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14. ABSTRACT

We proposed a novel approach which employs random sampling to generate an accurate non-uniform mesh for numerically solving Partial Differential Equation Boundary Value Problems (PDE-BVPs). From a uniform probability distribution U over a 1D domain, we considered a M discretization of size N where M>>N. The statistical moments of the solutions to a given BVP on each of the M ulta-sparse meshes provide insight into identifying highly accurate non-unuform meshes. We used the pointwise mean and variance of the coarse-grid solutions to construct a mapping Q(x) from uniformly to non-uniformly spaced mesh-points. The error convergence properties of the approximate solution to the PDE-BVP on the non-uniform mesh are superior to a uniform mesh for a certain class of BVPs. In particular, the mehod works well for BVPs with locally non-smooth solutions. We fully developed a framework for studying the sampled sparse-mesh solutions and provided numerical evidence for the utility of this approach as applied to a set of example BVPs.

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Solving Differential Equations with Random Ultra-Sparse Numerical Discretizations

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Final Report

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Abstract We proposed a novel approach which employs random sampling to generate an accurate non-uniform mesh for numerically solving Partial Differential Equation Boundary Value Problems (PDE-BVP's). From a uniform probability distribution $\mathcal{U}$ over a 1D domain, we considered M discretizations of size N where $M \gg N$. The statistical moments of the solutions to a given BVP on each of the M ultra-sparse meshes provide insight into identifying highly accurate non-uniform meshes. We used the pointwise mean and variance of the coarse-grid solutions to construct a mapping $Q(x)$ from uniformly to non-uniformly spaced mesh-points. The error convergence properties of the approximate solution to the PDE-BVP on the non-uniform mesh are superior to a uniform mesh for a certain class of BVP's. In particular, the method works well for BVP's with locally non-smooth solutions. We fully developed a framework for studying the sampled sparse-mesh solutions and provided numerical evidence for the utility of this approach as applied to a set of example BVP's.

Summary Over the duration of this grant, while developing our SMRT methodology for solving BVP-PDEs, the core of our research efforts have include the following: substantial refinement to our algorithm, extension of the algorithm to higher dimensions, and establishing the theoretical well-posedness of our approach [3,4]. All of these topics are linked by a desire to efficiently exploit the high paralellizability of our approach and future implementation on massively parallel multi-core technologies. Lastly, we have also been invited to contribute a review article on computing on GPU's to SIAM Review [5]. The focus of this effort is one type of computation which is substantially accelerated on GPU's.

We now give a brief summary of our progress.

Scandalously Paralellizable Mesh Generation The PI and his collaborator are developing an SMRT framework to generate non-uniform meshes for solving PDE's [3,4,5]. These discretizations can offer superior solution accuracy and convergence properties to that of uniform spacing. We offer a brief overview of our proposed algorithm as well as the establishment of a preliminary theoretical framework [3]. Also, in [4] we extended resutls in [2] to the identification of Q using an optimization technique using results from probability theory. However, we discovered that the approximation technique described below was substantially more efficient.

We consider a monotonically non-decreasing function $Q : \bar{\mathbf{I}} \to \bar{\mathbf{I}}$ which is absolutely continuous on a finite number of compact subsets of $\bar{\mathbf{I}}$ and restricted at the endpoints to $Q(0) = 0$, $Q(1) = 1$. The purpose of the function Q is to map the uniformly spaced mesh to a non-uniformly spaced one. The goal is to develop a strategy for identifying a Q such that, e.g., the approximate solution to the Poisson problem

$$u''(Q(x)) = f(Q(x)) \text{ s.t. } \quad u(Q(0)) = A\,; \quad u(Q(1)) = B\,,$$

has convergence properties (in n) superior to a uniform spacing.The core of our approach is to identify Q via a sparse stochastic approximation. We repeatedly sample from a distribution P and then use pointwise statistical moments of the coarse solutions to generate the desired non-uniform mesh function Q. Naturally, different classes of problems call for different strategies for generating Q. Our results, however, suggest that a more generalizable strategy may exist. Before presenting our conclusions, we briefly establish some notation.

Let p be a function taking a point $\xi \in \bar{\mathbf{I}}$ and a random vector of length n, and mapping them to a single random variable

$$p(\xi, \mathbb{X}_{(n)}(P)) \equiv \mathbb{E}_K \left[\left\{ U(\mathbb{X}_{(n)}(P)) \right\}_{K=k} \middle| X_{(k)} = \xi \right]. \tag{1}$$

The function U takes a discretization of the domain and solves the BVP. The operator $\mathbb{E}_K$ denotes expectation with respect to a uniform distribution on $\{1, \ldots, n\}$ where the distribution of the index random variable K and $\{\cdot\}_K$ denotes the Kth element of a vector. We note that this function returns a random variable for each ξ. Let the pointwise mean of p be defined for $\xi \in \bar{\mathbf{I}}$ as

$$\mu(\xi) \equiv \mathbb{E}_P \left[\mathbb{E}_K \left[\left\{ U(\mathbb{X}_{(n)}(P)) \right\}_{K=k} \middle| X_{(k)} = \xi \right] \right]. \tag{2}$$

