GTBench: Equations & Discretizations

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1 | Introduction

This document describes the equations solved and discretizations used by GTBench [5], a benchmark application based on GridTools [1] designed to mimic typical compute motifs of weather and climate applications. Thanks to GridTools, GTBench runs on all common CPU architectures as well as on AMD and NVIDIA GPUs. Much of the work was inspired by the dynamical core of the COSMO weather model[2, 3], the first weather model running in production on GPUs [4].

2 | Equations

GTBench solves the source-free three-dimensional advection-diffusion equation with on a periodic domain:

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi - \nabla \cdot (\mathbf{v} \phi), \tag{2.1}$$

diffusing the scalar field ϕ with the constant diffusion coefficient D and advecting it along the velocity field $\mathbf{v}$. The velocity field is spatially varying but constant in time. Similar to typical weather and climate codes, (first-order) operator-splitting is employed to solve the advection equation and diffusion equation separately:

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi \qquad \text{(diffusion)}, \tag{2.2}$$

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot (\mathbf{v} \phi) \qquad \text{(advection)}. \tag{2.3}$$

Additionally, first-order spatial splitting is used along the spatial dimensions. Typically, weather and climate codes differentiate between horizontal and vertical dimensions due to much larger horizontal than vertical grid spacing. Spatial splitting allows to use explicit discretizations on horizontal equations and implicit discretizations on vertical equations, to not restrict the time step size by the small vertical grid spacing. Thus, the fully split equations are

$$\frac{\partial \phi}{\partial t} = D \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \qquad \text{(horizontal diffusion)}, \tag{2.4}$$

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial z^2} \qquad \text{(vertical diffusion)}, \tag{2.5}$$

$$\frac{\partial \phi}{\partial t} = -\frac{\partial u \phi}{\partial x} - \frac{\partial v \phi}{\partial y} \qquad \text{(horizontal advection)}, \tag{2.6}$$

$$\frac{\partial \phi}{\partial t} = -\frac{\partial w \phi}{\partial z} \qquad \text{(vertical advection)}, \tag{2.7}$$

with $\mathbf{v} = [u, v, w]$.

3 | Numerics

3.1 Discretization

GTBench uses the finite difference method for discretizing all the equations. The passively transported variable ϕ, and the horizontal velocities u, and v are discretized at cell centers at time step n as $\phi^n_{i,j,k}$, $u^n_{i,j,k}$, and $v^n_{i,j,k}$. The vertical velocity field w is placed on the vertical cell faces, that is, staggered along the vertical dimension as $w^n_{i,j,k+\frac{1}{2}}$.

3.2 Horizontal Diffusion

The discretization of the horizontal diffusion equation (2.4) is a combination of a conservative flux-limited spatial discretization and forward-Euler time stepping[1]. The unlimited horizontal flux along x is:

$$\begin{aligned} f^n_{i+\frac{1}{2},j,k} = \frac{1}{\Delta x}\big(&\omega_1\phi^n_{i-2,j,k} + \omega_2\phi^n_{i-1,j,k} + \omega_3\phi^n_{i,j,k} \\ &+ \omega_4\phi^n_{i+1,j,k} + \omega_5\phi^n_{i+2,j,k} + \omega_6\phi^n_{i+3,j,k}\big), \end{aligned} \tag{3.1}$$

with the weights $\omega_1 = -\frac{1}{90}$, $\omega_2 = \frac{5}{36}$, $\omega_3 = -\frac{49}{36}$, $\omega_4 = \frac{49}{36}$, $\omega_5 = -\frac{5}{36}$, and $\omega_6 = \frac{1}{90}$. Equally, the unlimited flux along y is:

$$\begin{aligned} g^n_{i,j+\frac{1}{2},k} = \frac{1}{\Delta y}\big(&\omega_1\phi^n_{i,j-2,k} + \omega_2\phi^n_{i,j-1,k} + \omega_3\phi^n_{i,j,k} \\ &+ \omega_4\phi^n_{i,j+1,k} + \omega_5\phi^n_{i,j+2,k} + \omega_6\phi^n_{i,j+3,k}\big). \end{aligned} \tag{3.2}$$

[1] This is not the same as COSMO's horizontal diffusion operator, which is solving the higher-order diffusion equation $\frac{\partial\phi}{\partial t} = D\nabla^4\phi$.

The limited fluxes then are:

$$\hat{f}^n_{i+\frac{1}{2},j,k} = \begin{cases} f^n_{i+\frac{1}{2},j,k}, & \text{if } f^n_{i+\frac{1}{2},j,k}\left(\phi^n_{i+1,j,k} - \phi^n_{i,j,k}\right) > 0, \\ 0, & \text{otherwise,} \end{cases} \tag{3.3}$$

$$\hat{g}^n_{i,j+\frac{1}{2},k} = \begin{cases} g^n_{i,j+\frac{1}{2},k}, & \text{if } g^n_{i,j+\frac{1}{2},k}\left(\phi^n_{i,j+1,k} - \phi^n_{i,j,k}\right) > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{3.4}$$

Finally, the full discretization is

$$\phi^{n+1}_{i,j,k} = \phi^n_{i,j,k} + D\Delta t\left(\frac{\hat{f}^n_{i+\frac{1}{2},j,k} - \hat{f}^n_{i-\frac{1}{2},j,k}}{\Delta x} + \frac{\hat{g}^n_{i,j+\frac{1}{2},k} - \hat{g}^n_{i,j-\frac{1}{2},k}}{\Delta y}\right), \tag{3.5}$$

which is 6th order in space on smooth inputs and first order in time.

