Single-phase Fluid Finite-Difference Simulator using Python

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Current progress in the development is hosted at https://github.com/benjdewantara/fdressim

Abstract

The author presents the development of a basic finite-difference reservoir simulator using Python as the programming language. The simulator is similar to that of an old traditional simulator, that is to say that it is used to solve a single-phase fluid flow, in a homogeneous and isotropic medium, and discretized in a cartesian coordinate system using a finite-difference approach. The author then gives a few examples with different flow direction (1D, 2D, or 3D) and check the accuracy of the results against another simulator (MRST^{1xx}) or, if possible, against an analytical solution.

Introduction

Often, many undergraduate students majoring in petroleum engineering fail to understand how a reservoir simulator works behind the monitor. Most of these undergraduate students, if not all, must have taken introductory classes on programming, numerical method, and partial differential equations, but still fail to apply them to the field of reservoir simulation. This paper can hopefully give clear explanations on how to utilize those basic knowledges and put them in the form of actual computer program.

Since computers are not able to evaluate the continuous form of a differential equation, we need to approximate the solution to a differential mathematical expression into its discrete form. This method is also known as finite-difference method. Although most commercial reservoir simulators available nowadays no longer use the traditional finite-difference approach, it is still an eye-opening experience to understand how the governing equations are translated into their finite-difference forms. In fact, finite-difference is arguably more intuitive than other discretizing approaches (i.e. corner-point, control-volume).

After we derive the finite-difference form of the differential equation of interest, we then proceed with the presentation of how to put it in the form of computer program. Python is chosen as the programming language because it is easy to understand with its clear syntax and its human-readable trait.

Statement of Theory and Definitions (WHY YELLOW? BECAUSE THIS TITLE IS USUALLY LEFT OUT IN MOST PAPERS. DELETE THIS LATER!!)

Diffusivity Equation for Fluid Flow in Porous Media

In the field of reservoir engineering, the diffusivity equation governs the fluid flow and is derived using Darcy's law on the basis of conservation of mass. Firstly, one needs to choose the coordinate system that will represent the space. The choice of coordinate system is mainly influenced by the predicted nature of the flow. Due to the radial nature of the fluid flow, the diffusivity equation is usually derived using the cylindrical coordinate system with flow in θ and z direction neglected (see **Eq. 1**). However, in this paper we will only consider the cartesian coordinate system (see **Eq. 2**).

$$\phi \rho c_T \frac{\partial P}{\partial t} = -\frac{1}{r} \frac{\partial}{\partial r} \left(r \rho \frac{k_r}{\mu} \frac{\partial P}{\partial r} \right) \tag{1}$$

$$\phi \rho c_T \frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} \left(\rho \frac{k_x}{\mu} \frac{\partial P}{\partial x} \right) - \frac{\partial}{\partial y} \left(\rho \frac{k_y}{\mu} \frac{\partial P}{\partial y} \right) - \frac{\partial}{\partial z} \left(\rho \frac{k_z}{\mu} \left(\frac{\partial P}{\partial z} - \rho g \right) \right)$$
(2)

Finite-Difference Calculus

The concept of finite-difference forms the foundation of solving differential equations numerically. Instead of solving a differential equation that is supposed to be continuous everywhere in its domain, we look at discrete points and form difference equations. Another way to grasp this concept is that we are not evaluating the behavior of $\Delta f(x)$ as Δx gets closer to zero (see **Eq. 3**) as opposed to the actual definition of derivative (see **Eq. 4**). This method will introduce some error that depends on the chosen value of h.

$$\frac{df}{dx} \approx \frac{f_{x+\Delta x} - f_x}{h} \tag{3}$$

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x}$$
(4)

Appendix A presents the derivation of diffusivity equation in cartesian coordinate system.

More Numerical Methods

This section outlines the relevant numerical methods, particularly the ones dealing with matrix (solving a system of linear equations)

Python (programming language) and SciPy stack

This section outlines how Python is used and the libraries (NumPy and SciPy) used. You should mention the use of functions like scipy.linalg to solve a system of linear equations.

Description and Application of Equipment and Processes

Design Consideration

The first question we should address is how do we build the computer model? Or specifically, how do we represent the behavior of a **reservoir system** (consisting of **fluid** and **rock**) in a **3D** *cartesian* **space** using a computer program? Using this reasoning, the author declare objects as sketched in **Fig. x**.