The pointwise variance of p is defined for $\xi \in \bar{\mathbf{I}}$ as

$$v(\xi) \equiv \mathbb{V}_P \left[\mathbb{E}_K \left[\left\{ U(\mathbb{X}_{(n)}(P)) \right\}_{K=k} \middle| X_{(k)} = \xi \right] \right], \tag{3}$$

where $\mathbb{V}_P$ denotes variance with respect to P, $\mathbb{E}_K$ denotes expectation with respect to $\mathcal{U}\{1, \ldots, n\}$, the distribution of the index random variable K, and $\{\cdot\}_K$ denotes the Kth element of a vector.

Answers to the critical questions for this approach are depicted below

For each candidate Q, how many sample sparse grids need to be generated? The relationship between the mesh size n and the number of samples m is non-trivial. and Figure 1 illustrates this by depicting the error in $\bar{v}$ (relative to $\bar{v}$ computed with $m = 3000$ sampled from a uniform distribution on $\bar{\mathbf{I}}$) for a range of n and m values. For a given n, though, we do note that the error in the $\bar{v}$ computation is decreasing. In Figure 2 we depict the number of samples of vector size n which are needed to ensure three digits of accuracy in estimating the variance. Since the number was consistently below 1000 over a range of n, we let $m = 15000$ in all subsequent simulations (unless otherwise specified).

In what way do the random solutions converge to the actual solution? For a conventional finite difference discretization, we would consider the error E in the solution

$$\begin{aligned} \left\| E(Q, \mathbf{x}_n^0) \right\| &= \left\| u(Q(\mathbf{x}_n^0)) - U(Q(\mathbf{x}_n^0)) \right\| \\ &= \left\| A_{Q(\mathbf{x}_n^0)}^{-1} \left(A_{Q(\mathbf{x}_n^0)} u(Q(\mathbf{x}_n^0)) - f_{Q(\mathbf{x}_n^0)} \right) \right\| \\ &\leq \left\| A_{Q(\mathbf{x}_n^0)}^{-1} \right\| \left\| \tau_{Q(\mathbf{x}_n^0)} \right\|, \end{aligned}$$

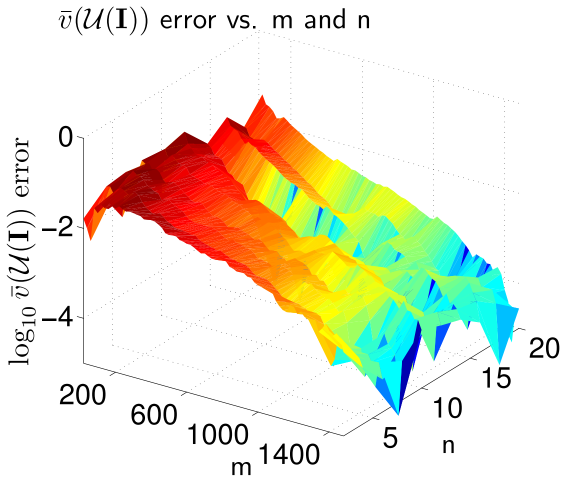

Figure 1: $\log_{10}$ of the error in the computation of $\bar{v}$ (sampling from a uniform distribution on $\bar{\mathbf{I}}$) as a function of m and n. Note the general downward trend along both the m and n axes.

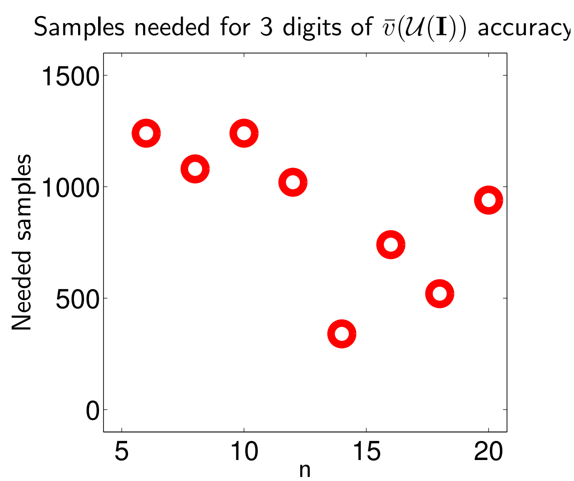

Figure 2: For each n, the vertical axis reflects the number of samples needed to compute the variance with 3 digits of accuracy relative to $\bar{v}$ (sampling from uniform distribution on $\bar{\mathbf{I}}$) with $m = 3000$.

which is bounded above by the spectral radius of the inverse of the finite difference operator $A^{-1}_{Q(\mathbf{x}^0_n)}$ and a truncation error $\tau_{Q(\mathbf{x}^0_n)}$. For the non-uniform three-point-stencil approximating the second derivative, the truncation error is $O(\max_k |h_k|)$. For our development, we consider a probabilistic version of this error, with the following conditions.

