ATM: Automated Testing for Numerical Simulation Program via Derivative Invariance

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I. Background

$$u'' + \omega^2 u = 0, \tag{1}$$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \tag{2}$$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \tag{3}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}, \tag{4}$$

Appendix A
Solution of PDEs

First, for the one-dimensional wave equation (2), we split the x domain and obtain

$$x_i = i\Delta x, i = 0, \ldots, N_x, \tag{5}$$

where x_i is one spatial point and Δx is the length of the step. We discrete both time and spatial domains into

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}, \tag{6}$$

where u_i^{n+1} represents for the value of u at time point $n+1$ and spatial point i. We do not know the value of u_0^n and $u_{N_x}^n$ when we at u_1^n and $u_{N_x-1}^n$ for discretization, respectively. Therefore, we need to define boundary conditions. We introduce two types of boundary conditions for wave equations as follows. Dirichlet conditions represent for specifications of u_0 and u_{N_x} at any time point. For instance, one Dirichlet conditions of the equation (2) could be

$$\begin{aligned} u(x_1, t) &= 0, \\ u(x_{N_x-1}, t) &= 0, \end{aligned} \tag{7}$$

Neumann conditions refer to declarations of $\partial u/\partial n$, such as $\partial u/\partial n = 0$. Specifically, we specify

$$\frac{u_0^n - u_2^n}{2\Delta x} = 0 \tag{8}$$

at $x = 1$ and $t = t_n$ while

$$\frac{u_{N_x}^n - u_{N_x-2}^n}{2\Delta x} = 0 \tag{9}$$

at x_{N_x-1} and $t = t_n$. Then we could substitute the formula from the two equations into equation (6) for the calculation of boundaries.

Second, as for the heat equation (3), after discretization, the ODE form could be

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}. \tag{10}$$

Finally, with respect to the one-dimensional burgers equation (4), the ODE form is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -u_i^n \frac{u_i^n - u_{i-1}^n}{\Delta x} + \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}. \tag{11}$$

To tackle the boundary problem, we introduce an another boundary condition, named periodic conditions. With regard to the case that we discuss before, we could set u_0^n as $u_{N_x-2}^n$ and $u_{N_x}^n$ as u_2^n, where the length of periodic is $N_x - 1$.

Appendix B
Soundness proof of PDEs

(1) One initial condition case We take the heat equation as an instance and we consider the second time step. Since u_1^2 and $u_{N_x-1}^2$ are the function f of our method, we have

$$u_1^2 = k(u_2^1 - 2u_1^1 + u_0^1) + u_1^1$$

$$u_{N_x-1}^2 = k(u_{N_x}^1 - 2u_{N_x-1}^1 + u_{N_x-2}^1) + u_{N_x-1}^1,$$

where we omit the term f_i^n and express $\alpha\Delta t/\Delta x^2$ with k for the sake of conciseness. As for $u_2^1, u_1^1, u_{N_x-1}^1, u_{N_x-2}^1$, we have

$$u_2^1 = k(u_3^0 - 2u_2^0 + u_1^0) + u_2^0$$

$$u_1^1 = k(u_2^0 - 2u_1^0 + u_0^0) + u_1^0$$

$$u_{N_x-1}^1 = k(u_{N_x}^0 - 2u_{N_x-1}^0 + u_{N_x-2}^0) + u_{N_x-1}^0$$

$$u_{N_x-2}^1 = k(u_{N_x-1}^0 - 2u_{N_x-2}^0 + u_{N_x-3}^0) + u_{N_x-2}^0$$

and $u_0^1, u_{N_x}^1$ depend on the boundary conditions. Regarding the Neumann conditions, they set values of $\partial u/\partial n$, such as $\partial u/\partial n = 0$, where $u_0^1 = u_2^1$ and $u_{N_x}^1 = u_{N_x-2}^1$. As for the periodic condition, we would have $u_0^1 = u_{N_x-2}^1$ and $u_{N_x}^1 = u_2^1$. Therefore, to check the boundary conditions, we could alter the valus of $u_0^0, u_1^0, u_2^0, u_3^0, u_{N_x-3}^0, u_{N_x-2}^0, u_{N_x-1}^0, u_{N_x}^0$ to compute the numerical derivatives of u_1^2 and $u_{N_x-1}^2$. Since these independent variables (*i.e.*, the values of u of the initial condition) could cover all instants in the iteration, ATM could ensure the soundness of **the core code block**.

