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Physics-Preserving Averaging Scheme based on Grunwald-Letnikov Formula for Gas Flow in Fractured Media

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Abstract

The heterogeneous natures of rock fabrics, due to the existence of multi-scale fractures and geological formations, led to the deviations from unity in the flux-equations fractional-exponent magnitudes. In this paper, the resulting non-Newtonian non-Darcy fractional-derivatives flux equations are solved using physics-preserving averaging schemes that incorporates both, original and shifted, Grunwald-Letnikov (GL) approximation formulas preserving the physics, by reducing the shifting effects, while maintaining the stability of the system, by keeping one shifted expansion. The proposed way of using the GL expansions also generate symmetrical coefficient matrices that significantly reduces the discretization complexities appearing with all shifted cases from literature, and help considerably in 2D and 3D systems. Systems equations derivations and discretization details are discussed. Then, the physics-preserving averaging scheme is explained and illustrated. Finally, results are presented and reviewed. Edge-based original GL expansions are unstable as also illustrated in literatures. Shifted GL expansions are stable but add a lot of additional weights to both discretization sides affecting the physical accuracy. In comparison, the physics-preserving averaging scheme balances the physical accuracy and stability requirements leading to a more physically conservative scheme that is more stable than the original GL approximation but might be slightly less stable than the shifted GL approximations. It is a locally conservative Single-Continuum averaging scheme that applies a finite-volume viewpoint.

Keywords: Grunwald-Letnikov, fractured porous media, fractional derivatives, physics preserving, average.

1 Introduction

Numerous geological formations and multi-scale fractures existing within rock fabrics affect the heterogeneity of the simulated systems. Also the fluids flows are affected by the porous medium and flow conditions such as system geometry, shear rates, shear stresses, durations of shearing, etc. (Chhabra and Richardson, 2011). Combining a collection of these properties, we end up with a Non-Newtonian Non-Darcy flow equations system (Amir and Sun, 2017). That system can easily be simplified into the typical Newtonian Darcy flow system through substituting each superscript n and α

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by 1 (Amir and Sun, 2017) such that each possible n range within the viscosity described using the “power-law” or “Ostwald de Waele” establishes some indications as follows: (1) $n < 1 \rightarrow$ shear-thinning fluid; (2) $n = 1 \rightarrow$ Newtonian fluid; and (3) $n > 1 \rightarrow$ shear- thickening fluid (Chhabra and Richardson, 2011) along with some other multi-scale heterogeneous-diffusion uncertainties (Albinali and Ozkan, 2016; Holy and Ozkan, 2016) that can be indicated by α ranges within the temporal and spatial flux equations as follows: (1) $\alpha < 1 \rightarrow$ Anomalous Sub-Diffusion; (2) $\alpha = 1 \rightarrow$ Normal Diffusion; and (3) $\alpha > 1 \rightarrow$ Anomalous Super-Diffusion (Obembe et al., [2017a, 2017b, and 2017c]; Raghavan and Chen, [2013 and 2017]).

Many numerical schemes were developed over the years to simulate fractures heterogeneity effects using the typical Newtonian Darcy-flow equations that included: (1) *Single-Continuum* models (Civan et al., 2011) that specify fractures and matrices positions explicitly within the grid cells by their permeabilities, porosities, and mesh sizes, and require large mesh sizes that might impose using some complicated linear solvers (e.g. the multigrid solvers) adding an additional degree of complexity to the system. (2) *Dual-Continuum* models (Kasiri and Bashiri, 2011; Clarkson et al., 2012; Hao and Carrigan, 2013; Moynfar et al., 2013; Li et al., 2015) introduced by Warren and Root (1963) define two detached overlapping continua, for fracture networks homogenizing actual fracture shapes and acting as the major flow routes and porous rock matrices serving as the main storage, and the interaction between each two overlapping grids from them is coordinated using a flux exchange parameter that needs to be specified according to some physical properties adding an additional degree of complexity to the system. (3) *Discrete Fracture Network* models (Cipolla et al., 2010; Zhang et al., 2009) generate huge numbers of elements that are dealt with using an enormous numerical system that imposes significant CPU times even for single well tests simulations making it neither practical nor beneficial to model dense fractured systems. Using any of the previous numerical schemes would require considering a way to deal with the additional complexities accompanying each and taking into account most of the possible complex fractures properties that include their directions, shapes, lengths, angles, ... etc.

One way around this would be by using the fractional derivatives to indicate fluxes anomalous diffusions within Non-Newtonian Non-Darcy flow equations within a *Single-Continuum* (Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Atangana and Vermeulen, 2014; Ghanam et al., 2014). Such methodology adds supplementary degrees of freedoms to the system signifying the natural system heterogeneities and uncertainties. Resulting temporal and/or spatial flux derivatives are substituted by expansion formulas that are used in generating the numerical system solution.

Several expansion formulas were introduced (Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014) that include: (1) Riemann-Liouville formula (Munkhammar, 2004) that was rigorously investigated by Liouville within a series of papers between 1832-1837 and as a result, the first fractional integration operator was defined. Later investigation by Riemann led to the generation of the integral-based Riemann-Liouville fractional integral operator as a generalization of Cauchy's formula. However, it was particularly used for analytical solutions since it describes a continuous domain by integral-based forms. (2) Grunwald-Letnikov (GL) formula (Cafagna, 2007) was a discretization proposed by Anton Karl Grunwald (1867) as a finite difference method generalization for fractional derivatives. Latter Letnikov (1868) suggested a similar approach with different discretization definitions that were proven to be equivalent to Grunwald (1867) formula (Podlubny et al., 1997). However, both discretization's, even if applied correctly, were not mathematically rigorous (i.e unstable) and were latter known as Grunwald-Letnikov expansions. To overcome the instability issue, the resulting right-hand side and left-hand side space-fractional GL expansions weights were shifted by a certain number of grid cells (Samko, 1993; Su et al., 2009). Such shifts for both sides improved the stability significantly but affected the accuracy of the physical effects that required the grid-cells closer to the grid-cell considered to have higher weights than further ones. The shifts for both sides also generated complex non-symmetric numerical systems for 1D let alone 2D and 3D systems (Su et al., 2009; Sweilam et al., 2011).

In this paper, a physics-preserving averaging discretization scheme is proposed for the Non-Newtonian Non-Darcy flow equations at which one side is discretized using the original GL expansions and the other side is discretized using the shifted GL expansions. This way the original side preserves more physical properties and the shifted side preserves the stability forming a certain balancing act. Comparing to literature approaches (Samko, 1993; Su et al., 2009; Sweilam et al., 2011), the physics-preserving averaging scheme balances the physical accuracy and stability requirements leading to a

more physically conservative scheme that is more stable than the original GL approximation but might be slightly less stable than the shifted GL approximations. It is however a locally conservative Single-Continuum averaging scheme that applies a finite-volume viewpoint.

The proposed averaging scheme also generates symmetrical coefficient matrices for the system making it much simpler to apply in 1D, 2D, and 3D, as well as in multi-point flux approximation cases and also significantly reduces the discretization complexities appearing with literature two-side shift cases. Other instability causes from literature (Samko, 1993; Meerschaert and Tadjeran, [2004 and 2006]; Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Su et al., 2009; Sweilam et al., 2011; Ahmed and Nieto, 2012; Atangana and Vermeulen, 2014; Ghanam et al., 2014; Vance, 2014) are discussed in Section 2 and corrected in the proposed physics-preserving averaging scheme. Systems equations derivations and discretization details are discussed. Then, the physics-preserving averaging scheme is explained and illustrated. Finally, examples are tested for two gas-flow equations and results are presented and reviewed.

2 Fractional order physics-preserving averaging scheme

Fractional derivatives are actually generalizations of classical derivatives. They tend to generate full coefficient matrices in 1D. In larger dimensions, they generate denser coefficient matrices such that each cell is affected by the whole row and column intersecting with that cell at each dimension according to the scheme considered. In other words, the spatial fractional-flux expansion at each position, for example, gives an indication for the fluid flow on the global spacial distribution of each property in the porous media matrix, not only in that position. Meaning that the solution at each grid-cell of the domain is solved for as a system along with all the other grid-cells effects in the domain as coefficients. So, each cell depends on the global values at all cells.

