**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. As a result, many of them accept the results at face value without knowing what has happened inside the box. 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. One method that was widely used is 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 and direction neglected (see **Eq. 1**). However, in this paper we will only consider the cartesian coordinate system (see **Eq. 2**).

|  |  |
| --- | --- |
|  | **(1)** |
|  | **(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 as 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 .

|  |  |
| --- | --- |
|  | **(3)** |
|  | **(4)** |

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

## 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.

**Python** is a programming language designed by Guido van Rossum in 1991. Python is widely known for its neat design, code readability, and its syntax which allows programmers to express concepts in fewer lines of code. It supports object-oriented programming paradigm which enables programmers to express their thinking as objects that interact with each other. Each object may have their own methods to interact with other objects or to perform specific operations.

This simulator makes use of the **SciPy stack**. SciPy stack is a Python-based ecosystem of open-source software for mathematics, science, and engineering. Two of the core packages which are used in this simulator are **NumPy** and **SciPy library**. NumPy provides numerical array objects, and routines to manipulate them. It has also become fundamental package for scientific computing with Python. SciPy library provides numerical routines and is used hand in hand with NumPy.

# Description and Application of Equipment and Processes

# Designing the Data Structures

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 classes as sketched in **Fig. 1**. These classes form the core data structures that model the reservoir

Node

Grid

Fluid

Rock

Reservoir

BoundaryCondition

contains

contains

contains

contains

(optional) assigned to

Figure 1 - Schematic of classes

## Node and Grid Classes

Node objects will be used to represent a point in space. Node will contain information such as the flattened index, the coordinate index (, , notation), whether or not a node is a boundary node, and whether or not a node is a source/sink. Flattened index, in contrast to 3D coordinate index, is a 1D array index. For instance, a Grid object with a dimension of (1, 2, 5) will have one gridblock with respect to direction, two gridblocks with respect to direction, and five gridblocks with respect to direction. Each gridblock is bound to a Node object. **Fig. 2** explains how flattened index and coordinate index are assigned to each gridblock for a (1, 2, 5) Grid. This indexing scheme will later be useful when setting up a 2D matrix that consists of linear equations describing pressure relationship among all points at a time level.

A Grid object will contain list of node objects. A Grid class will be instantiated with the specification of its grid dimension (not actual reservoir dimension). Below is the code for the \_\_init\_\_ function for the Node and Grid classes:

class Node(object):

def \_\_init\_\_(self, nodeIndx, dims):

self.nodeIndx = int(nodeIndx)

self.coordIndx = np.unravel\_index(self.nodeIndx, dims)

self.qsrc = 0

self.initBoundaryNode(dims)

class Grid(object):

