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 $M$ 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 BVPs. In particular, the method 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.
Solving Differential Equations with Random Ultra-Sparse Numerical Discretizations

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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 parallelizability 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 Parallelizable 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 results 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 $Q : \bar{I} \rightarrow \bar{I}$ which is absolutely continuous on a finite number of compact subsets of $I$ 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

$$u''(Q(x)) = f(Q(x)) \ s.t. \ u(Q(0)) = A; \ u(Q(1)) = B,$$
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 \(\xi \in \bar{I}\) and a random vector of length \(n\), and mapping them to a single random variable

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

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 \(K\)th element of a vector. We note that this function returns a random variable for each \(\xi\). Let the pointwise mean of \(p\) be defined for \(\xi \in \bar{I}\) as

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

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

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

where \(\mathbb{V}_P\) denotes variance with respect to \(P\), \(\mathbb{E}_K\) denotes expectation with respect to \(\mathbb{U}\{1, \ldots, n\}\), the distribution of the index random variable \(K\), and \(\{\cdot\}_K\) denotes the \(K\)th 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 \(\tilde{v}\) (relative to \(\tilde{v}\) computed with \(m = 3000\) sampled from a uniform distribution on \(\mathbb{I}\)) for a range of \(n\) and \(m\) values. For a given \(n\), though, we do note that the error in the \(\tilde{v}\) 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

\[
\| E(Q, x^0_n) \| \leq \| u(Q(x^0_n)) - U(Q(x^0_n)) \|
\]

\[
\leq \left\| A^{-1} Q(x^0_n) \left( A_{Q(x^0_n)} u(Q(x^0_n)) - f_{Q(x^0_n)} \right) \right\|
\]

\[
\leq \left\| A^{-1} Q(x^0_n) \right\| \left\| T_{Q(x^0_n)} \right\| ,
\]

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Figure 1: $\log_{10}$ of the error in the computation of $\bar{v}$ (sampling from a uniform distribution on $\bar{I}$) 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 $\bar{I}$) with $m = 3000$. 
which is bounded above by the spectral radius of the inverse of the finite difference operator $A^{-1}_{Q(x_0^n)}$ and a truncation error $\tau_{Q(x_0^n)}$. 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 $A^{-1}_{X(n)}(P)$ 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

$$Q(x) = \left[ \begin{array}{c} q_1(x) \\ q_1(1) \end{array} \right]^{-1}(x),$$

where

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

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

$$Q(x) = \left[ \begin{array}{c} q_2(x) \\ q_2(1) \end{array} \right]^{-1}(x),$$

where

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

and $v$ 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 $\mu'$ may converge faster than $\mu$. 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 $\mu''$ may not converge quickly, the product $\mu''v$ does. We also found that multiplication by an extra $v$ dramatically improves the computed $Q$, though an explanation is not immediately clear. A deeper understanding of the spectrum of $A_{X(n)}(P)$ 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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References


Publications


Personnel Supported by Grant During 10-11
D.M. Bortz, Assistant Professor, University of Colorado, Boulder
A. J. Christlieb, Associate Professor, Michigan State University

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University of Graz, Invited speaker for summer school on mathematical methods in mathematical biology 2009
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