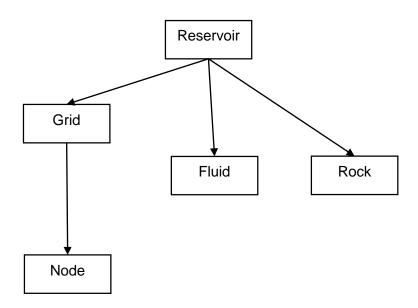


Figure 1 - Schematic of objects

Defining Each Objects

Applying the Finite-difference Diffusivity Equation

Let us first consider the finite-difference form of the diffusivity equation (derived in Appendix A)
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Presentation of Data and Results
Conclusions
Acknowledgments
Nomenclature
References
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Appendix

Possible list of appendices:

- 1. Finite-difference derivation of Diffusivity Equation
- 2. Analytical solution to a 1D flow problem

Appendix A - Finite-difference Derivation of Diffusivity Equation

We begin by observing the conservation of mass equation,

$$\frac{d(m_{cv})}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{m}_{sc} \tag{A1}$$

Evaluating the right-hand side, for simplicity, we consider mass rate (\dot{m}_x) that only flows in x direction, with term \dot{m} being ρuA ,

$$\begin{split} \dot{m}_{in} &= \rho u_{x-\frac{\Delta x}{2}} A_{x-\frac{\Delta x}{2}} \\ \dot{m}_{out} &= \rho u_{x+\frac{\Delta x}{2}} A_{x+\frac{\Delta x}{2}} \\ \dot{m}_{in} - \dot{m}_{out} + \dot{m}_{sc} &= \rho u_{x-\frac{\Delta x}{2}} A_{x-\frac{\Delta x}{2}} - \rho u_{x+\frac{\Delta x}{2}} A_{x+\frac{\Delta x}{2}} + \dot{m}_{sc} \end{split}$$

Using the derivative definition as follows,

$$\frac{\partial(\rho u_x A_x)}{\partial x} = \frac{\left(\rho u_x A_x\right)_{x - \frac{\Delta x}{2}} - \left(\rho u_x A_x\right)_{x + \frac{\Delta x}{2}}}{\left(x - \frac{\Delta x}{2}\right) - \left(x + \frac{\Delta x}{2}\right)}$$
$$-\Delta x \frac{\partial(\rho u_x A_x)}{\partial x} = \left(\rho u_x A_x\right)_{x - \frac{\Delta x}{2}} - \left(\rho u_x A_x\right)_{x + \frac{\Delta x}{2}}$$

Thus, the right-hand side of the equation becomes,

$$\dot{m}_{in} - \dot{m}_{out} + \dot{m}_{sc} = -\Delta x \frac{\partial (\rho u_x A_x)}{\partial x} + \dot{m}_{sc}$$

Evaluating the left-hand side of the equation, noticing that $m_{cv} = \phi \rho V_b$, with term V_b being $\Delta x \Delta y \Delta z$,

$$\frac{d(m_{cv})}{dt} = \frac{d(\phi \rho V_b)}{dt}$$

Coming back to the earlier mass conservation equation,

$$\frac{d(m_{cv})}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{m}_{sc}$$

$$\frac{d(\phi \rho V_b)}{dt} = -\Delta x \frac{\partial (\rho u_x A_x)}{\partial x} + \dot{m}_{sc}$$

Since V_b and A_x are constants,

$$V_{b} \frac{d(\phi \rho)}{dt} = -A_{x} \Delta x \frac{\partial(\rho u_{x})}{\partial x} + \dot{m}_{sc}$$

$$\frac{d(\phi \rho)}{dt} = \frac{-A_{x} \Delta x}{V_{b}} \frac{\partial(\rho u_{x})}{\partial x} + \frac{\dot{m}_{sc}}{V_{b}}$$

$$\frac{d(\phi \rho)}{dP} \frac{\partial P}{\partial t} = \frac{-A_{x} \Delta x}{V_{b}} \frac{\partial(\rho u_{x})}{\partial x} + \frac{\dot{m}_{sc}}{V_{b}}$$

$$\phi \rho c_{T} \frac{\partial P}{\partial t} = \frac{-A_{x} \Delta x}{V_{b}} \frac{\partial(\rho u_{x})}{\partial x} + \frac{\dot{m}_{sc}}{V_{b}}$$

