

## Parallel, Scalable, and Robust Multigrid on Structured Grids

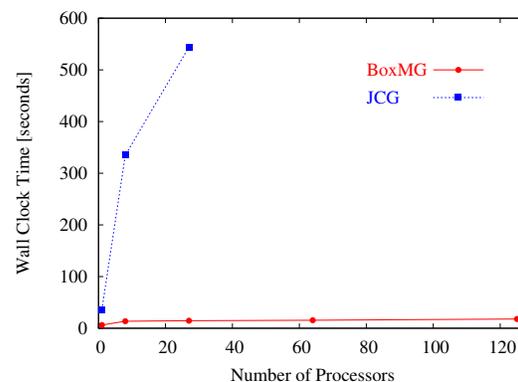
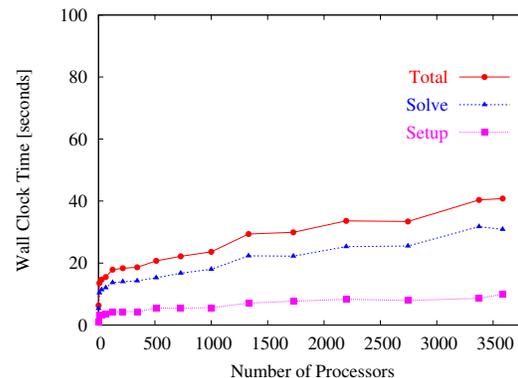
T. Austin, M. Berndt, B. K. Bergen, J. E. Dendy, Jr., and J. D. Moulton

### Introduction:

Robust and efficient multilevel iterative solvers are vital for the predictive simulation of complex multiscale and multicomponent nonlinear applications. Specifically, diffusive phenomena play a significant role in wide range of applications, including radiation transport, flow in porous media, and composite materials. In fact, the solution of the diffusive component (elliptic component) of these systems frequently dominates the simulation cost because it is characterized by a discontinuous diffusion coefficient with fine-scale spatial structure. Thus, efficient multilevel iterative methods are crucial because their solution cost scales linearly with the number of unknowns (i.e., optimal algorithmic scaling). In particular, this optimal scaling facilitates the efficient three-dimensional multiscale simulations of linear problems. It also expands the applicability and enhances the effectiveness of large three-dimensional multicomponent nonlinear simulations that advance implicitly in time (e.g., matrix-free Newton-Krylov methods) through efficient and robust preconditioning of the Krylov iteration.

### Robust Multigrid Algorithms:

Multigrid methods gained recognition in the late 1970's as an efficient algorithm for the solution of the discrete linear systems that arise from models of diffusive phenomena (e.g., heat conduction, neutron diffusion, single-phase saturated flow). These methods achieve their efficiency through the recursive use of successively coarser discrete problems (i.e., a sequence of coarse-grid discrete operators) in conjunction with smoothing on each level (e.g., a single Gauss-Seidel iteration on each level) to damp the highly oscillatory



*A scalability study of the three-dimensional BoxMG code on QB for a standard discretization of a Poisson problem on the unit cube is shown in the top plot. The local problem size of  $100 \times 100 \times 100$  is kept fixed while the global problem size grows with the increasing number of processors. In the bottom plot the scalability of BoxMG is contrasted with the poor scaling of Jacobi preconditioned conjugate gradient iterations.*

errors associated with each grid. Unfortunately, early multigrid algorithms were fragile, with their efficiency strongly dependent on the variability of the model's coefficients. Considerable research in the early 1980's, much of it in T-7, led to the first multigrid algorithms that could be used reliably for a large class of practical problems. The key to the success of these robust *Black Box* methods, was the use of the fine-scale discrete model to construct, through a variational principle, the successively coarser coarse-grid operators. More

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recently this class of practical problems has been expanded further by using multigrid methods as preconditioners for various Krylov methods.

## A Parallel Scalable Implementation:

Multilevel iterative methods may be classified as either multiplicative or additive. Additive methods are inherently more parallel as they allow corrections to be computed on all levels simultaneously, thereby minimizing the impact of interprocessor communication. However, this flexibility comes at the price of robustness and sub-optimal algorithmic scaling with problem size. In contrast multiplicative methods such as multigrid are more robust and achieve optimal scaling with problem size, but have an unavoidable sequential aspect to the iteration cycle. Early work on parallel multilevel solvers suggested that despite this algorithmic advantage over additive methods, the communication overhead of multigrid was too severe to be competitive. However, this view has been challenged by several advances in modern supercomputers, including improvements in the interconnect, the increasing size of local memory, and the increasing speed of the individual processors.

We implemented an MPI-based parallel version of the Dendy's Black Box Multigrid Code for structured grids [1, 2] in both two and three dimensions that scales well over one sector of the supercomputer Q (3584 processors). In particular, we developed a customized version of the Message Passing for Structured Grid Toolkit (MSG) from netlib, created the necessary data structures, and established the necessary communication patterns to facilitate the reuse of the core computational kernels from the serial BoxMG code. At present these codes have been tested on several supercomputers at LANL, including QSC, Q, and Theta, as well as T-7's Linux-based Beowulf clusters. As part of the SC&S Q milestone we demonstrated the scalability of these codes for a standard finite difference discretization of the Poisson equation. Specifically, for the three-dimensional case, shown in the Figure, we considered a fixed local problem size of  $100 \times 100 \times 100$ , growing the global problem size by increasing the number of processors. A common measure of parallel efficiency for this type

of scalability study is the ratio of the time to solution on one processor to the time on  $N$  processors. For perfect scaling the ratio is one, very poor scaling is near zero. When solving a problem with over 3 billion unknowns to a relative residual in the 2-norm of  $10^{-12}$  in 40 seconds, the three-dimensional BoxMG code achieved a parallel efficiency of 15.5%. A similar study in two dimensions achieved a parallel efficiency of 25.8%.

We anticipate that the BoxMG solvers will have a positive impact on several code projects at LANL. Thus far, we have integrated the two-dimensional parallel BoxMG code into the ZATHRAS gray thermal radiation transport equation solver. Although ZATHRAS is designed primarily for simulation on unstructured grids, it is also used for computations on structured grids. For this case we created the necessary interface routines to map the unstructured storage to the structured data structures of BoxMG. The initial timing results on small problems are very promising, and likely to improve with larger problems on more processors. Based on this success we plan to continue this collaboration and integrate the three-dimensional parallel BoxMG code into ZATHRAS in an analogous fashion. In addition, we plan on making a publicly available release in the near future that will extend the accessibility of the code to projects outside of LANL.

## References

- [1] J. E. DENDY. Black box multigrid. *J. Comput. Phys.*, 48:366–386, 1982.
- [2] J. E. DENDY. Two multigrid methods for three-dimensional problems with discontinuous and anisotropic coefficients. *SIAM J. Sci. Stat. Comput.*, 8(2):673–685, 1987.

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## Contact

For further information e-mail [moulton@lanl.gov](mailto:moulton@lanl.gov) or see <http://math.lanl.gov/~moulton>