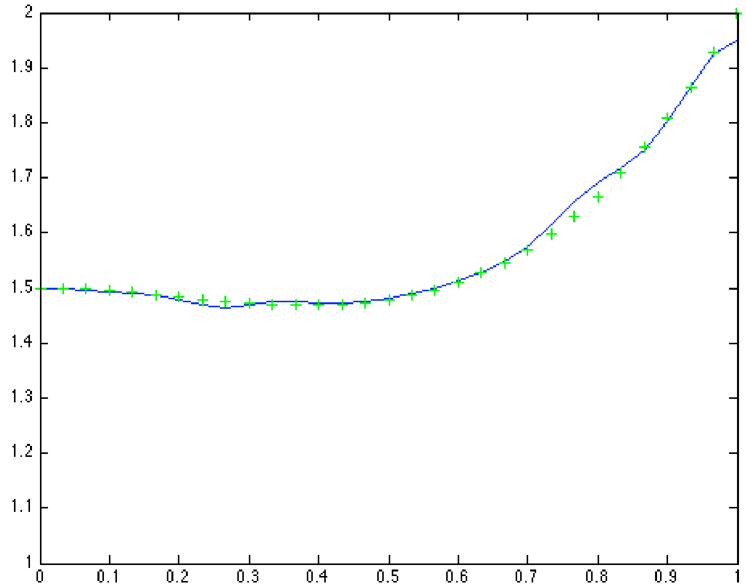


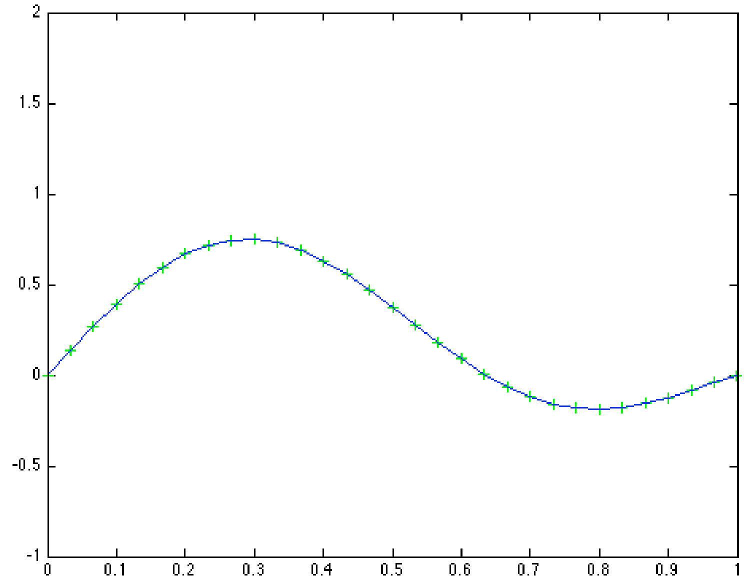
Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 1$

