Emergent Numerical Algorithms

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Outline

1. Introduction
   - Goals
   - Plan
2. Progress
   - Core algorithm
   - Analysis
   - Results
3. Summary

Motivation

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Non-Uniform Mesh Generation Example

- Identifying optimal change of independet variable $Q^*(x)$ such that approximate solution to PDE has convergence properties superior to $Q(x) \equiv x$.
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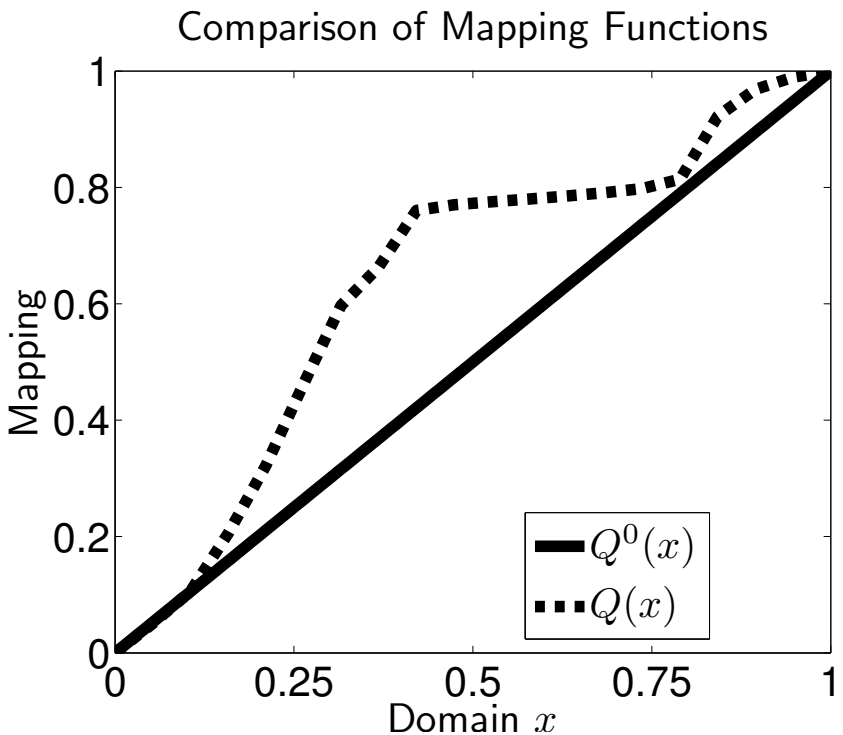

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- Identify P^* via sparse sampling:
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  - Perform m solves of coarse solutions (discretization order n)
  - Compute pointwise statistical moments of the coarse solutions
  - Improve candidate P?

Plan

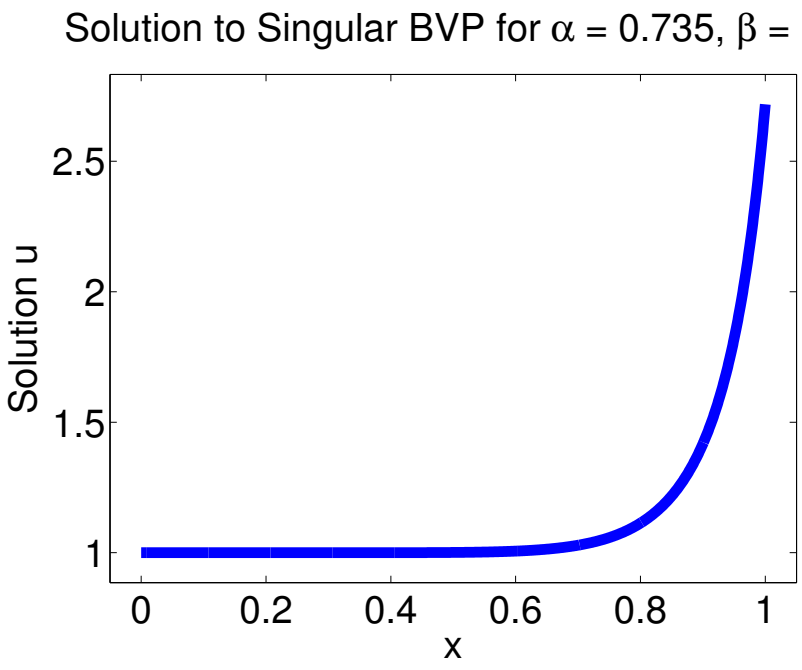
1. Core algorithm
2. Analysis
3. Test problems
4. Results

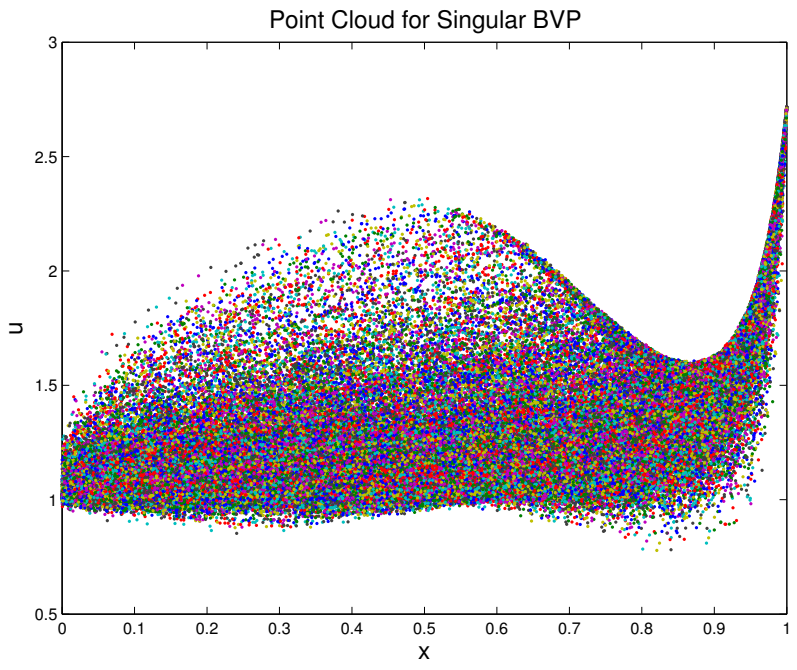
1D mesh generation: DMB & Christlieb, *SIAM J. Sci. Comp.*, in revision.
Theory: DMB & Byrne, *Inverse Problems*, in revision.
2D mesh generation: DMB & Christlieb, in prep.

- All simulations performed on a Tesla C2070 using matlab's GPU toolbox (**arrayfun**).

Core Algorithm

Sampling and Solving





$$(x^{\alpha}u')' = \beta x^{\alpha+\beta-2}((\alpha+\beta-1)+\beta x^{\beta})u \qquad ; 0 \leq x \leq 1$$

$$u(0) = A\,,\; u(1) = B$$

$$Q^*(x) = x^{1-\alpha}$$

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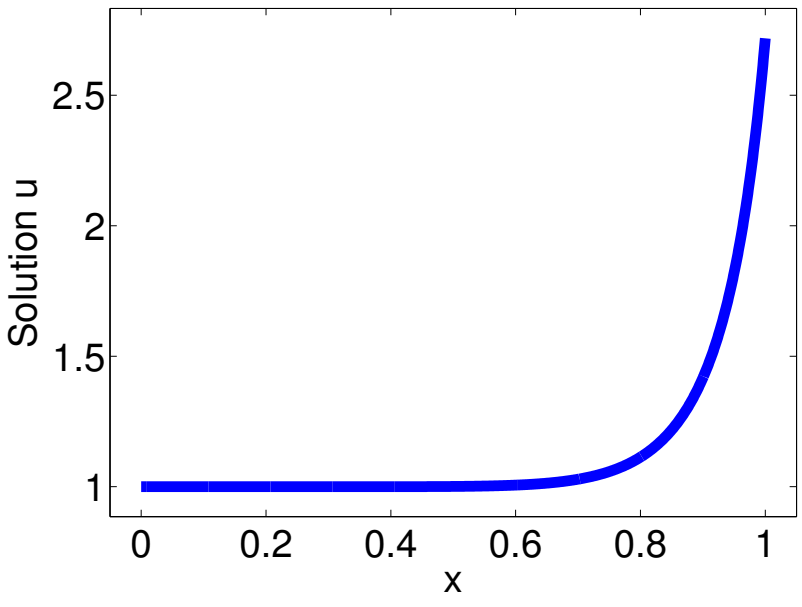