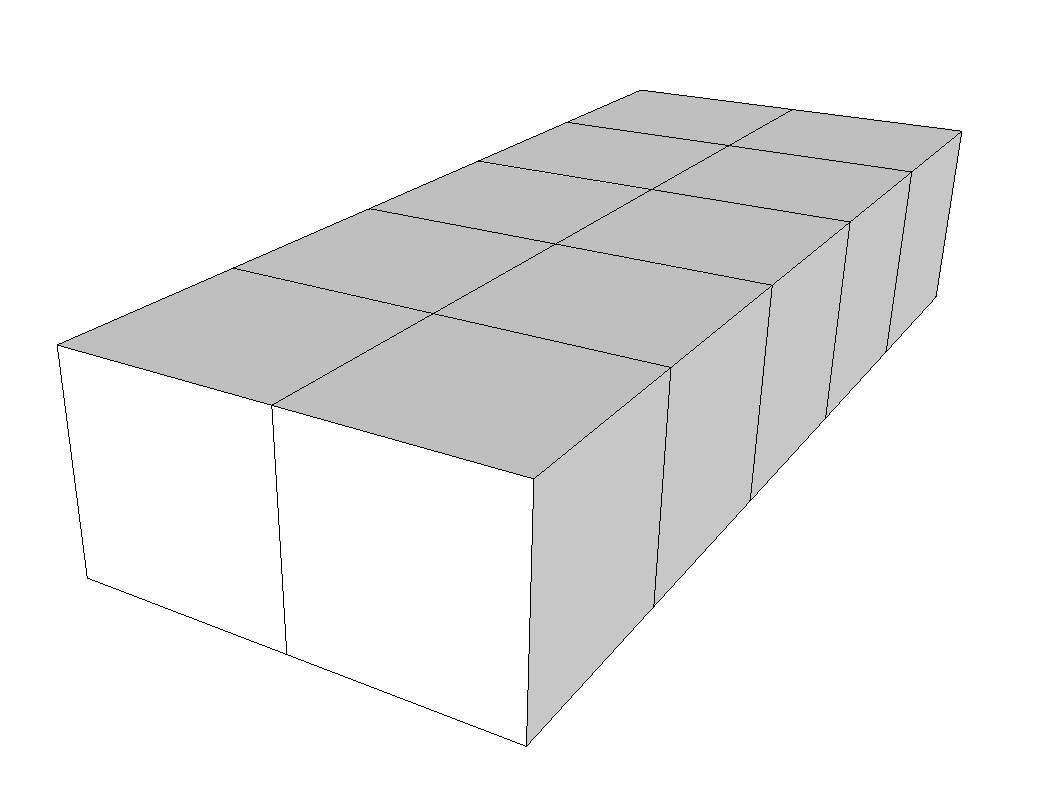
def \_\_init\_\_(self, dims):

nz, ny, nx = dims

self.dims = dims

self.numOfNodes = nz\*ny\*nx

self.nodes = self.initNodes()



(0, 0, 4)

(0, 0, 3)

(0, 0, 2)

(0, 0, 1)

(0, 0, 0)

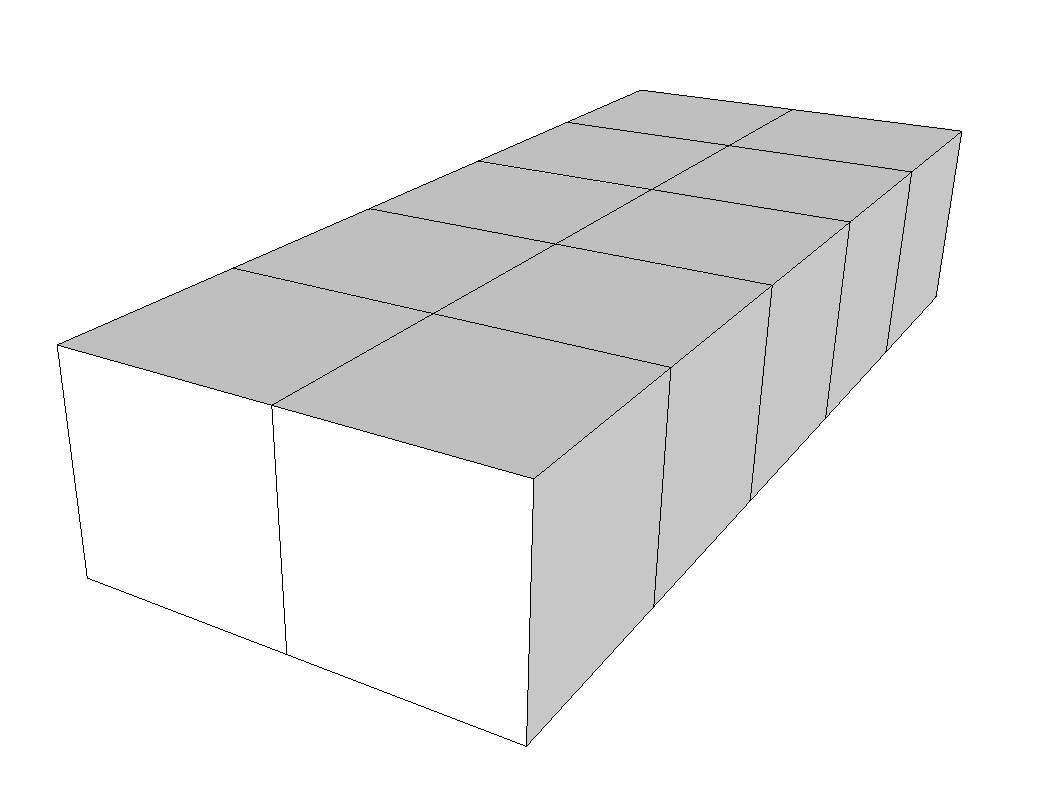
(0, 1, 4)