3.3 Vertical Diffusion

The discretization of the vertical diffusion equation (2.5) follows straightly the implementation of COSMO [3]. It is based on the (2nd-order in time and space) Crank-Nicolson scheme

$$\phi^{n+1}_{i,j,k} = \phi^n_{i,j,k} + \Delta t \frac{1}{2}\left[A\left(\phi^n\right) + A\left(\phi^{n+1}\right)\right], \tag{3.6}$$

$$A(\phi) = D\frac{\phi_{i,j,k-1} - 2\phi_{i,j,k} + \phi_{i,j,k+1}}{\Delta z^2}. \tag{3.7}$$

Which can be rewritten as the tridiagonal linear system of equations

$$a\phi^{n+1}_{i,j,k-1} + b\phi^{n+1}_{i,j,k} + c\phi^{n+1}_{i,j,k+1} = d, \tag{3.8}$$

with the diagonal and right hand side entries defined as

$$a = -D\frac{1}{2}\frac{1}{\Delta z^2}, \tag{3.9}$$

$$b = \frac{1}{\Delta t} + D\frac{1}{\Delta z^2}, \tag{3.10}$$

$$c = -D\frac{1}{2}\frac{1}{\Delta z^2}, \tag{3.11}$$

$$d = \frac{\phi^n_{i,j,k}}{\Delta t} + D\frac{1}{2}\frac{\phi^n_{i,j,k-1} - 2\phi^n_{i,j,k} + \phi^n_{i,j,k+1}}{\Delta z^2}. \tag{3.12}$$

3.4 Horizontal Advection

GTBench uses the COSMO 5th-order upwind advection scheme [3] for the discretization of the horizontal advection equation (2.6). Along the x-direction, the fluxes are

$$\begin{aligned}f^{-n}_{i,j,k} = -\frac{1}{\Delta x}\big(&\omega_1\phi^n_{i-3,j,k} + \omega_2\phi^n_{i-2,j,k} + \omega_3\phi^n_{i-1,j,k} \\ &+ \omega_4\phi^n_{i,j,k} + \omega_5\phi^n_{i+1,j,k} + \omega_6\phi^n_{i+2,j,k}\big),\end{aligned} \tag{3.13}$$

$$\begin{aligned}f^{+n}_{i,j,k} = \frac{1}{\Delta x}\big(&\omega_6\phi^n_{i-2,j,k} + \omega_5\phi^n_{i-1,j,k} + \omega_4\phi^n_{i,j,k} \\ &+ \omega_3\phi^n_{i+1,j,k} + \omega_2\phi^n_{i+2,j,k} + \omega_1\phi^n_{i+3,j,k}\big),\end{aligned} \tag{3.14}$$

with the weights $\omega_1 = \frac{1}{30}$, $\omega_2 = \frac{-1}{4}$, $\omega_3 = 1$, $\omega_4 = \frac{-1}{3}$, $\omega_5 = \frac{-1}{2}$, and $\omega_6 = \frac{1}{20}$. Selecting the upwind flux yields

$$f^n_{i,j,k} = \max\left(u_{i,j,k}, 0\right) f^{-n}_{i,j,k} + \min\left(u_{i,j,k}, 0\right) f^{+n}_{i,j,k}. \tag{3.15}$$

Equally along the y-direction:

$$\begin{aligned}g^{-n}_{i,j,k} = -\frac{1}{\Delta y}\big(&\omega_1\phi^n_{i,j-3,k} + \omega_2\phi^n_{i,j-2,k} + \omega_3\phi^n_{i,j-1,k} \\ &+ \omega_4\phi^n_{i,j,k} + \omega_5\phi^n_{i,j+1,k} + \omega_6\phi^n_{i,j+2,k}\big),\end{aligned} \tag{3.16}$$

$$\begin{aligned}g^{+n}_{i,j,k} = \frac{1}{\Delta y}\big(&\omega_6\phi^n_{i,j-2,k} + \omega_5\phi^n_{i,j-1,k} + \omega_4\phi^n_{i,j,k} \\ &+ \omega_3\phi^n_{i,j+1,k} + \omega_2\phi^n_{i,j+2,k} + \omega_1\phi^n_{i,j+3,k}\big),\end{aligned} \tag{3.17}$$

$$g^n_{i,j,k} = \max\left(u_{i,j,k}, 0\right) g^{-n}_{i,j,k} + \min\left(u_{i,j,k}, 0\right) g^{+n}_{i,j,k}. \tag{3.18}$$

