A Generalized Multilevel Adaptive Solver for PDEs with Fast Transitions

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Date: December 8th, 2006
Type: Dissertation Proposal
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Summary

Whether tracking the eye of a storm, the leading edge of a wildfire, or the front of a chemical reaction, one finds that significant change occurs at the thin edge of an advancing line. The tracking of such change-fronts comes in myriad forms with a wide variety of applications. Our research over the past two years combines fast multiresolution methods with the freedom of gridless techniques to arrive at a robust and accurate PDE solver for systems exhibiting fast transitions. Our method is unique because it unifies collocation, mesh refinement and solution strategy under one underlying wavelet-like representation. These attributes, as well as the method's inherent parallelizability, make it ideally suitable for scientific inquiry via in silico experiments.

INTELLECTUAL MERIT—We have developed a numerical solver capable of detecting sharp transition regions and refining its own computational domain and linear solver while maintaining a uniform generalized multiresolution analysis. Our method does not require expensive tiling of the computational domain, and its front tracking and coarsening strategies are inherently parallelizable. Both of these features make our adaptive multilevel solver ideal for HPC applications.

BROADER IMPACT—Our research culminates with a software package suitable for exploration of discontinuous and multiscale phenomena. Preliminary results have

already been achieved in nano-electronics and computational finance [29, 30, 31, 32]. In addition to its scientific merits, our method is ideally suited for further theoretical development, as it maps $\mathbb{R}^n \to \mathbb{R}$. This feature also makes the method easily incorporable into numerical curricula at both the graduate and undergraduate level, thus further disseminating key ideas developed throughout this research venture.

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1 Introduction

Our research over the past two years on multiresolution methods [24, 25, 29] is being integrated with quadrature techniques [9, 15, 18, 20] to arrive at a robust adaptive PDE solver designed for systems exhibiting fast transitions. Multiresolution methods naturally capture variations in the solution, but their extension to higher-dimensions are non-trivial due to numerous stability conditions imposed on the tiling of the computational domain [8, 37, 38]. Quadrature (or meshless) methods have natural extensions to higher dimensions and have become ever more present in the modern development of numerical PDE solvers [4, 13, 16, 19, 21, 23, 26, 27, 28, 34, 36]. In recent years, these meshless techniques have been combined with mesh refinement methods to form adaptive PDE solvers [11, 16, 26, 34]; however, no uniform treatment of mesh refinement and compact function representation has been undertaken. It is this synergy—between variation capturing techniques and compact radial basis function methods—which we are developing.

The development of this synergetic research focuses on the generalized multiresolution analysis of A. Harten [1, 17, 35]. His method and its extensions are used to capture variations in the solution and translate those variations into wavelet coefficients, which are then used to refine the mesh via coefficient thresholding [10]. Moreover, wavelets form a natural basis for the solution and can be interpreted as a compact alternative to radial basis functions (RBF) by extending the notion of a distance function [5, 6, 7]. In this way, the representation of the solution is better conditioned and its behavior can be tailored to the local features of the computational domain, which is not possible using traditional RBF approaches. This method captures adaptation and representation in a uniform multiresolution framework that tightly couples the interplay between mesh refinement and accurate depiction of the solution.

KEYWORDS: *Generalized Multiresolution Analysis, Mesh Coarsening, Radial Basis Functions, and Distance Wavelets.*

2 Planned Investigation

Our investigation of variation capturing techniques and compact radial basis function methods has three primary components. These components are: mesh coarsening via generalized multiresolution analysis, adaptive multi-quadratic radial bases, and distance wavelets as radial bases. The initial study, which involved the analysis and development of a two-dimensional coarsening strategy for discontinuous applications, is complete [25]. The results of this study have yielded insight into a parallel implementation of the coarsening algorithm that could be useful for data mining and large image processing applications. Our research agenda is currently focused on the development of adaptive multi-quadratic radial basis functions; this research is delineated in Section 2.1 after a short background discussion on multi-quadratic functions. The final component of the research concentrates on the development and implementation of compact radial basis analogs for PDE applications with fast transitions (see Section 2.2).

2.1 Adaptive Multi-Quadratic Radial Basis Functions

Multi-quadratic functions have been used since the early 1970's for topographical and scattered data fitting applications [15, 18]. More recently, Kansa [20, 21] began using these methods for the numerical solution of PDEs. In the last ten years, the growth in the theoretical understanding of radial bases has contributed to the explosion in RBF methods for PDEs [4, 11, 13, 16, 19, 21, 23, 26, 27, 28, 34, 36]. However, there are important issues that need to be resolved [22], and primary among these is lowering the condition number of the resulting linear system.

The condition number increases when large numbers of radial bases are used to approximate the solution, as well as when the coupling involves all radial basis functions within a computational domain (see Table 1). Therefore, the condition number can be decreased by lowering the number of nodes used in the approximation and decoupling long-range effects. The first can be accomplished by coarsening the computational domain, the second by limiting the range of interaction between radial basis functions (via parameter tuning), or by using compactly supported basis functions (refer to Section 2.2).

Domain Size	16×16	32×32	64×64
Condition Number	6.2 E06	2.9 E08	1.5 E10

Table 1: Doubling domain size increases condition number by two orders of magnitude.