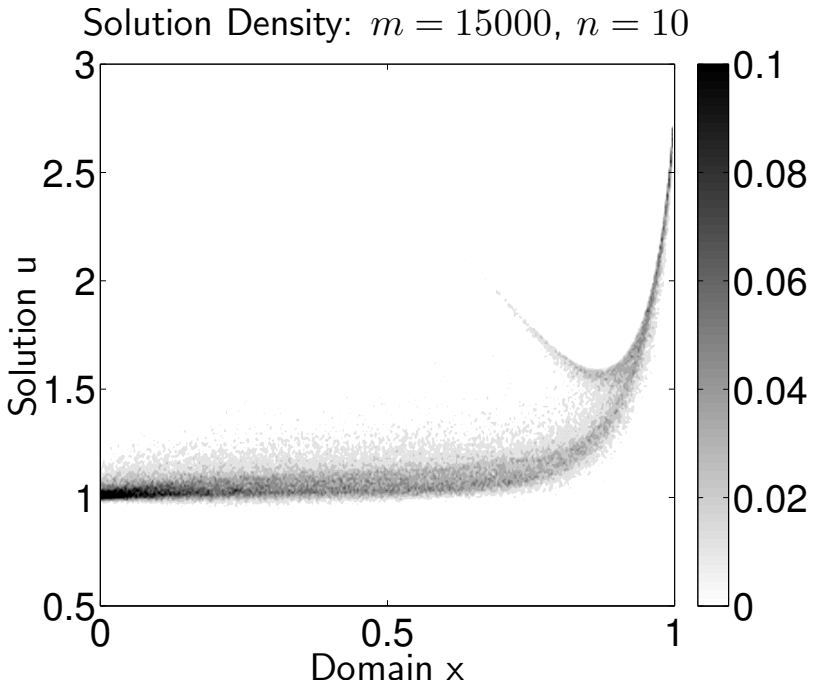

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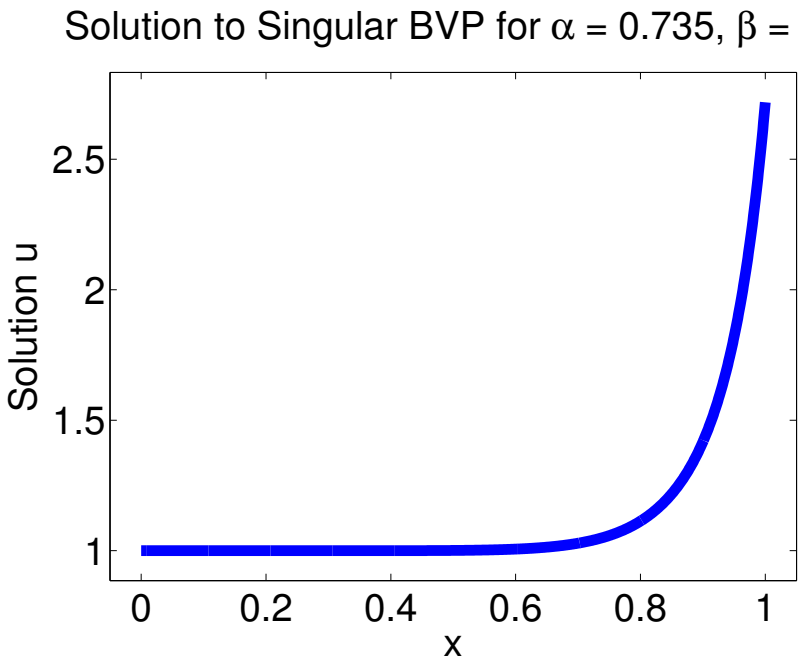
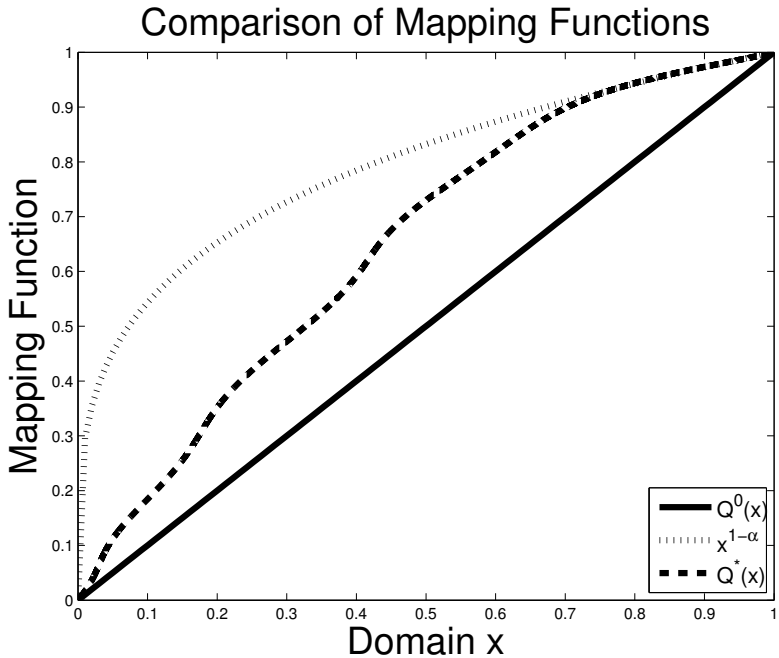
Sparse-Mesh Solutions (Aziz & Kumar, JCAM 2001)





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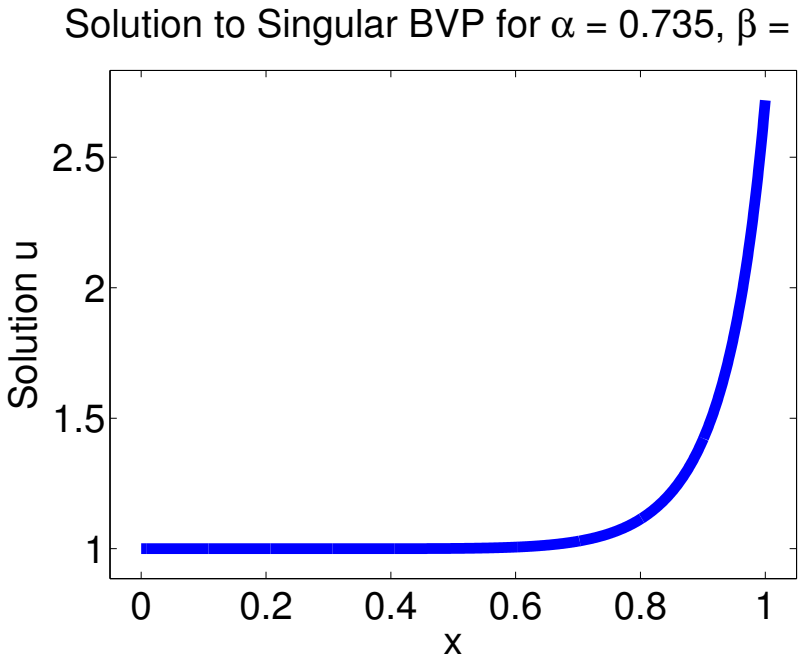

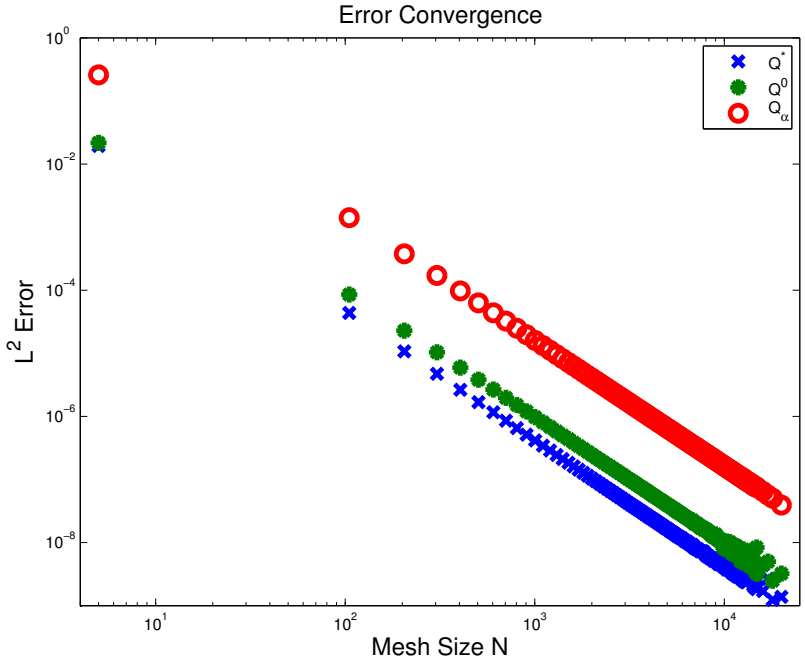

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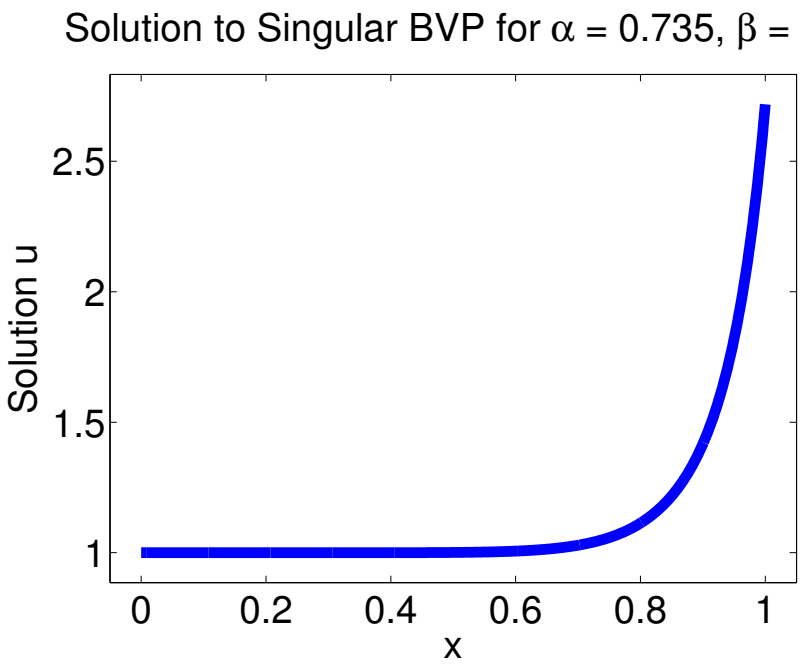

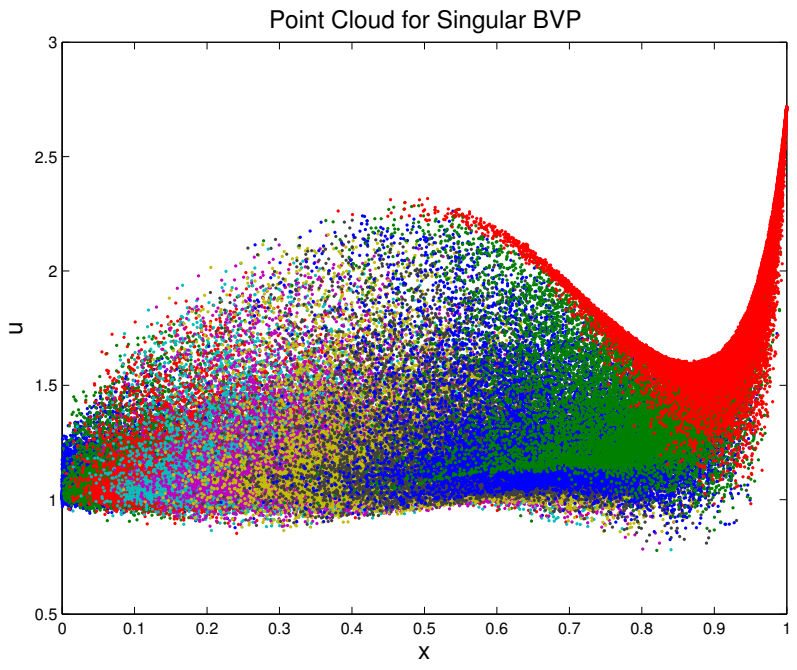

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$$\begin{aligned} \Pr\left[K = k : X_{(k)} \leq \xi\right] &= \Pr\left[\left(\bigcap_{j=1}^{k-1}\{X_{(j)} < \xi\}\right) \cap \left(\bigcap_{j=k+1}^{n}\{X_{(j)} > \xi\}\right)\right] \\ \text{CDF} &= \binom{n-1}{k-1} P(\xi)^{i-1}(1 - P(\xi))^{n-(i-1)}, \end{aligned}$$

