Halfar Model Numerics Example

Drisana Iverson (dmosaphir@sift.net) and Dan Bryce (dbryce@sift.net)

January 18, 2024

1 Discretized PDEs as continuous Petrinets

We discretize and solve PDEs expressed with partial derivatives $\frac{\partial u}{\partial t}$ and $\frac{\partial u}{\partial x}$ over time t and space x by encoding discrete approximations of the PDE as continuous Petrinets. Our method relies upon the semantics of continuous Petrinets wherein transitions and the associated transition rates describe flow along the PDE gradient. A single Petrinet transition of the form

$$\{u_1\} \xrightarrow{r} \{u_2\}$$

corresponds to

$$\frac{\partial u_1}{\partial t} = -r \qquad \frac{\partial u_2}{\partial t} = r$$

and encodes a flow from u_1 to u_2 with rate r. Similarly, partial derivatives

$$\frac{\partial u_3}{\partial t} = r_1 + r_2 \qquad \frac{\partial u_4}{\partial t} = r_1 - r_2$$

correspond to transitions

$$\{u_4\} \xrightarrow{r_2} \{u_3\} \qquad \{\} \xrightarrow{2r_1} \{u_3, u_4\}$$

where the *aggregate* flow rate for each variable is identical to the partial derivative with respect to time. We encode discretized PDEs as a Petrinet, where states correspond to each variable at different spatial points and the rates encode the partial derivatives.

We define the discretizations of space and time respectively as

$$u_i^k = u(x_i, t_k)$$

where

$$\begin{aligned} x_i &= i\Delta x, \qquad i \in [0, I) \\ t_k &= k\Delta t, \qquad k \in [0, K] \end{aligned}$$

Then we refer to the definitions of the partial derivatives with the function F.

$$\frac{\partial u}{\partial t}(x_i, t_k) = F_{ut}(x_i, t_k) \tag{1}$$

$$\frac{\partial u}{\partial x}(x_i, t_k) = F_{ux}(x_i, t_k) \tag{2}$$

The subscripts identify the partial derivative with respect to t and x, respectively. We also denote by $\mathtt{F}$, the discretization of a partial derivative, for example, the forward derivative:

$$\begin{aligned} \frac{\partial u}{\partial t}(x_i, t_k) = F_{ut}(x_i, t_k) \approx \mathtt{F}_{ut}(x_i, t_k) = \frac{u_i^{k+1} - u_i^k}{\Delta t} \\ \frac{\partial u}{\partial x}(x_i, t_k) = F_{ux}(x_i, t_k) \approx \mathtt{F}_{ux}(x_i, t_k) = \frac{u_{i+1}^k - u_i^k}{\Delta x} \end{aligned} \tag{3}$$

In the following, we discretize the definitions of partial derivatives F by substituting the chosen discretization $\mathtt{F}$. While Equation 3 illustrates using a particular approximation of the partial derivative, this choice is an arbitrary, but important, decision. We discuss several possible definitions in the following section.

Solving for u_i^{k+1} in Equation 3 allows us to define:

$$u_i^{k+1} = u_i^k + \mathtt{F}_{ut}(x_i, t_k)\Delta t \tag{4}$$

where $\mathtt{F}$ is the discretization of an arbitrary expression F that includes, for example, additional partial derivatives. If the expression $F_{ut}(x_i, t_k)$ includes a partial derivative term F', then we substitute $\mathtt{F}'$, recursively. For example, the advection operator applied to a vector field a:

$$(\mathbf{u} \cdot \nabla)a = -u\frac{\partial a}{\partial x} - v\frac{\partial a}{\partial y} - w\frac{\partial a}{\partial z}$$

defines the equation:

$$\frac{\partial a}{\partial t} = -u\frac{\partial a}{\partial x} - v\frac{\partial a}{\partial y} - w\frac{\partial a}{\partial z}$$

The partial deriviative of a wrt. to time at point $p_i = (x_{i_1}, y_{i_2}, z_{i_3})$ and time t_k is:

$$\begin{aligned} \frac{\partial a}{\partial t}(p_i, t_k) &= F_{at}(p_i, t_k) \\ &= -uF_{ax}(p_i, t_k) \\ &\quad - vF_{ay}(p_i, t_k) \\ &\quad - wF_{az}(p_i, t_k) \end{aligned} \tag{5}$$

