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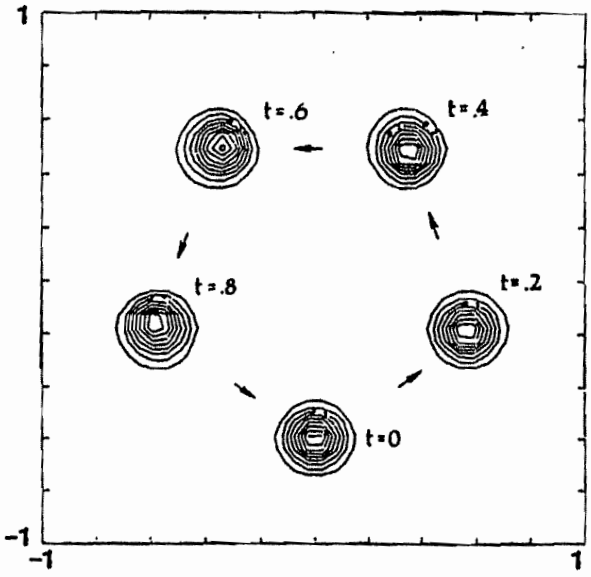

Figure 2. Concentration contours for the purely advective rotating plume problem at various time levels. Contour interval is 0.1.

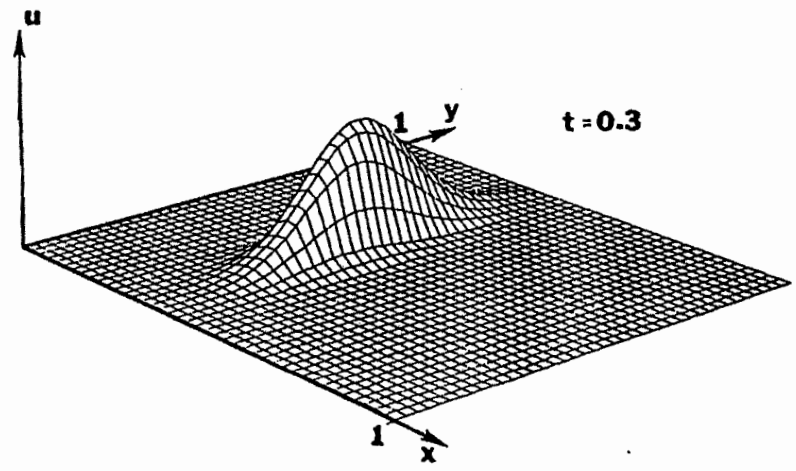

Figure 3. Plot of concentration distribution at $t = 0.3$ for an advection-diffusion prob with potential flow.

ADJOINT PETROV-GALERKIN METHODS FOR MULTI-DIMENSIONAL FLOW PROBLEMS

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ABSTRACT

Adjoint Petrov-Galerkin (APG) methods are a general class of Petrov Galerkin methods that derive from the general theories of Herrera ([1]-[6]). Practical implementation of these methods has been achieved for one-dimensional problems ([4],[7]). Application to problems in more than one space dimension requires additional developments. This paper develops a family of Adjoint Petrov-Galerkin methods for two-dimensional flow problems. The general behavior of the schemes is discussed, and the methods are compared to other standard approximations.

1. INTRODUCTION

Simulation of multi-dimensional flow and transport equations is required in many engineering problems. Of particular interest in this paper are potential flows and advective-diffusive transport of passive scalars in low dispersivity fields. This paper develops the Adjoint Petrov-Galerkin (APG) methods of Herrera and coworkers ([1]-[7]) for multi-dimensional flow and transport problems. Specific difficulties introduced by the dimensionality of the problem are discussed, and several approximations for model flow and transport equations in two dimensions are given.