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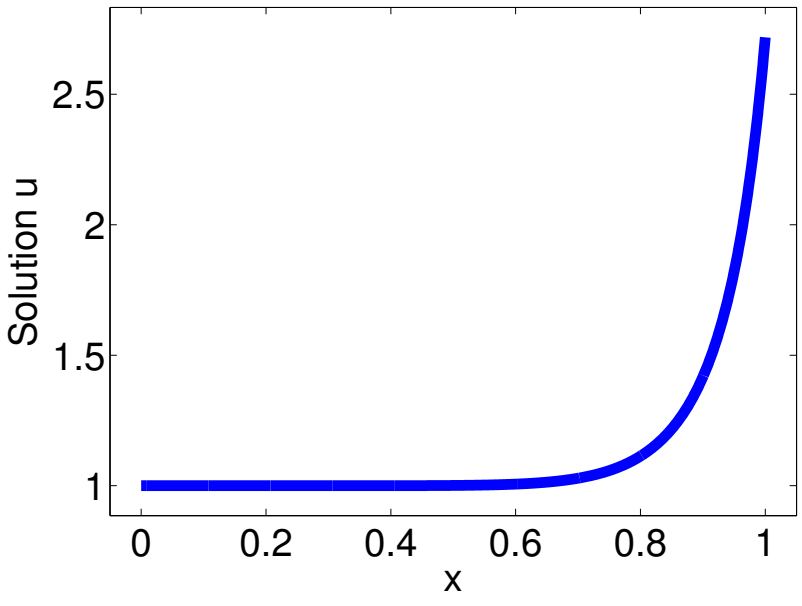
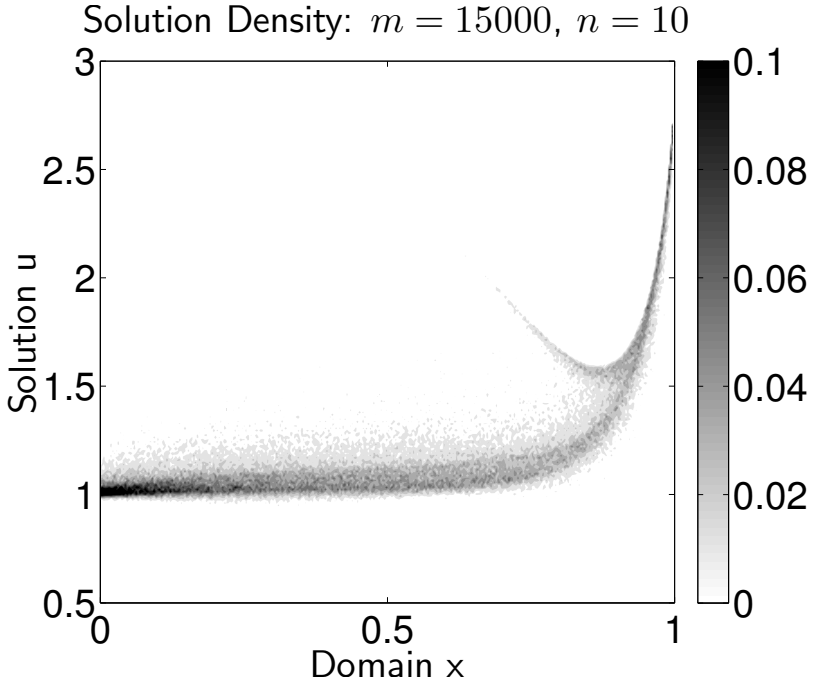
$$U(\mathbf{x}) = \text{takes a vector } \mathbf{x} \text{ and generates numerical solution}$$

Theoretical Framework?





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Definition

Pointwise probability density function

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Pointwise variance

$$v(\xi) \equiv \mathbb{V}_P \left[\mathbb{E}_K \left[\left\{ U(\mathbb{X}_{(n)}(P)) \right\}_{K=k} \middle| X_{(k)} = \xi \right] \right] ,$$

Theory

Theorem

Expected error converges pointwise to zero.

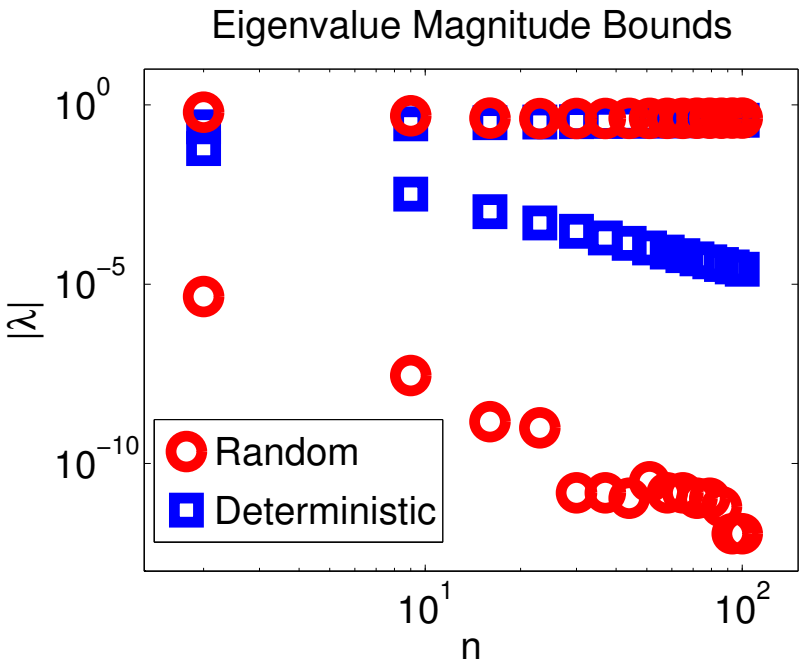
Proof.

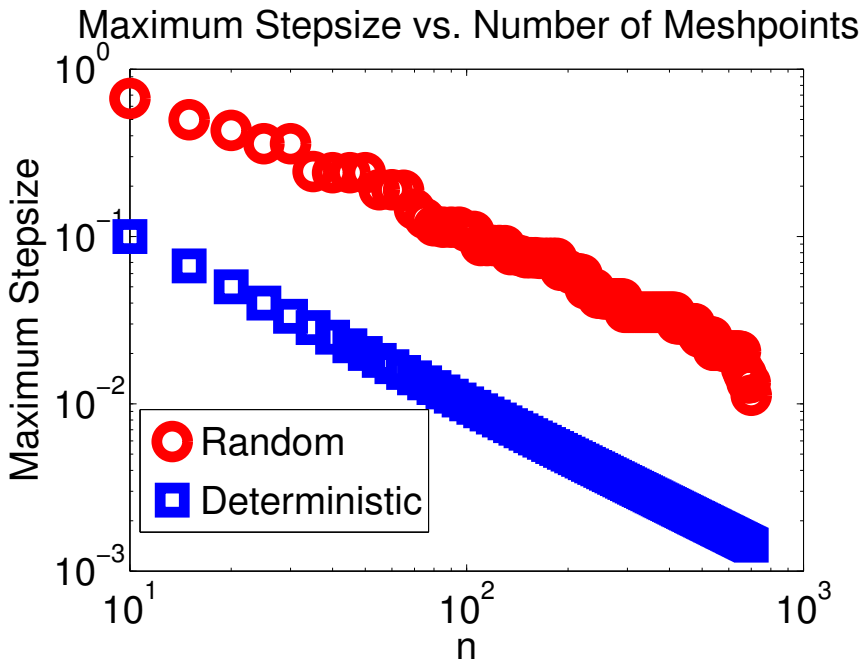
$$\left\| u(\xi) - \mu(\xi; U(\mathbb{X}_{(n)}(P))) \right\| \leq \mathbb{E}_P \left[\left\| A^{-1}_{\mathbb{X}_{(n)}(P)} \right\| \cdot \mathcal{O}(\max_{i=1,\ldots,n-1} |X_{(i)} - X_{(i+1)}|) \right]$$

□

DMB & AJC, *SIAM J. Sci. Comp.*, in revision.

"Proof"


Eigenvalue Magnitude Bounds
10^0
10^{-5}
10^{-10}
$|\lambda|$
Random
Deterministic
10^1
10^2
n


Maximum Stepsize vs. Number of Meshpoints
10^0
10^{-1}
10^{-2}
10^{-3}
Maximum Stepsize
Random
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10^1
10^2
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$$m = 1000$$

Expected Least Squares $\mathbb{E}[J]$

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- Optimize variance of U as a surrogate for error?
- SQP with Hessian Lagrangian updated via BFGS?

Theory

Theorem

Hausdorf distance convergence as $m, n \to \infty$ for

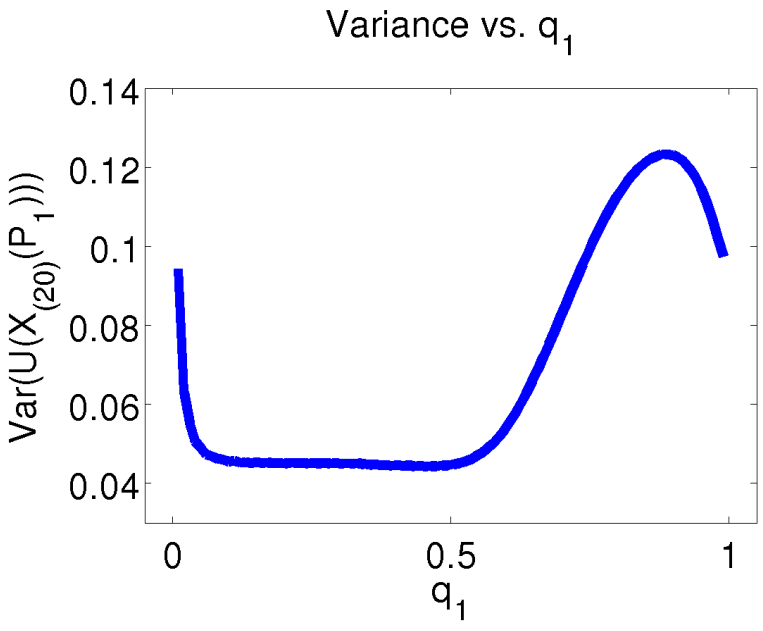
- *set of optimal distributions for approximate solution*
- *set of optimal distributions for exact solution*

Corollary

Well-posedness of inverse problem of P^* identification.