Number of Monte Carlo samples $= M = 100$



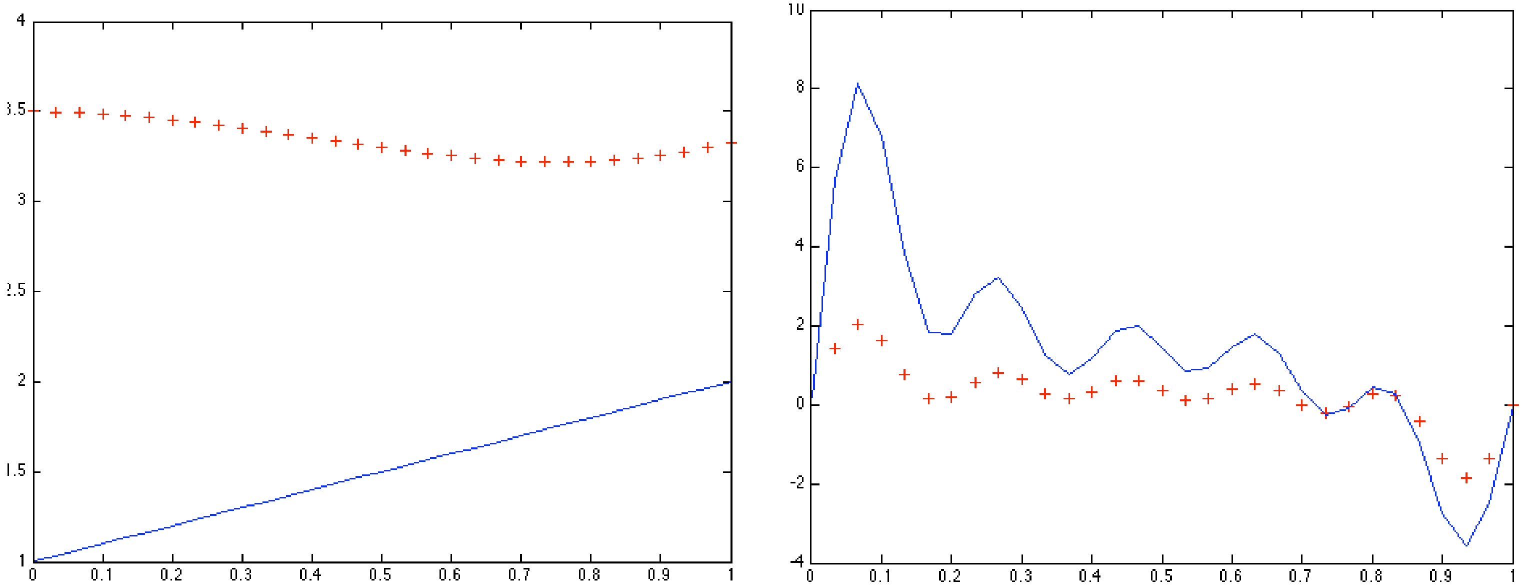


Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 1$

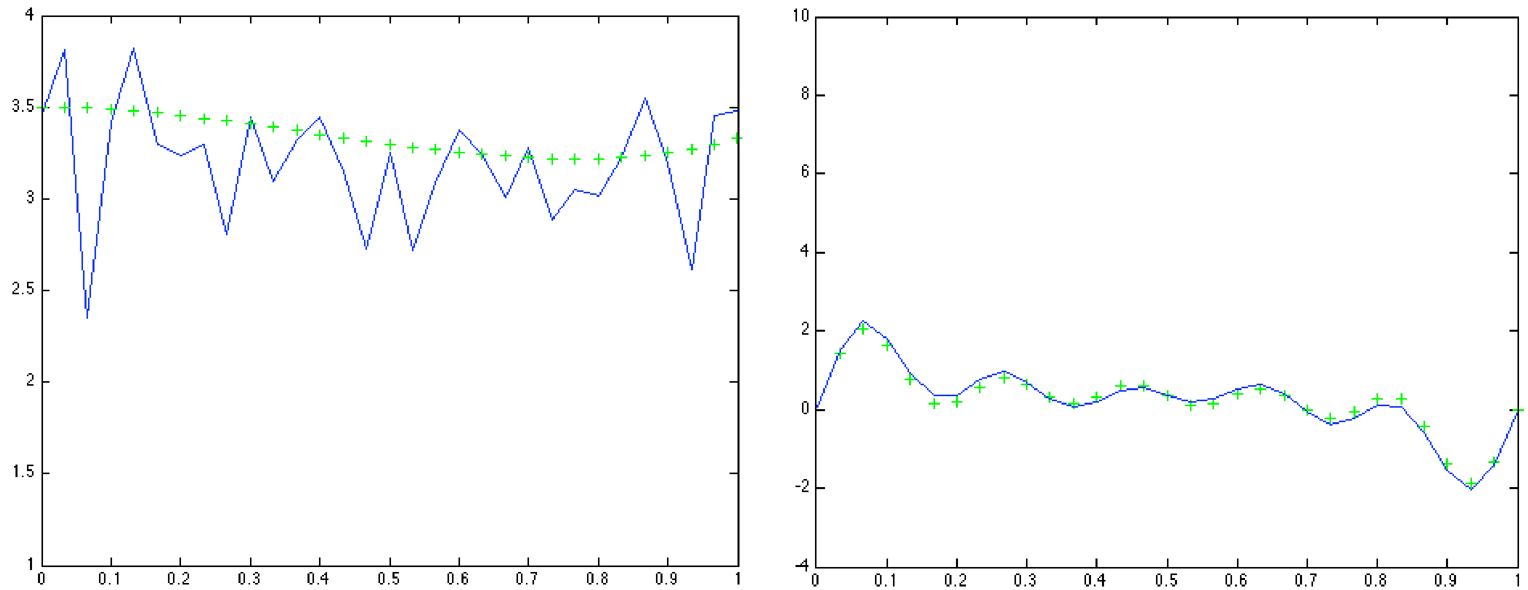
Number of anisotropic Smolyak collocation points $= M = 1$



