

# **Numerical Methods for Forward and Inverse Problems in Discontinuous Media**

**Final Scientific/Technical Report**

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by

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## Abstract

The research emphasis under this grant's funding is in the area of algebraic multigrid methods. The research has two main branches: 1) exploring interdisciplinary applications in which algebraic multigrid can make an impact and 2) extending the scope of algebraic multigrid methods with algorithmic improvements that are based in strong analysis.

The work in interdisciplinary applications falls primarily in the field of biomedical imaging. Work under this grant demonstrated the effectiveness and robustness of multigrid for solving linear systems that result from highly heterogeneous finite element method models of the human head. The results in this work also give promise to medical advances possible with software that may be developed.

Research to extend the scope of algebraic multigrid has been focused in several areas. In collaboration with researchers at the University of Colorado, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory, the PI developed an adaptive multigrid with subcycling via complementary grids. This method has very cheap computing costs per iterate and is showing promise as a preconditioner for conjugate gradient. Recent work with Los Alamos National Laboratory concentrates on developing algorithms that take advantage of the recent advances in adaptive multigrid research.

The results of the various efforts in this research could ultimately have direct use and impact to researchers for a wide variety of applications, including, astrophysics, neuroscience, contaminant transport in porous media, bi-domain heart modeling, modeling of tumor growth, and flow in heterogeneous porous media. This work has already led to basic advances in computational mathematics and numerical linear algebra and will continue to do so into the future.

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## Executive Summary

Research under this grant focused on the analysis, development and implementation of algebraic multigrid methods. Such methods show great promise in increasing the efficiency of modern computational science. Moreover, such work targeted applications stemming from forward and inverse problems in discontinuous media.

The analysis and development of such methods has concentrated on adaptive multigrid which automatically adjusts the multigrid components to improve efficiency. Success in such an area would vastly expand the use of multigrid into the engineering and scientific community where such users are generally not multigrid experts but require fast linear solvers in computational experimentation.

Work under this grant led to the development of an adaptive algebraic multigrid method that uses, so called, complementary grids. The method is notably cheap computationally per iteration and shows promise as an efficient preconditioner, which is a common role for multigrid methods. This work led to developing projects with two researchers at Los Alamos National Laboratory which are made possible by recent advances in adaptive multigrid research.

The work funded under this grant demonstrated the efficiency of multigrid on a biomedical application in brain topography. Algebraic multigrid methods were marketably faster than the preexisting methods being used. If such 3-D current distributions can be computed and visualized within an hour, clinical applications become possible. If it can be done in real time, clinical utility will be ensured. The work under this grant demonstrated that an efficient numerical solution based on algebraic multigrid is a promising direction in this field of research. Moreover, multigrid methods are also noteworthy for their scalability on a large class of problems. As such, multigrid methods have the potential to solve the currents and fields in a whole head model (800,000 nodes) within a few seconds on a fast computer. Such a result would benefit the field of brain modeling research.

Recent work with Los Alamos National Laboratory concentrates on developing algorithms that take advantage of the recent advances in adaptive multigrid research. Current work in the BoxMG implementation will be adding a general Full Approximation Scheme (FAS) based simulation framework. FAS and linear multigrid are equivalent for linear problems. As such, FAS is developed for nonlinear problems which are of importance to many DOE applications. More specifically, in FAS the coarse-grid problem is solved for the full approximation rather than the error equation. Existing research on adaptive AMG methods provides an excellent starting point for adaption of the operators in the FAS hierarchy. The work on BoxMG promises to leverage the direct connection to the physical problem, to aid in the development and analysis of new techniques and error estimation.

The results of the various efforts in this research could ultimately have direct use and impact to researchers for a wide variety of applications, including, astrophysics, neuroscience, contaminant transport in porous media, bi-domain heart modeling, modeling of tumor growth, and flow in heterogeneous porous media. This work has already led to basic advances in computational mathematics and numerical linear algebra and will continue to do so into the future.