DMB & Byrne, *Inverse Problems*, in revision.

In Practice...



- Sufficient sampling addresses smoothness.
- Problems with optimization:
  - initial P guess.
  - discretization resolution N
  - number of samples M.
- Inference from moments of coarse solutions?

Distribution Construction

Eilliptic

$$q_1(x) = \int_0^x \sqrt{\left|\mu'(\xi; U(\mathbb{X}_{(n)}(P))\right|} d\xi \,,$$

Hamilton-Jacobi

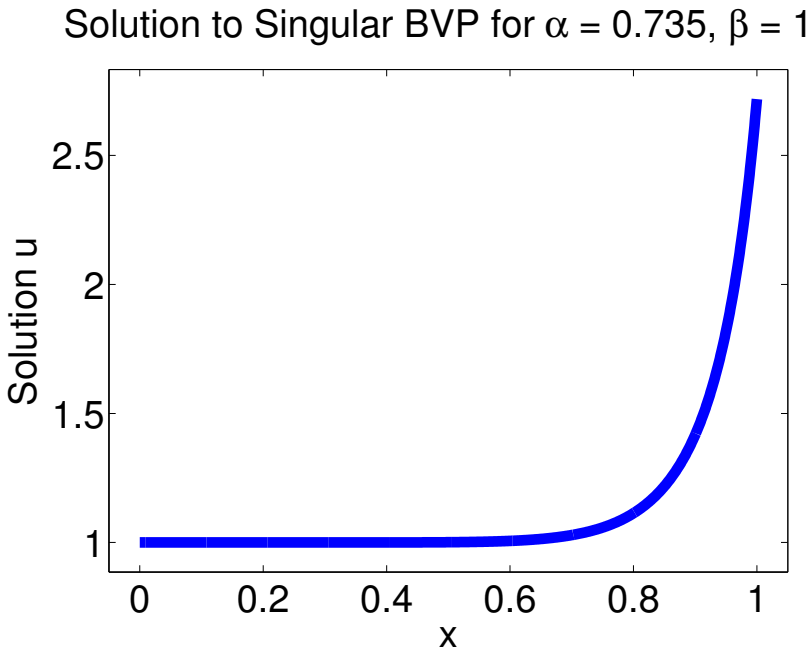
$$q_2(x) = \int_0^x \mu''(\xi; U(\mathbb{X}_{(n)}(P))^2 \, v(\xi; U(\mathbb{X}_{(n)}(P))^2 d\xi \,,$$

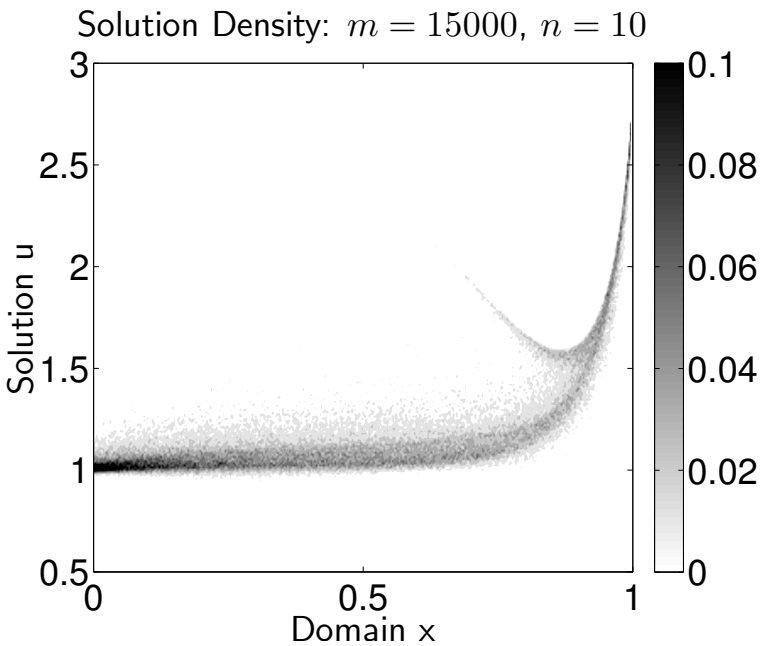
$$Q(x) = \left[\frac{q_i(\cdot)}{q_i(1)}\right]^{-1}(x)$$

Results[1]

[1] Simulations from runs on a Tesla C2070 using matlab's GPU toolbox (**arrayfun**).

Singular BVP





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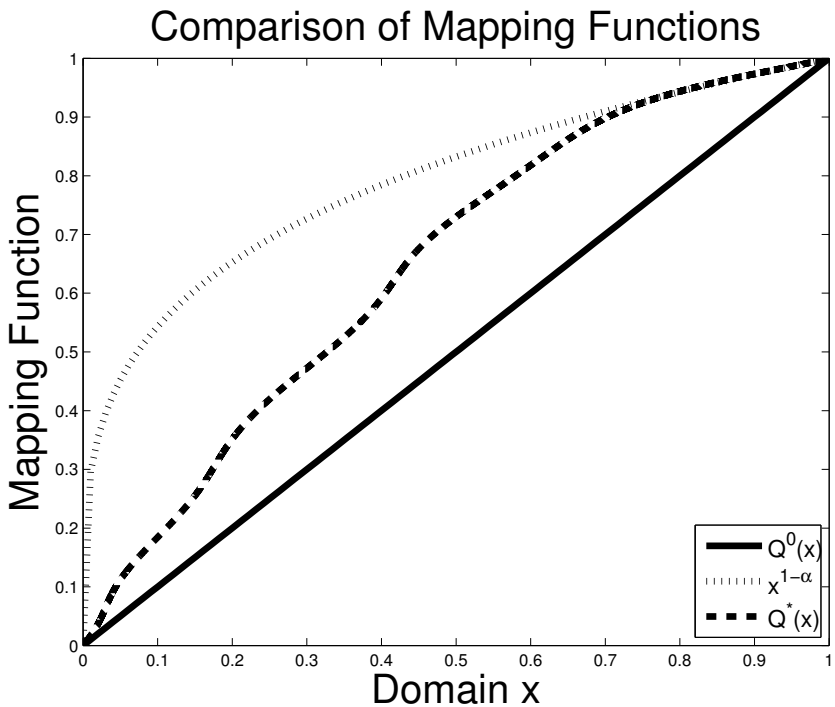

