Advanced Discretization Methods

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Summary

Numerical solution of PDEs is a mission critical enabling technology for many applications throughout the DOE complex. A key component of this technology is the discretization that replaces the PDE by a finite dimensional algebraic problem. Discretization is accompanied by losses of information about the PDE and its structure. Unless properly accounted for, these losses can lead to unstable discrete models with spurious solutions that hamper predictive numerical simulations. The main research driver of this project is the need to develop advanced compatible and stabilized algebraic models that yield stable, accurate, and physically meaningful approximate solutions and support validated computer simulations of processes that involve multiple physics and multiple scales.

During this fiscal year we pursued two main research directions. One was directed at applications of the algebraic topology framework for compatible discretizations, developed as part of this project, to prototype PDE models arising in applications such as device modeling, nanofluids and oil reservoir simulations. We used this framework to formulate new compatible methods for second order PDEs using the idea of *weak material laws*. This approach is motivated by our choice of the natural inner product to be the primary discrete operation.

To apply this approach, a PDE such as the Darcy flow problem is transformed into an equivalent, 4 field constrained optimization problem, given by

$$\min \frac{1}{2}\left(\left\| \sqrt{\alpha}\left(*_{\alpha^{-1}} w - v \right) \right\|^2 + \left\| \sqrt{\beta}\left(*_{\beta^{-1}} q - p \right) \right\|^2 \right)$$

subject to $dw = -d_t q$ and $dp = v$

In this problem the constitutive laws are minimized subject to constraints given by the differential equations expressing mass conservation and kinematic equilibrium.

We proved that such four field formulations give rise to primal and dual mixed Galerkin methods and a *compatible least-squares method* that is equivalent to *simultaneous solution of both the primal and the dual Galerkin methods*. This is a first of its kind theoretical result that demonstrates previously unknown connection between Ritz-Galerkin and Mixed Galerkin methods (deemed “natural” for the problem) and least-squares principles (deemed “artificial” or “external” to the problem). In particular, our approach allows to interpret compatible least-squares methods as leading to a particular realization of a *discrete Hodge * operator*.

Figure 1 demonstrates the compatible least-squares method for a Darcy flow with discontinuous permeability. A collocated method gives rise to a spurious *y*-velocity component due to the incompatibility of C^0 finite element spaces with velocity fields that can have jumps in their tangential

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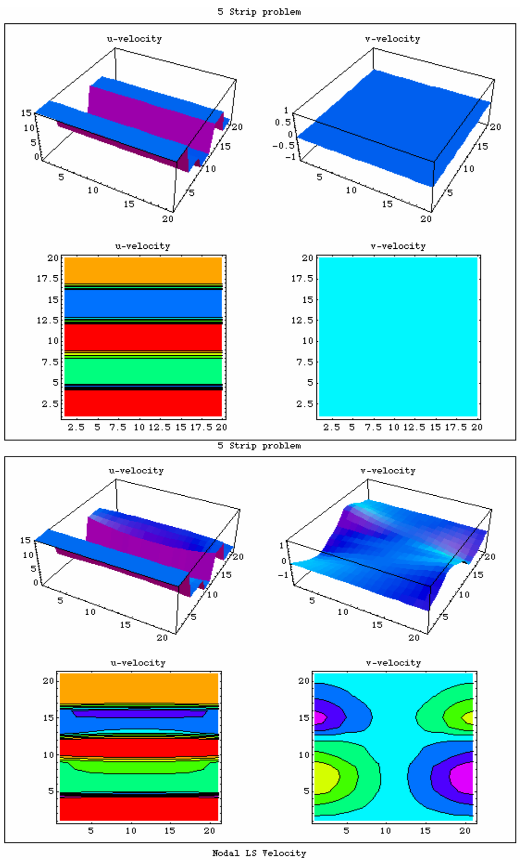

Figure 1. Velocity component plots for a mimetic least-squares method with weak material laws (top) and collocated least-squares method (bottom) for Darcy flow problem with discontinuous permeability. (Problem formulation courtesy of T.J.R. Hughes, J. Wan and A. Masud)

components. Pollution from this spurious component prevents the method from recovering the exact pressure, despite the fact that it belongs to the discrete space!

A second, complementary research direction focused on stabilized methods for time dependent PDEs. The main thrust of this work was to investigate the impact of combining implicit time discretization with spatially stabilized mixed variational formulations. Our analysis concentrated on consistently stabilized methods for unsteady incompressible viscous flows. This choice was driven by small time step instabilities observed in simulations of chemically reacting flows by using Sandia's massively parallel reacting flows/transport code MP Salsa.

We established theoretically that such methods, obtained by a method of lines approach, may experience difficulty when the time step is small relative to the spatial grid size. Using as a model problem the unsteady Stokes equations, we were able to prove that the semi-discrete pressure operator associated with such methods is not uniformly (with respect to the mesh size h) coercive. Our results also demonstrate that for sufficiently large (relative to the square of the spatial grid size) time steps, implicit time discretizations contribute terms that stabilize this operator. However, we also proved that if the time step is sufficiently small, then the fully discrete problem necessarily leads to unstable pressure approximations. In addition we have also studied stability of finite element upwinding methods such as SUPG. Our analysis shows that in contrast to stabilization of saddle-point problems, the small time step instability does not occur in this class of methods. This research, carried jointly with M. Gunzburger (FSU) and R. Lehoucq (SNL) has significant impact for several Sandia application codes, including the new transport-reaction code CHARON, which is based on stabilized Galerkin finite element technology.

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