Literature fractional expansion formulas (Samko, 1993; Meerschaert and Tadjeran, [2004 and 2006]; Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Su et al., 2009; Sweilam et al., 2011; Ahmed and Nieto, 2012; Atangana and Vermeulen, 2014; Ghanam et al., 2014; Vance, 2014) were edge-based as illustrated is Table A.1 of the Appendix. They were used in literature assuming that pressures and velocities exist at the same point causing instabilities that needed to be taken care of. In this paper, velocities are assumed to be on edges and pressured at cell-centers. In such cases, literature edge based GL expansions from Table A.1 are not applicable. This led to the derivation of the cell-centered GL expansions in Table A.2 as illustrated by examples in section A of the Appendix. The most important equations from them are listed in Table 1.

<i>Original Grunwald-Letnikov formula</i>	
Left side	$\left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) \Big _{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma p_{i+0.5-k} \quad (1)$
Right side	$\left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \Big _{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k} \quad (2)$
<i>Shifted Left Grunwald-Letnikov at x_{i-1}</i>	
Right side:	$\left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \Big _{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k} \quad (3)$
<i>Shifted Right Grunwald-Letnikov at x_{i+1}</i>	
Left side:	$\left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) \Big _{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k} \quad (4)$

Table 1: cell-centered GL fractional order derivatives expansions. The g_k^γ used is illustrated in section 2.3.

The previously developed fractional schemes dealt with permeability k in the mass conservation law as a constant and simplified the equation respectively (Wang et al., 2010; Wang and Du, 2014). This affected the physical conservation laws significantly causing porous media permeabilities to change greatly between locations according to the rock fabric at each of these locations causing discontinuous jumps in values. Then, discretization was done using the shifted GL approximation for all of the

fractional derivatives to reach mathematical stability (Wang et al., 2010; Wang and Du, 2014). Such approaches give physically non-conservative results due to two reasons: (1) GL approximation formula expands the solution of the derivative at any mesh point x_i depending on all of its surrounding points from $x_0, x_1 \dots x_M$ for a 1D mesh that spans from 0, 1, ... M giving higher weights to the grid cells close to x_i . In general, weights keep decreasing as we move further from x_i . Shifting all approximations will decrease the weight of the grid cell of interest (x_i in this case) and increase the weights of one of its surroundings causing a slight deviation than the desired numerical effects. (2) Permeability varies with locations and even at the same location according to the direction in porous media causing discontinuous jumps. To overcome these physically non-conservative effects, a Physics-Preserving Averaging (PPA) scheme is proposed and derived in this paper and its results are illustrated and discussed.

2.1 Systems Equations Derivation

According to the laws of physics for mass conservation, mass cannot change quantity if it is not added or removed. In other words, mass in an isolated system is neither created nor destroyed by physical transformations or chemical reactions (Boundless, 2016). On the other hand, fractional derivatives reflect anomalous dissipations for non-conservative systems accounting for the possible non-local effects on dissipations (Chen and Holm, 2003; Loverro, 2004).

This gives an indication that in order to preserve the physics in flow simulations, mass conservation laws need to be used without fractional derivatives to conserve the mass properly. However, friction (also referred to as mass flow or flow velocity) is affected significantly by the non-local porous media heterogeneities. Since fluid velocities are effected by the non-local strong heterogeneities resulting from the fractures and pores existence, their dissipations can be reflected using fractional derivatives within Darcy's law. Many resources from literature used fractional order derivatives to recover fractured porous media heterogeneities for Darcy's law either analytically or using pure *shifted Grunwald-Letnikov* formulas (Clout and Botha, 2006; Ochoa-Tapia et al., 2007; Atangana and Vermeulen, 2014; Ghanam et al., 2014).

Two cases are tested in this paper, a simplified case that assumes constant permeability for a physically non-conservative case that was used in a lot in literature illustrations. The second equation is a physically conservative case applied in the mass conservation equation for a single-phase slightly compressible fluid case. The analytical derivation of the source term for both cases is illustrated in details in Section B of the Appendix.

Starting from the mass conservation equation:

$$\frac{\partial(\rho\varphi)}{\partial t} + \nabla \cdot (\rho u) = Q \quad (5)$$

$$\left(\rho \frac{\partial \varphi}{\partial p} + \varphi \frac{\partial \rho}{\partial p} \right) \frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = Q \quad (6)$$

Such that: $\rho \rightarrow$ density; $\varphi \rightarrow$ porosity; $u \rightarrow$ velocity; $Q \rightarrow$ source term; $t \rightarrow$ time; $p \rightarrow$ total head that is the total amount of pressure when fluid is flowing in a system. It is computed by adding vertical rise (elevation head) and friction loss (pressure head). Focusing on horizontal planes, pressure head will be the most effective. In 1D, Equation (6) becomes:

$$\left(\rho \frac{\partial \varphi}{\partial p} + \varphi \frac{\partial \rho}{\partial p} \right) \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (7)$$

Such that $u_x \rightarrow$ velocity discussed latter. Deriving both, the simple case and the compressible fluid case, from Equation (7) we end up with:

Simple case

Assuming constant density: $\rho = 1 \rightarrow \partial \rho / \partial p = 0$ and let $\partial \varphi / \partial p = 1$. Equation (7) becomes:

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (u_x) = Q \quad (8)$$

This can also be written as:

$$C \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (9)$$

Such that $C = \left(\rho \frac{\partial \varphi}{\partial p} + \varphi \frac{\partial \rho}{\partial p} \right) = 1$ and $\rho = 1$. The source term Q is derived analytically in section B of

the Appendix giving Equation (B.14) that is:

$$Q = \pm 4 \exp(-t) \left\{ x^2(2-x)^2 + K \left[4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} [(x)^{1-\gamma} + (2-x)^{1-\gamma}] - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} [(x)^{2-\gamma} + (2-x)^{2-\gamma}] + \frac{\Gamma(5)}{\Gamma(4-\gamma)} [(x)^{3-\gamma} + (2-x)^{3-\gamma}] \right] \right\} \quad (10)$$

Slightly compressible fluid case

Assuming a slightly compressible fluid using Taylor series: $\rho = \rho^0 \exp(c_f[p - p^0])$ and non-compressible rock properties: $\partial\phi/\partial p = 0$ and applying the thermodynamic properties: (11)

$$c_f = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial p} \right)_T \rightarrow \frac{\partial \rho}{\partial p} = c_f \rho \quad (12)$$

Such that: $c_f \rightarrow$ fluid compressibility; $\rho^0 \rightarrow$ density at p^0 pressure; $V \rightarrow$ volume. Substituting $\partial\phi/\partial p = 0$ and Equation (12) in Equation (7):

$$(\phi c_f \rho) \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (13)$$

This can also be written as:

$$C \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (14)$$

Such that $C = \phi c_f \rho$. The source term Q is derived analytically in section B of the Appendix giving Equation (B.45) that is:

$$Q = \pm 4 \exp(-t) \left\{ \phi c_f \rho x^2(2-x)^2 + 4K_{const} \left[\rho \left\{ \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-8 + 12x - 6x^2 + 2x^3] \right\} + \rho^0 c_f \exp(4c_f[\exp(-t) - 1][4x^2 - 4x^3 + x^4])[\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \right] \right\} \quad (15)$$

Generalization

Looking at Equation 9 and Equation 14, it can be concluded that for both cases the discretization scheme can be developed for the generalized form:

$$C \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (16)$$

Such that:

$$\left[\begin{array}{ll} \text{simple case} \rightarrow & C = 1; \rho = 1 \\ \text{compressible case} \rightarrow & C = \phi c_f \rho; \rho = \rho^0 \exp(c_f[p - p^0]) \end{array} \right] \quad (17)$$

2.2 Scheme discretization details

Discretizing Equation 16 in Cell-Centered Finite Difference (CCFD) scheme from a finite volume viewpoint as illustrated in Figure 1 such that:

- (1) Velocities reside on the grid cell edges: $x_0, x_1 \dots x_i \dots x_{M-1}, x_M$ with $i = 0, 1, \dots M$.
- (2) Pressures reside on cell centers: $x_{0.5}, x_{1.5}, \dots x_{i-0.5}, x_{i+0.5}, x_{i+1.5} \dots x_{M-0.5}$.