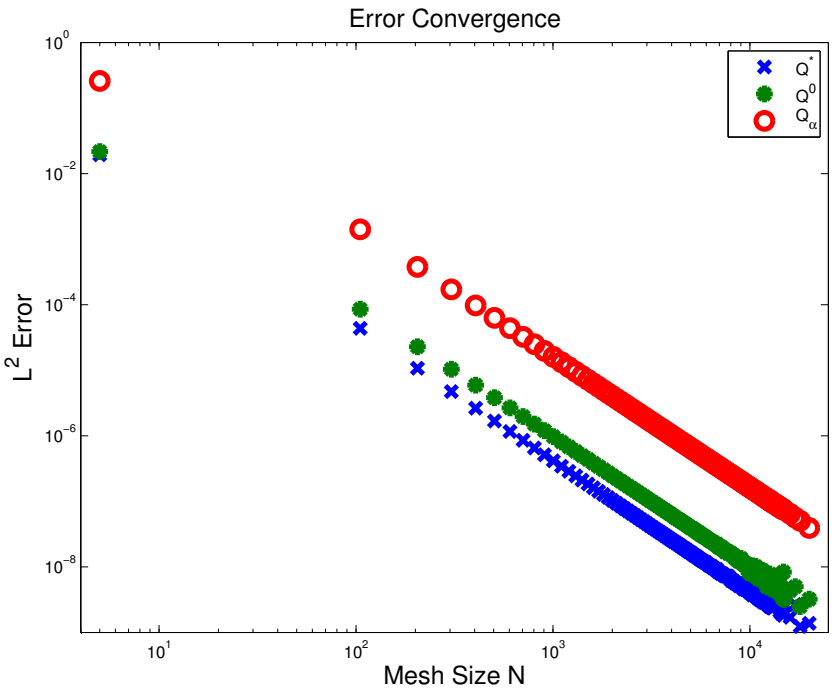

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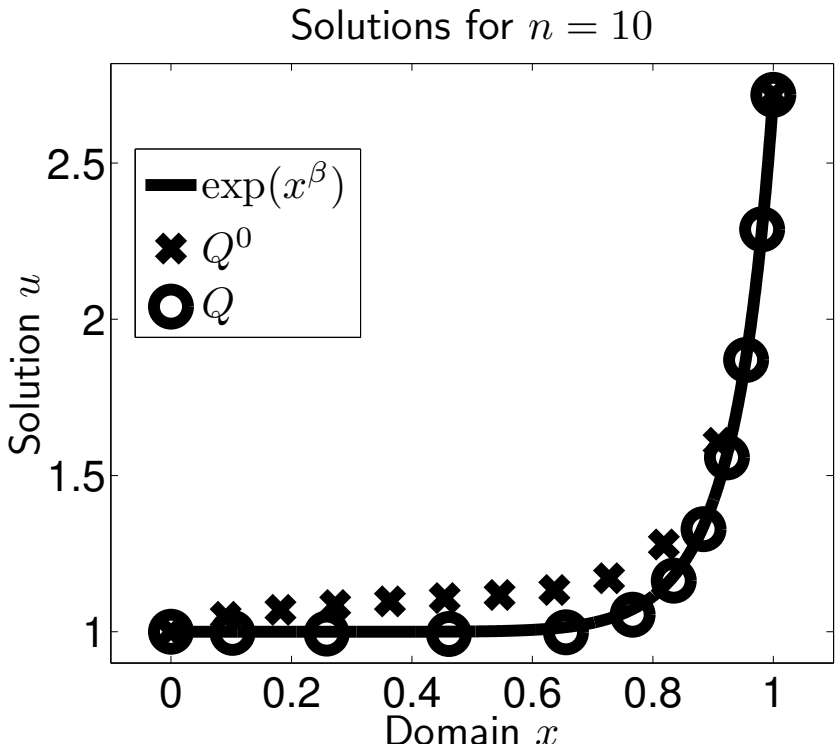
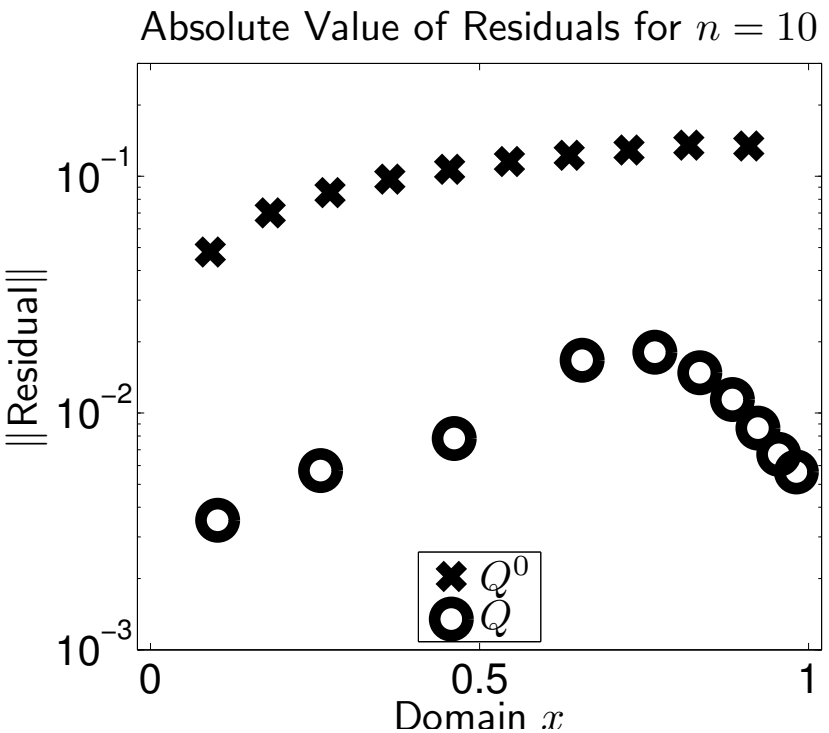
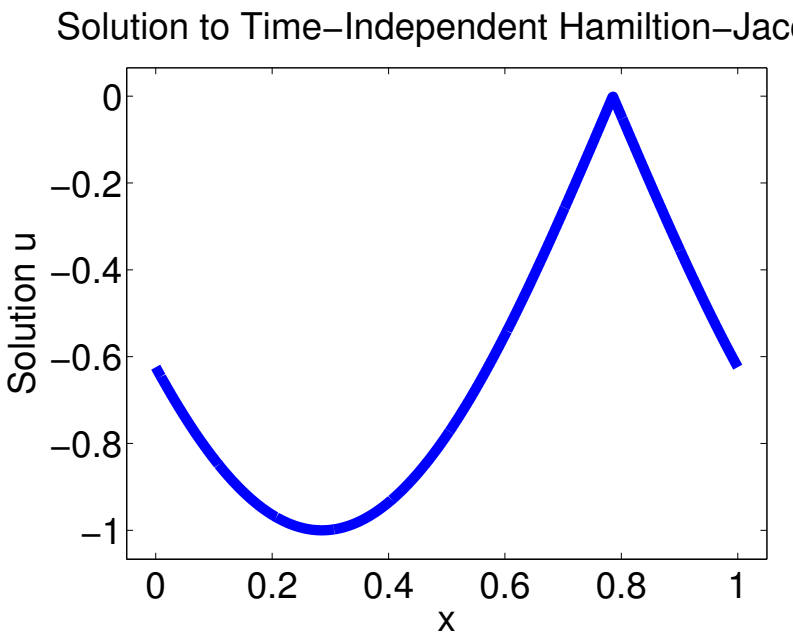
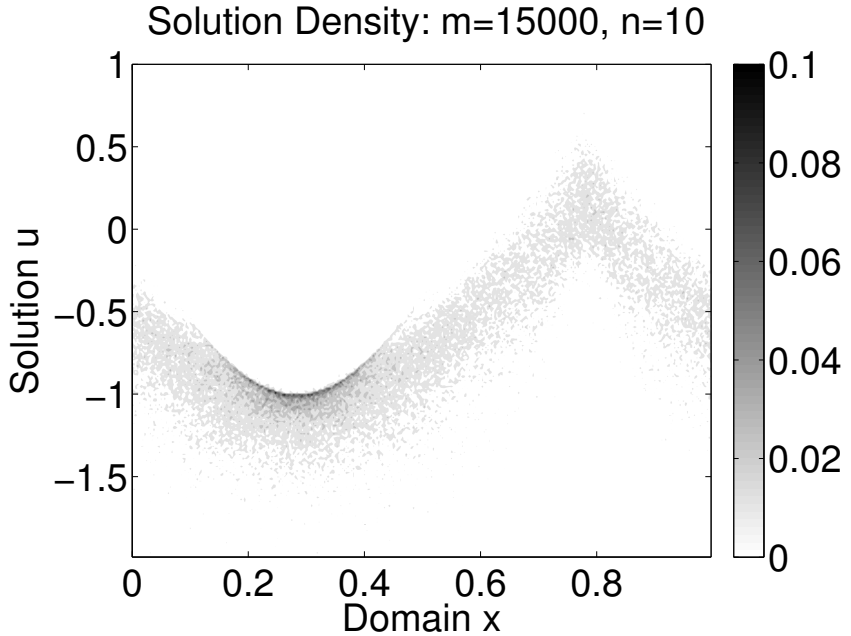




Time-Invariant Hamilton-Jacobi Equation



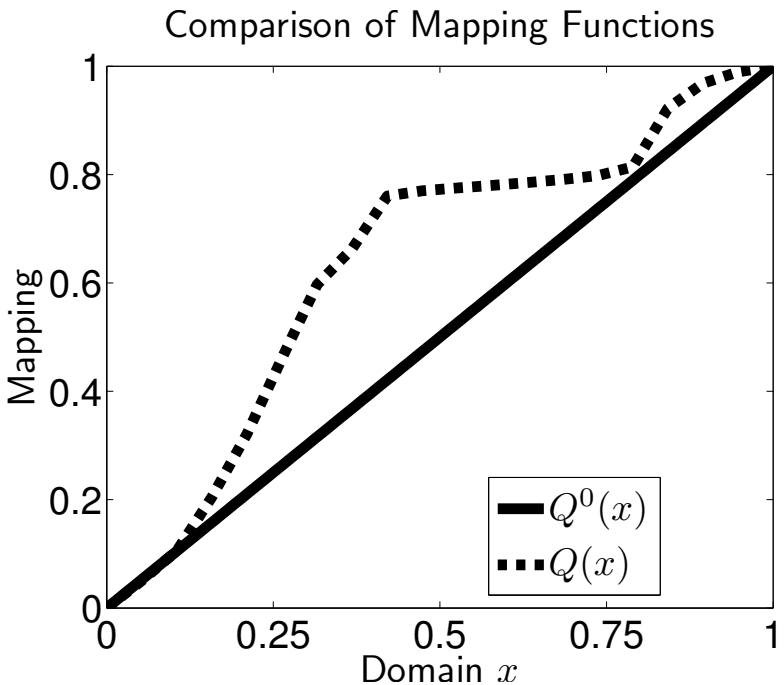


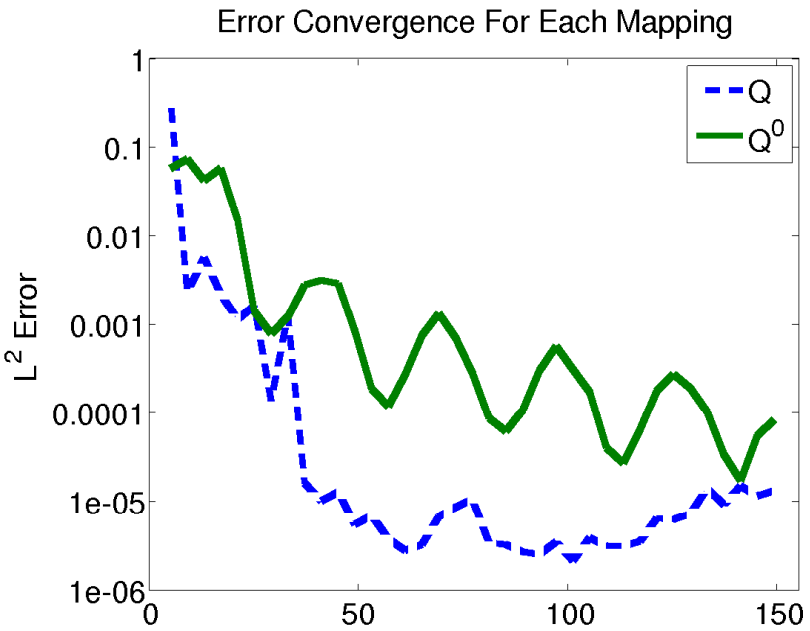
$$u + (u_x)^2/\pi^2 = -\left|\sin(\pi(x - \frac{\pi}{4}))\right| + \cos^2(\pi(x - \frac{\pi}{4})), \qquad (1)$$

$$\text{Solution: } u(x) = -\left|\sin\left(\pi\left(x - \frac{\pi}{4}\right)\right)\right|$$