We now have the general continuity equation. One can generalize the equation further by taking into account the flow in y and z direction as follows,

$$\phi \rho c_T \frac{\partial P}{\partial t} = \frac{-A_x \Delta x}{V_h} \frac{\partial (\rho u_x)}{\partial x} + \frac{-A_y \Delta y}{V_h} \frac{\partial (\rho u_y)}{\partial y} + \frac{-A_z \Delta z}{V_h} \frac{\partial (\rho u_z)}{\partial z} + \frac{\dot{m}_{sc}}{V_h}$$
(A2)

The moment we evaluate the velocity term (u_s) , using Darcy's law, we will arrive at the diffusivity equation. Again, for clarity we shall derive the equation further by considering only the flow in x direction. Recall the equation for Darcy's law in some s direction,

$$u_s = \frac{-k}{u} \left(\frac{\partial P}{\partial s} - \rho g \frac{\partial z}{\partial s} \right)$$

For flow only in x direction, the continuity equation becomes,

$$\phi \rho c_T \frac{\partial P}{\partial t} = \frac{-A_x \Delta x}{V_b} \frac{\partial}{\partial x} \left(\rho \frac{-k}{\mu} \frac{\partial P}{\partial x} \right) + \frac{\dot{m}_{sc}}{V_b}$$

We begin translating any $\frac{\partial}{\partial x}$ term (spatial derivative) using finite-difference method,

$$\begin{split} \phi \rho c_{T} \frac{\partial P}{\partial t} &= \frac{A_{x} \Delta x}{V_{b}} \frac{\partial}{\partial x} \left(\rho \frac{k}{\mu} \frac{\partial P}{\partial x} \right) + \frac{\dot{m}_{SC}}{V_{b}} \\ &= \frac{A_{x} \Delta x}{V_{b}} \frac{1}{\Delta x} \left[\left(\rho \frac{k}{\mu} \frac{\partial P}{\partial x} \right)_{x + \frac{\Delta x}{2}} - \left(\rho \frac{k}{\mu} \frac{\partial P}{\partial x} \right)_{x - \frac{\Delta x}{2}} \right] + \frac{\dot{m}_{SC}}{V_{b}} \\ &= \frac{A_{x}}{V_{b}} \left[\left(\frac{\rho k}{\mu} \right)_{x + \frac{\Delta x}{2}} \left(\frac{\partial P}{\partial x} \right)_{x + \frac{\Delta x}{2}} - \left(\frac{\rho k}{\mu} \right)_{x - \frac{\Delta x}{2}} \left(\frac{\partial P}{\partial x} \right)_{x - \frac{\Delta x}{2}} \right] + \frac{\dot{m}_{SC}}{V_{b}} \\ &= \left[\left(\frac{\rho k A_{x}}{\mu V_{b}} \right)_{x + \frac{\Delta x}{2}} \frac{1}{\Delta x} \left(P_{x + \Delta x} - P_{x} \right) - \left(\frac{\rho k A_{x}}{\mu V_{b}} \right)_{x - \frac{\Delta x}{2}} \frac{1}{\Delta x} \left(P_{x} - P_{x - \Delta x} \right) \right] + \frac{\dot{m}_{SC}}{V_{b}} \\ \phi \rho c_{T} \frac{\partial P}{\partial t} &= \left[\left(\frac{\rho k A_{x}}{\mu V_{b} \Delta x} \right)_{x + \frac{\Delta x}{2}} \left(P_{x + \Delta x} - P_{x} \right) - \left(\frac{\rho k A_{x}}{\mu V_{b} \Delta x} \right)_{x - \frac{\Delta x}{2}} \left(P_{x} - P_{x - \Delta x} \right) \right] + \frac{\dot{m}_{SC}}{V_{b}} \end{split}$$