Discretizing F_{at} involves substituting $\mathtt{F}_{ax}$, $\mathtt{F}_{ay}$, and $\mathtt{F}_{az}$ so that:

$$F_{at}(p, t_k) \approx \mathtt{F}_{at}(p_i, t_k) = -u\mathtt{F}_{ax}(p_i, t_k) - v\mathtt{F}_{ay}(p_i, t_k) - w\mathtt{F}_{az}(p_i, t_k) \tag{6}$$

Expanding each derivative term $\mathtt{F}$ will result in the expression:

$$\begin{aligned} \mathtt{F}_{at}(p_i, t_k) &= -u\mathtt{F}_{ax}(p_i, t_k) - v\mathtt{F}_{ay}(p_i, t_k) - w\mathtt{F}_{az}(p_i, t_k) \\ \frac{a_i^{k+1} - a_i^k}{\Delta t} &= -u\frac{a_{i_{x^+}}^k - a_i^k}{\Delta x} - v\frac{a_{i_{y^+}}^k - a_i^k}{\Delta y} - w\frac{a_{i_{z^+}}^k - a_i^k}{\Delta z} \end{aligned} \tag{7}$$

where i_{x^+} corresponds to $(x_{i_1+1}, y_{i_2}, z_{i_3})$, and similarly for i_{y^+} and i_{z^+}. Solving 7 for a_i^{k+1} provides a state-update expression:

$$a_i^{k+1} = a_i^k + \left(-u\frac{a_{i_{x^+}}^k - a_i^k}{\Delta x} - v\frac{a_{i_{y^+}}^k - a_i^k}{\Delta y} - w\frac{a_{i_{z^+}}^k - a_i^k}{\Delta z}\right)\Delta t \tag{8}$$

Our main observation is that the state-update expression can be expressed as a linear combination of terms (which we refer to as rates r):

$$\begin{aligned} a_i^{k+1} =& a_i^k + \left(-u\frac{a_{i_{x^+}}^k - a_i^k}{\Delta x} - v\frac{a_{i_{y^+}}^k - a_i^k}{\Delta y} - w\frac{a_{i_{z^+}}^k - a_i^k}{\Delta z}\right)\Delta t \\ =& a_i^k + \left(-u\frac{a_{i_{x^+}}^k}{\Delta x} - u\frac{-a_i^k}{\Delta x} - v\frac{a_{i_{y^+}}^k}{\Delta y} - v\frac{-a_i^k}{\Delta y} - w\frac{a_{i_{z^+}}^k}{\Delta z} - w\frac{-a_i^k}{\Delta z}\right)\Delta t \\ =& a_i^k + \left(r_{x^+} - r_x + r_{y^+} - r_y + r_{z^+} - r_z\right)\Delta t \end{aligned} \tag{9}$$

Rewriting Equation 9, we can recover the partial derivative expressed in terms of rates:

$$\begin{aligned}\frac{a_i^{k+1} - a_i^k}{\Delta t} &= r_{x^+} - r_x + r_{y^+} - r_y + r_{z^+} - r_z \\ &\approx \frac{\partial a}{\partial t}(p_i, t_k)\end{aligned} \tag{10}$$

Petrinets expressing mass action kinetics use the same format, whereby positive terms are the rates associated with incoming transitions and negative, outgoing transitions. We denote by $src \xrightarrow{r} dest$ a transition from states in src to states in $dest$ with rate r. We express Equation 10 as the transitions:

$$\begin{aligned}\{a_{i_{x^+}}\} &\xrightarrow{r_{x^+}} \{a_i\} \\ \{a_i\} &\xrightarrow{r_x} \{a_{i_{x^-}}\} \\ \{a_{i_{y^+}}\} &\xrightarrow{r_{y^+}} \{a_i\} \\ \{a_i\} &\xrightarrow{r_y} \{a_{i_{y^-}}\} \\ \{a_{i_{z^+}}\} &\xrightarrow{r_{z^+}} \{a_i\} \\ \{a_i\} &\xrightarrow{r_z} \{a_{i_{z^-}}\}\end{aligned} \tag{11}$$

where i_{x^-} corresponds to $(x_{i_1-1}, y_{i_2}, z_{i_3})$, and similarly for i_{y^-} and i_{z^-}. The transitions refer to these neighboring locations because they share common rate terms. Aggregating the transitions allows us to express $\frac{\partial a}{\partial t}$ for all locations.