Cockburn & Yenikaya 2005

Hamilton-Jacobi





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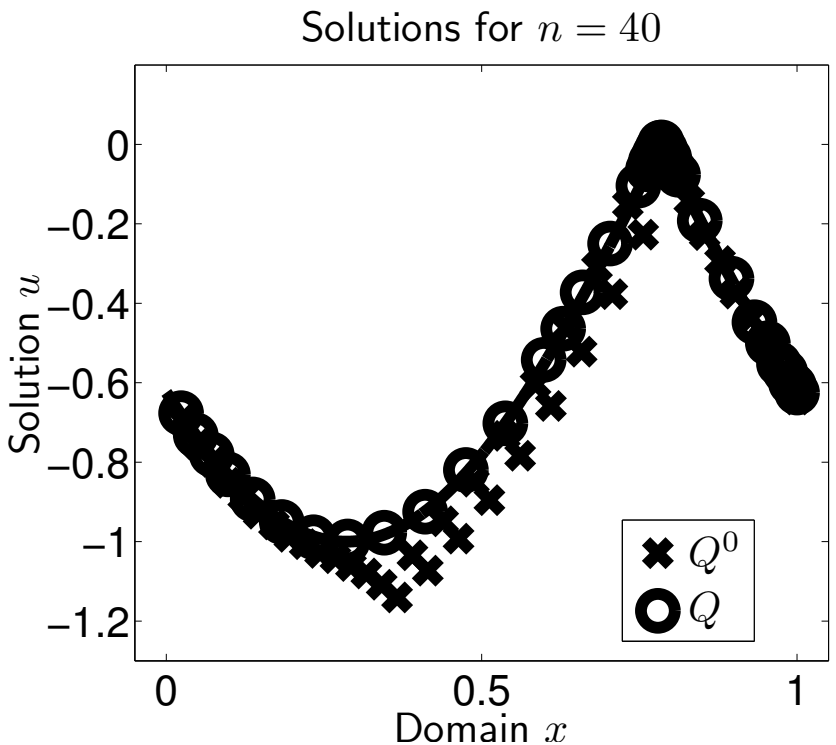
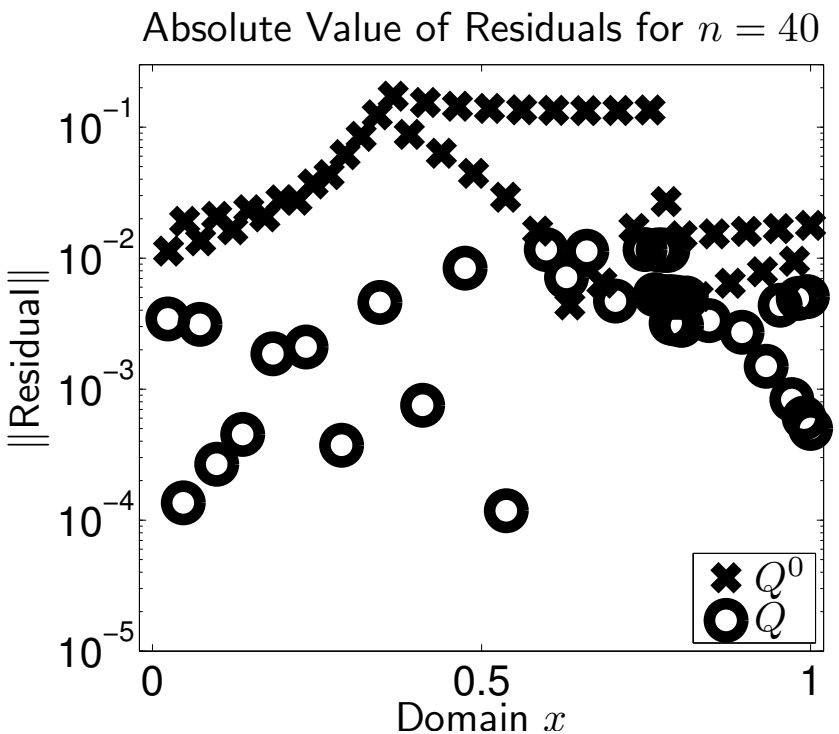
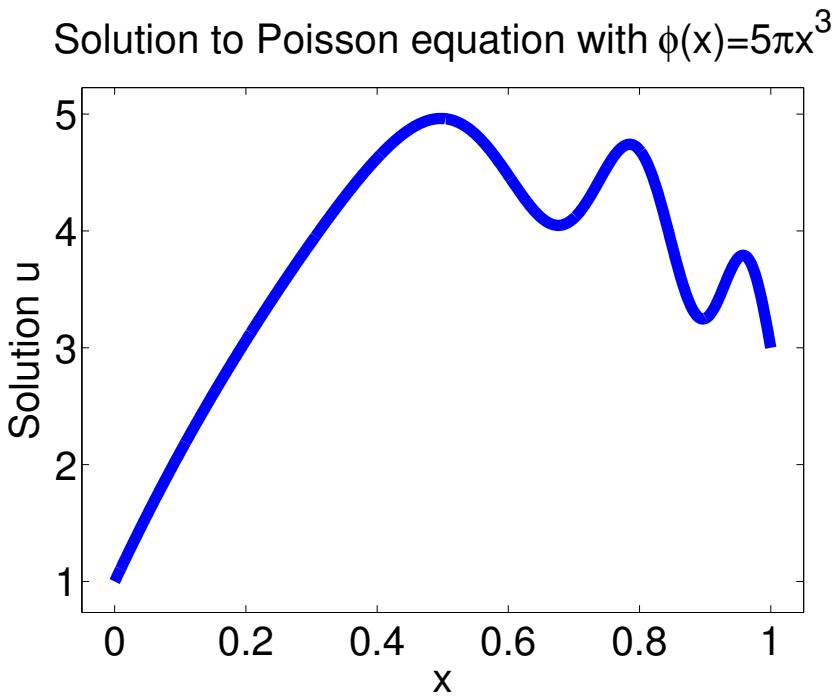
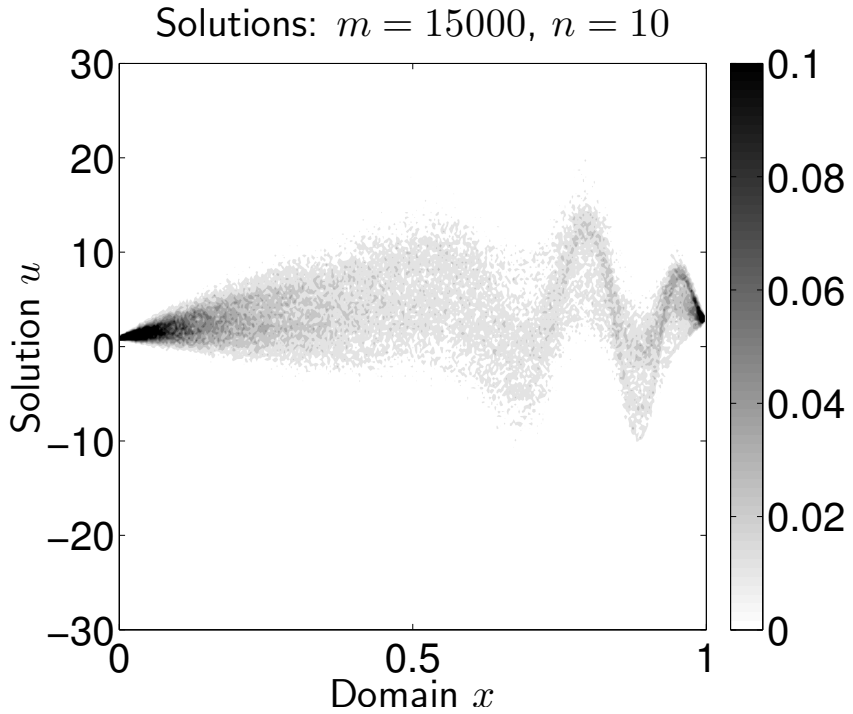




Oscillatory BVP



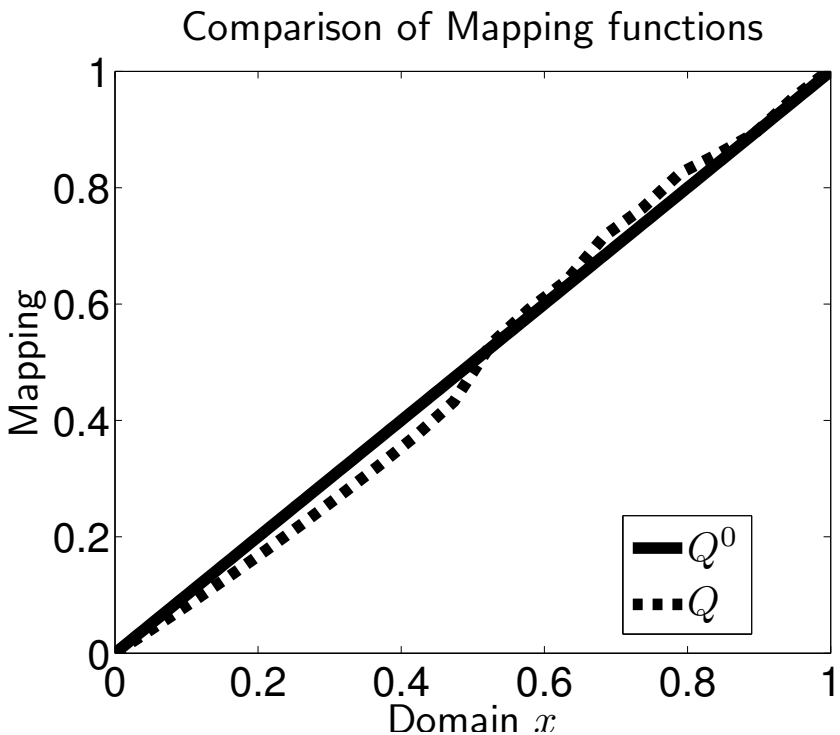


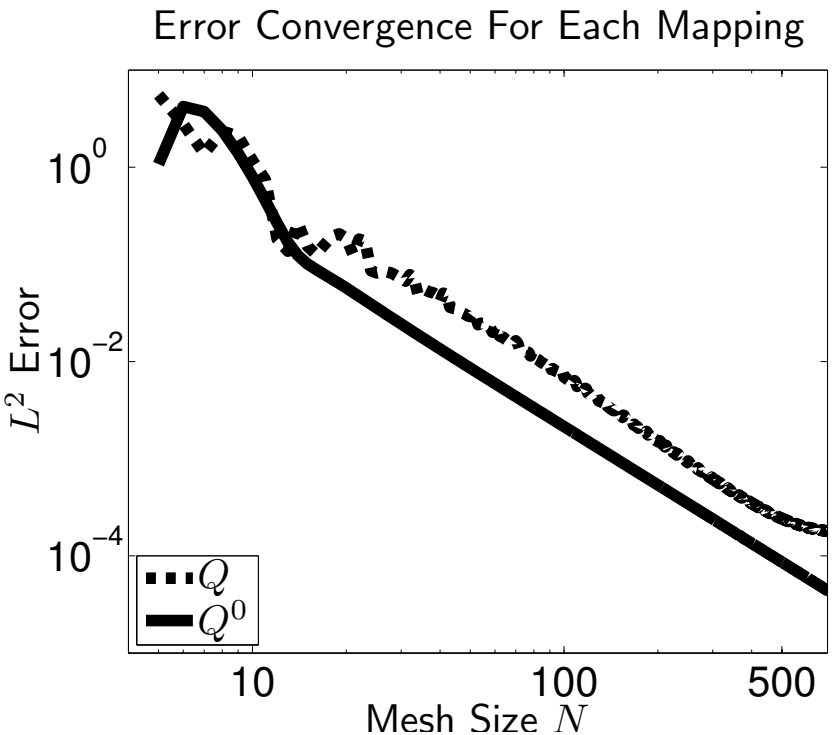
$$u''(x) = -20 + 0.5\phi''(x)\cos(\phi(x)) - 0.5(\phi'(x))^2 \sin(\phi(x))$$