(2) Two initial conditions case We use the wave equation as an illustrative example, where we take $\{u_1^2, u_{N_x-1}^2, u_1^3, u_{N_x-1}^3\}$ as the functions f. Regarding the second time step, we have

$$u_1^2 = (2 - 2g)u_1^1 - u_1^0 + gu_2^1 + gu_0^1$$

$$u^2_{N_x-1} = (2-2g)u^1_{N_x-1} - u^0_{N_x-1} + gu^1_{N_x} + gu^1_{N_x-2},$$

where

$$\begin{aligned}
u^1_2 &= u^0_2 + 0.5g(u^0_3 - 2u^0_2 + u^0_1) \\
u^1_1 &= u^0_1 + 0.5g(u^0_2 - 2u^0_1 + u^0_0) \\
u^1_{N_x-1} &= u^0_{N_x-1} + 0.5g(u^0_{N_x} - 2u^0_{N_x-1} + u^0_{N_x-2}) \\
u^1_{N_x-2} &= u^0_{N_x-2} + 0.5g(u^0_{N_x-1} - 2u^0_{N_x-2} + u^0_{N_x-3})
\end{aligned}$$

and $u^1_0, u^1_{N_x}$ depend on the boundary condition. We abbreviate $c^2\Delta t^2/\Delta x^2$ as g. In a manner akin to the **one initial condition case**, ATM could test all parts of **the core code block** and the boundary condition of the computation for the first step if we alter the value of $\{u^0_0, u^0_1, u^0_2, u^0_3, u^0_{N_x-3}, u^0_{N_x-2}, u^0_{N_x-1}, u^0_{N_x}\}$ and calculate the numerical derivatives, respectively. If all parts above are correct, we utilize the third time step $\{u^3_1, u^3_{N_x-1}\}$ to test the boundary condition of **the main iteration**, which is the last portion. We now have

$$\begin{aligned}
u^3_1 &= (2-2g)u^2_1 - u^1_1 + gu^2_2 + gu^2_0 \\
u^3_{N_x-1} &= (2-2g)u^2_{N_x-1} - u^1_{N_x-1} + gu^2_{N_x} + gu^2_{N_x-2}
\end{aligned}$$

where

$$\begin{aligned}
u^2_2 &= (2g-2g^2)u^0_3 + (3g^2-4g+1)u^0_2 + \\
&\quad (2g-2g^2)u^0_1 + 0.5g^2u^0_4 + 0.5g^2u^0_0 \\
u^2_1 &= (g-g^2)u^0_0 + (2.5g^2-4g+1)u^0_1 + \\
&\quad (-2g^2+2g)u^0_2 + 0.5g^2u^0_3 + gu^1_0 \\
u^2_{N_x-2} &= (2g-2g^2)u^0_{N_x-1} + (3g^2-4g+1)u^0_{N_x-2} + \\
&\quad (2g-2g^2)u^0_{N_x-3} + 0.5g^2u^0_{N_x} + 0.5g^2u^0_{N_x-4} \\
u^2_{N_x-1} &= (g-g^2)u^0_{N_x} + (2.5g^2-4g+1)u^0_{N_x-1} + \\
&\quad (-2g^2+2g)u^0_{N_x-2} + 0.5g^2u^0_{N_x-3} + gu^1_{N_x}
\end{aligned}$$

and $\{u^1_0, u^1_{N_x}, u^2_0, u^2_{N_x}\}$ depend on the boundary condition. In a similar manner, $\{u^0_0, u^0_1, u^0_2, u^0_3, u^0_4, u^0_{N_x-4}, u^0_{N_x-3}, u^0_{N_x-2}, u^0_{N_x-1}, u^0_{N_x}\}$ are independent variables of u^3_1 and $u^3_{N_x-1}$. If we alter these variables and calculate the numerical derivatives, we could detect the bug of boundary condition which specify in **the main iteration**.