Figure 1: PPA-CCFD finite volume viewpoint with velocities at edges and pressures at centers.

$$C \frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) = Q \quad (18)$$

The discretization at each cell with center position $(i + 0.5)$ is computed with:

$$C_{i+0.5} \left[\frac{(p_{i+0.5}^{n+1} - p_{i+0.5}^n)}{\Delta t} \right] + \frac{1}{\Delta x_{i+0.5}} [\rho_{i+1} u_{i+1} - \rho_i u_i] = Q_{i+0.5} \quad (19)$$

Such that n indicates the time step. This can be simplified as:

$$p_{i+0.5}^{n+1} + \frac{\Delta t}{C_{i+0.5} \Delta x_{i+0.5}} [\rho_{i+1} u_{i+1} - \rho_i u_i] = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (20)$$

Each velocity u is defined using a fractional Darcy law (Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Atangana and Vermeulen, 2014; Ghanam et al., 2014; Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014). Ignoring gravity, the fractional Darcy law becomes: $u = -K (\partial^\gamma p / \partial x^\gamma)$. From this equation, it can be noticed that Darcy's law depends essentially on the pressures. Pressures in the proposed physics-preserving averaging scheme introduced in this paper are cell-centered values. So, the velocities need to be averaged for the cell-centered versions of the fractional derivatives to be applicable directly. In other words, since velocities reside on edges, their surrounding cell-centered velocities are used in the computations in an approach similar to the following 1D CCFD examples:

$$\rho_i u_i = (\rho_{i-0.5} u_{i-0.5} + \rho_{i+0.5} u_{i+0.5}) / 2 \quad (21)$$

$$\rho_{i+1} u_{i+1} = (\rho_{i+0.5} u_{i+0.5} + \rho_{i+1.5} u_{i+1.5}) / 2 \quad (22)$$

Substituting Equations (21) and (22) into Equation (20):

$$p_{i+0.5}^{n+1} + \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}} [(\rho_{i+0.5} u_{i+0.5} + \rho_{i+1.5} u_{i+1.5}) - (\rho_{i-0.5} u_{i-0.5} + \rho_{i+0.5} u_{i+0.5})] = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (23)$$

Substituting each u by its fractional Darcy's law, Equation (23) becomes:

$$\begin{aligned} & p_{i+0.5}^{n+1} - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}} \left\{ \left[\rho_{i+0.5} \left(K_{i+0.5} \frac{\partial^\gamma p}{\partial x^\gamma} \right)_{i+0.5} \right] + \rho_{i+1.5} \left(K_{i+1.5} \frac{\partial^\gamma p}{\partial x^\gamma} \right)_{i+1.5} \right] - \left[\rho_{i-0.5} \left(K_{i-0.5} \frac{\partial^\gamma p}{\partial x^\gamma} \right)_{i-0.5} \right] + \right. \\ & \left. \rho_{i+0.5} \left(K_{i+0.5} \frac{\partial^\gamma p}{\partial x^\gamma} \right)_{i+0.5} \right] \} = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \end{aligned} \quad (24)$$

Each fractional derivative is split using two-sides fractional derivatives formulas as illustrated in Equation (25) that are discretized for each grid-cell. One-way to discretize is to use the GL approximations discussed in Section A of the appendix. In Section A, the well-known fractional derivatives formulas, their uses, their discretization approaches, and literature edge-based *Original and Shifted GL* formulas are listed in Table A.1; this paper proposed slightly different cell-centered-based *Original and Shifted GL* formulas are documented in Table A.2; their expansions, fractional derivatives expansions in time are listed in Table A.3, along with lists of most of the heavily used equations for such applications in Section A of the appendix.

$$\begin{aligned} & p_{i+0.5}^{n+1} - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}} \left\{ \left[\rho_{i+0.5} \left(K_{i+0.5}^+ \frac{\partial^\gamma p}{\partial_{+x}^\gamma} \right)_{i+0.5} + K_{i+0.5}^- \frac{\partial^\gamma p}{\partial_{-x}^\gamma} \right]_{i+0.5} \right] + \rho_{i+1.5} \left(K_{i+1.5}^+ \frac{\partial^\gamma p}{\partial_{+x}^\gamma} \right)_{i+1.5} + \right. \\ & \left. K_{i+1.5}^- \frac{\partial^\gamma p}{\partial_{-x}^\gamma} \right]_{i+1.5} \right] - \left[\rho_{i-0.5} \left(K_{i-0.5}^+ \frac{\partial^\gamma p}{\partial_{+x}^\gamma} \right)_{i-0.5} + K_{i-0.5}^- \frac{\partial^\gamma p}{\partial_{-x}^\gamma} \right]_{i-0.5} \right] + \rho_{i+0.5} \left(K_{i+0.5}^+ \frac{\partial^\gamma p}{\partial_{+x}^\gamma} \right)_{i+0.5} + \right. \\ & \left. K_{i+0.5}^- \frac{\partial^\gamma p}{\partial_{-x}^\gamma} \right]_{i+0.5} \right] \} = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \end{aligned} \quad (25)$$

Using the *Original GL* formula for all derivatives would cause a lot of instability issues as illustrated in literature (Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014; Liao, 2014; Jacobs, 2015). In order to overcome this difficulty and preserve the physics while maintaining the stability of the system, we expand some velocity parts from Equation (25) using the *original GL formula* and expand other velocity parts using the *shifted GL formulas*. This way, we keep half the weight of the grid cell of interest untouched and slightly increase the other half preserving more physical properties in the process. The type of the GL derivative expansion used for each pressure derivative in Equation (25) defines the mixed physics-preserving averaging (PPA) scheme introduced in this paper.

2.3 Applying the Physics-Preserving Averaging (PPA) scheme

When solving any equations system, a coefficients matrix needs to be generated for each grid-cell in the domain considering the effects of the surrounding grid-cells according to the equations and the

discretization approach chosen. In Equation (25), it is obvious that each $(i + 0.5)^{th}$ grid-cell center is affected by the fractional derivatives discretization of three cells as illustrated in Figure 2 such that global domain especially in 1D affects each fractional derivative discretization.

Figure 2: illustration of the 3 local cells that need to be considered with respect to the global domain when solving Equation (25) for each grid cell at position $(i + 0.5)$.

As discussed before, some derivatives from Equation (25) need to be expanded using the original GL formula and other derivatives using the shifted GL formula to preserve the physics to a certain point while maintaining the stability of the system also to a certain point. In this paper, the GL expansions formulas are selected in a way that generates symmetrical coefficient matrices as illustrated in Figures 4-5 and Table 2.

Figure 2 shows that for each grid-cell center $(i + 0.5)$ considered for discretization, there are two edges surrounding it in 1D CCFD that are (i) and $(i + 1)$. Velocities reside on these edges, but pressures solved for directly within the system reside on the grid-cell centers. So, for each velocity edge, pressure derivatives averages from both surrounding (left and right) grid-cell centers are used as illustrated in Figure 3. For example, velocity at edge $(i + 1)$ depends on the pressure derivatives at grid-cell centers $(i + 0.5)$ and $(i + 1.5)$ as demonstrated in Figure 2. Similarly, velocity at edge (i) depends on the pressure derivatives at grid-cell centers $(i - 0.5)$ and $(i + 0.5)$. Due to the domain heterogeneities discussed before, the pressure derivatives within the velocities are fractional derivatives. That is, each one of them needs to be expanded and solved for globally.

Table 1 lists the most important left side and right side cell-centered GL expansions derived in this paper. Figure 3 summarizes Figure 2 discussion by abbreviating that each edge has two grid-cell centers surrounding it: right grid-cell center and left grid-cell center. Each grid-cell center has a fractional derivative that is discretized in both sides, left side and right side as illustrated in Figures 3.

For example, in Figure 4 the edge $(i + 1)$ has two cell centers surrounding it that are: *Left-cell center* and *Right-cell center*. Each has *left side* and *right side* expansions as illustrated in Figure 3. The *Left-cell left-side* uses right shift expansion and *right-side* uses GL original expansion. On the other hand, the *right-cell left-side* uses GL original expansion and *right-side* uses left shift expansion. Derivative choices are applied on Table 1 and the resulting expansions used in the PPA scheme are illustrated in Table 2. Similar approach is used for the i^{th} edge and any other edge.

Figure 3: Each edge fractional derivatives expansion parts illustration.

Figure 4: Edge $(i + 1)$ surrounding cells expansions illustration.

Figure 5: Edge (i) surrounding cells expansions illustration.