# Final Scientific/Technical Report

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## 1 Adaptive Algebraic Smoothers

Chartier spent the month of June 2007 at Los Alamos National Laboratory. A majority of his time was spent in research collaboration with Bobby Philip a research scientist in the Mathematical Analysis and Modeling Group. Chartier and Philip made considerable progress on a new multigrid method that uses Local Sensitivity Analysis (LSA) to identify blocks of variables in a linear system that are strongly coupled. With such information regarding the coupling of variables, we construct stationary block iterative methods that can be used, for instance, as smoothers in multigrid methods. The smoothers so constructed can be used in the context of both geometric and algebraic multigrid methods. The method is suitable for both constant and variable coefficient problems. Furthermore, the method has been applied to systems arising from both scalar and coupled system partial differential equations (PDEs), as well as linear systems not arising from PDEs. The simplicity of the method will allow it to be easily incorporated into existing multigrid codes. Furthermore, it is possible to adaptively vary the size and strength of the blocks leading to the construction of a parametrized family of block iterative smoothers which can be tuned to the problem based on efficiency or convergence criteria.

Giving the details of this method are beyond the scope of this progress report but are available upon request. Chartier and Philip expect to submit a paper for peer review within the coming month. The next subsection gives numerical results on a variety of problems to emphasize the robustness of the method.

### 1.0.1 Varying anisotropy within the domain

The first example is from Section 1.3 in [19]. The underlying PDE is:

$$-(au_x)_x - (bu_y)_y + cu_{xy} = f(x, y) \quad (1)$$

defined on a unit square with full Dirichlet boundary conditions. The problem is defined such that  $a = b = 1$  everywhere except in the upper left quarter of the unit square where  $b = 10^3$  and the lower right quarter where  $a = 10^3$ . To split the domain into four regions with varying anisotropies,  $c = 0$  except in the upper right quarter where  $c = 2$ .

The discretized system is formed using a standard 5-point stencil and a (left-oriented) 7-point stencil for the diffusion and mixed derivative points of the PDE, respectively. As a result of these varying coefficients, the system is isotropic in the lower left quarter of the unit square but strongly anisotropic in the remaining quarters. The direction, however, of the anisotropy varies in the remaining three quarters of the unit square with the direction of strong connection lying in the  $x$ ,  $y$  and diagonal directions for the upper left, lower right, and upper right quarters, respectively. The varying directions of these anisotropies are reflected in the smooth error produced after four iterations of pointwise Gauss-Seidel seen in Figure

Pointwise		Block	
$\ r\ $	Conv. Fac.	$\ r\ $	Conv. Fac.
1.704e+007	1.00000	1.704e+007	1.00000
2.580e+006	0.15138	2.908e+003	0.00017
7.049e+005	0.27318	9.142e+002	0.31444
3.736e+005	0.53000	6.060e+002	0.66285
2.666e+005	0.71357	4.764e+002	0.78607

Table 1: Pointwise and block smoothing results for PDE given in 1 defined with full Dirichlet boundary conditions. Algebraic block smoothing created 285 blocks.

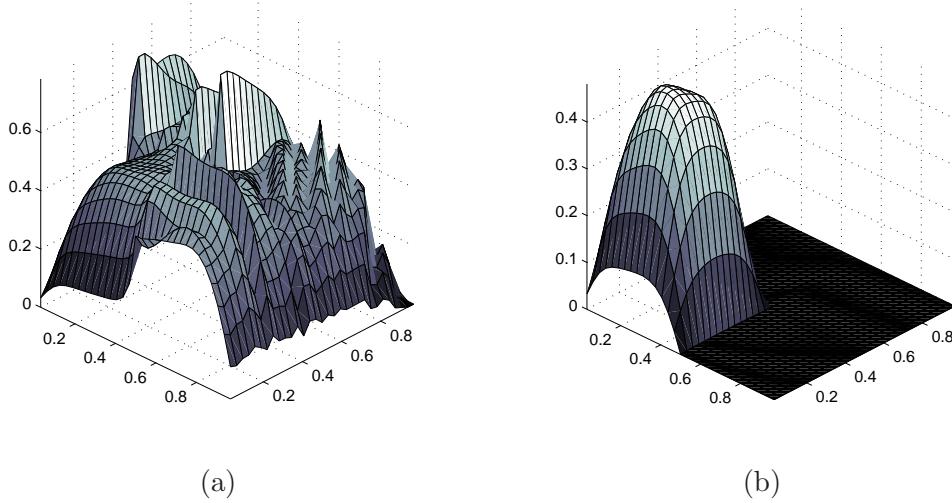


Figure 1: Algebraically smooth error after four iterations of (a) pointwise smoother and (b) block smoother for the scalar PDE (1).