2. ADJOINT PERTOV-GALERKIN METHODS

Adjoint Petrov-Galerkin (APG) methods are based on the pioneering work of Herrera ([1]-[6]). One result of Herrera's general theory is a selection criterion for test functions in a general Petrov-Galerkin framework. For a given operator equation, the criterion to be satisfied is that each test function should satisfy the homogeneous adjoint operator locally (within each element). This choice of test function effectively concentrates information at element boundaries, thereby eliminating integrations over element interiors. In one dimension, this means that all information is concentrated directly at node points. One-dimensional versions of APG have been developed and applied to ordinary differential equations [4] and to one-dimensional transient partial differential equations [7]. In the latter case, APG was applied in space to obtain a semidiscrete systems of ordinary differential

equations in time, which was then solved using standard time-stepping algorithms.

Extension on the APG method to multiple dimensions is complicated by the fact that the solution space of the homogeneous adjoint equation is now infinite-dimensional, so that there is no unique choice of test functions. In addition, concentration of information at element boundaries produces line integrals (two-dimensional problems) or surface integrals (three-dimensional problems) rather than the simple nodal evaluation of one dimension. Each of these complications can be overcome in several different ways.

As an example, consider the Poisson equation in two dimensions, defined on a closed rectangular domain Ω, with suitable boundary conditions specified along $\partial\Omega$,

$$\mathfrak{L}u \equiv \nabla^2 u = f(x,y), \qquad (x,y)\in\Omega \tag{1}$$

Application of APG proceeds as follows. Let Ω be partitioned into E rectangular subintervals, $\{\Omega^e\}_{e=1}^{E}$. A weighted form of equation (1) is then written as

$$\int_\Omega (\nabla^2 u)\, w_k(x,y)\, dx\, dy = \int_\Omega f(x,y)\, w_k(x,y)\, dx\, dy \tag{2}$$

For simplicity, assume $u\in C^1$ (this is for simplicity of presentation only; Herrera's general theory treats fully discontinuous functions). Then equation (2) can be written equivalently as

$$\int_\Omega (\nabla^2 u)\, w_k(x,y)\, dx\, dy = \sum_{e=1}^{E} \int_{\Omega^e} (\nabla^2 u)\, w_k(x,y)\, dx\, dy = \int_\Omega f\, w_k\, dx\, dy \tag{3}$$

Integration by parts (Green's theorem) can be applied to each elemental integral in equation (3),

$$\sum_{e=1}^{E} \int_{\Omega^e} (\nabla^2 u)\, w_k(x,y)\, dx\, dy = \sum_{e=1}^{E} \Big\{ \int_{\partial\Omega^e} [(\underset{\sim}{\nabla} u\cdot \underset{\sim}{n}^e) w_k - u(\underset{\sim}{\nabla} w_k \cdot \underset{\sim}{n}^e)]\, ds + \int_{\Omega^e} u(\nabla^2 w_k)\, dx\, dy \Big\} \tag{4}$$

where $\underset{\sim}{n}^e$ is the unit normal along the boundary of element e. Choice of $w_k(x,y)$ such that $\mathfrak{L}^* w_k \equiv \nabla^2 w_k = 0$ within each Ω^e eliminates the interior integrals in equation (4), thereby concentrating information along element boundaries. Approximation of the boundary integrals in terms of nodal values of the unknown function then produces the approximating equations of interest.

One of the simplest choices of test function is a tensor product form in which each directional component is required to satisfy its respective one-dimensional component of the operator $\mathcal{L}^*$. For the Poisson equation, this leads to definition of $w_k(x,y)$ as the standard piecewise bilinear Lagrange polynomial, centered at node $\underset{\sim}{x}_k$. For this choice of test function, $\nabla^2 w_k = 0$ within each Ω^e, e=1,2,....,E. Furthermore, the contributions from the first term in the boundary integral of equation (4) sum to zero because both $(\underset{\sim}{v}\cdot\underset{\sim}{n}^e)$ and w_k are continuous ($\mathbb{C}^0[\Omega]$), and contributions to $\sum_{e=1}^{E} \int_{\partial\Omega^e} (\underset{\sim}{v}\cdot\underset{\sim}{n}^e) w_k \, ds$ from adjoining elements cancel. The second term is nonzero because $\underset{\sim}{v} w_k \cdot \underset{\sim}{n}^e$ is discontinuous across element boundaries.

