New Discretization Methodology for Diffusion Problems on Polyhedral Meshes

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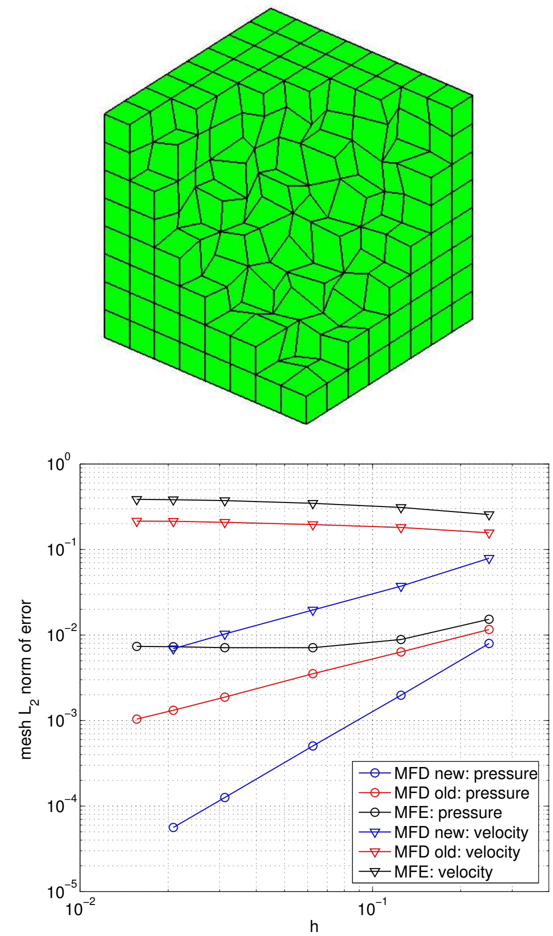
For decades, tetrahedral and hexahedral meshes were used in majority of engineering simulations; they are relatively easy to generate and there exist enormous amount of numerical methods oriented on these meshes. Nowadays, a growing number of complex simulations show advantage of using polyhedral meshes. Here are just two examples. In the simulation of flow through a water jacket of an engine [1], the results obtained on a polyhedral mesh are more accurate than the results obtained on a tetrahedral mesh with a comparable number of cells. In oil reservoir simulations, the polyhedral meshes offer unlimited possibilities: cells can be automatically joined, split, or modified by introducing additional points, edges and faces to model different geological features. Unfortunately, most of the existing numerical methods cannot be extended to polyhedral meshes, especially to meshes with cells having strongly curved (non-planar) faces. In [2], we considered a diffusion problem, which appears in computational fluid dynamics, heat conduction, radiation transport, etc., and developed a new discretization methodology that has no analogs in literature.

To design the new discretization method, we followed the general principle of the mimetic finite difference (MFD) method — to mimic the essential underlying properties of the original continuum differential operators such as the conservation laws, solution symmetries, and the fundamental identities and theorems of vector and tensor calculus. The mixed form of the diffusion problem is

$$\vec{F} = -K \operatorname{grad} p, \qquad \operatorname{div} \vec{F} = b$$



A logically cubic mesh with randomly perturbed interior points (top picture). The part of the unit cube was cut out to show the interior mesh. The convergence graphs for a smooth solution and the identity diffusion tensor (bottom picture) show optimal convergence rates for the new MFD method (blue), and the lack of convergence for the mixed finite element (black) and the old MFD (red) methods.

where the first equation is the constitutive equation relating the scalar function p (pressure in flow simulations) to the velocity field $\vec{F}$ and the second one is the mass conservation law. The material properties are described by the full symmetric tensor K, and b is the source function. For this problem, the MFD method mimics the

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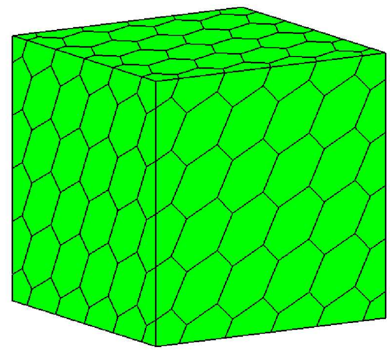
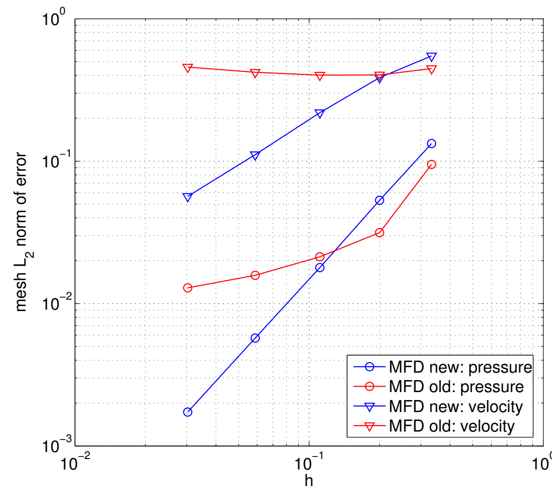
Gauss divergence theorem, the symmetry between the continuous gradient and divergence operators, and the null spaces of these operators. Therefore, it produces the discretization scheme which is always symmetric and locally conservative.

The previously developed (old) MFD method [3] used one degree of freedom per cell to approximate the pressure and one degree of freedom per mesh face to approximate the average normal component of the velocity. The same degrees of freedom are used in the mixed finite element (MFE) method on tetrahedral and hexahedral meshes. The new discretization methodology uses three degrees of freedom, three average velocity components, to approximate velocity on strongly curved faces. As shown on figures, it improves drastically the capabilities of the existing methods.

When faces of mesh cells are plane segments, or slightly perturbed plane segments, the new discretization method is reduced to method from [3]. Necessity to use three velocity components on strongly curved faces is possibly the intrinsic difficulty and the reason why nobody succeeded in doing a reasonable job on meshes with such cells. The theoretical analysis of the convergence rates is done in [2].

Another advantage of the developed methodology is that its practical implementation is simple and follows roughly the path described in [4]. In particular, we get a family of discretization schemes with similar properties. This family may be used to attack other computational problems, e.g., to enforce the discrete maximum principle.





A polyhedral mesh where the mixed finite element method can not be used (top picture). Note that 68% of interior mesh faces are non-planar. The convergence graphs (bottom picture) for the same problem as above show optimal convergence rates for the new MFD method (blue) and lack of convergence for the old MFD method (red).

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