Derivative	Selected equation type	Derivative expansion
$[A] = \frac{\partial^\gamma p}{\partial_+ x^\gamma} \Big _{i+0.5}$	Shifted right	$\frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}$
$[B] = \frac{\partial^\gamma p}{\partial_- x^\gamma} \Big _{i+0.5}$	Original	$\frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}$
$[C] = \frac{\partial^\gamma p}{\partial_+ x^\gamma} \Big _{i+1.5}$	Original + substituting each (i) by $(i + 1)$	$\frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}$
$[D] = \frac{\partial^\gamma p}{\partial_- x^\gamma} \Big _{i+1.5}$	Shifted left + substituting each (i) by $(i + 1)$	$\frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}$
$[E] = \frac{\partial^\gamma p}{\partial_+ x^\gamma} \Big _{i-0.5}$	Shifted right + substituting each (i) by $(i - 1)$	$\frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma p_{i+0.5-k}$
$[F] = \frac{\partial^\gamma p}{\partial_- x^\gamma} \Big _{i-0.5}$	Original + substituting each (i) by $(i - 1)$	$\frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}$
$[G] = \frac{\partial^\gamma p}{\partial_+ x^\gamma} \Big _{i+0.5}$	Original	$\frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma p_{i+0.5-k}$
$[H] = \frac{\partial^\gamma p}{\partial_- x^\gamma} \Big _{i+0.5}$	Shifted left	$\frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}$

Table 2: derivative expansions selected for Equation (25) applying the PPA scheme.

Substituting each expansion from Table 2 into Equation (25):

$$p_{i+0.5}^{n+1} - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}} \left\{ \left[\rho_{i+0.5} \left(K_{i+0.5}^+ \left[\frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1} \right] + K_{i+0.5}^- \left[\frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1} \right] \right) + \rho_{i+1.5} \left(K_{i+1.5}^+ \left[\frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1} \right] + K_{i+1.5}^- \left[\frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1} \right] \right) \right\} -$$

$$\left[\rho_{i-0.5} \left(K_{i-0.5}^+ \left[\frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1} \right] + K_{i-0.5}^- \left[\frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1} \right] \right) + \rho_{i+0.5} \left(K_{i+0.5}^+ \left[\frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1} \right] + K_{i+0.5}^- \left[\frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1} \right] \right) \right] = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (26)$$

This can be simplified and rearranged as:

$$p_{i+0.5}^{n+1} - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} \left\{ \left[(\rho_{i+0.5} K_{i+0.5}^+ + \rho_{i+1.5} K_{i+1.5}^+) (\sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1}) - (\rho_{i-0.5} K_{i-0.5}^+ + \rho_{i+0.5} K_{i+0.5}^+) (\sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1}) \right] + \left[(\rho_{i+0.5} K_{i+0.5}^- + \rho_{i+1.5} K_{i+1.5}^-) (\sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1}) - (\rho_{i-0.5} K_{i-0.5}^- + \rho_{i+0.5} K_{i+0.5}^-) (\sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1}) \right] \right\} = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (27)$$

Equation (27) can be expanded as:

$$p_{i+0.5}^{n+1} - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} \left(\rho_{i+0.5} K_{i+0.5}^+ + \rho_{i+1.5} K_{i+1.5}^+ \right) (\sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1}) + \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i-0.5} K_{i-0.5}^+ + \rho_{i+0.5} K_{i+0.5}^+) (\sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1}) - \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i+0.5} K_{i+0.5}^- + \rho_{i+1.5} K_{i+1.5}^-) (\sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1}) + \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i-0.5} K_{i-0.5}^- + \rho_{i+0.5} K_{i+0.5}^-) (\sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1}) = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (28)$$

Let:

$$S_R^+ = \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i+0.5} K_{i+0.5}^+ + \rho_{i+1.5} K_{i+1.5}^+) \quad (29)$$

$$S_L^+ = \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i-0.5} K_{i-0.5}^+ + \rho_{i+0.5} K_{i+0.5}^+) \quad (30)$$

$$S_R^- = \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i+0.5} K_{i+0.5}^- + \rho_{i+1.5} K_{i+1.5}^-) \quad (31)$$

$$S_L^- = \frac{\Delta t}{2 C_{i+0.5} \Delta x_{i+0.5}(h^\gamma)} (\rho_{i-0.5} K_{i-0.5}^- + \rho_{i+0.5} K_{i+0.5}^-) \quad (32)$$

Using Equations (29-32), Equation (28) can be rewritten as:

$$p_{i+0.5}^{n+1} - S_R^+ (\sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1}) + S_L^+ (\sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1}) - S_R^- (\sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1}) + S_L^- (\sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1}) = \frac{\Delta t}{C_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n \quad (33)$$

Equation (33) is used to generate the system $Ap = b$ solved as $p = A/b$. Vector b is the set of all constants collected. Vector p indicates the cell centered pressures we solve for by implicit time step $(n+1)$ or pressures taken from the explicit previous time step (n) . Matrix A is formed as:

$$A_{i,j} = \begin{cases} 1 - S_R^+ g_1^\gamma + S_L^+ g_0^\gamma - S_R^- g_0^\gamma + S_L^- g_1^\gamma & \text{if } j = i \\ -S_R^+ g_0^\gamma - S_R^- g_1^\gamma + S_L^+ g_2^\gamma & \text{if } j = i+1 \\ -S_R^+ g_2^\gamma + S_L^+ g_1^\gamma + S_L^- g_0^\gamma & \text{if } j = i-1 \\ -S_R^- g_{j-1}^\gamma + S_L^- g_j^\gamma & \text{if } j > i+1 \\ -S_R^+ g_j^\gamma + S_L^+ g_{j-1}^\gamma & \text{if } j < i-1 \end{cases} \quad (34)$$

The coefficients that take the shape g_k^γ indicate the fractional binomial coefficient weights. They are computed at each grid cell as: $g_k^\gamma = (-1)^k \binom{\gamma}{k}$. The value $\binom{\gamma}{k}$ indicate the fractional binomial coefficient. Several ways have been used to define these weights in literature (Meerschaert and Tadjeran, [2004, 2006]; Wang et al., 2010; Wang and Du, 2014). We use the recursive way (Wang et al., 2010) to define them in this paper as:

$$g_0^\gamma = 1, g_1^\gamma = -\gamma, \quad g_k^\gamma = \left(1 - \frac{\gamma+1}{k} \right) g_{k-1}^\gamma \quad \text{for } k \geq 2 \quad (35)$$

An expansion of Equation (33) GL formulas is illustrated by example in Appendix C with $M = 5$ in a 1D domain along with the created A matrix for such an assumption.

The generated symmetrical coefficient matrix illustrated in Equation (34) for 1D Cell-Centered Finite Difference (CCFD) indicates the simplicity of expanding the proposed PPA scheme to 2D or 3D within the (X, Y, Z) axis's. Similarly, PPA scheme simplifies implementing the generalization of the

CCFD discretization as a Multi-Point Flux Approximation (MPFA). MPFA (Chen et al., 2007; Aavatsmark, 2002) requires extending the scheme to 3D in (X, Y, Z) in addition to all the other sub dimensions XY, XZ, YX, YZ, ZX , and ZY . At each possible extension, concepts are similar but numerical details change slightly accordingly.

3 Results illustration and discussion

To investigate the characteristic and benefits of the Physics Preserving Averaging (PPA) scheme, Equation (33) is used with the proper substitutions from Section 2 according to the simulation cases considered. Since this paper basically focuses on introducing the PPA scheme concept, small domain and interval ranges are zoomed on. So, assuming 1D reservoirs that cover domain ranges between $[a, b] = [0, 2]$ over the time interval $[0, T] = [0, 1]$. Consider the exact solution to be $p_{true}(x, t) = 4 \exp(-t) x^2(2 - x)^2$. This makes the initial pressure equation: $p_{true}(x, 0) = 4 x^2(2 - x)^2$. So, at the domain interval midpoint $x = 1$, the equation gives the pressure $p_{init}(1, 0) = 4$. Similarly, at the final time-step $t = 1$ the midpoint value is computed as $p_{true}(1, 1) = 4 \exp(-1) = 1.4715$ such that $\exp(x)$ computes the exponent e^x . This gives an indication that the numerical results should convert to 1.4715.