for $\phi(x) = 5\pi x^3$, $u(0) = 1$, and $u(1) = 3$ with solution

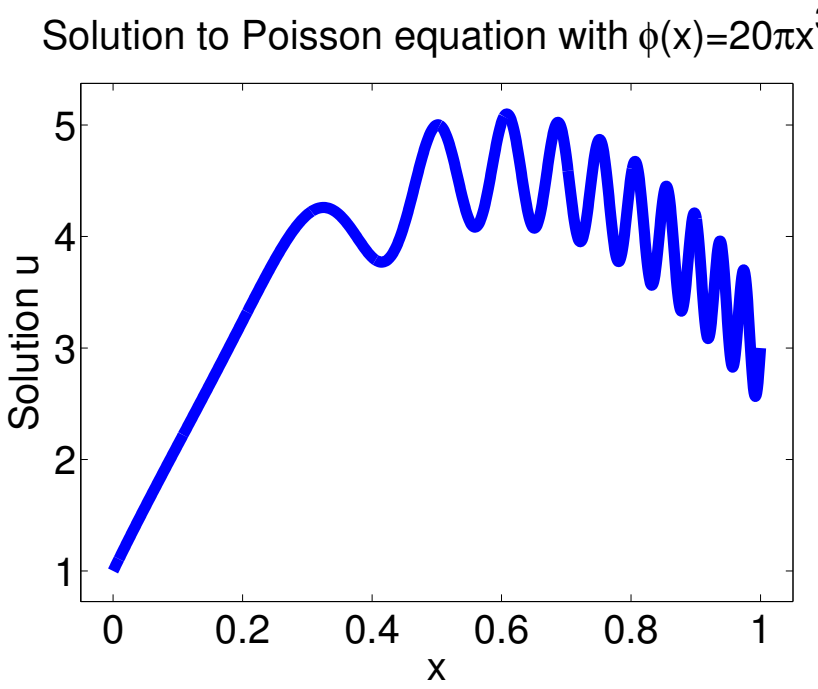
$$u(x) = 1 + 12x - 10x^2 + a\sin(\phi(x))$$

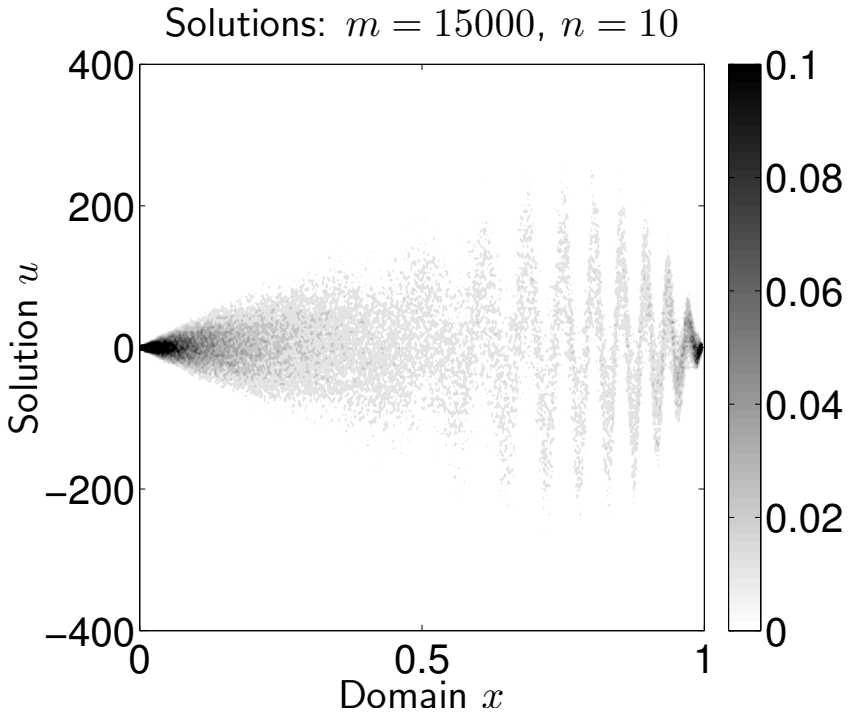
Oscillatory BVP





Highly Oscillatory BVP





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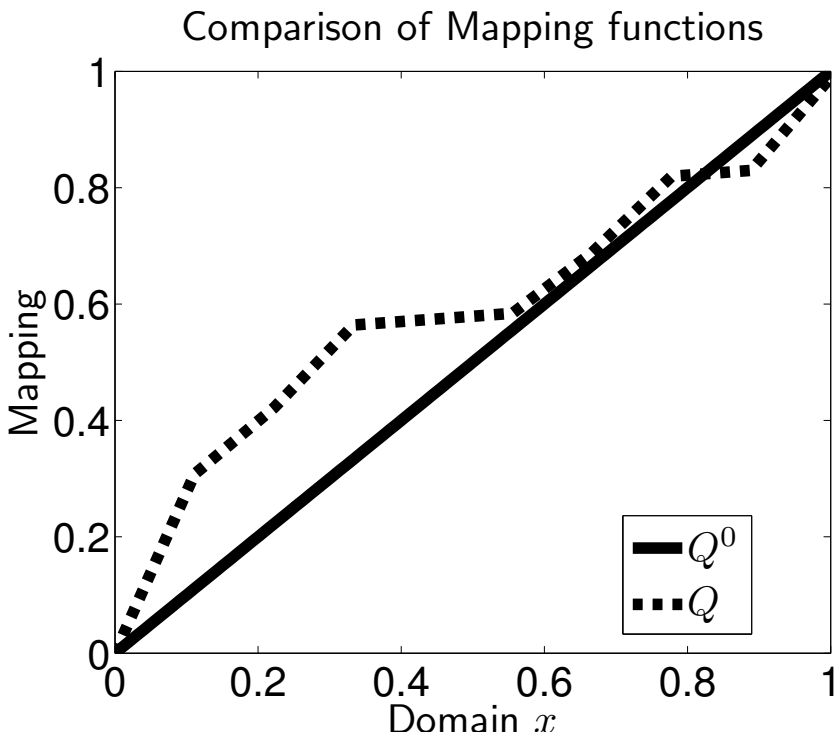
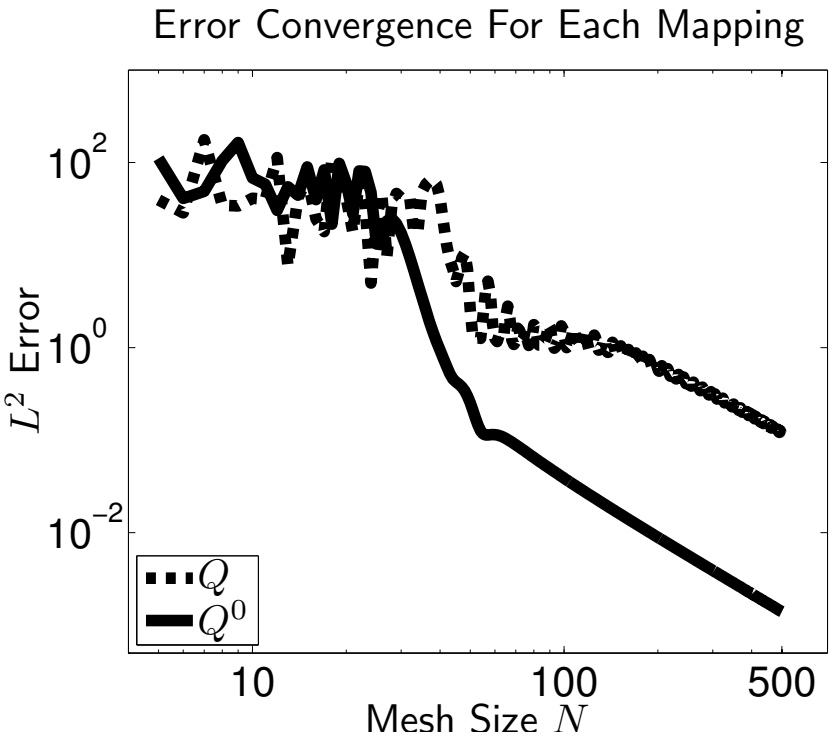
Highly Oscillatory BVP