1 (a). Note that the numerics use the discretized system which included both  $A$  and  $\mathbf{f}$  were supplied by Klaus Stüben.

In Table 1, pointwise Gauss-Seidel converges toward the solution. However, the adaptive algebraic smoother performs much better particularly in the first iteration which is important for multigrid methods. The adaptive algebraic smoother forms blocks that geometrically follow the anisotropies within each region, which results in geometrically smooth error, as seen in Figure 1 (b), suggesting its usefulness for geometric multigrid methods. Note that the largest error occurs in the quarter of the domain that is isotropic which is where the block smoother chooses only pointwise smoothing.

## 1.1 Systems of Partial Differential Equations

System PDEs are traditionally difficult problems for algebraic multigrid methods. This section demonstrates the ability of the adaptive algebraic smoother to define strong couplings for such problems and its affect on the block smoothing iteration. For simplicity the examples presented in this section are  $2 \times 2$  coupled systems of PDEs where AMG is known to have

Pointwise		Block	
$\ r\ $	Conv. Fac.	$\ r\ $	Conv. Fac.
33.43388	1.00000	33.43388	1.00000
4.91278	0.14694	0.06436	0.00193
1.32823	0.27036	0.02394	0.37189
0.73113	0.55045	0.00427	0.17855
0.53874	0.73686	0.00204	0.47660

Table 2: For  $\alpha = 0.1$ , algebraic block smoothing created 66 blocks for  $\epsilon = 0.01$  and  $k = 0.01$  in system (2).

Pointwise		Block	
$\ r\ $	Conv. Fac.	$\ r\ $	Conv. Fac.
2.68835e+003	1.00000e+000	2.68835e+003	1.00000
2.89686e+009	1.07756e+006	2.65285e-001	0.00010
1.06165e+014	3.66484e+004	2.61072e-005	0.00010
3.94519e+018	3.71608e+004	2.56705e-009	0.00010
1.47601e+023	3.74130e+004	2.51757e-013	0.00010

Table 3: For  $\alpha = 0.1$ , the adaptive algebraic smoother created 1089 blocks for  $\epsilon = 0.01$  and  $k = 100$  in system (2).

trouble.

We consider two model systems where the anisotropy in each variable differs. These systems were provided by Jim E. Jones [13]. In order to introduce the system of interest, define

$$-\Delta_{\epsilon:x} \equiv \begin{pmatrix} -1 & & \\ -\epsilon & 2+2\epsilon & -\epsilon \\ & -1 & \end{pmatrix} \quad \text{and} \quad -\Delta_{\epsilon:y} \equiv \begin{pmatrix} -\epsilon & & \\ -1 & 2+2\epsilon & -1 \\ & -\epsilon & \end{pmatrix}.$$

Therefore, this section considers the linear system:

$$\begin{pmatrix} -\Delta_{\epsilon:x} & kI \\ -kI & -\Delta_{\epsilon:y} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}. \quad (2)$$

For the numerics to follow, we will set  $\epsilon = 0.01$ .

In the first system, the diagonal blocks have the 5-point anisotropic Laplacian with  $\epsilon = 0.01$ . Again, the direction of the anisotropy differs between the blocks. In order to have a coupled system, we set  $k = 0.01$ .

In Table 2, pointwise Gauss-Seidel converges toward the solution. However, the adaptive algebraic smoother performs much better both in early and later iterations. The system is  $2178 \times 2178$  with a total of 66 blocks where each block contains 33 variables.