In this paper, we consider two numerical cases as illustrated in Section 2:

- (3.1) Simple case with constant permeability, $C = 1, \rho = 1$, initial pressure follows $p(x, 0) = 4 x^2(2 - x)^2$, and the source term Q follows Equation (10).
- (3.2) Slightly compressible flow case with $C = \varphi c_f \rho, \rho = \rho^0 \exp(c_f[p - p^0])$, the source term Q follows Equation (15), the permeability is a function of the x position within the domain, and the initial pressure follows $p(x, 0) = 4 x^2(2 - x)^2$ too.

3.1 Simple case

As demonstrated before, in this simple case we have a constant permeability, $C = 1, \rho = 1$, the initial pressure follows $p(x, 0) = 4 x^2(2 - x)^2$, and the source term Q follows Equation (10). The reservoir is discretized along its 1D length with a control volume of size $\Delta x = 1/145$. The time step is $\Delta t = 1/125$ and the total simulation length is 1. The remaining properties include the fractional derivative order $\gamma = 0.7$, the constant permeability $K = 5E - 10$ (constant), and the left and right boundaries permeabilities $K_{BL} = 0$ and $K_{BR} = 0$.

Figure 6 shows the pressure profiles along the $x -$ axis for the numerical result in the simple case and compares it to the analytical solution for exactly similar conditions.

Figure 6: comparison between numerical model simulation results and analytical solution results.

The excellent overlap observed between the solutions of the numerical pressure systems and the predicted analytical results in Figure 5 establish the accuracy of the proposed PPA scheme discretization applied in this paper. It can also be noted that at the midpoint of the domain interval $x = 1$, the pressure result converges toward the true solution at that point given by $p_{true}(1, 1) = 4 \exp(-1) = 1.4715$ as illustrated before that further establishes the proposed scheme accuracy.

However, the numerical pressure values needs to converge over time throughout the interval $[0, T] = [0, 1]$ starting from the initial pressures illustrated in Figure 7, then converging from the second time-step illustrated in black within Figure 8, until the final step illustrated in blue in Figure 8.

Figure 7: initial numerical pressure values.

Figure 8: numerical pressure convergence over time towards the final pressure starting from the second time-step.

A lot of simplifications are assumed for the simple case as clarified in Section 2 considering $C = 1$, $\rho = 1$, and K is constant, we end up with the equations:

$$S_R^+ = \frac{\Delta t}{\Delta x_{i+0.5}(h^\gamma)} K_{i+0.5}^+ \quad (36)$$

$$S_L^+ = \frac{\Delta t}{\Delta x_{i+0.5}(h^\gamma)} K_{i+0.5}^+ \quad (37)$$

$$S_R^- = \frac{\Delta t}{\Delta x_{i+0.5}(h^\gamma)} K_{i+0.5}^- \quad (38)$$

$$S_L^- = \frac{\Delta t}{\Delta x_{i+0.5}(h^\gamma)} K_{i+0.5}^- \quad (39)$$

Equations (36-39) demonstrate that the coefficients residing within the same side either (L or R) are subjected to exactly similar effects since they cover similar $\Delta x_{i+0.5}$ ranges and the permeability $K_{i+0.5}$ is constant. This gives the relations $S_R^+ = S_R^-$ and $S_L^+ = S_L^-$, that are clearly noticed in Figure 9.

It is customary to investigate the error convergence for several possible grid-cell sizes to check the accuracy of the proposed mathematical schemes. So, in this simple example too, the grid-cell sizes $\Delta x_{i+0.5} = [1/50, 1/60, 1/70, 1/80, 1/90, 1/100, 1/110, 1/120]$ are used such that the mesh grid-cell sizes vary within the specified range. Error converges with each cases as illustrated in Figure 10. It can be noticed from Figure 10 that the error norms decrease as the grid-cell sizes decrease and vise-versa. This gives an indication that small size meshes give better numerical results.

Figure 11 parts (A-D) zoom the investigation into four examples grid-cell mesh sizes ranging within the values: $\Delta x_{i+0.5} = [1/50, 1/75, 1/100, 1/145]$. Focusing on parts (A-D), it can be noticed that for the same time steps $\Delta t = 1/125$ at the final step with time $T = 1$, as the mesh size decreases the final step numerical result converges more toward the true solution.

Figure 9: Simple case coefficients with $S_R^+ = S_R^-$ and $S_L^+ = S_L^-$ due to the similar computation values resulting from the constant assumptions.

Figure 10: (norm_2 error) convergence with respect to the actual mesh sizes show that the errors decrease as the mesh size decreases.

Starting from mesh size $1/145$ and going to smaller mesh sizes, the convergence remains the same. So, using the best smallest possible mesh size is better from CPU and memory points of view, that is $1/145$ for this example.

Figure 11: Zooming into examples with $\Delta x_{i+0.5} = [1/50, 1/75, 1/100, 1/145]$, it can be noticed that for the same time steps $\Delta t = 1/125$ at the final step ($T = 1$), numerical results converge better as mesh size decrease.

To further analyze the convergence, relations between $\log_{10}(\text{mesh size})$ and $\log_{10}(\text{norm}_2 \text{ error})$ are sketched in Figure 12. The general shape of both scatter plots from Figure 10 and Figure 12 are similar, but values in Figure 12 of the best line fitting the data points has slopes that range approximately between $[1: 2]$ that is to be expected according to Saad (2003).

Figure 12: Error convergence using the vlaues of $\log_{10}(\text{mesh size})$ and $\log_{10}(\text{norm}_2 \text{ error})$ show scatter plots similar in behavior to Figure 10 but give slops that range between $[1: 2]$.

Figure 13: error norms decrease as the number of cell-centered pressure variables increase in consistent with the previous discussion.

In such systems, the number of variables, that are the cell-centered pressures here, are proportional to the mesh size. So, as the mesh sizes decrease, the number of cells increase. As a result, the number of cell-centered pressure variables increase and with that the error norm decrease in consistent with the previous discussion as illustrated in Figure 13. This relation can be refered to as: $\#vars \propto 1/(\Delta x_{i+0.5})^2$.

Finding the relation between $\log(\#vars)$ and $\log(\text{norm}_2 \text{ error})$ with mesh sizes ranging within the values $\Delta x_{i+0.5} = [1/50, 1/60, 1/70, 1/80, 1/90, 1/100, 1/110, 1/120]$ also gives slops within the range $[1: 2]$ that is to be expected too according to Saad (2003).

Figure 14: Error convergence using the vlaues of $\log_{10}(\# vars)$ and $\log_{10}(\text{norm}_2 \text{ error})$ show scatter plots similar in behavior to Figure 13 but give slops that range between $[1: 2]$.

3.2 Compressible case

As illustrated before within Section 2 and the Appendix derivations, the slightly compressible case uses Equation (33) with $C = \varphi c_f \rho$, $\rho = \rho^0 \exp(c_f[p - p^0])$, the source term Q follows Equation (15), the permeability is a function of the x position within the domain defined as $K_+ = K_{const} x^\gamma$, $K_- = K_{const} (x_{end} - x)^\gamma \rightarrow K_- = K_{const} (2 - x)^\gamma$ within the domain $[a, b] = [0, 2]$ and the initial pressure follows $p(x, 0) = 4x^2(2 - x)^2$ too.

In this example too, the reservoir is discretized along its 1D length with a control volume of size $\Delta x = 1/145$. The time step is $\Delta t = 1/125$ and the total simulation length is $T = 1$. The remaining properties include: fractional derivative order $\gamma = 0.7$, constant permeability used within both permeabilities definitions $K_{const} = 5E - 10$, initial rock porosity $\varphi_R = 0.3$, initial fluid density $\rho_f^0 = 1.0726$, compressibility factor $c_f = 0.8259$, and the left and right boundaries conditions are: $(K_{BL} = 0, K_{BR} = 0, \rho_{BL} = 0, \rho_{BR} = 0)$.

Figure 15 shows the pressure profiles along the x – axis for the numerical result in the slightly compressible case and compares it to the analytical solution for exactly similar conditions.

Figure 15: comparison between numerical model simulation results and analytical solution results.

