PDE test descriptions

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1 Parabolic solver test problem

A PDE test parabolic problem that is useful is a simple heat equation describing the evolution of temperature $T(z,t)$ in space and time subject to uniform thermal conduction:

$$\frac{\partial T}{\partial t} - \lambda \frac{\partial^2 T}{\partial z^2} = 0. \tag{1}$$

For purposes of testing we solve this equation on the *bounded* domain $0 \leq x \leq 1$. Invoking separation of variables we presume $T(z,t) = Z(z)\mathcal{T}(t)$ and substitute back into the original equation:

$$\frac{1}{\lambda \mathcal{T}} \frac{\partial \mathcal{T}}{\partial t} - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = 0. \tag{2}$$

Each term depends solely on one of the independent variables x, t, which implies that for this relation to be valid for all x, t then each term must be equal to a constant.

$$\frac{1}{\lambda \mathcal{T}} \frac{d\mathcal{T}}{dt} = -k^2 \tag{3}$$

$$-\frac{1}{Z} \frac{d^2 Z}{dz^2} = k^2. \tag{4}$$

Note also that since we have dependence on only one variable that we have converted the derivatives into *ordinary* derivatives. The solutions to these ODEs read:

$$\mathcal{T}(t) = A e^{-k^2 \lambda t} \tag{5}$$

$$Z(z) = A' \sin kz + B' \cos kz \tag{6}$$

The elemental solution (k arbitrary) is given by:

$$\tilde{T}(z,t) = Z(z)\mathcal{T}(t) = e^{-k^2 \lambda t} \left(A'' \sin kz + B'' \cos kz \right) \tag{7}$$

From this equation it is seen that the time scale for decay of a mode with wavenumber k is given by

$$\tau = \frac{1}{k^2 \lambda} \tag{8}$$

Further progress toward a general solution requires specific initial and boundary conditions. For our test problem we assume that the temperature goes to zero on the boundaries ($z \in \{0, 1\}$). Let us also assume that the initial temperature of the system is given by: $T(z,0) = f(z)$. First employing the condition $T(0,t) = 0$, we find that $B'' = 0$. The other boundary condition $T(1,t) = 0$ sets restrictions on the argument/eigenvalues of the sine function, namely that $k = n\pi, n \in \mathbb{Z}^+$ is a set of roots for the sine function. The elemental solution is then:

$$\tilde{T}_n(z,t) = A_n e^{-n^2 \pi^2 \lambda t} \sin(n\pi z) \tag{9}$$

Any integer value chosen for n results in a legitimate solution for the original partial differential equation; therefore, the general solution is a linear superposition of all such solutions.

$$T(z,t) = \sum_{n=1}^{\infty} A_n \, e^{-n^2 \pi^2 \lambda t} \sin(n\pi z). \tag{10}$$

The initial condition can now be applied to solve for the coefficients A_n by leveraging orthogonality of the sine functions. That is by making use of the fact that:

$$\left\langle \sin(n\pi z) \middle| \sin(n'\pi z) \right\rangle = \int_0^1 \sin(n\pi z)\sin(n'\pi z)dz = \frac{1}{2}\delta_{nn'}, \tag{11}$$

we may produce a solution for A_n from the series solution. The initial condition is represented in summation form (a Fourer sine series) as:

$$T(z,0) = f(z) = \sum_{n=1}^{\infty} A_n \ \sin\left(n\pi z\right). \tag{12}$$

Taking the scalar product of both sides with $\sin(n'\pi z)$ gives:

$$\left\langle f(z) \middle| \sin(n'\pi z) \right\rangle = \sum_{n=1}^{\infty} A_n \ \left\langle \sin(n\pi z) \middle| \sin(n'\pi z) \right\rangle = \sum_n = \frac{A_n}{2}\delta_{nn'} = \frac{A_{n'}}{2} \tag{13}$$

Thus the coefficients are:

$$A_{n'} = 2\left\langle f(z) \middle| \sin(n'\pi z) \right\rangle = 2\int_0^1 f(z)\sin(n'\pi z)dz \tag{14}$$

For purposes of testing it is easiest to pick a test problem with boundary conditions that are represented by a finite sum - one way this can be accomplished is by choosing a boundary condition that is an eigenfunction for this particular problem. Additionally to fully test the algorithms we should should several different modes in order to illustrate different decay times, for example:

$$f(z) = \sin(2\pi z) + \sin(8\pi z). \tag{15}$$

From this, and orthogonality of the sine function it follows that:

$$A_{n'} = \begin{cases} 2 & n \in \{2,8\} \\ 0 & \text{otherwise} \end{cases}, \tag{16}$$

and that the general solution for this specific set of boundary and initial conditions is:

$$T(z,t) = e^{-4\pi^2\lambda t}\sin\left(2\pi z\right) + e^{-64\pi^2\lambda t}\sin\left(8\pi z\right) \tag{17}$$