In the second system, we keep  $\epsilon = 0.01$ . However, we create a large off-diagonal element by setting  $k = 100$ . In fact, the linear system is no longer (and far from being) diagonally dominant. The adaptive algebraic smoother's success on problems difficult for pointwise Gauss-Seidel is clearly seen in this example. In Table 3 we see clear divergence for pointwise Gauss-Seidel. The adaptive algebraic smoother performs with low convergence rates. Again,

the system is  $2178 \times 2178$ . The block smoother chooses 1089 blocks with each being a  $2 \times 2$  block.

## 2 Forward-inverse computations of bioelectric and biomagnetic fields of human head and torso

Chartier continued collaboration with Ceon Ramon of the Electrical Engineering Department at the University of Washington on problems involving magnetoencephalography to detect neuronal activity in the brain. The discretized system

$$Ax = b, \quad (3)$$

is generated from MEG (magnetoencephalography) and EEG (electroencephalography) data of the head and/or torso, where  $A$  is a sparse matrix with approximately 1.5 million degrees of freedom.

The linear systems in this project stem from highly heterogeneous finite element method (FEM) models of the human head. Such models have recently become increasingly popular for EEG (electroencephalography) simulations and inverse reconstructions of the electrical sources in the cortex. Recent work [17] has studied how the FEM models influence the forward and inverse simulations. For more information, see [10, 18, 11].

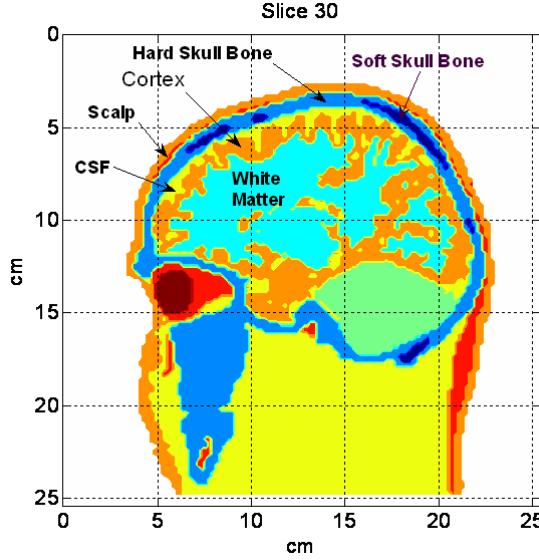


Figure 2: A segmented slice, marked as slice number 30, used in the FEM model. Note the detailed structure of the ears, eye sockets, sinus and oral cavities, and occipital hole. This is the 30th slice starting from the left side of the subject and is located 1.7 cm to the right from the midline of the brain.

Under this grant funding, Chartier along with undergraduate Tim Rankin demonstrated the effective role multigrid methods can play in such simulations. The sparse matrix

equations of interest result from a FEM model of the head that produces the necessary electric potentials and fluxes. A 3-D view of the model and the coordinate system is given in Figure 3.

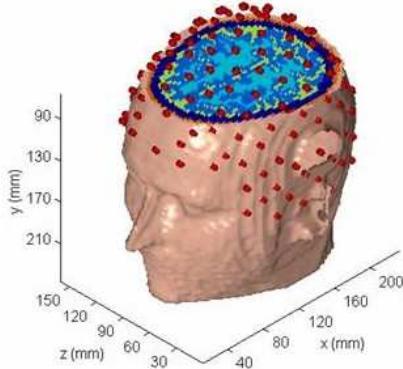


Figure 3: A three dimensional view of the head model superimposed with 145 EEG electrode positions.

Such a FEM model results in a sparse matrix equation that involves over 1.5 million variables. The research demonstrated the effectiveness of SAMG multigrid algorithm, which is an algebraic multigrid package produced by the Fraunhofer-Institute for Algorithms and Scientific Computing [19, 20]. The results were compared to the existing FEM solver used by Ramon’s group in their simulation code. SAMG was found to perform with comparable speeds for Ramon’s set of model problems. Further, SAMG performed at a rate at least 30 times faster than the method previously used in Ramon’s FEM code.