(0, 1, 3)

(0, 1, 2)

(0, 1, 1)

(0, 1, 0)



4

3

2

1

0

9

8

7

6

5

Figure 2 - Flattened index and 3D coordinate index in a 1×2×5 Grid

## Fluid and Rock Classes

Fluid in the diffusivity equation presents itself as variables density () and viscosity (). Whereas the porous medium (rock) presents as variables porosity () and absolute permeability (). One should notice that density, viscosity, and porosity are functions of time. Density and porosity can further be combined to form total compressibility (), which is equal to compressibility of fluid and compressibility of rock, .

|  |  |
| --- | --- |
|  | **(5)** |

As given by **Eq. 5**, for any given pressure value, one can determine the value of density and porosity using the following expression:

We need to include a reference density or reference porosity with their reference pressure value. For *slightly compressible* fluid model, this equation of state (EOS) is sufficient. However, for *highly compressible* fluid, such as gas, the model must take into account other factors such as -factor. Also, for this simulator, we will consider a constant value of viscosity () at any given pressure value. The code for \_\_init\_\_ function for Fluid and Rock classes are as follows:

class Rock(object):

def \_\_init\_\_(self, refPoro, refPres, compress, perm):

self.refPoro = refPoro

self.refPres = refPres

self.compress = compress

self.perm = perm

class Fluid(object):

def \_\_init\_\_(self, refRho, refPres, compress, mu):

self.refRho = refRho

self.refPres = refPres

self.compress = compress

self.mu = mu

## Reservoir class

All the information on Grid, Fluid, and Rock objects will then be passed into a Reservoir object. In addition, when instantiating a Reservoir object, one must also specify the actual dimension of the reservoir (in feet).

## BoundaryCondition class

There are two types of boundary condition used in this simulator, Neumann condition (pressure gradient specified) and Dirichlet condition (pressure specified). **Appendix B** explains how each condition is implemented on a boundary node. By default, this simulator will specify a no-flow Neumann condition () at every boundary node when a Grid object is instantiated.

## Applying the Finite-difference Diffusivity Equation

Let us first consider the finite-difference form of the diffusivity equation (derived in **Appendix A**)

# Presentation of Data and Results (EXAMPLES!!)

# Conclusions

# Acknowledgments

# Nomenclature

# References

Ertekin, T., Abou-Kassem, J. H., and King, G. R. 2001. ***Basic Applied Reservoir Simulation***. Richardson, Texas: Society of Petroleum Engineers, Inc.

Kreyszig, E., Kreyszig. H., and Norminton, E. J. 2011. ***Advanced Engineering Mathematics (10th Edition)***. Jefferson City, Missouri: John Wiley & Sons, Inc.

Lie, K.-A. 2014. ***An Introduction to Reservoir Simulation Using MATLAB***. Oslo, Norway: SINTEF ICT, Department of Applied Mathematics.

# 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,

|  |  |
| --- | --- |
|  | **(A1)** |

Evaluating the right-hand side, for simplicity, we consider mass rate () that only flows in direction, with term being ,

Using the derivative definition as follows,

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

Evaluating the left-hand side of the equation, noticing that , with term being ,

Coming back to the earlier mass conservation equation,

Since and are constants,

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

|  |  |
| --- | --- |
|  | **(A2)** |

The moment we evaluate the velocity term (), 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 direction. Recall the equation for Darcy’s law in some direction,

For flow only in direction, the continuity equation becomes,

We begin translating any term (spatial derivative) using finite-difference method,

We can group the term and define them as transmissibility, ,

We then proceed by translating the term (time derivative) using finite-difference. We also assign superscript or to any variable to specify the time level.

|  |  |
| --- | --- |
|  | **(A3)** |

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

|  |  |
| --- | --- |
|  | **(A4)** |

where:

# 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 , , and direction. However, this is not the case for a boundary gridblock. This situation is best described using a 3D grid sketch (**Fig. B1**). For a boundary gridblock, a special treatment based on either Dirichlet or Neumann boundary condition needs to be made.