We handle boundary conditions implicitly by using transitions with an empty src or $dest$, and a rate that substitutes references to the value of boundary locations with an expression. For example, if a_i^k appears in a rate expression and location i is a boundary location (e.g., $i = -1$ or $i = I$, in the one dimensional case), then we replace a_i^k with the boundary condition $b(a, t)$. The Petrinet does not represent boundary locations with state variables because, otherwise, the semantics for the Petrinet would cause those state variables to be updated. It is sufficient to leak the boundary rate expressions into locations on the upper boundaries and out from locations on the lower boundaries to ensure the appropriate rate terms impact the state variables with transitions of the form $\{\} \xrightarrow{r_b} \{a_{I-1}\}$ (upper) and $\{a_0\} \xrightarrow{r_b} \{\}$ (lower).

2 Discretizing Partial Derivatives

We consider three primary methods for computing partial derivatives from a discretization: forward, backward, and centered. The definitions in Equation 3 correspond to the forward derivative, calculating the derivative at u_i^k by considering the next greater point along the respective dimension, u_{i+1}^k or u_i^{k+1}. We define the backward derivative as:

$$\begin{aligned}\mathtt{F}_{ut}(x_i, t_k) &= \frac{u_i^k - u_i^{k-1}}{\Delta t} \\ \mathtt{F}_{ux}(x_i, t_k) &= \frac{u_i^k - u_{i-1}^k}{\Delta x}\end{aligned} \tag{12}$$

and the centered derivative as:

$$\begin{aligned}\mathtt{F}_{ut}(x_i, t_k) &= \frac{u_i^{k+1} - u_i^{k-1}}{2\Delta t} \\ \mathtt{F}_{ux}(x_i, t_k) &= \frac{u_{i+1}^k - u_{i-1}^k}{2\Delta x}\end{aligned} \tag{13}$$

The primary difference between these methods of calculating the derivative is how the Petrinet transitions connect the states.

3 Examples

We illustrate several examples from climate modeling to show how to transform a PDE model into a Petrinet.

3.1 Halfar Equation

The original Halfar dome equation is given by

$$\frac{\partial h}{\partial t} = \frac{2}{n+2} A(\rho g)^n \frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\left|\frac{\partial h}{\partial x}\right|^{n-1} h^{n+2}\right). \tag{14}$$

Substituting $\Gamma = \frac{2}{n+2} A(\rho g)^n$ (this is a constant) and $n = 3$ (also a constant), we get

$$\frac{\partial h}{\partial t} = \Gamma \frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\left|\frac{\partial h}{\partial x}\right|^{2} h^{5}\right). \tag{15}$$

We can start by substituting $\frac{\partial h}{\partial t}$ with the forward derivative $\mathtt{F}_{ut}$ (Equation 3) and $\frac{\partial h}{\partial x}$ with the centered derivative $\mathtt{F}_{ux}$ (Equation 13):

$$\frac{h_i^{k+1} - h_i^k}{\Delta t} = \Gamma \frac{\partial}{\partial x}\left(\frac{h_{i+1}^k - h_{i-1}^k}{2\Delta x}\left|\frac{h_{i+1}^k - h_{i-1}^k}{2\Delta x}\right|^2 (h_i^k)^5\right) \tag{16}$$

Then, to simplify the expression, we can define

$$w_i^k = \frac{h_{i+1}^k - h_{i-1}^k}{2\Delta x}\left|\frac{h_{i+1}^k - h_{i-1}^k}{2\Delta x}\right|^2 (h_i^k)^5 \tag{17}$$

Substituting Equation 17, we get

$$\frac{h_i^{k+1} - h_i^k}{\Delta t} = \Gamma \frac{\partial}{\partial x} w_i^k \tag{18}$$