During the 2007–2008 academic year, Chartier met with Ramon to discuss testing publicly available AMG codes on these sets of problems and comparing their performance to SAMG. Further, Ramon and Chartier intend to pursue implementing such ideas in Matlab so they can be explored by researchers and students in biomedical engineering.

### 3 BoxMG: Robust variational multigrid on structured grids

The Black Box Multigrid (BoxMG) (introduced in [7] and further developed in [8, 9]) is a robust variationally based multigrid solver for symmetric elliptic PDEs discretized on logically structured two- or three-dimensional grids. Much like AMG the user is only required to provide the fine-grid discretization and an initial guess for the solution. It uses standard coarsening, so it coarsens the problem by a factor of 4 in two dimensions and 8 in three dimensions. The interpolation in BoxMG is constructed from the discrete operator such that it approximately preserves the continuity of the normal flux (i.e., with discontinuous coefficients it is not the gradient of the solution is not continuous). Using this operator-induced technique in conjunction with the variational construction of coarse-grid operators BoxMG constructs the entire hierarchy of operators that are needed. Relaxation is either colored Gauss-Seidel, or alternating-line relaxation in two dimensions and alternating-plane relaxation in three dimensions. BoxMG was recently released as an open source project under the Lesser GNU

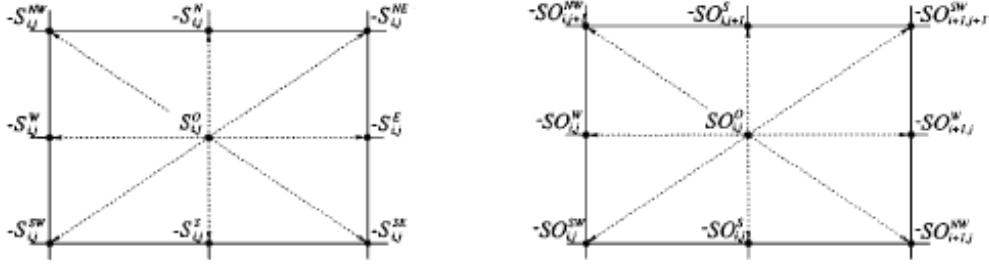


Figure 4: A compass-based definition of an arbitrary 9-point stencil (left). A 9-point symmetric stencil defined using a cell-based nomenclature (right).

Public License (LGPL), and is available on the web (<https://software.lanl.gov/boxmg>). The software is already being used by researchers for a wide variety of applications, including, bi-domain heart modeling [2], modeling of tumor growth [12], and flow in heterogeneous porous media [14, 15, 16]. Both OpenMP and MPI-based parallel versions are available as well, so users that find it useful can migrate their codes to these platforms easily.

Current work in the BoxMG implementation will be adding a general Full Approximation Scheme (FAS) based simulation framework. FAS and linear multigrid are equivalent for linear problems. As such, FAS is developed for nonlinear problems which are of importance to many DOE applications. More specifically, in FAS the coarse-grid problem is solved for the full approximation rather than the error equation. For more information, see ([6], chapter 6 or [21], section 5.3). Existing research on adaptive AMG methods [4, 3, 5] provides an excellent starting point for adaption of the operators in the FAS hierarchy.

To this end, Chartier along with David Moulton (Los Alamos National Laboratory) and Scott MacLachlan (Tufts University) continue their collaborative work to integrate existing research on adaptive AMG methods into BoxMG. The hope is to leverage the direct connection to the physical problem, to aid in the development and analysis of new techniques and error estimation.

In November 2008, Chartier visited Tufts University where Moulton also visited in order for MacLachlan, Moulton and Chartier to begin work on building the common infrastructure necessary to integrate adaptive multigrid ideas into BoxMG. By the end of the visit, the framework was in place for continued development of the code.

While work and discussions continued, a visit by Chartier to Tufts in the fall of 2009 accelerated development. Chartier and MacLachlan were able to complete one implementation of BoxMG with adaptive ideas. The following gives a short overview of the method.