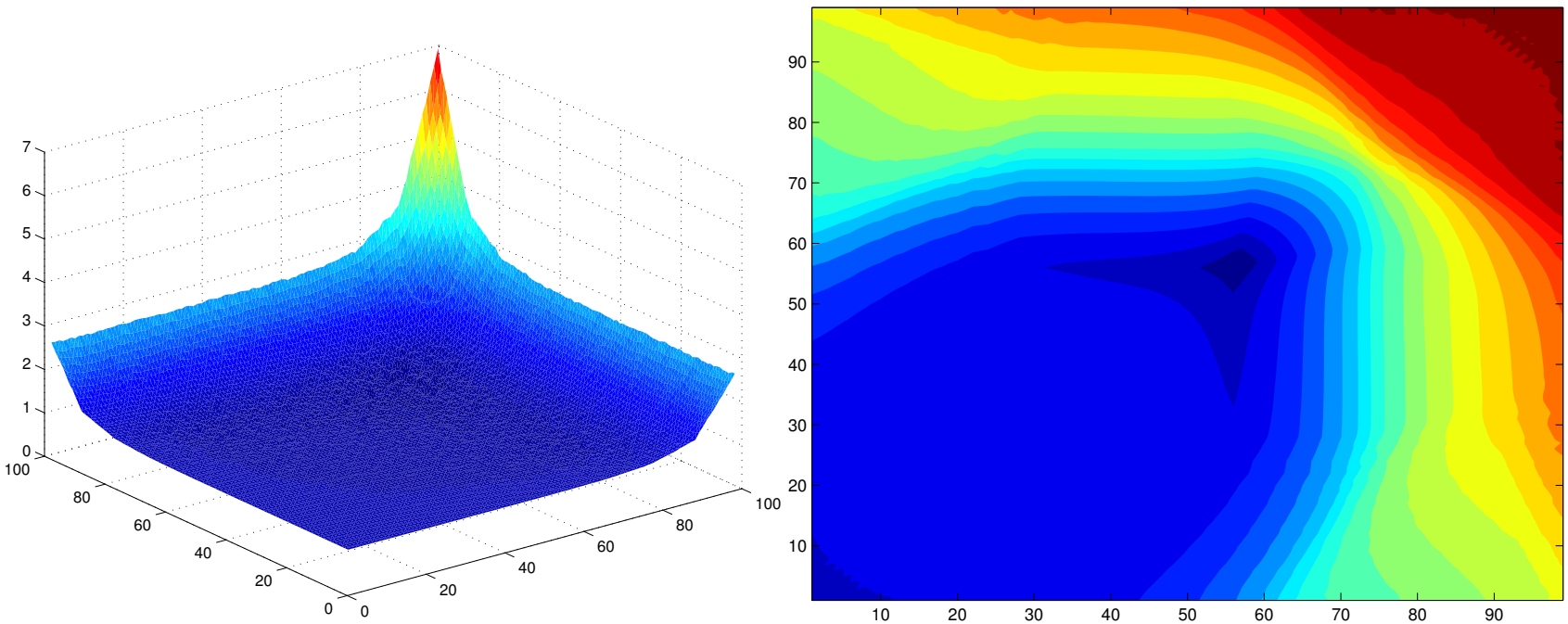
Summary

- Methodology exploiting massively-multicore architecture:
  - Minimizing variance of solutions is not robust
  - Use moments of sparse-mesh solutions to create superior nonuniform mesh
  - Promising for problems with local features
  - Disappointing for problems with oscillations
- Theory
  - First moment convergence (in expectation)
  - Consistency and Stability (in expectation)
  - Inverse Problem well-posedness
- 1D mesh generation: DMB & AJC, *SIAM J. Sci. Comp.*, in revision.
- Theory: DMB & Byrne, *Inverse Problems*, in revision.

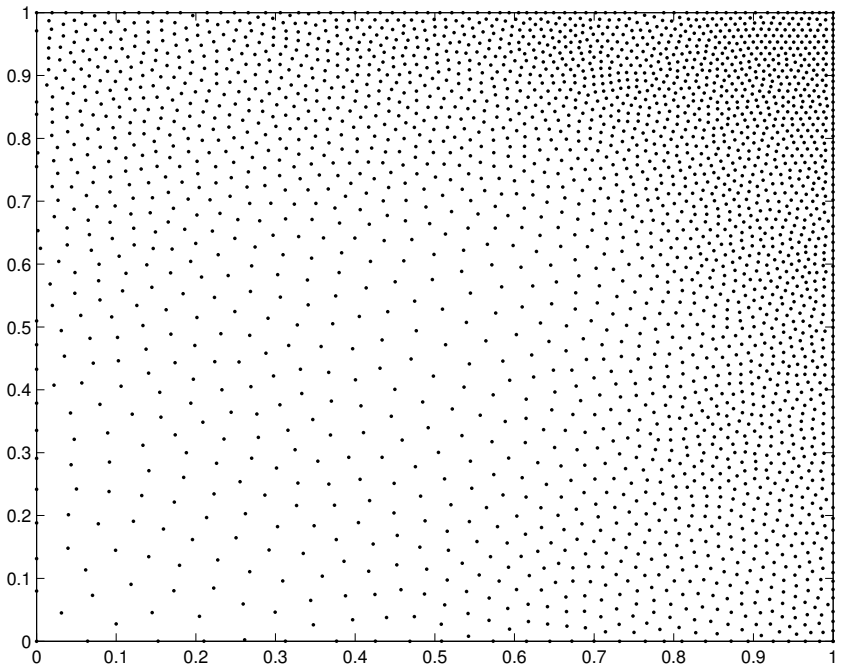
Work in Progress

- Framework for creating Q from moments.
- 2D investigation
  - Standard FEM solve
  - Comparison with moving meshes
  - DMB & AJC, in prep.
- Moving Mesh Methods
  - Monitor functions

Singular BVP

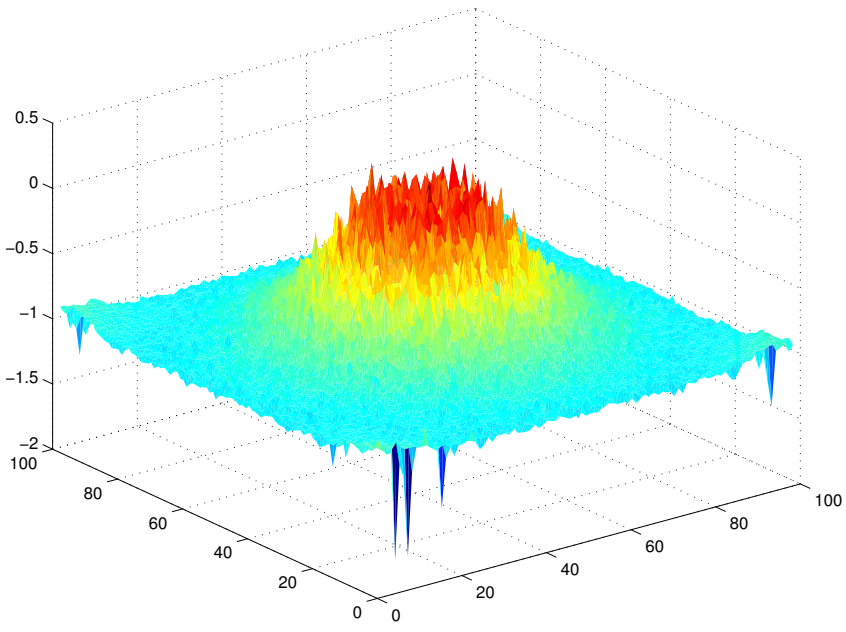


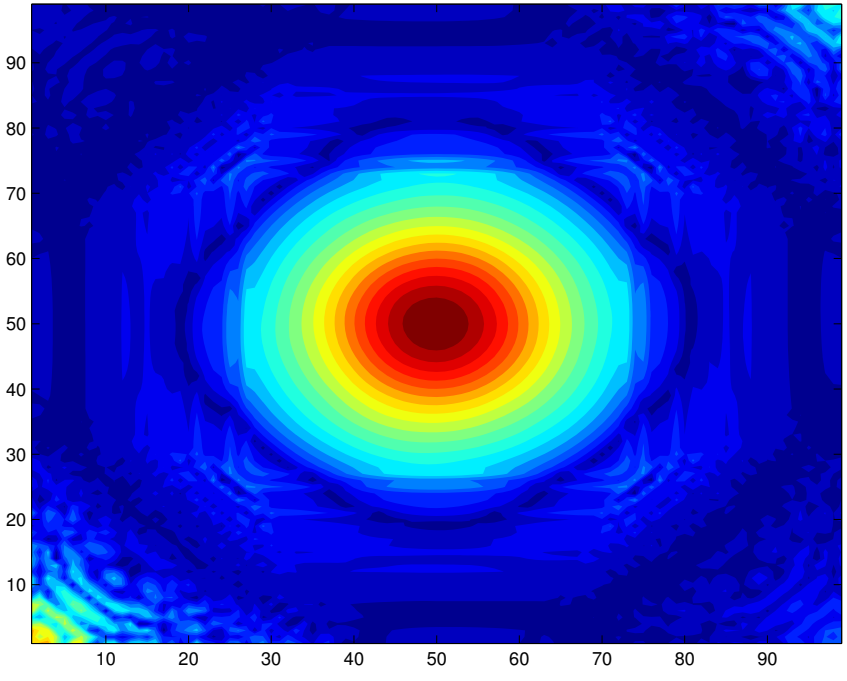
Singular BVP



$$h_{min} = 0.01$$

Hamilton-Jacobi





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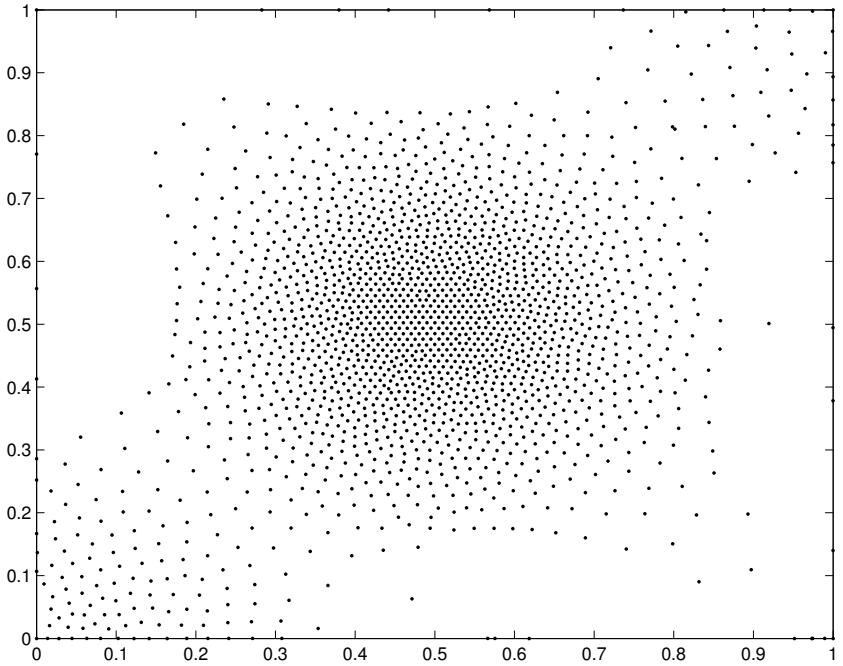

Acknowledgments

Comp. Math. FA9550-09-1-0403

Academic Partnership Program