The excellent overlapping observed between the solutions of the numerical pressure systems and the predicted analytical results in the slightly compressible case too within Figure 15 establishes the accuracy of the proposed PPA scheme discretization for this case too. It can also be noted that at the midpoint of the domain interval $x = 1$, the pressure result converges toward the true solution at that point given by $p_{true}(1, 1) = 4 \exp(-1) = 1.4715$ as illustrated before that further establishes the proposed scheme accuracy.

However, the numerical pressure values needs to converge over time, in the compressible case too, throughout the interval $[0, T] = [0, 1]$ starting from the initial pressures illustrated in Figure 16, then converging from the second time-step illustrated in black within Figure 17, until the final step illustrated in blue in Figure 17.

As a result, density that is computed by equation $\rho = \rho^0 \exp(c_f[p - p^0])$ is effected by the pressure and changes over time as illustrated in Figure 18. To further investigate the accuracy of density, we can use the domain midpoint pressure found before to check if the analytic density is close to the numerical density, that is: $\rho = \rho^0 \exp(c_f[p - p^0]) \rightarrow \rho = 1.0726 \exp(0.8259[1.4715 - 4]) = 0.1329$. This value seems to be very adjacent to Figure 18 midpoint density. A similar approach can be used to check the numerical accuracy of ρ at any time step using the pressure of that step.

The value C within Equations (29-32) is computed by $C = \varphi c_f \rho$, meaning that it uses the density ρ that changes over time. So it also changes over time as illustrated in Figure 19. Since C depends mainly on ρ changes while the remaining variables are constants, its curves take a shape similar to ρ shapes from Figure 18 with different values. Checking the midpoint C with ρ from Figure 18 discussion gives $C = \varphi c_f \rho = (0.3)(0.8259)(0.1329) = 0.0329$, that is adjacent to Figure 19 results. In this case too, a similar approach can be used to check the numerical accuracy of C at any time step using ρ of that step.

Figure 16: initial numerical pressure values.

Figure 17: numerical pressure $p_{i+0.5}$ convergence over time towards the final $p_{i+0.5}$ starting from the second time-step in black.

Figure 18: numerical density $\rho_{i+0.5}$ convergence over time towards the final $\rho_{i+0.5}$ starting from the second time-step in black.

Figure 19: numerical $C_{i+0.5}$ value convergence over time towards the final $C_{i+0.5}$ starting from the second time-step in black.

Since the permeability depends on the x position within the domain defined using the relations $K_+ = K_{const} x^\gamma$, $K_- = K_{const} (2 - x)^\gamma$, such that K_{const} and γ are constant over time, the permeability values take the shape illustrated in Figure 20. Within the figure, left and right cells around each edge of the same side (plus or minus) have approximately similar permeability behaviors. Drops in values start to appear as an effect of the boundary conditions when the domain limits are reached, like the right cell of the right direction or the plus direction (K_R^+), or the left cell of the left direction or the minus direction (K_L^-). Permeabilities are not affected over time according to this case assumptions and conditions. So, they are used directly in Equations (29-32) computations of S_R^+ , S_L^+ , S_R^- and S_L^- .

The computations of S_R^+ , S_L^+ , S_R^- and S_L^- include a multiplication between ρ and $1/C$ changing over time, and K constant over time but changing over domain space. Finding the value of $1/C$ for each $C_{i+0.5}$ flips the shapes of the curves at each time step as illustrated in Figure 22.

As a result, we end up with multiplying an upward concave for ρ (Figure 18) by downward concave for $1/C$ (Figure 22) by a slightly less concaving curve facing left or right corners for K (Figure 20). The upward concave cancels a fair amount of the downward concave, giving more weight to the slightly less concaving curve effects. This can be realized from few facts seen in Figure 21 that include: (A) the final shape of each S curve (Figure 21) looks like as if it is connecting the largest value with the lowest value of the K used (Figure 20) drawn respectively with the same color. (B) The effects of reaching the domain limits are also inherited to the final resulting S , like the right cell of the right direction or the plus direction ($K_R^+ \rightarrow S_R^+$), or the left cell of the left direction or the minus direction ($K_L^- \rightarrow S_L^-$).

As discussed before, it is customary to investigate the error convergence for several possible grid-cell sizes to check the accuracy of the proposed mathematical schemes. So, in the slightly compressible case too, the grid-cell sizes used are:

$\Delta x_{i+0.5} = [1/50, 1/60, 1/70, 1/80, 1/90, 1/100, 1/110, 1/120]$ such that the mesh grid-cell sizes vary within the specified range. Error converges with each cases as illustrated in Figure 23. It can be noticed from Figure 23 that the error norms decrease as the grid-cell sizes decrease and vice-versa. This gives an indication that small size meshes give better numerical results.

Figure 26 parts (A-D) zoom the investigation into four examples of the grid-cell mesh sizes ranging within the values: $\Delta x_{i+0.5} = [1/50, 1/75, 1/100, 1/145]$. Focusing on parts (A-D), it can be noticed that for the same time steps $\Delta t = 1/125$ at the final step with time $T = 1$, as the mesh size decreases the final step numerical result converges more toward the true solution. It can also be noticed that starting from mesh size $1/145$ and going into smaller mesh sizes, the convergence remains the same. So, it would be better from the CPU and memory points of view to use the best smallest possible mesh size, that is $1/145$ for this example.

To further analyze the convergence, relations between $\log_{10}(\text{mesh size})$ and $\log_{10}(\text{norm2 error})$ are outlined in Figure 24. The general shape of both scatter plots from Figure 23 and Figure 24 are similar, but values in Figure 24 of the best line fitting the data points has slopes that range approximately between $[1:2]$ that is to be expected according to Saad (2003) in this case too.

In this system too and any similar system, the number of variables, that are the cell-centered pressures here, are proportional to the mesh size. So, as the mesh sizes decrease, the number of cells increase. As a result, the number of cell-centered pressure variables increase and with that the error norm decrease in consistent with the previous discussion as illustrated in Figure 25. This relation can be referred to as: $\#vars \propto 1/(\Delta x_{i+0.5})^2$.

Finding the relation between $\log(\#vars)$ and $\log(\text{norm2 error})$ with mesh sizes ranging within the values $\Delta x_{i+0.5} = [1/50, 1/60, 1/70, 1/80, 1/90, 1/100, 1/110, 1/120]$ also gives slopes within the range $[1:2]$ that is to be expected too according to Saad (2003) as illustrated in Figure 27.

So, applying the proposed Physics Preserving Averaging (PPA) scheme on both scenarios, one for a simple case (Figure 6) that assumes constant values (permeability, C , and ρ) and another one for slightly compressible fluids (Figure 15) with (C , and ρ) changing with time steps and permeability changing with position on the domain space, produces an excellent overlap between the numerical pressure solutions and the predicted analytical results.

One more way to investigate the privileges of using the PPA scheme is to discretize Equation (16) using the two-side edge-based shifted fractional derivatives illustrated in Table A.1 of the Appendix and used in literature (Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Atangana and Vermeulen, 2014; Ghanam et al., 2014; Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014) to compare the numerical results with the PPA scheme numerical results. Figure 28 shows the simple case PPA scheme numerical results vs. the typical two-side shifted scheme results and Figure 29 applies a similar comparison for the slightly compressible case. Both figures illustrate that the PPA scheme gives more adjacent results to the analytical true solutions that are more obvious in the slightly compressible case. This gives an indication that the physical complexity of the system distinguishes the PPA scheme benefits more. In other words, as the physical system complexity increase, the variation between the PPA scheme results and the typical two-side edge-based shifted scheme results manifest more.

Figure 20: permeabilities using the relations $K_+ = K_{const} x^\gamma$ and $K_- = K_{const} (2 - x)^\gamma$ for both left and right cells around each edge in both plus and minus sides of the domain.

Figure 21: S_R^+ , S_L^+ , S_R^- , and S_L^- shapes considering the effects of ρ and C changing over time, and K constant over time but changing over domain space.

Figure 22: S_R^+ , S_L^+ , S_R^- , and S_L^- computations include a multiplication by $1/C_{i+0.5}$, that is the result of flipping Figure 19.

Figure 23: (norm_2 error) convergence with respect to actual mesh sizes show that errors decrease as mesh size decreases in the slightly compressible case too.

Figure 24: Error convergence using the values of $\log_{10}(\text{mesh size})$ vs. $\log_{10}(\text{norm}_2 \text{ error})$ give slopes that range between $[1: 2]$.