### 3.0.1 Adaptive Process

Let  $\text{BoxMG}(\mathbf{x}, \mathbf{b})$  denote one call to the standard BoxMG solver with initial guess  $\mathbf{x}$  and right-hand side  $\mathbf{b}$ . Assume that the vector  $\mathbf{b}$  is supplied by the user. Then the adaptive process for BoxMG follows

1. Let  $\mathbf{x}$  be a random vector and run  $\text{BoxMG}(\mathbf{x}, \mathbf{0})$ .
2. Let  $k = \text{NOG}$  be the index of the finest grid and set  $\mathbf{x}^{(k)} = \mathbf{x}$ .

3. Relax on  $A^{(k)}\mathbf{x}^{(k)} = \mathbf{0}$  until  $(\mathbf{x}^{(k)})^T A^{(k)}\mathbf{x}^{(k)} = (\mathbf{x}^{(k)})^T \mathbf{r}^{(k)}$  is “stable”.
4. Redefine interpolation  $P_{k-1}^k$  and coarse grid operator  $A^{(k-1)} = (P_{k-1}^k)^T A^{(k)} P_{k-1}^k$ .
5. If  $k > 1$ , let  $\mathbf{x}^{(k-1)} = (\mathbf{x}^{(k)})_c$  (that is, inject  $\mathbf{x}^{(k)}$  onto grid  $k-1$ ), set  $k = k-1$ , and go to Step (3). Otherwise, continue.
6. Let  $\mathbf{x}$  be a random vector and run BoxMG( $\mathbf{x}, \mathbf{0}$ ). If cycling is inefficient, go to Step (2), passing the present  $\mathbf{x}$  as a smooth prototype. Otherwise, continue.
7. Run BoxMG( $\mathbf{y}, \mathbf{b}$ ) where  $\mathbf{y}$  be a random vector until convergence is achieved.

### 3.0.2 Interpolation

From above, Step (4) takes the most time, care and effort from MacLachlan, Moulton and Chartier. Suppose  $\mathbf{x}^{(k)}$  is a smooth error prototype obtained in Step (3) above. We wish to adjust the interpolation operator  $P_{k-1}^k$  to accommodate  $\mathbf{x}^{(k)}$ .

Partition the fine grid  $k$  as  $F \cup C$ , where  $C$  consists of the coarse grid nodes from grid  $k-1$  and  $F$  contains the remaining fine grid nodes. As in standard BoxMG, the values at the nodes in  $C$  are simply injected onto the fine grid. Standard coarsening implies that we must consider the following three cases when interpolating to the  $F$ -nodes. An  $F$ -node has coarse grid neighbors

- (a) to the North and South,
- (b) to the East and West, or
- (c) neither, in which case the  $F$ -node has coarse neighbors to the Northwest, Northeast, Southeast, and Southwest.

In what follows, we consider (a). An analogous interpolation scheme would be used for (b). The final case is handled exactly as in standard BoxMG, using, of course, the newly interpolated values obtained in (a) and (b). As such, we implicitly assume that the necessary adaptivity for (c) is already sufficiently built into the nodes interpolated in (a) and (b). For (a), we use the prototype error vector produced through the adaptive process given above to adjust the interpolation weights to the node associated with the stencil entry  $-Sij^W$ , for example. In particular, the weights for interpolation to this point are now adjusted from the prototype error vector.

Initial numerical results produced increased robustness of BoxMG. However, if we take

$$A\mathbf{u} = \mathbf{0}.$$

and alter this to:

$$SAS\mathbf{x} = \mathbf{0}, \quad (4)$$

where  $S$  is a diagonal matrix with  $s_{ii} = 10^{d_i}$  and  $d_i \in (0, 10^3)$ , adaptive cycling methods found in [4, 3, 5] recover suitable interpolation weights even with the drastic change in the geometric nature of the algebraic smooth error.

This was not the case for the first implementation of an adaptive BoxMG algorithm. The group suspects that using a standard BoxMG definition for interpolation of  $F$ -nodes with

Northwest, Northeast, Southeast and Southwest neighbors is potentially the culprit. More analytical study of the algorithm will uncover the truth of this suspicion or lead to insight into another algorithmic decision that limits the algorithm in this way.