The final update step is then:

$$\phi^{n+1}_{i,j,k} = \phi^n_{i,j,k} - \Delta t\left(f^n_{i,j,k} + g^n_{i,j,k}\right). \tag{3.19}$$

3.5 Vertical Advection

The discretization of the vertical advection equation (2.7) follows again closely the COSMO implementation [3]. That is, it uses the Crank-Nicolson discretization scheme

$$\phi^{n+1}_{i,j,k} = \phi^n_{i,j,k} + \Delta t\frac{1}{2}\left[A\left(\phi^n\right) + A\left(\phi^{n+1}\right)\right], \tag{3.20}$$

$$A(\phi) = -\frac{1}{2}\left[\frac{w_{i,j,k-\frac{1}{2}}\left(\phi_{i,j,k} - \phi_{i,j,k-1}\right)}{\Delta z} + \frac{w_{i,j,k+\frac{1}{2}}\left(\phi_{i,j,k+1} - \phi_{i,j,k}\right)}{\Delta z}\right]. \tag{3.21}$$

$$\tag{3.22}$$

This leads to the tridiagonal linear system

$$a\phi_{i,j,k-1}^{n+1} + b\phi_{i,j,k}^{n+1} + c\phi_{i,j,k+1}^{n+1} = d, \tag{3.23}$$

with

$$a = -\frac{1}{4}\frac{w_{i,j,k-\frac{1}{2}}}{\Delta z}, \tag{3.24}$$

$$b = \frac{1}{\Delta t} + \frac{1}{4}\frac{w_{i,j,k-\frac{1}{2}} - w_{i,j,k+\frac{1}{2}}}{\Delta z}, \tag{3.25}$$

$$c = \frac{1}{4}\frac{w_{i,j,k+\frac{1}{2}}}{\Delta z}, \tag{3.26}$$

$$d = \frac{\phi_{i,j,k}^{n}}{\Delta t} - \frac{1}{4}\left[\frac{w_{i,j,k-\frac{1}{2}}\left(\phi_{i,j,k}^{n} - \phi_{i,j,k-1}^{n}\right)}{\Delta z} + \frac{w_{i,j,k+\frac{1}{2}}\left(\phi_{i,j,k+1}^{n} - \phi_{i,j,k}^{n}\right)}{\Delta z}\right]. \tag{3.27}$$

3.6 Periodic Tridiagonal System Solver

Equations (3.8) and (3.23) in combination with the periodic boundary conditions lead to a linear systems of equations of the form

$$\begin{bmatrix} b_1 & c_1 & & & a_1 \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & b_{n-1} & c_{n-1} \\ c_n & & & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_{n-1} \\ d_n \end{bmatrix}. \tag{3.28}$$

Dropping the last equation and subtracting the last columns times x_n yields

$$\begin{bmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-2} \\ x_{n-1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_{n-2} \\ d_{n-1} \end{bmatrix} - x_n \begin{bmatrix} a_1 \\ 0 \\ \vdots \\ 0 \\ c_{n-1} \end{bmatrix}. \tag{3.29}$$

With $\mathbf{x} = [x_1, \cdots, x_{n-1}]^{\mathrm{T}}$, $\mathbf{d} = [d_1, \cdots, d_{n-1}]^{\mathrm{T}}$, and $\mathbf{e} = [a_1, 0, \cdots, 0, c_{n-1}]^{\mathrm{T}}$, this is $\mathbf{Ax} = \mathbf{d} - x_n\mathbf{e}$. Splitting $\mathbf{x} = \mathbf{y} - x_n\mathbf{z}$, we solve the two tridiagonal systems $\mathbf{Ay} = \mathbf{d}$ and $\mathbf{Az} = \mathbf{e}$ with the Thomas algorithm for $\mathbf{y}$ and $\mathbf{z}$, respectively. From the last row of (3.28), we further have $c_n x_1 + a_n x_{n-1} + b_n x_n = d_n$. Thus $c_n(y_1 - x_n z_1) + a_n(y_{n-1} - x_n z_{n-1}) + b_n x_n = d_n$. Solving for x_n gives

$$x_n = \frac{d_n - c_n z_1 - a_n y_{n-1}}{b_n - c_n z_1 - a_n z_{n-1}}. \tag{3.30}$$

3.7 Time Stepping

GTBench uses the following 3-stage Runge-Kutta time stepping scheme for advection that is also available in COSMO [6]:

$$\phi^{*} = \phi^{n} + \frac{1}{3}\Delta t \mathcal{L}\left(\phi^{n}\right), \tag{3.31}$$

$$\phi^{**} = \phi^{n} + \frac{1}{2}\Delta t \mathcal{L}\left(\phi^{*}\right), \tag{3.32}$$

$$\phi^{n+1} = \phi^{n} + \Delta t \mathcal{L}\left(\phi^{**}\right). \tag{3.33}$$

In each time step, horizontal diffusion is applied first, followed by the Runge-Kutta advection scheme (that is, three applications of horizontal advection and vertical advection) and finally one application of vertical advection.

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