CONDITION C1. *For a given P, the spectrum of* $A^{-1}_{\mathbb{X}_{(n)}(P)}$ *is bounded in* $[0,1]$.

CONDITION C2. *For a given P, the truncation error induced by a finite difference approximation to the second derivative is first order in the largest step-size h.*

THEOREM 1. Under Condition C1 and C2, the expected error converges pointwise to zero.

See [3] for support of these conditions as well as a proof of the theorem.

How should Q be constructed? The function Q is created using the statistical moments of the sampled sparse-mesh solutions and based on results in [1]. For the problems with second derivatives we define Q as

$$Q(x) = \left[\frac{q_1(\cdot)}{q_1(1)}\right]^{-1}(x),$$

where

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

and the superscript -1 is an inverse function operator. Essentially, this definition will pile up points in regions with a steep solution in an effort to provide higher order accuracy for the nonuniform second derivative discretization.

For the problem with a second power of the first derivative, we define Q as

$$Q(x) = \left[\frac{q_2(\cdot)}{q_2(1)}\right]^{-1}(x),$$

where

$$q_2(x) = \int_0^x \mu''(\xi; U(\mathbb{X}_{(n)}(P))^2 \nu(\xi; U(\mathbb{X}_{(n)}(P))^3 d\xi,$$

and ν is defined above. Evidence for improvement in error convergence is depicted in Figures 3-4
.

We hypothesize that the reason $q_1(x)$ works well is that the μ' may converge faster than μ. We also hypothesize that the function $q_2(x)$ works well because the second derivative (when cast as the local curvature) is inversely proportional to the local variance of a random variable (a result which is well known in the semi-parametric nonlinear regression literature). Essentially, while the μ'' may not converge quickly, the product $\mu''\nu$ does. We also found that multiplication by an extra ν dramatically improves the computed Q, though an explanation is not immediately clear. A deeper understanding of the spectrum of $A_{\mathbb{X}_{(n)}(P)}$ and how it depends upon the choice of P will be essential to explaining the efficiency of $q_2(x)$. We plan to explore both of these issues in a future paper [4].

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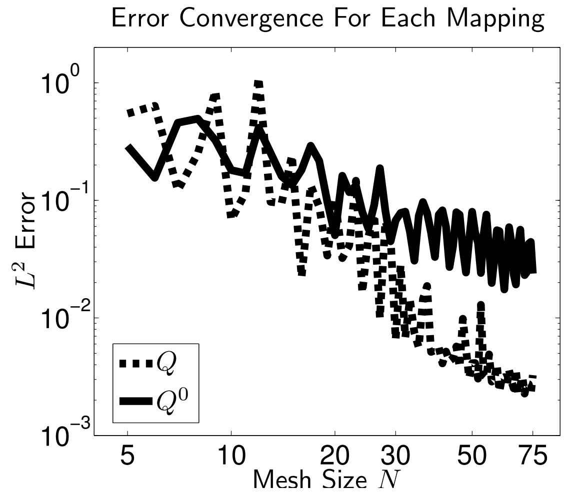

Figure 3: Error convergence for uniformly and non-uniformly spaced points for the steady-state Hamilton-Jacobi BVP.

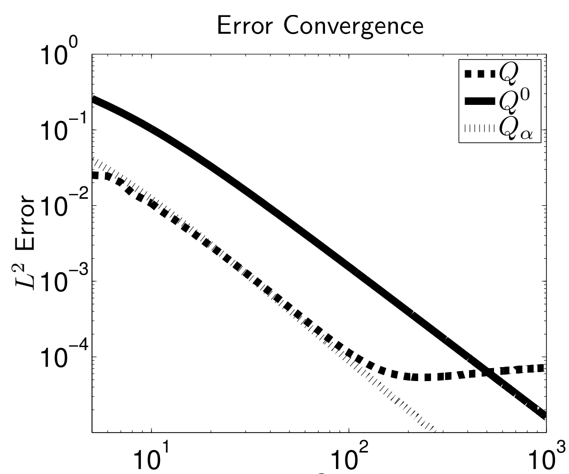

Figure 4: Error convergence of the different mesh mappings for the singular BVP.

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Publications

3. D.M. Bortz and A.J. Christlieb, "Scandalously Parallelizable Mesh Generation," in revision SIAM J. Scientfic Computation.

4. D.M. Bortz and E.C. Byrne, "Identification of Conditional Probability Measures," in revision Inverse Problems.

5. D.M. Bortz and A.J. Christlieb, "Analysis of Random Mesh Generation Methods," in preparation.

6. D.M. Bortz, A.J. Christlieb, J. Cohen, and F. Fahroo, "Computations on GPU's," in preparation.

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