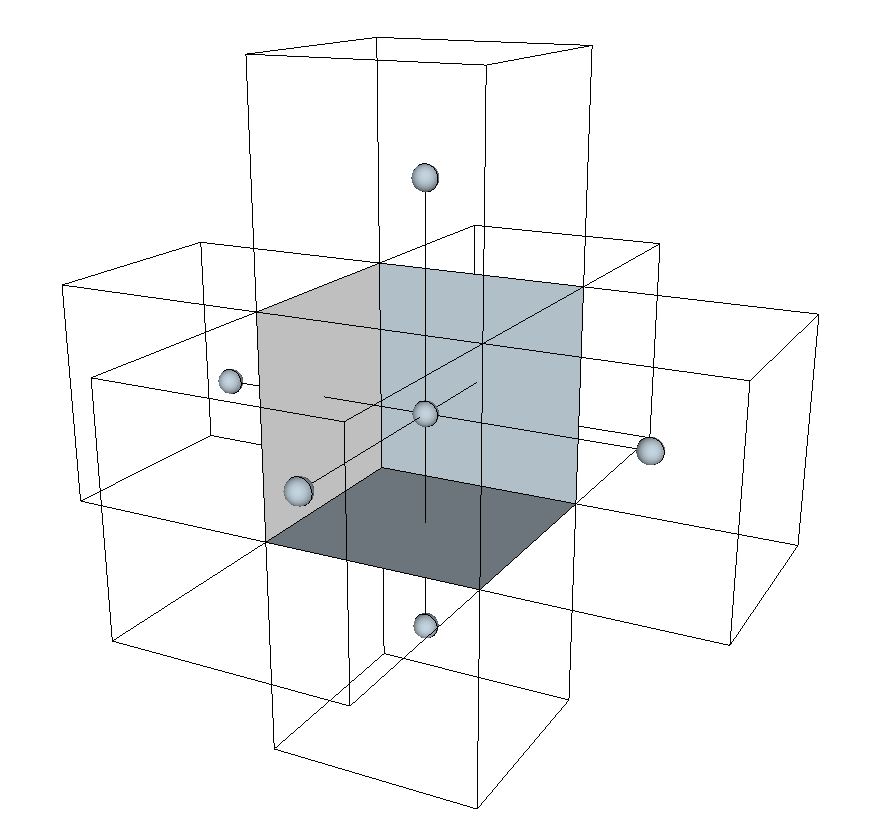
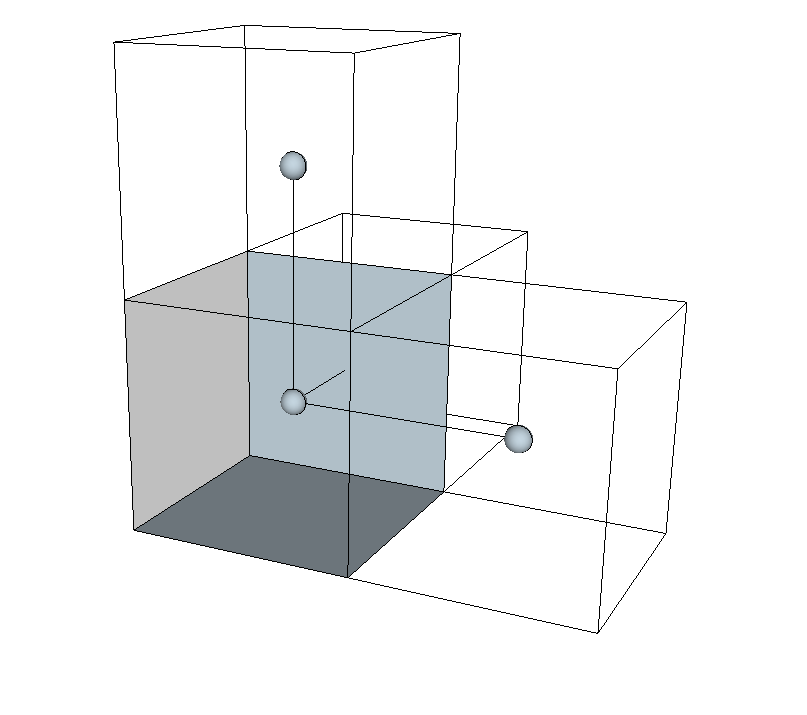