We can then use Eq. 13 a second time to get

$$\frac{h_i^{k+1} - h_i^k}{\Delta t} = \Gamma \left(\frac{w_{i+1}^k - w_{i-1}^k}{2\Delta x}\right) \tag{19}$$

Solving for h_i^{k+1} gives the step update equation:

$$h_i^{k+1} = h_i^k + \Gamma \Delta t \left(\frac{w_{i+1}^k - w_{i-1}^k}{2\Delta x}\right). \tag{20}$$

Re-writing equation 20, we can define for each $i = [0, I)$:

$$\begin{aligned} h_i^{k+1} &= h_i^k + \left(\frac{\Gamma}{2\Delta x} w_{i+1}^k - \frac{\Gamma}{2\Delta x} w_{i-1}^k\right)\Delta t \\ &= h_i^k + (r_{i+1} - r_{i-1})\Delta t \end{aligned} \tag{21}$$

where we drop the time index k so that

$$\begin{aligned} r_i &= \frac{\Gamma}{2\Delta x} w_i \\ &= \frac{\Gamma}{2\Delta x}\frac{h_{i+1} - h_{i-1}}{2\Delta x}\left|\frac{h_{i+1} - h_{i-1}}{2\Delta x}\right|^2 (h_i)^5 \end{aligned} \tag{22}$$

for $i \in [0, I)$ and $r_{-1} = r_I = B(t)$, where $B(t)$ is the boundary condition, assumed to be $B(t) = 0$ in the Halfar model.

Expressing Equation 21 as a Petrinet, results in the transitions:

$$\{h_{i+1}\} \xrightarrow{r_i} \{h_{i-1}\} \quad : i \in [-1, I] \tag{23}$$

where the source and target states are $\{\}$ when $i = I$ or $i = -1$, respectively. Figure 1 (Centered Difference) illustrates the Petrinet for the Halfar model when $I = 5$.