Figure 25: error norms decrease as the number of cell-centered pressure variables increase in consistent with the previous discussions.

Figure 26: Zooming into examples with $\Delta x_{t+0.5} = [1/50, 1/75, 1/100, 1/145]$, it can be noticed that for the same time steps $\Delta t = 1/125$ at the final step ($T = 1$), numerical results converge better as mesh size decrease.

Figure 27: Error convergence using the values of $\log_{10}(\# vars)$ and $\log_{10}(\text{norm}_2 \text{ error})$ show scatter plots similar in behavior to Figure 25 but give slopes that range between $[1: 2]$.

Figure 28: Simple case: comparing PPA scheme vs. typical two-side shifted scheme show that PPA scheme gives more adjacent results to the analytical true solutions.

Figure 29: Slightly compressible case: comparing PPA scheme vs. typical two-side shifted scheme shows that PPA scheme gives more adjacent results to the analytical true solutions.

4 Conclusion

In this paper, the non-Newtonian non-Darcy fractional derivatives within velocity flux equations are discretized using a Physics Preserving Averaging (PPA) scheme. It expands one side with the original cell-centered GL formula preserving the physics by reducing the shifting effects, and the other side with the shifted cell-centered GL formula to overcome the instability issues of the typical original edge-based fractional derivatives.

PPA scheme is expected to be more stable than the original edge-based GL derivatives but might be slightly less stable than the shifted edge-based GL derivatives. However, physical results are expected to be more accurate as demonstrated by examples in Figures 28-29.

PPA discretization generates symmetrical coefficient matrices as illustrated in Equation (34). This reduces a lot of computational complexities that used to appear within typical shifted edge-based GL formulas. As a result, this helps significantly in developing 2D-3D or Multi-Point Flux Approximation (MPFA) computational codes. Also, it can be noticed that as the considered system complexity increase, the variation between the PPA scheme results and the typical edge-based shifted GL scheme results manifest more.

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Appendix

Section A of the Appendix discusses: the well-known GL fractional derivatives formulas, their uses, their discretization approaches, literature edge-based *Original and Shifted GL* formulas (Table A.1), this paper cell-centered-based *Original and Shifted GL* formulas (Table A.2), their expansions, fractional derivatives expansions in time (Table A.3), and lists most of the heavily used equations for such applications. Section B of the Appendix derives the analytical source term Q for both: the simple case and the compressible fluid case assuming an analytical value for the pressure p . Section C of the Appendix illustrates an example for GL formulas expansions in PPA scheme.

A. Grunwald-Letnikov (GL) Approximations

Fractional derivative formulas include Riemann-Liouville formulas, Grunwald-Letnikov formulas, Caputo formulas, Riesz-Feller formulas (Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014). Many discretization approaches have been investigated for the Riemann-Liouville space fractional derivatives within the mass conservation law (Cloot and Botha, 2006; Ochoa-Tapia et al., 2007; Atangana and Vermeulen, 2014; Ghanam et al., 2014; Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014). *Grunwald-Letnikov (GL)* approximation improved in this paper was one of these discretization approaches.

Table A.1 and the 1D illustrative Figures A.1-A.3 explain how the Literature edge-based GL expansions span edges from $0, 1, \dots, M$ such that $0 \leq x_i \leq M$. According to Table A.1 definitions, the derivative at each mesh point x_i depends on all of its surrounding mesh points from $x_0, x_1 \dots x_M$. For example, to find the fractional derivative of any function $u(x)$ defined at mesh point x_i , it will include a left-side and a right-side derivatives approximations as illustrated in Table A.1. Both left-side and right-side derivatives are either used in their original form or in their shifted form. The original GL formula for both sides are Equations (A.1a) and (A.2a).

Applying Equation (A.1a) expansion for $u(x)$ shifted a single shift to the left at mesh point x_{i-1} gives Equation (A.3a) and $u(x)$ shifted a single shift to the right at mesh point x_{i+1} gives Equation (A.4a). Similarly, Equation (A.2a) expansion for $u(x)$ shifted a single shift to the left at mesh point x_{i-1} gives Equation (A.5a) and $u(x)$ shifted a single shift to the right at mesh point x_{i+1} gives Equation (A.6a). These shifted equations can be used to find the derivative at the point x_i . However, the left side equation (A.3a) and the right side equation (A.6a) are considered unstable to solve for the derivative at x_i since the expansion approximation is missing the most important effect that is $u(x_i)$.

Literature studies (Meerschaert and Tadjeran, [2004 and 2006]; Ahmed and Nieto, 2012; Vance, 2014) proved that using the original edge-based GL expansion formulas give instable fractional derivatives discretization. While on the other hand, the shifted edge-based GL expansion formulas give mathematically stable fractional derivatives discretization that is significantly effected in physically accuracy due to shifting the weights of the most important edge of interest as illustrated in Figures 28-29.

Figure A.1: Edges included with each side in the *Original GL* approximation.

Figure A.2: Edges included with each side in the *Shifted-left GL* approximation starting at edge x_{i-1} for the derivative at point x_i . So, the left side doesn't include $u(x_i)$, that is, it can not be used to solve for it.

Figure A.3: Edges included with each side in the *Shifted-right GL* approximation starting at edge x_{i+1} for the derivative at point x_i . So, the right side doesn't include $u(x_i)$, that is, it can not be used to solve for it.

Edge-based	Original Grunwald-Letnikov formula	
Left side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma u_{i-k} \quad (\text{A.1a})$	
Right side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma u_{i+k} \quad (\text{A.2a})$	
	<i>Shifted Left Grunwald-Letnikov at x_{i-1}</i>	<i>Shifted Right Grunwald-Letnikov at x_{i+1}</i>
Left side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^{i-1} g_k^\gamma u_{i-k-1} \quad (\text{A.3a}) \rightarrow \text{unstable}$	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma u_{i-k+1} \quad (\text{A.4a})$
Right side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i+1} g_k^\gamma u_{i+k-1} \quad (\text{A.5a})$	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma u_{i+k+1} \quad (\text{A.6a}) \rightarrow \text{unstable}$

Table A.1: Original GL and both Left-Side and Right-Side Shifted GL approximation formulas.

Further illustration is provide by an example in 1D that spans the domain $[0,6]$ edges at $x_0, x_1 \dots x_6$ with $M = 6$. Finding the fractional derivatives at the forth edge $u(x_4)$, the GL derivation formulas are expanded as:

1) Original left-side:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_4 + g_1^\gamma u_3 + g_2^\gamma u_2 + g_3^\gamma u_1 + g_4^\gamma u_0] = \frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma u_{i-k}$
2) Left-side single left-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_3 + g_1^\gamma u_2 + g_2^\gamma u_1 + g_3^\gamma u_0] = \frac{1}{h^\gamma} \sum_{k=0}^{i-1} g_k^\gamma u_{i-k-1}$
3) Left-side single right-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_5 + g_1^\gamma u_4 + g_2^\gamma u_3 + g_3^\gamma u_2 + g_4^\gamma u_1 + g_5^\gamma u_0] = \frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma u_{i-k+1}$
4) Original right-side:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_4 + g_1^\gamma u_5 + g_2^\gamma u_6] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma u_{i+k}$
5) Right-side single left-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_3 + g_1^\gamma u_4 + g_2^\gamma u_5 + g_3^\gamma u_6] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i+1} g_k^\gamma u_{i+k-1}$
6) Right-side single right-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_i} = \frac{1}{h^\gamma} [g_0^\gamma u_5 + g_1^\gamma u_6] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma u_{i+k+1}$

Literature *Edge-based* GL expansions from Table A.1 assume both velocities and pressures residing on edges. This might be part of the instability issue rising in this scheme. In this paper, velocities are assumed to be residing on edges and pressures are cell centers. When solving for pressures, the Edge-

based Table A.1 discretization is inapplicable. New modified sets of discretization formulas are introduced for such cases that are illustrated in Figures A.4-A.6.

Left side

Figure A.4: Cell-centers included with each side in the Original GL approximation

Left side

Figure A.5: Cell-centers included with each side in the *Shifted-left GL* approximation starting at edge $x_{i-0.5}$ for the derivative at point $x_{i+0.5}$. So, the left side doesn't include $u(x_{i+0.5})$, that is, it cannot be used to solve for it.