Figure B1 - Sketch of a boundary node (left) and a regular node (right) with their neighboring gridblocks

We restrict further discussion on the flow equation only looking at flow in direction for simplicity. For instance, consider a boundary gridblock at that does not have both gridblocks at and to interact with. This means with respect to , either or 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 , for Dirichlet condition, one can directly specify the boundary pressure,

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

1. **Neumann condition (pressure gradient specified)**

For this condition, we are given the gradient value, , which is equal to . We can then translate this gradient into the following,

Similarly, if the boundary pressure is , the gradient expression can be approximated as follows,

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

# Appendix C - Forming a Linear Equation on a Grid Node

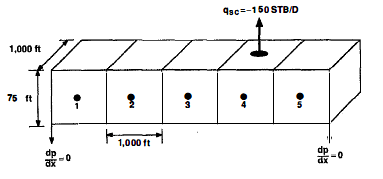
Again we consider **Eq. A4**, with a bit rearrangement,

Each of these differential terms (with respect to , , , and ) is translated accordingly to form the diffusivity equation for one particular point. This will form a linear equation with some unknown terms and known variables. Notice that we will get the term only when performing differential with respect to . Also, we will get a known term when performing differential with respect to . Therefore, we rearrange the equation further as follows,

where:

We can form the following matrices,

# Appendix D - Analytical Solution to 1D Single-phase Fluid Flow



For the 1D, block-centered grid shown above, determine the pressure distribution during the first year of production. The initial reservoir pressure is . The rock and fluid properties for this problem are , , , , , , , , and .

Consider the following equation (as derived in **App. A**) with its initial and boundary condition

|  |  |
| --- | --- |
| Partial differential equation (PDE) | |
|  | |
|  | |
| Initial condition (IC) | Boundary condition (BC) |
|  |  |
|  |  |
| Other specification |  |
|  |  |

First, we need to assume that the only variable that changes with respect to and is . All else are constants. We can group variable and define it as . Similarly, we define as . The PDE then becomes

Recognize that the equation is a non-homogeneous PDE of the form , with being constant for every and . We can apply **Laplace transform** in this case. Recall the following definition of Laplace transform for some function of and

*Remark*. We are performing Laplace transform **with respect to** .

Applying that to the PDE

For clarity, let denote

Similarly, perform Laplace transform to BC and IC. We are now given the following specification

|  |  |
| --- | --- |
| Partial differential equation (PDE) | |
|  | |
|  |  |
| Initial condition (IC) | Boundary condition (BC) |
|  |  |

Now we have an ordinary differential equation (ODE) with that varies only with respect to . It is still a non-homogeneous ODE however. We need to break down its form into homogeneous and particular form as follows

It follows that

Suppose has a solution of the form

The characteristic equation is . The roots are and . Therefore

As for , we use **method of undetermined coefficients**. We take a solution of the polynomial form, .

It follows that

We obtain the general form of , which is

Now we need to look into . The behavior of is still unknown. Since it will affect the variable , i.e. if , we will get an imaginary number.

1. **Assuming**

In order to obtain , we need to perform inverse transform

The above general expression satisfies the initial condition. But we still need to determine coefficient by cross-checking it with boundary condition.

We get a trivial solution.

1. **Assuming .**

By **Euler’s formula**, we can evaluate any term as described by the following formula

Since is some negative number, we can rewrite it as . Our earlier general expression of can then be rewritten into the following,

**to be continued..**