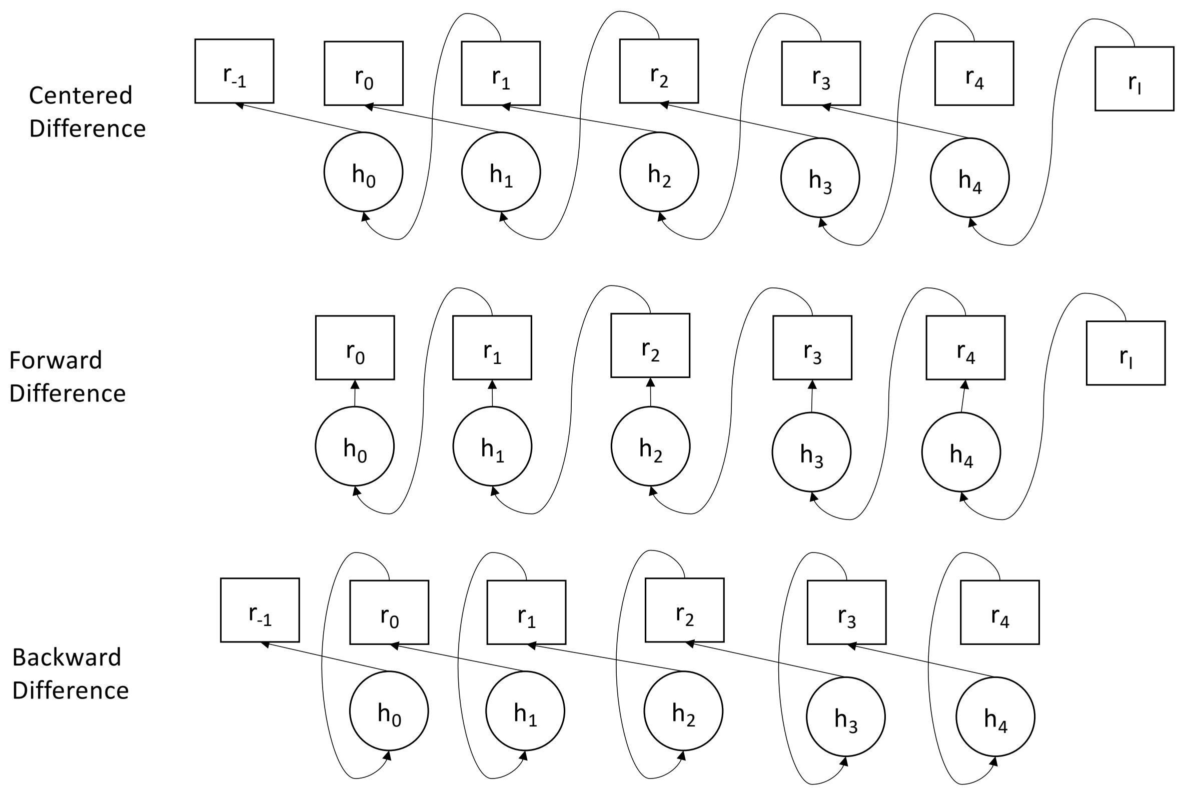

Figure 1: Petrinets for the Halfar model when $I = 5$, using different derivatives. Circles denote states and rectangles denote transitions.

3.2 Advection Equation

The 1d advection equation (1d version of the Oceananigans equation, from Scenario 4), is given by

$$\frac{\partial a}{\partial t} + u\frac{\partial a}{\partial x} = 0 \tag{24}$$

After substituting the forward derivative for $\mathtt{F}_{at}$ (Equation 3) and backward derivative (Equation 12) for $\mathtt{F}_{ax}$, the state-update equation simplifies to:

$$\begin{aligned} a_i^{k+1} &= a_i^k - u\left(\frac{a_i^k - a_{i-1}^k}{\Delta x}\right)\Delta t \\ &= u_i^k + \left(\frac{-ua_i^k}{\Delta x} - \frac{-ua_{i-1}^k}{\Delta x}\right)\Delta t \\ &= a_i^k + (r_i - r_{i-1})\Delta t \end{aligned} \tag{25}$$

where, in the following $r_i = \dfrac{-ua_i}{\Delta x}$ for all $i \in [0, I)$.

The boundary condition defines:

$$b(a,t) = 0.0 \tag{26}$$

The above scheme is stable when $\left|\frac{u\Delta t}{\Delta x}\right| \leq 1$ or equivalently when $\Delta t \leq \frac{\Delta x}{|u|}$.
Translating this model to a Petrinet results in transitions of the form:

$$\begin{aligned}
\{a_0\} &\xrightarrow{r_b=0} \{\} \\
\{a_1\} &\xrightarrow{r_1=\frac{-ua_1}{\Delta x}} \{a_0\} \\
&\dots \\
\{a_{I-1}\} &\xrightarrow{r_{I-1}=\frac{-ua_{I-1}}{\Delta x}} \{a_{I-2}\} \\
\{\} &\xrightarrow{r_b=0} \{a_{I-1}\}
\end{aligned} \tag{27}$$

so that the Petrinet expresses the step updates:

$$\begin{aligned}
a_0^{k+1} &= a_0^k + (r_1 - r_b)\Delta t \\
a_1^{k+1} &= a_1^k + (r_2 - r_1)\Delta t \\
&\dots \\
a_{I-1}^{k+1} &= a_{I-1}^k + (r_b - r_{I-1})\Delta t
\end{aligned} \tag{28}$$

3.3 Discretization using Sympy (LaTeX to discretized equation)

We start with Equation 14 in LaTeX, then parse it into SymPy, where it becomes the equation (as printed in LaTeX by SymPy):

$$\frac{d}{dt} h = \frac{2A\left(g\rho\right)^{n} \frac{\partial}{\partial x} h^{n+2} \left|\frac{d}{dx} h\right|^{n-1} \frac{d}{dx} h}{n+2} \tag{29}$$

We specify the time and space dimensions by replacing h with $h(x,t)$:

$$\frac{\partial}{\partial t} h(x,t) = \frac{2A\left(g\rho\right)^{n} \frac{\partial}{\partial x} h^{n+2}(x,t) \left|\frac{\partial}{\partial x} h(x,t)\right|^{n-1} \frac{\partial}{\partial x} h(x,t)}{n+2} \tag{30}$$

