Aerospace Computational Engineering Field Exam

Consider a reaction-diffusion equation:

$$u_t = \alpha u + \nu u_{xx}$$

with $\alpha \leq 0$ and $\nu \geq 0$. The objective is to develop an efficient numerical algorithm to calculate the temporal evolution of u from an initial condition $u(t = 0, x) = u_0(x)$.

1. Determine the eigenvalues and eigenmodes for this equation for the following two sets of boundary conditions:

   (a) Periodic: $u(t, x - 1) = u(t, x + 1)$ on a domain from $-\infty < x < \infty$.

   (b) Dirichlet: $u(t, \pm 1) = 0$ on a domain from $-1 < x < 1$.

   Compare the eigenvalues for these two cases.

2. Consider a finite difference discretization of the periodic problem with N divisions from $-1 < x < 1$ such that the spacing between nodes is $h = 2/N$. Write down a second-order accurate, central-difference discretization for this problem keeping the temporal derivative in analytic form (i.e. write down a semi-discrete method). Compare the eigenvalues of this semi-discrete discretization to the exact eigenvalues derived in the first question.

3. Now consider a three-dimensional reaction-diffusion problem,

   $$u_t = \alpha u + \nu \left(u_{xx} + u_{yy} + u_{zz} \right).$$

   Assume a second-order accurate central difference in space and an implicit time-integration method are used. Describe solution approaches for the resulting system of equations. In particular, what solution approaches would you recommend when the discrete system has a large number of unknowns? How is your choice affected by α and ν?

4. As another discretization option, derive a finite element discretization for the three-dimensional reaction-diffusion problem with homogenous boundary conditions ($u = 0$) on the boundary $\partial\Omega$ of the domain Ω. Use continuous linear finite elements and derive the semi-discrete weak form in which only the spatial terms are discretized.

5. Describe the differences (if any) that arise in the implementation of a time-integration method for the finite difference and finite element methods. Consider both explicit and implicit methods.

Solution

1. Eigenvalues/eigenmode pairs (λ^k, u^k) must satisfy,

$$\lambda^k u^k = \alpha u^k + \nu u^k_{xx},$$

as well as the associated periodicity/boundary conditions. For the periodic case, the eigenmodes are:

$$u^k(x) = \exp[i\pi kx] \qquad \text{for integer } k$$

Note: could also write the modes as $\sin \pi kx$ and $\cos \pi kx$ with non-negative k though this complex mode is more compact notation. In either case, the corresponding eigenvalues can be easily found,

$$\lambda^k = \alpha - \nu(\pi k)^2$$

giving repeated eigenvalues for positive/negative k.

For the Dirichlet case, only the $\sin \pi kx$ satisfy the b.c.'s, so

$$u^k(x) = \sin \pi kx \qquad \text{for integer } k \geq 0$$

And, the eigenvalues are unchanged (though not repeated and without the $k = 0$ mode).

2.

$$(u_t)_j = \alpha u_j + \frac{\nu}{h^2}\left(u_{j+1} - 2u_j + u_{j-1}\right).$$

The eigenmodes are just the nodal samples of the exact (analytic) eigenmodes, though there are only N of them,

$$u^k_j = \exp[i\pi k x_j] \qquad \text{for } -N/2 < k < N/2 - 1$$

This assume even N; for odd N the range on k is $-(N-1)/2 < k < (N-1)/2$. The range is arbitrary because of aliasing but the above choices are traditional. The eigenvalues can be found by substitute the eigenmodes into the discretization:

$$\lambda^k = \alpha + 2\frac{\nu}{h^2}\left(\cos \pi kh - 1\right)$$

The well-resolved eigenmodes correspond to $kh << 1$. In this limit,

$$\lambda^k = \alpha - \nu(\pi k)^2 + O((kh)^2),$$

which is second-order accurate. For the inaccurate (underresolved) mode, $kh \approx 1$ gives,

$$\lambda^k = \alpha - 4\frac{\nu}{h^2}$$

3. Expected discussion points:

   (a) System of equations is a banded 9-diagonal system.

   (b) For large DOF's, direct solve will be impractical. need to use some kind of iterative method.

   (c) If $|\alpha|h^2/\nu$ is large, then system is dominated by reaction term. Thus, coupling is weak and a point-iterative technique (Jacobi or Gauss-Seidel) should work well. Note that as accuracy of simulation is increased (such that h is decreased) then diffusion eventually dominates.

   (d) In the diffusion dominated case, multigrid should work well since the system is elliptic. If the grid is isotropic, a point-iterative smoother should work well.

   (e) Another option would be conjugate gradient or GMRES, but this would require a preconditioner; in this case, might use the multigrid as a preconditioner.

4. FEM: weak form: Find $U \in X_h$ such that $(U_t, V) = \alpha(U, V) + \nu(\nabla U, \nabla V)$ for all $V \in X_h$.

5. FEM gives rise to mass matrix. Even for explicit schemes this requires inversion of a matrix. For implicit algorithms, the impact is not significant since mass matrix just modifies the matrix arising from the spatial derivative terms (and the right-hand side).

Some additional follow-ups depending on time

1. Consider the following second-order accurate, implicit methods (in a form to solve $u_t = f(u,t)$):

   (a) Trapezoidal method

   $$u^{n+1} - u^n = \frac{1}{2}\Delta t \left[f(u^n, t^n) + f(u^{n+1}, t^{n+1}) \right]$$

   (b) Second-order backwards differentiation

   $$u^{n+1} - \frac{4}{3}u^n + \frac{1}{3}u^{n-1} = \frac{2}{3}\Delta t f(u^{n+1}, t^{n+1}).$$

   Applying these methods to the finite-difference discretization of the reaction-diffusion, compare their behavior for large magnitude eigenvalues. Which methods behavior is more representative of the exact analytic behavior?

   Solution: To analyze this, consider $f = \lambda u$ and determine amplification factors for the two methods:

(a) Trapezoidal method

$$g = \frac{1 + \lambda\Delta t/2}{1 - \lambda\Delta t/2}$$

which for large magnitude (and negative) $\lambda\Delta t$ gives $g \to -1$. Thus, these modes will oscillate but should be heavily damped.

(b) Second-order backwards differentiation. The characteristic equation for the amm-plification factor is,

$$(1 - \frac{2}{3}\lambda\Delta t)g^2 - \frac{4}{3}g + \frac{1}{3} = 0.$$

In the limiting case with $\lambda\Delta t \to -\infty$, this can be shown to give $g \to 0$ which is rapidly damped, and more consistent with analytic behavior.