We can group the term $\left(\frac{\rho k A_{\chi}}{\mu V_b \Delta x}\right)_{\chi}$ and define them as transmissibility, T_{χ} ,

$$\begin{split} \phi \rho c_T \frac{\partial P}{\partial t} &= \left[T_{x + \frac{\Delta x}{2}} (P_{x + \Delta x} - P_x) - T_{x - \frac{\Delta x}{2}} (P_x - P_{x - \Delta x}) \right] + \frac{\dot{m}_{sc}}{V_b} \\ &= \left[T_{x + \frac{\Delta x}{2}} P_{x + \Delta x} - \left(T_{x + \frac{\Delta x}{2}} + T_{x - \frac{\Delta x}{2}} \right) P_x + T_{x - \frac{\Delta x}{2}} P_{x - \Delta x} \right] + \frac{\dot{m}_{sc}}{V_b} \end{split}$$

We then proceed by translating the $\frac{\partial}{\partial t}$ term (time derivative) using finite-difference. We also assign superscript t or $t + \Delta t$ to any variable to specify the time level.

$$\begin{split} \phi\rho c_T \left(\frac{P_x^{t+\Delta t} - P_x^t}{\Delta t} \right) &= \left[T_{x+\frac{\Delta x}{2}}^t P_{x+\Delta x}^{t+\Delta t} - \left(T_{x+\frac{\Delta x}{2}}^t + T_{x-\frac{\Delta x}{2}}^t \right) P_x^{t+\Delta t} + T_{x-\frac{\Delta x}{2}}^t P_{x-\Delta x}^{t+\Delta t} \right] + \frac{\dot{m}_{sc}}{V_b} \\ \frac{\phi\rho c_T}{\Delta t} \left(P_x^{t+\Delta t} - P_x^t \right) &= \left[T_{x+\frac{\Delta x}{2}}^t P_{x+\Delta x}^{t+\Delta t} - \left(T_{x+\frac{\Delta x}{2}}^t + T_{x-\frac{\Delta x}{2}}^t \right) P_x^{t+\Delta t} + T_{x-\frac{\Delta x}{2}}^t P_{x-\Delta x}^{t+\Delta t} \right] + \frac{\dot{m}_{sc}}{V_b} \end{split}$$
(A3)

We have arrived at the final finite-difference form of diffusivity equation for flow only in x direction. One should notice that any P_x term encountered so far is actually P at some x, y, z coordinate (i.e. $P_{x,y,z}$). Similarly, the term $P_{x+\Delta x}$ actually denotes $P_{x+\Delta x,y,z}$. The subscript y, z is left out for brevity when considering the differential with respect to x. We can further generalize this form and factor in the flow terms for y and z direction as follows,

$$\begin{bmatrix} \text{differential} \\ \text{in } t \end{bmatrix} = \begin{bmatrix} \text{differential} \\ \text{in } x \text{ direction} \end{bmatrix} + \begin{bmatrix} \text{differential} \\ \text{in } y \text{ direction} \end{bmatrix} + \begin{bmatrix} \text{differential} \\ \text{in } z \text{ direction} \end{bmatrix} + \frac{\dot{m}_{sc}}{V_b}$$
(A4)

where:

$$\begin{array}{ll} \text{differential} &= T_{x+\frac{\Delta x}{2}}^t P_{x+\Delta x}^{t+\Delta t} - \left(T_{x+\frac{\Delta x}{2}}^t + T_{x-\frac{\Delta x}{2}}^t\right) P_x^{t+\Delta t} + T_{x-\frac{\Delta x}{2}}^t P_{x-\Delta x}^{t+\Delta t} \\ \text{differential} &= T_{y+\frac{\Delta y}{2}}^t P_{y+\Delta y}^{t+\Delta t} - \left(T_{y+\frac{\Delta y}{2}}^t + T_{y-\frac{\Delta y}{2}}^t\right) P_y^{t+\Delta t} + T_{y-\frac{\Delta y}{2}}^t P_{y-\Delta y}^{t+\Delta t} \\ \text{differential} &= T_{z+\frac{\Delta z}{2}}^t P_{z+\Delta z}^{t+\Delta t} - \left(T_{z+\frac{\Delta z}{2}}^t + T_{z-\frac{\Delta z}{2}}^t\right) P_z^{t+\Delta t} + T_{z-\frac{\Delta z}{2}}^t P_{z-\Delta z}^{t+\Delta t} + \left(-T_{z+\frac{\Delta z}{2}}^t + T_{z-\frac{\Delta z}{2}}^t\right) \rho g \Delta z \\ \text{differential} &= \frac{\phi \rho c_T}{\Delta t} \left(P_{x,y,z}^{t+\Delta t} - P_{x,y,z}^t\right) \\ T_S &= \left(\frac{\rho k A_S}{\mu V_b \Delta S}\right)_S \end{array}$$

