Benchmarking Diffusion Discretizations on Polyhedral Meshes

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The flexibility of polyhedral meshes, in conjunction with recent advances in robust diffusion discretizations, has created significant interest from both the computational science community and ASC-related applications. Specifically, polyhedral meshes simplify grid generation for complex geometries, readily treat cell- or patch-based adaptively refined meshes (AMR) as degenerate polyhedra, and simplify mesh reconnection algorithms for moving meshes. Simulations of fluid flow in complex geometries indicate that a polyhedral mesh may provide a more accurate solution than a tetrahedral mesh with the same number of elements. Recent progress in Mimetic Finite Difference (MFD) methods has produced a number of accurate and robust discretizations of the time-dependent diffusion equations on polyhedral meshes [1].

Although, these new discretizations lead to linear systems of equations that may be treated by state-of-the-art multilevel linear solvers, issues of efficiency and robustness must still be characterized and addressed. The objective of this work is to engineer an integrated, performance-oriented computational method for the diffusion equation on polyhedral meshes through the development of an automated benchmarking tool.

Discretization on Polyhedral Meshes

We consider the steady-state diffusion equation written in a conservative form:

$$\mathbf{u} = -\mathrm{D}\nabla p \quad \text{and} \quad \operatorname{div} \mathbf{u} = b,$$

where D is the symmetric diffusion tensor, and b is the source term. We shall refer to p as the pressure and $\mathbf{u}$ as the velocity. We consider three MFD methods that use the same degrees of freedom: two unknowns per mesh face (average normal velocity and average pressure) and one unknown per mesh zone (average pressure). The KLS [2] and BLS [3] methods result in a symmetric indefinite linear system. In contrast, the Morel method [4] results in a nonsymmetric indefinite linear system. In [1], we explain how the elimination of velocity and zone-based pressure unknowns lead to a smaller system involving face-based pressures. We use a Krylov iteration preconditioned with the Los Alamos algebraic multigrid (LAMG) to solve these systems.

Numerical Results

Polyhedral mesh generation, discretization methods, and multilevel iterative solvers are all under active development, while the underlying implementations may require additional tuning on new architectures. Consequently, we have developed a flexible testing framework in Python (a modern, easy-to-read, object-oriented scripting language), to perform the setup, execution, and report creation for these diffusion problems.

In this study we focus on bottom-line performance, with points appearing closer to the origin corresponding to lower error and less overall computation time. The first case uses a severely distorted structured mesh, dubbed the Kershaw mesh (Fig. 1). This highlights the higher construction cost of the KLS method, as well as its lower accuracy, with an error more than 6 times greater than BLS and Morel. The second case (Fig. 2) uses a spherical mesh with AMR style refinement leading to many degenerate polyhedral zones. Here, the setup cost plays a significant role in KLS trailing as its accuracy at a given resolution is between Morel and BLS. Overall the BLS discretization appears to provide the best balance of discretization error and solution time for the meshes and solvers considered thus far.

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[3] F. Brezzi, et al., *Math. Mod. Meth. Appl. S.* **15** (10) 1533–1551 (October 2005).
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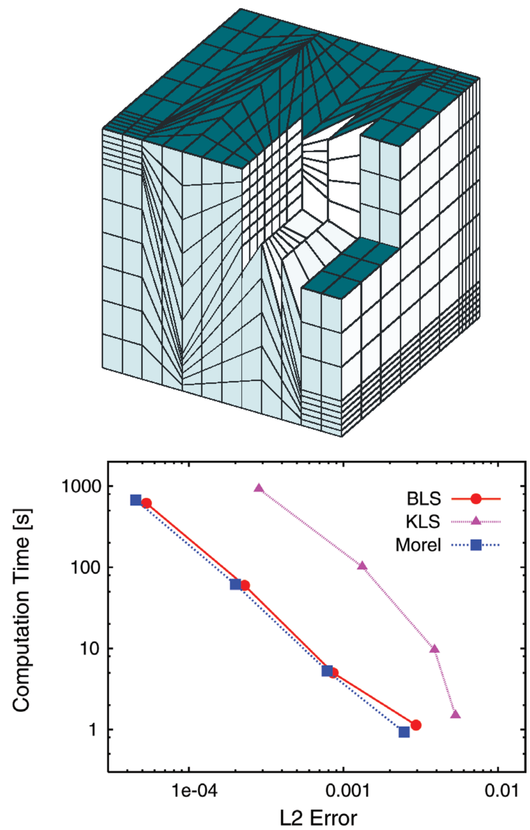

Fig. 1.
A series of N x N x N *logically structured meshes* (N = 10, 20, 40, 80), *with Kershaw style perturbations were used in this study. A* 12 x 12 x 12 *Kershaw mesh with a cutaway of zones lying near the front-right-top corner is shown at the top. The achieved accuracy, measured in the* L_2 *norm of the error in zone-based pressures, vs total CPU time is shown in the bottom plot. The BLS and Morel discretizations are significantly more efficient than the KLS discretization.*

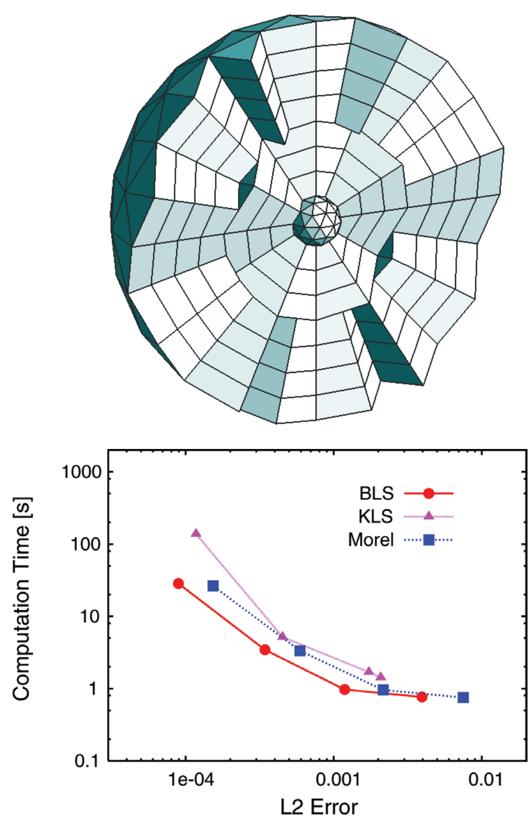

Fig. 2.
A series of locally refined meshes consisting of prismatic zones with five faces and refined zones with eight faces were used in this study. The zones have approximately an even volume distribution. A cutaway view of a sample mesh is shown at the top. The achieved accuracy in the zone-based pressure, measured in the L_2 *norm, vs total CPU time is also shown in the bottom plot.*