Left: expected value of initial (blue) and target (red) coefficient κ

Right: expected value of initial and target solution u

Number of random variables $= N = 5$

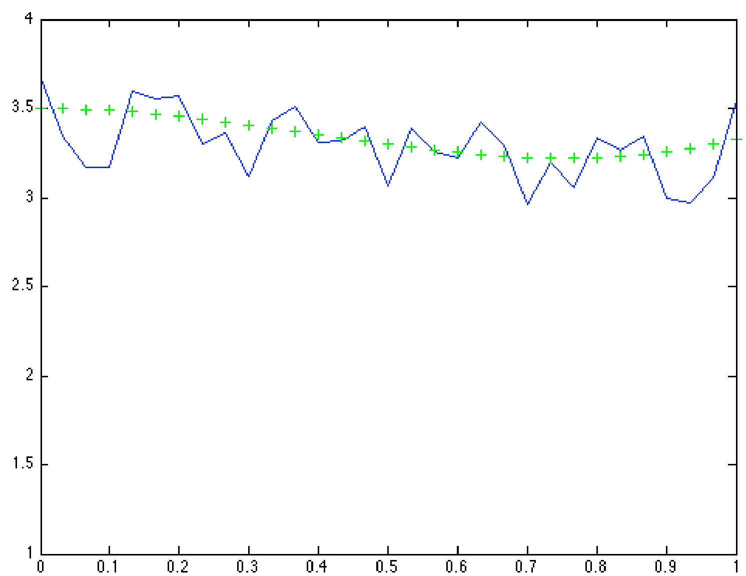


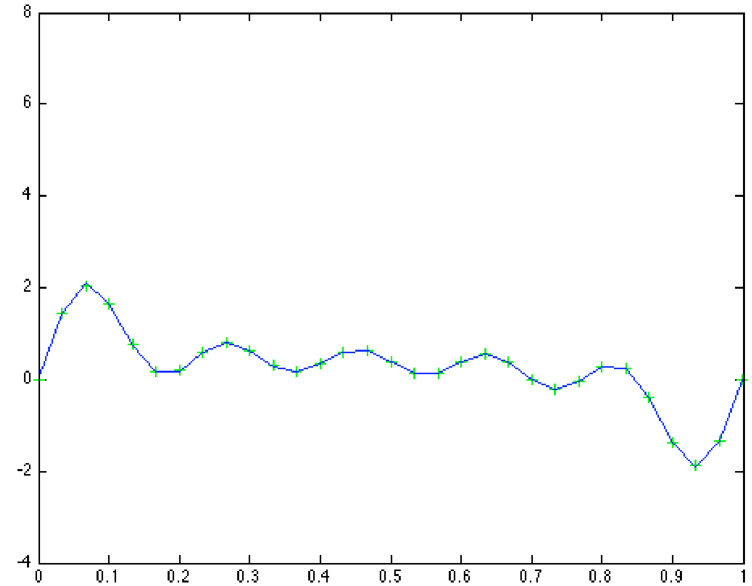
Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 5$

Number of Monte Carlo samples $= M = 11$





Left: expected value of optimal and target coefficient κ

Right: expected value of optimal and target solution u

Number of random variables $= N = 5$

Number of anisotropic Smolyak collocation points $= M = 11$

N	MC	AS
5	7e+03	801
10	9e+06	1581
20	8e+09	11561

For N random parameters, the number of Monte Carlo samples and the number of anisotropic Smolyak collocation points required to reduce the original error in the expected values of both the solution u and coefficient κ by a factor of 10^6