Appendix B - Implementing Boundary Condition

The finite-difference derivation as described in **Appendix A** is based on the central difference scheme. This type of scheme is only applicable to a gridblock which has neighboring gridblocks in its x, y, and z direction. However, this is not the case for a boundary gridblock. This situation is best described using a 2D grid sketch (**Fig. B1**). For a boundary gridblock, a special treatment based on either Dirichlet or Neumann boundary condition needs to be made.

Figure Bx goes here

Figure B1 - Figure's caption!!

We restrict further discussion on the flow equation only looking at flow in x direction for simplicity. For instance, consider a boundary gridblock at x that does not have both gridblocks at $x-\frac{\Delta x}{2}$ and $x+\frac{\Delta x}{2}$ to interact with. This means with respect to x, either $P_{x+\Delta x}$ or $P_{x-\Delta x}$ is missing and the diffusivity equation (**Eq. A4**) cannot be completed. Either one of them is the boundary pressure. We need to evaluate how Dirichlet or Neumann condition is imposed on this boundary pressure.

1. Dirichlet condition (pressure specified)

Suppose the boundary pressure is $P_{x-\Delta x}$, for Dirichlet condition, one can directly specify the boundary pressure,

$$P_{r-\Lambda r} = C$$

The value of C is some constant but can also be a function of time. But we will assume it is constant throughout the time.

2. Neumann condition (pressure gradient specified)

For this condition, we are given the gradient value, $\frac{\partial P}{\partial x}$, which is equal to C. We can then translate this gradient into the following,

$$\frac{\partial P}{\partial x} = C$$

$$\frac{\partial P}{\partial x} = \frac{P_x - P_{x - \Delta x}}{\Delta x}$$

$$P_{x-\Delta x} = P_x - C\Delta x$$

Similarly, if the boundary pressure is $P_{x+\Delta x}$, the gradient expression can be approximated as follows,

$$\frac{\partial P}{\partial x} = \frac{P_{x+\Delta x} - P_x}{\Delta x}$$

$$P_{x+\Delta x} = P_x + C\Delta x$$

For a no-flow condition, the gradient is zero (C = 0), thus the boundary pressure is directly equal to P_x .

Appendix C - Imposing the Finite-difference Flow Equation on a Grid Node

Again we consider Eq. A4, with a bit rearrangement,

$$\begin{bmatrix} \text{differential} \\ \text{in } t \end{bmatrix} - \begin{bmatrix} \text{differential} \\ \text{in } x \text{ direction} \end{bmatrix} - \begin{bmatrix} \text{differential} \\ \text{in } y \text{ direction} \end{bmatrix} - \begin{bmatrix} \text{differential} \\ \text{in } z \text{ direction} \end{bmatrix} = \frac{\dot{m}_{sc}}{V_b}$$

$$\begin{array}{ll} \text{differential} &= T_{x+\Delta x}^t P_{x+\Delta x}^{t+\Delta t} - \left(T_{x+\Delta x}^t + T_{x-\Delta x}^t \right) P_x^{t+\Delta t} + T_{x-\Delta x}^t P_{x-\Delta x}^{t+\Delta t} \\ \text{differential} &= T_{y+\Delta y}^t P_{y+\Delta y}^{t+\Delta t} - \left(T_{y+\Delta y}^t + T_{y-\Delta y}^t \right) P_y^{t+\Delta t} + T_{y-\Delta y}^t P_{y-\Delta y}^{t+\Delta t} \\ \text{differential} &= T_{y+\Delta y}^t P_{y+\Delta y}^{t+\Delta t} - \left(T_{y+\Delta y}^t + T_{y-\Delta y}^t \right) P_y^{t+\Delta t} + T_{y-\Delta y}^t P_{y-\Delta y}^{t+\Delta t} \\ \text{differential} &= T_{z+\Delta z}^t P_{z+\Delta z}^{t+\Delta t} - \left(T_{z+\Delta z}^t + T_{z-\Delta z}^t \right) P_z^{t+\Delta t} + T_{z-\Delta z}^t P_{z-\Delta z}^{t+\Delta t} + \left(-T_{z+\Delta z}^t + T_{z-\Delta z}^t \right) \rho g \Delta z \\ \text{differential} &= \frac{\phi \rho c_T}{\Delta t} \left(P_{x,y,z}^{t+\Delta t} - P_{x,y,z}^t \right) \\ \text{in } t &= \left(\frac{\rho k A_s}{\mu V_b \Delta s}\right)_s \end{array}$$