Consider a rectangular array of nodes, with indices i and j referring respectively to x and y position, so that $\underset{\sim}{x}_k \equiv (x_i, y_j)$. The following equation results from equations (3) and (4), with the choice of w_k as a piecewise bilinear Lagrange polynomial centered at $\underset{\sim}{x}_k$ and constant node spacing assumed in both x and y.

$$\int_{y_{j-1}}^{y_{j+1}} \left[\left(\frac{1}{\Delta x}\right)u(x_{i-1},y) - \left(\frac{2}{\Delta x}\right)u(x_i,y) + \left(\frac{1}{\Delta x}\right)u(x_{i+1},y)\right] dy +$$

$$\int_{x_{i-1}}^{x_{i+1}} \left[\left(\frac{1}{\Delta y}\right)u(x,y_{j-1}) - \left(\frac{2}{\Delta y}\right)u(x,y_j) + \left(\frac{1}{\Delta y}\right)u(x,y_{j+1})\right] dx = \int_{y_{j-1}}^{y_{j+1}} \int_{x_{i-1}}^{x_{i+1}} f\, w_k \, dx\, dy \tag{5}$$

The final step is approximation of the line integrals in terms of nodal values of u(x,y). Three examples are provided to demonstrate the approximations that may be derived.

1. Each line integral is approximated using a constant value of u, defined as the midpoint value (this is equivalent to a one-point integration rule). This leads to the standard five-point finite difference approximation,

$$\frac{1}{(\Delta x)^2}[\delta_x^2 u_{i,j}] + \frac{1}{(\Delta y)^2}[\delta_y^2 u_{i,j}] = f_{i,j} \tag{6}$$

where $\delta_x^2 u_{i,j} \equiv u_{i-1,j} - 2u_{i,j} + u_{i+1,j}$ and $\delta_y^2 u_{i,j} \equiv u_{i,j-1} - 2u_{i,j} + u_{i,j+1}$ are the usual second order difference operators, and the right side integral is also approximated with a one-point rule.

2. Piecewise linear Lagrange polynomial approximation of u in each line integral leads to

$$\frac{1}{6(\Delta x)^2}\{\delta_x^2 [u_{i,j-1}+4u_{i,j}+u_{i,j+1}]\} + \frac{1}{6(\Delta y)^2}\{\delta_y^2 [u_{i-1,j}+4u_{i,j}+u_{i+1,j}]\}$$

$$= \frac{1}{(\Delta x)(\Delta y)} \int_{y_{j-1}}^{y_{j+1}} \int_{x_{i-1}}^{x_{i+1}} f\, w_k \, dx\, dy \qquad (7)$$

This approximation is identical to the usual piecewise bilinear finite element approximation to the Poisson equation

3. Quadratic Lagrange polynomial approximation of u using the three nodes associated with each line integral leads to

$$\frac{1}{12(\Delta x)^2}\{\delta_x^2 [u_{i,j-1}+10u_{i,j}+u_{i,j+1}]\} + \frac{1}{12(\Delta y)^2}\{\delta_y^2 [u_{i-1,j}+10u_{i,j}+u_{i+1,j}]\}$$

$$= \frac{1}{(\Delta x)(\Delta y)} \int_{y_{j-1}}^{y_{j+1}} \int_{x_{i-1}}^{x_{i+1}} f\, w_k \, dx\, dy \qquad (8)$$

This is an enhanced nine-point approximation to the Poisson equation. The approximation (8) is $O(h^4)$ on uniform grids ($h=\Delta x=\Delta y$), while the previous two approximations are $O(h^2)$. When $f=0$, equation (8) becomes an $O(h^6)$ approximation. Furthermore, Collatz [8] has shown that it is not possible to obtain a higher order approximation to the Laplace operator using nine points. In this sense, the method leads to an optimal approximation.

These three examples illustrate one possible family of approximations based on the APG approach.