The group continues to study this method and discusses a method in which interpolation follows a more AMG style of interpolation. Comparing both efficiency and robustness of such methods is the goal of the group. Chartier anticipates working with an undergraduate student during the summer of 2010 to continue work on this project.

## 4 Summary

The results of the various efforts in this research could ultimately have direct use and impact to researchers for a wide variety of applications, including, astrophysics, neuroscience, contaminant transport in porous media, bi-domain heart modeling, modeling of tumor growth, and flow in heterogeneous porous media. This work has already led to basic advances in computational mathematics and numerical linear algebra and will continue to do so into the future.

## 5 Conference Presentations and Journal Articles

### 5.1 Conferences and talks

1. Session Co-organizer – *Adaptive Algebraic Multigrid Methods*, SIAM Annual Meeting, Denver, Colorado, July 2008.
2. Department of Mathematics Colloquium, Wake Forest University, Winston-Salem, North Carolina. October 2008. *Improving on your Mistakes: solving linear systems iteratively*.
3. Department of Applied Mathematics Seminar, University of Washington, Seattle, Washington, April, 2008. *Adaptive Block Smoothing*.
4. Department of Mathematics Seminar, Willamette University, Salem, Oregon. April 2008. *Improving on your Mistakes: solving linear systems iteratively*.
5. Department of Mathematics Colloquium, Western Michigan University, Kalamazoo, Michigan. March 2009. *Adaptive Block Smoothing*.
6. Invited lecture. Math Colloquium, Appalachian State University, Boone, North Carolina. October 2009. *Improving on your Mistakes: solving linear systems iteratively*.
7. Invited lecture by undergraduate assistant, Southeastern Ranking and Clustering Workshop, August 2009. *Fiedler's Method*.
8. Florida Institute of Technology, Melbourne, Florida. March 2010. *Improving on your Mistakes: solving linear systems iteratively*.

### Journal articles

1. *Efficiency of Multigrid Algorithms for Head Models on Electroencephalography Simulations* (with T. Rankin\* and C. Ramon), International Journal of Pure and Applied Mathematics **45** (2008) 3, 349–357.
2. *Spectral element agglomerate AMGe* (with R. D. Falgout, V. E. Henson, J. E. Jones, T. A. Manteuffel, S. F. McCormick, J. W. Ruge, and P. S. Vassilevski), in Domain Decomposition Methods in Science and Engineering XVI, 513–521, Lecture Notes in Computational Science and Engineering **55**, Springer, Berlin, 2007.
3. Philip, Bobby and Timothy Chartier, *Adaptive Algebraic Smoothers* (with B. Philip), submitted.
4. *Adaptive multigrid via subcycling on complementary grids* (with D. Orr), in progress.
5. *Robust and Adaptive Multigrid Methods: comparing structured and algebraic approaches* (with S. MacLachlan and D. Moulton)

## 6 Students supported

1. Undergraduate, Spring 2009 – Implementing and testing algebraic block smoothers within Algebraic Multigrid.
2. Undergraduate, Spring 2009 – Studying robustness and efficiency of block smoothers to solve linear system formulation of PageRank.
3. Undergraduate, Summer 2009 – Analyzed the use of algebraic block smoothing methods as clustering methods and also the use of clustering methods to form algebraic blocks for iterative relaxation.
4. Undergraduate, Summer 2009 – Analyzed the use of a measure of algebraic strength from research in algebraic block smoothers in the context of classical AMG.
5. Undergraduate Fall 2009 - Improvement of MATLAB implementation of AMG and potential of AMG as a solver for M-matrices stemming from ranking problems.
6. Undergraduate Fall 2008, Spring 2009 – Studied robustness and efficiency of block smoothers to solve linear system formulation of PageRank.
7. Undergraduate Summer 2008 – Performed algorithm development of adaptive BoxMG for LANL.
8. Undergraduate Summer 2008 – Analyzed preconditioning and adaptive multigrid via subcycling.
9. Undergraduate, Summer 2007 – Continued analysis of adaptive multigrid method as a preconditioner and inclusion of preconditioning into the adaptive cycling.

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