Each of these differential terms (with respect to t, x, y, and z) is translated accordingly to form the diffusivity equation for one particular point. This will form a linear equation with some unknown $P^{t+\Delta t}$ terms and known P^t variables. Notice that we will get the term P^t only when performing differential with respect to t. Also, we will get a known term when performing differential with respect to z. Therefore, we rearrange the equation further as follows,

$$\frac{\phi \rho c_T}{\Delta t} \left(P_{x,y,z}^{t+\Delta t} \right) - \begin{bmatrix} \text{differential} \\ \text{in } x \text{ direction} \end{bmatrix} - \begin{bmatrix} \text{differential} \\ \text{in } y \text{ direction} \end{bmatrix} - \begin{bmatrix} \text{differential'} \\ \text{in } z \text{ direction} \end{bmatrix} = \begin{bmatrix} \text{known} \\ \text{right hand side} \end{bmatrix}$$

where:

$$\begin{bmatrix} \text{differential'} \\ \text{in } z \text{ direction} \end{bmatrix} = T_{z+\frac{\Delta z}{2}}^t P_{z+\Delta t}^{t+\Delta t} - \left(T_{z+\frac{\Delta z}{2}}^t + T_{z-\frac{\Delta z}{2}}^t \right) P_z^{t+\Delta t} + T_{z-\frac{\Delta z}{2}}^t P_{z-\Delta z}^{t+\Delta t}$$

$$\begin{bmatrix} \text{known} \\ \text{right hand side} \end{bmatrix} = \frac{\dot{m}_{SC}}{V_b} + \frac{\phi \rho c_T}{\Delta t} \left(P_{x,y,z}^t \right) + \left(T_{z+\frac{\Delta z}{2}} - T_{z-\frac{\Delta z}{2}} \right) \rho g \Delta z$$

We can form the following matrices,

$$\begin{array}{ll} \text{differential} & = \begin{bmatrix} T^t_{x+\Delta x} & -\left(T^t_{x+\Delta x} + T^t_{x-\Delta x}\right) & T^t_{x-\Delta x} \end{bmatrix} \begin{bmatrix} P^{t+\Delta t}_{x+\Delta x} \\ P^{t+\Delta t}_{x-\Delta x} \end{bmatrix} \\ P^{t+\Delta t}_{x-\Delta x} & P^{t+\Delta t}_{x-\Delta x} \end{bmatrix} \\ \text{differential} & = \begin{bmatrix} T^t_{y+\Delta y} & -\left(T^t_{y+\Delta y} + T^t_{y-\Delta y}\right) & T^t_{y-\Delta y} \end{bmatrix} \begin{bmatrix} P^{t+\Delta t}_{y+\Delta y} \\ P^{t+\Delta t}_{y+\Delta y} \end{bmatrix} \\ P^{t+\Delta t}_{y-\Delta y} & P^{t+\Delta t}_{y-\Delta y} \end{bmatrix} \\ \text{differential}' & = \begin{bmatrix} T^t_{z+\Delta z} & -\left(T^t_{z+\Delta z} + T^t_{z-\Delta z}\right) & T^t_{z-\Delta z} \end{bmatrix} \begin{bmatrix} P^{t+\Delta t}_{z+\Delta z} \\ P^{t+\Delta t}_{z+\Delta z} \end{bmatrix} \\ P^{t+\Delta t}_{z-\Delta z} & P^{t+\Delta t}_{z-\Delta z} \end{bmatrix} \\ P^{t+\Delta t}_{z-\Delta z} & P^{t+\Delta t}_{z-\Delta z} \end{bmatrix}$$