A similar approach may be followed for the advection-diffusion transport equation. Consider, for example, the two-dimensional equation

$$\mathfrak{L}u \equiv \underset{\sim}{V}\cdot\underset{\sim}{\nabla}u - D\nabla^2 u = f(x,y), \quad (x,y)\in\Omega \qquad (9)$$

In this case $\mathfrak{L}^* w_k = -\underset{\sim}{V}\cdot\underset{\sim}{\nabla} w_k - D\nabla^2 w_k$, with local tensor product homogeneous solutions given by

$$w_k(x,y) = \alpha_i(x)\beta_j(y), \qquad (10)$$

where

$$\alpha_i(x) = \begin{cases} \frac{1-f_1(x)}{1-F}, & x_{i-1}\le x\le x_i \\ \frac{f_2(x)-F}{1-F}, & x_i\le x\le x_{i+1} \\ 0, & x\le x_{i-1},\ x\ge x_{i+1} \end{cases} \qquad \beta_j(y) = \begin{cases} \frac{1-g_1(y)}{1-G}, & y_{j-1}\le y\le y_j \\ \frac{g_2(y)-G}{1-G}, & y_j\le y\le y_{j+1} \\ 0, & y\le y_{j-1},\ y\ge y_{j+1} \end{cases}$$

with $f_1(x)\equiv\exp[-V_x(x-x_{i-1})/D]$, $f_2(x)\equiv\exp[-V_x(x-x_i)/D]$, $g_1(y)\equiv\exp[-V_y(y-y_{j-1})/D]$, $g_2(y)\equiv\exp[-V_y(y-y_j)/D]$, $F\equiv\exp[-V_x(\Delta x)/D]$, and $G\equiv\exp[-V_y(\Delta y)/D]$. Calculation of the appropriate line integrals in equation (4) then leads to a nine-point, upsteam-weighted approximation for the nodal estimates of u. Different interpolations for u in the line integrals again lead to different approximations.

3. COMPARISON TO OTHER METHODS

Equations (6)-(8) show that the APG method applied to the Poisson equation leads to a general family of approximations which includes the standard 5-point finite difference approximation, the standard 9-point finite element approximation, and an enhanced 9-point approximation that attains optimal order. Equation (5) can be viewed as a general statement of a C^0, tensor product APG approximation which subsumes the standard approximations for this equation. Other choices of test function definition (under the restriction that $\mathcal{L}^* w=0$) lead to other families of approximations.

The APG approximation to the transport equation (9) using the tensor product form (10) can be viewed as maintaining a sense of optimality in each coordinate direction, since w(x,y) is required to satisfy each directional component of the adjoint equation. The approach is therefore analogous to other methods that use one-dimensional optimality to develop multi-dimensional approximations. Examples of this approach include the tensor product version of the Quadratic Petrov-Galerkin (QPG) method [9] and to some extent the Streamline Upwind Petrov Galerkin (SUPG) method of Hughes and coworkers [10], as well as the two-dimensional Allen and Southwell [11] scheme. Under certain interpolation choices (quadratic interpolation in the line integrals), APG becomes nearly equal to QPG and SUPG. Other more general approximations can again be derived by including the advective term in the general equation (5).

4. SUMMARY OF RESULTS

For highly advective transport problems, the APG method using quadratic interpolation produces results the are very similar to the two-dimensional QPG methods [9]. Two-dimensional steady state test problems have also shown that APG produces results similar to SUPG except that APG is better able to resolve boundary layers.

Similar results have been observed for transient multi-dimensional problems when the Petrov-Galerkin methods are applied in space only. For the transient problem, our results indicate that a a variant of Dick's [12] Cubic Petrov-Galerkin (CPG) method produces results far superior to any other nine-point Eulerian approximation. The APG, QPG, and SUPG yield results that are very similar and generally overly-dissipative, while CPG results are significantly less dissipative and more accurate. Numerical results to support these claims will be presented at the conference.

5. CONCLUSIONS

A multi-dimensional Adjoint Petrov-Galerkin computational algorithm was developed for problems of flow and transport. The development leads to general families of approximations. Definition of appropriate tensor product test functions leads to standard finite difference and finite element approximations for both the flow and transport problem. Standard numerical approximations can therefore be viewed as examples of the general APG formulation.

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