AMCS 312. Course project

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Introduction

The aim of this study is to explore how efficient could be Krylov-iterative methods implemented in PETSc solving hyperbolic equations with implicit time stepping, such as wave equations.

As a particular example we consider a simplified case, because it is sufficient for the performance comparison purposes. The framework is as follows:

Equation: Strong form of equation of motion

Discretization: Finite differences in time domain (FDTD)

Time stepping: Implicit

Accuracy: 2nd order schemes in space and time

Model: Homogeneous isotropic media with constant velocity

Programming: C/C++ with PETSc 3.7.3

3D acoustic wave equation

Acoustic wave equation for homogeneous media in strong formulation could be expressed as follows

$$\frac{\partial^2 u}{\partial t^2} - c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = f \tag{1}$$

We discretize with 2nd order of accuracy both in space and time. Implicit time stepping requires backward time derivative approximation, whereas spacial derivatives are approximated with centered scheme.

$$\frac{2U_{i,j,k}^{n+1} - 5U_{i,j,k}^{n} + 4U_{i,j,k}^{n-1} - U_{i,j,k}^{n-2}}{\Delta t^{2}} = c_{i,j,k}^{2} \frac{U_{i+1,j,k}^{n+1} - 2U_{i,j,k}^{n+1} + U_{i-1,j,k}^{n+1}}{\Delta x^{2}} + c_{i,j,k}^{2} \frac{U_{i,j+1,k}^{n+1} - 2U_{i,j,k}^{n+1} + U_{i,j-1,k}^{n+1}}{\Delta y^{2}} + c_{i,j,k}^{2} \frac{U_{i,j,k+1}^{n+1} - 2U_{i,j,k}^{n+1} + U_{i,j,k-1}^{n+1}}{\Delta z^{2}} + f_{i,j,k}$$
(2)

Hence,

$$\begin{split} U_{i,j,k}^{n+1} \left(2\Delta x \Delta y \Delta z + 2c_{i,j,k}^2 \Delta t^2 \left(\frac{\Delta y \Delta z}{\Delta x} + \frac{\Delta x \Delta z}{\Delta y} + \frac{\Delta x \Delta y}{\Delta z} \right) \right) + \\ U_{i+1,j,k}^{n+1} \left(-c_{i+1,j,k}^2 \Delta t^2 \frac{\Delta y \Delta z}{\Delta x} \right) + \\ U_{i-1,j,k}^{n+1} \left(-c_{i-1,j,k}^2 \Delta t^2 \frac{\Delta y \Delta z}{\Delta x} \right) + \\ U_{i,j+1,k}^{n+1} \left(-c_{i,j+1,k}^2 \Delta t^2 \frac{\Delta x \Delta z}{\Delta y} \right) + \\ U_{i,j-1,k}^{n+1} \left(-c_{i,j-1,k}^2 \Delta t^2 \frac{\Delta x \Delta z}{\Delta y} \right) + \\ U_{i,j,k+1}^{n+1} \left(-c_{i,j,k+1}^2 \Delta t^2 \frac{\Delta x \Delta y}{\Delta z} \right) + \\ U_{i,j,k-1}^{n+1} \left(-c_{i,j,k-1}^2 \Delta t^2 \frac{\Delta x \Delta y}{\Delta z} \right) = \Delta x \Delta y \Delta z \left(5U_{i,j,k}^n - 4U_{i,j,k}^{n-1} + U_{i,j,k}^{n-2} + \Delta t^2 f_{i,j,k} \right) \end{split}$$

$$(3)$$

4th order:

$$\frac{2U_{i,j,k}^{n+1} - 5U_{i,j,k}^{n} + 4U_{i,j,k}^{n-1} - U_{i,j,k}^{n-2}}{\Delta t^{2}} = c_{i,j,k}^{2} - \frac{-U_{i+2,j,k}^{n+1} + 16U_{i+1,j,k}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i-1,j,k}^{n+1} - U_{i-2,j,k}^{n+1}}{12\Delta x^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j+2,k}^{n+1} + 16U_{i,j+2,k}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j-1,k}^{n+1} - U_{i,j-2,k}^{n+1}}{12\Delta y^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - 30U_{i,j,k}^{n+1} + 16U_{i,j,k-1}^{n+1} - U_{i,j,k-2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - \frac{-U_{i,j,k+2}^{n+1} + 16U_{i,j,k+1}^{n+1} - U_{i,j,k+2}^{n+1}}{12\Delta z^{2}} + c_{i,j,k}^{2} - U_{i,j,k+2}^{n+1} - U_{i,$$

$$\begin{split} U_{i,j,k}^{n+1} \left(2\Delta x \Delta y \Delta z + 30 \ c_{i,j,k}^2 \Delta t^2 \left(\frac{\Delta y \Delta z}{12\Delta x} + \frac{\Delta x \Delta z}{12\Delta y} + \frac{\Delta x \Delta y}{12\Delta z} \right) \right) + \\ U_{i+2,j,k}^{n+1} \left(c_{i+2,j,k}^2 \Delta t^2 \ \frac{\Delta y \Delta z}{12\Delta x} \right) + \\ U_{i+1,j,k}^{n+1} \left(-16 \ c_{i+1,j,k}^2 \Delta t^2 \ \frac{\Delta y \Delta z}{12\Delta x} \right) + \\ U_{i-1,j,k}^{n+1} \left(-16 \ c_{i-1,j,k}^2 \Delta t^2 \ \frac{\Delta y \Delta z}{12\Delta x} \right) + \\ U_{i-2,j,k}^{n+1} \left(c_{i-2,j,k}^2 \Delta t^2 \ \frac{\Delta x \Delta z}{12\Delta y} \right) + \\ U_{i,j+2,k}^{n+1} \left(c_{i,j+2,k}^2 \Delta t^2 \ \frac{\Delta x \Delta z}{12\Delta y} \right) + \\ U_{i,j+1,k}^{n+1} \left(-16 \ c_{i,j+1,k}^2 \Delta t^2 \ \frac{\Delta x \Delta z}{12\Delta y} \right) + \\ U_{i,j-2,k}^{n+1} \left(c_{i,j-2,k}^2 \Delta t^2 \ \frac{\Delta x \Delta z}{12\Delta y} \right) + \\ U_{i,j,k+2}^{n+1} \left(c_{i,j,k+2}^2 \Delta t^2 \ \frac{\Delta x \Delta y}{12\Delta z} \right) + \\ U_{i,j,k+1}^{n+1} \left(-16 \ c_{i,j,k+1}^2 \Delta t^2 \ \frac{\Delta x \Delta y}{12\Delta z} \right) + \\ U_{i,j,k-1}^{n+1} \left(-16 \ c_{i,j,k-1}^2 \Delta t^2 \ \frac{\Delta x \Delta y}{12\Delta z} \right) + \\ U_{i,j,k-1}^{n+1} \left(-16 \ c_{i,j,k-1}^2 \Delta t^2 \ \frac{\Delta x \Delta y}{12\Delta z} \right) + \\ U_{i,j,k-2}^{n+1} \left(c_{i,j,k-2}^2 \Delta t^2 \ \frac{\Delta x \Delta y}{12\Delta z} \right) = \\ \Delta x \Delta y \Delta z \left(5 U_{i,j,k}^n - 4 U_{i,j,k}^{n+1} + U_{i,j,k}^{n-2} + \Delta t^2 f_{i,j,k} \right) \end{split}$$