We then substitute constant values $g = 9.8101$, $\rho = 910.0$, and $n = 3.0$:

$$\frac{\partial}{\partial t} h(x,t) = 284580063236.609A \frac{\partial}{\partial x} h^{5.0}(x,t) \left|\frac{\partial}{\partial x} h(x,t)\right|^{2.0} \frac{\partial}{\partial x} h(x,t) \tag{31}$$

We can then replace the derivative expressions by using the `as_finite_difference` function. In this example, we chose to evaluate x at the points $x-1$ and x, indicating a backwards difference in space, and evaluate t at the points t and $t+dt$, indicating a forward difference in time:

$$\begin{aligned}
-\frac{h(x,t)}{dt} + \frac{h(x,dt+t)}{dt} =& 284580063236.609A\Big(\\
&\left(h(x,t) - h(x-1,t)\right) h^{5.0}(x,t) \left|h(x,t) - h(x-1,t)\right|^{2.0} \\
&- \left(-h(x-2,t) + h(x-1,t)\right) h^{5.0}(x-1,t) \left|h(x-2,t) - h(x-1,t)\right|^{2.0} \\
&\Big)
\end{aligned} \tag{32}$$

The `solve` function can then be used to solve for the solution at the next time step $h(x,t+dt)$ in terms of expressions at the current time t.

$$
\begin{aligned}
h(x,t+dt) = & h(x,t) + \Big(\\
& \quad 284580063236.609 A h^6(x,t) \left|h(x,t) - h(x-1,t)\right|^2 \\
& - 284580063236.609 A h^5(x,t) h(x-1,t) \left|h(x,t) - h(x-1,t)\right|^2 \\
& + 284580063236.609 A h(x-2,t) h^5(x-1,t) \left|h(x-2,t) - h(x-1,t)\right|^2 \\
& - 284580063236.609 A h^6(x-1,t) \left|h(x-2,t) - h(x-1,t)\right|^2 \\
& \Big) dt
\end{aligned}
\tag{33}
$$

For each value of $i \in [0,4]$, we substitute i for x, for example if $i = 2$:

$$
\begin{aligned}
h(2,t+dt) = & h(2,t) + \Big(\\
& \quad 284580063236.609 A h^6(2,t) \left|h(1,t) - h(2,t)\right|^2 \\
& - 284580063236.609 A h(1,t) h^5(2,t) \left|h(1,t) - h(2,t)\right|^2 \\
& + 284580063236.609 A h(0,t) h^5(1,t) \left|h(0,t) - h(1,t)\right|^2 \\
& - 284580063236.609 A h^6(1,t) \left|h(0,t) - h(1,t)\right|^2 \\
& \Big) dt
\end{aligned}
\tag{34}
$$

For each $i \in [0,4]$, we define a Petrinet state x_i with transitions of the form $\{x_{i+1}\} \xrightarrow{r_i} \{x_i\}$ and $\{x_i\} \xrightarrow{r_{i-1}} \{x_{i-1}\}$, where if $i = 2$, then in transition $\{x_3\} \xrightarrow{r_2} \{x_2\}$, r_2 corresponds to:

$$
\begin{aligned}
r_2 &= 284580063236.609 A h^6(2,t) \left|h(1,t) - h(2,t)\right|^2 - 284580063236.609 A h(1,t) h^5(2,t) \left|h(1,t) - h(2,t)\right|^2 \\
&= 284580063236.609 A \left(h(2,t) - h(1,t)\right) \left|h(1,t) - h(2,t)\right|^2 h^5(2,t)
\end{aligned}
\tag{35}
$$

and in transition $\{x_2\} \xrightarrow{r_1} \{x_1\}$, r_1 corresponds to:

$$
\begin{aligned}
r_1 &= -\Big(284580063236.609 A h(0,t) h^5(1,t) \left|h(0,t) - h(1,t)\right|^2 - 284580063236.609 A h^6(1,t) \left|h(0,t) - h(1,t)\right|^2\Big) \\
&= 284580063236.609 A \left(h(1,t) - h(0,t)\right) \left|h(0,t) - h(1,t)\right|^2 h^5(1,t)
\end{aligned}
\tag{36}
$$

References