In this first study, we explore a family of multi-quadratic functions which have a positive parameter that can be used to prescribe long-range coupling between basis functions. This parameter can be chosen to coincide with the local mesh refinement measure, thereby prescribing different coupling constants depending on the local behavior of the computational domain. In this way, we arrive at a preliminary adaptive collocation method, which we can use to refine our multiresolution mesh coarsening strategy in two dimensions and test the method's robustness against different types of applications.

DIFFICULTIES—The coupling between the grid refinement measure, expressed in terms of wavelet coefficients, and the parameter in the multi-quadratic family may not be fully compatible. Therefore, a simple scaling function might not be sufficient to correctly capture the solution in regions exhibiting fast transitions.

2.2 Compactly Supported RBF Analogs

The next stage in the development of our adaptive collocation method is to replace the ad-hoc parameter based radial basis functions with compactly supported multiresolution bases. This is a novel approach, as compactly supported basis functions have traditionally been constructed by simply truncating the basis' domain [14, 39, 40]. This simplistic compactification approach produces a scheme which is sparse, but whose condition number is comparable to that of a non-compact scheme. Moreover, these simple compact schemes suffer from instabilities produced by the truncation of the basis' domain.

More recently, compactly supported basis functions have been constructed using multiresolution techniques [2, 3, 5, 6, 7, 12, 33]. These techniques allow for a better representation of the underlying function in terms of scales, thus capturing the function accurately while maintaining a sparse representation, a feature crucial to the development of fast numerical methods. In addition, it has been shown that multilevel methods play an important role in the development of iterative solvers by preconditioning the resulting RBF system [13]. Therefore, our adaptive multiresolution approach will be sparse and robust to charges in scales, and will result in better conditioned systems.

DIFFICULTIES—Defining distance wavelets that are computationally efficient and couple well to the coarsening algorithm already developed in terms of generalized wavelets.

3 Evaluation Criteria

The research as it has been presented has two components: function representation, and PDE solution. The first of these is simple to evaluate, because an energy norm or wavelet measure suffices to verify the approximation properties of the compactly supported basis functions. This static representation portion of the evaluation process is presently being conducted on discontinuous test functions (see sample function in Figure 1). The second of these components, the PDE solution, will be tested against analytic and numerical solutions of elliptic and hyperbolic systems.

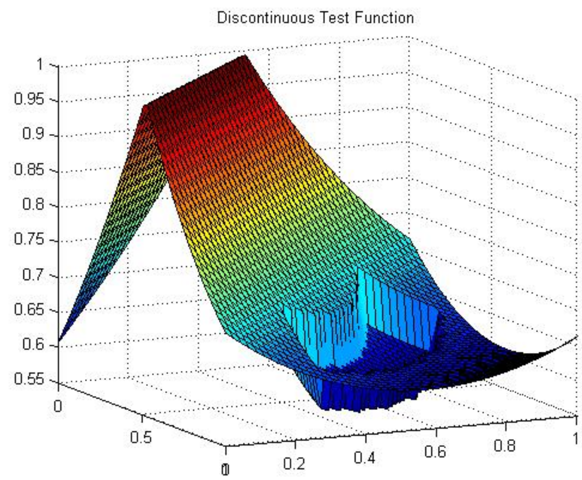

Figure 1: Sample test function with jumps in its values and first derivatives.

Elliptic systems have a natural representation based on multiresolution techniques; thus, they are a natural first test case for our adaptive collocation method. We will first reproduce some of the results for elliptic operators, both linear and non-linear, in the RBF literature [13, 16]. Once we have successfully reproduced the literature, our plan is to apply our method to more interesting applications in nano-electronics—where the PDEs become coupled and non-linear, with internal layers and general boundary conditions.

Hyperbolic applications such as those described in [4, 11, 26, 27] are an excellent test bench for the adaptive portion of our method, and we expect these tests to challenge the accuracy and robustness of our compact basis functions. Perhaps the most difficult portion of benchmarking our collocation solver against hyperbolic systems will involve errors in time integration, as we do not yet have an integrator that fully respects the multiresolution structure. Further investigations and development of a robust multiresolution integrator is left as a future research venture.

DIFFICULTIES—Testing our adaptive collocation method against time marching solutions, because our current research does not have an integration technique that couples to the multilevel structure of our solver.

4 Timeline

The remaining portion of this research revolves around the collocation portion of the solver. This research involves the transition from traditional to compactly supported RBFs and their representation properties in terms of elliptic and hyperbolic PDEs. A large amount of time will be spent on the RBF representation portion of the method, and the remaining time on application development and research dissemination.

To date, we have developed a thin-plate spline collocation method that is being extended to utilize multi-quadratic RBFs. This new family of RBF functions essentially expands the method by allowing us to adaptively change the coupling neighborhood of each RBF independently (refer to Section 2.1). The next task is to move from these parameter based multi-quadratic RBFs to fully compact analogs based on multiresolution methods (refer to Section 2.2). Testing of our adaptive collocation method against the literature is expected to be finished by February; from February to April, the research results will be compiled into a manuscript.

TIMELINE:

November	–	Thin-Plate Splines to Multi-Quadratic Radial Basis Functions
December	–	MQ RBFs to Compactly Supposed Analogs
February	–	Test Applications
March	–	Complete Dissertation

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