2 Elliptic solver test problem

The elliptic potential solver can tested using a simplified 2D test problem, Laplace's equation:

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0, \tag{18}$$

on the domain $0 \leq x \leq 1, 0 \leq y \leq 1$ with the boundary conditions $\Phi(x,0) - = \Phi(0,y) = \Phi(1,y) = 0, \Phi(x,1) = f(x)$. Exploying separation of variables $\Phi(x,y) = X(x)Y(y)$ we find the ODE solutions for $X(x)$ and $Y(y)$ to be:

$$X(x) = A \sin kx + B \cos kx \tag{19}$$

$$Y(y) = A' \sinh ky + B' \cosh ky \tag{20}$$

The boundary conditions dictate the following constraints: $\Phi(0,y) = 0 \implies B = 0, \Phi(x,0) \implies B' = 0, \Phi(1,y) = 0 \implies k = n\pi$. Thus we have the general solution:

$$\Phi(x,y) = \sum_n A_n \sinh(n\pi y) \sin(n\pi x) \tag{21}$$

Again choosing our boundary conditions for this test problem so that only one term in the series survives we may choose:

$$f(x) = \sin(2\pi x). \tag{22}$$

Which gives:

$$f(x) = \sum_n A_n \sinh(n\pi) \sin(n\pi x), \tag{23}$$

for the potential evaluated at the non-grounded boundary. By orthogonality the coefficients are:

$$A_n = \frac{2}{\sinh(n\pi)} \langle f(x) | \sin(n\pi x) \rangle ; \tag{24}$$

however the only nonzero coefficient occurs for $n = 2$:

$$A_2 = \frac{2}{\sinh(2\pi)} \langle \sin(2\pi x) | \sin(2\pi x) \rangle = \frac{1}{\sinh(2\pi)}; \tag{25}$$

The solution for this set of boundary conditions is, thus:

$$\Phi(x,y) = \frac{\sinh(2\pi y)}{\sinh(2\pi)} \sin(2\pi x) \tag{26}$$

All potential solutions currently in GEMINI are two-dimensional so this particular test problem is representative of each.

3 Hyperbolic solver test problem

The advection (hyperbolic) solver deals with problems of the form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z} (\rho v) = 0, \tag{27}$$

and higher dimensional equivalents (implemented through directional splitting). For constant velocity (assumed to be given) a simpler equation, which can be solved analytically, results.

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial z} = 0, \tag{28}$$

This equation can be seen to be equivalent to the wave equation by differentiating with respect to time and space respectively giving:

$$\frac{\partial^2 \rho}{\partial t^2} + v\frac{\partial^2 \rho}{\partial t \partial z} = 0 \tag{29}$$

$$\frac{\partial^2 \rho}{\partial z \partial t} + v\frac{\partial^2 \rho}{\partial z^2} = 0 \tag{30}$$

Eliminating the cross partial derivatives from these equations gives the familiar wave equation.

$$\frac{\partial^2 \rho}{\partial t^2} - v^2\frac{\partial^2 \rho}{\partial z^2} = 0, \tag{31}$$

The solution to this particular equation is a wave of the form:

$$\rho(z,t) = f(z - vt), \tag{32}$$

where the function f is arbitrary, generally speaking, but dictated by the specific initial conditions of the problem of interest. This solution can be verified by direct substitution, or derived by separation of variables - analogous to the test problems above. For an initial condition given by:

$$\rho(z,0) = e^{-\frac{z^2}{2\sigma_z^2}} \tag{33}$$

The solution at later times is:

$$\rho(z,t) = e^{-\frac{(z-vt)^2}{2\sigma_z^2}} \tag{34}$$

For testing purposes it is useful to numerical solve this on a periodic domain, e.g. $0 \leq x \leq 1$.

GEMINI advects mass, momentum, and energy in all three dimensions, representative of the equation:

$$\frac{\partial \rho}{\partial t} + v_x\frac{\partial \rho}{\partial x} + v_y\frac{\partial \rho}{\partial y} + v_z\frac{\partial \rho}{\partial z} = 0 \tag{35}$$

For initial conditions given by:

$$\rho(z,0) = e^{-\frac{x^2}{2\sigma_x^2}} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{z^2}{2\sigma_z^2}} \tag{36}$$

the solution at later time is:

$$\rho(z,t) = e^{-\frac{(x-v_x t)^2}{2\sigma_x^2}} e^{-\frac{(y-v_y t)^2}{2\sigma_y^2}} e^{-\frac{(z-v_z t)^2}{2\sigma_z^2}} \tag{37}$$