Left side

Figure A.6: Cell-centers included with each side in the *Shifted-right GL* approximation starting at edge $x_{i+1.5}$ for the derivative at point $x_{i+0.5}$. So, the right side doesn't include $u(x_{i+0.5})$, that is, it cannot be used to solve for it.

In general, the indices of the Edge-based cases in Table A.1 need to change to fit the Cell-Centered based cases. Applying the indices changes on Table A.1 equations [indicated by (A.xa)], we end up with Table A.2 equations [indicated by (A.xb) respectively for similar version from (A.xa)].

Table A.2 and the 1D illustrative Figures A.4-A.6 explain how the Cell-Centered based GL expansions span cell-centers from $0.5, 1.5, \dots (M - 0.5)$ such that $0 \leq x_{i+0.5} \leq M$. According to Table A.2 definitions, the derivative at each cell-center $x_{i+0.5}$ depends on all of its surrounding cell-centered points from $x_{0.5}, x_{1.5} \dots x_{M-0.5}$. For example, to find the fractional derivative of any function $u(x)$ defined at cell-center $x_{i+0.5}$, it will include a left-side and a right-side derivatives approximation as illustrated in Table A.2. Both left-side and right-side derivatives are either used in their original form or in their shifted form. The original GL formula for both sides are Equations (A.1b) and (A.2b).

Applying Equation (A.1b) expansion for $u(x)$ shifted a single shift to the left at mesh point $x_{i-0.5}$ gives Equation (A.3b) and $u(x)$ shifted a single shift to the right at mesh point $x_{i+1.5}$ gives Equation (A.4b). Similarly, Equation (A.2b) expansion for $u(x)$ shifted a single shift to the left at mesh point $x_{i-0.5}$ gives Equation (A.5b) and $u(x)$ shifted a single shift to the right at mesh point $x_{i+1.5}$ gives Equation (A.6b). These shifted equations can be used to find the derivative at the point $x_{i+0.5}$. However, the left side equation (A.3b) and the right side equation (A.6b) are considered unstable to solve for the derivative at $x_{i+0.5}$ since their expansion approximations are missing the most important effect that is $u(x_{i+0.5})$.

Cell-Centered	Original Grunwald-Letnikov formula	
Left side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma u_{i+0.5-k} \quad (A.1b)$	
Right side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma u_{i+0.5+k} \quad (A.2b)$	
	Shifted Left Grunwald-Letnikov at $x_{i-0.5}$	Shifted Right Grunwald-Letnikov at $x_{i+1.5}$
Left side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{i-1} g_k^\gamma u_{i-k-0.5} \quad (A.3b) \rightarrow \text{unstable}$	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma u_{i-k+1.5} \quad (A.4b)$
Right side	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma u_{i+k-0.5} \quad (A.5b)$	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-2} g_k^\gamma u_{i+k+1.5} \quad (A.6b) \rightarrow \text{unstable}$

Table A.2: Cell-Centered Original and shifted Grunwald-Letnikov approximation formulas

Further illustration is provided by an example in 1D here too that spans the mesh $[0,6]$ grid cell centers at $x_{0.5}, x_{1.5} \dots x_{5.5}$ with $M = 6$. Finding the derivatives at $x_{i+0.5}$ such that $i = 3$ (cell-center) $\rightarrow x_{3.5}$, the GL derivation formulas are expanded as:

1) Original left-side:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{3.5} + g_1^\gamma u_{2.5} + g_2^\gamma u_{1.5} + g_3^\gamma u_{0.5}] = \frac{1}{h^\gamma} \sum_{k=0}^i g_k^\gamma u_{i+0.5-k}$
2) Left-side single left-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{2.5} + g_1^\gamma u_{1.5} + g_2^\gamma u_{0.5}] = \frac{1}{h^\gamma} \sum_{k=0}^{i-1} g_k^\gamma u_{i-k-0.5}$
3) Left-side single right-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{L \rightarrow x} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{4.5} + g_1^\gamma u_{3.5} + g_2^\gamma u_{2.5} + g_3^\gamma u_{1.5} + g_4^\gamma u_{0.5}] = \frac{1}{h^\gamma} \sum_{k=0}^{i+1} g_k^\gamma u_{i-k+1.5}$
4) Original right-side:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{3.5} + g_1^\gamma u_{4.5} + g_2^\gamma u_{5.5}] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-1} g_k^\gamma u_{i+0.5+k}$
5) Right-side single left-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{2.5} + g_1^\gamma u_{3.5} + g_2^\gamma u_{4.5} + g_3^\gamma u_{5.5}] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i} g_k^\gamma u_{i+k-0.5}$
6) Right-side single right-shift:	$\left(\frac{\partial^\gamma u}{\partial x^\gamma}\right)_{x \rightarrow R} \Big _{x_{i+0.5}} = \frac{1}{h^\gamma} [g_0^\gamma u_{4.5} + g_1^\gamma u_{5.5}] = \frac{1}{h^\gamma} \sum_{k=0}^{M-i-2} g_k^\gamma u_{i+k+1.5}$

Notes:

- Both (Table A.1 and Table A2) display four possible shifts, either left or right for each side. However, Table A.1 finds the discretization around edge x_i and Table A.2 finds the discretization around cell-center $x_{i+0.5}$.
- Equations (A.3a) and (A.6a) are unstable to use since they are missing $u(x_i)$ computations part and Equations (A.3b) and (A.6b) are unstable to use since they are missing $u(x_{i+0.5})$ computations. That is the most important part for this part (edge or cell-center) solution.
- Equations (A.4b) and (A.5b) are used for the shifted cell-centered pressure derivatives and Equations (A.4a) and (A.5a) are used for the shifted edge-based pressure derivatives.

Derivative solutions were investigated with respect to time using: *Explicit Euler method*, *Implicit Euler method*, *Crank-Nicolson method* (averages *Explicit Euler* and *Implicit Euler methods*), and *A weighted difference method* (considered a generalization for the *Explicit*, *Implicit*, and *Crank-Nicolson methods*). Generalizing all the GL approximations from Tables A.1-A.2, they can be written as:

$$\frac{\partial^\gamma u}{\partial x^\gamma} = \frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega \quad \begin{aligned} & \text{[Such that } \delta \text{ and } \omega \text{ can take any of the following indices:} \\ & \omega = i - k, i - k + 1, i - k - 1, i + k, i + k - 1, i + k + 1; \delta = \\ & i, i + 1, i - 1, M - i, M - i + 1, M - i - 1, i - 0.5, i + 0.5, i - \\ & 1.5, M - i - 0.5, M - i + 0.5, M - i - 1.5] \end{aligned} \quad (\text{A.7})$$

As a result, each expansion from Tables A.1 and A.2 can be expressed in time as illustrated in Table A.3:

<i>Explicit Euler method</i>	<i>Implicit Euler method</i>	<i>Crank-Nicolson method</i>
$\frac{\partial^\gamma u}{\partial x^\gamma} = \frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega^n$	$\frac{\partial^\gamma u}{\partial x^\gamma} = \frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega^{n+1}$	$\frac{\partial^\gamma u}{\partial x^\gamma} = \frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega^{n+0.5}$
<i>Weighted difference method: generalization for the Explicit, Implicit, and Crank-Nicolson methods</i>		
$\begin{aligned} \frac{\partial^\gamma u}{\partial x^\gamma} &= \left((1 - \theta) \left(\frac{\partial^\gamma u}{\partial x^\gamma} \right)^{n+1} + \theta \left(\frac{\partial^\gamma u}{\partial x^\gamma} \right)^n \right) \\ &= \left((1 - \theta) \left(\frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega^{n+1} \right) + \theta \left(\frac{1}{h^\gamma} \sum_{k=0}^{\delta} g_k^\gamma u_\omega^n \right) \right) \end{aligned}$		

Table A.3: GL expansions in time.

Using Riemann-Liouville derivative of order $\gamma > 0$ with $n - 1 < \gamma < n$ of the power function $f(x) = x^p$ for $p \geq 0$ (Meerschaert and Tadjeran 2006, Ahmed and Nieto 2012, Vance 2014), the Riemann-Liouville derivative of power $\gamma > 0$ is:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{1}{\Gamma(n - \gamma)} \left(\frac{\partial}{\partial x} \right)^n \int_0^x (x - u)^{n-\gamma-1} u^p du \quad (\text{A.8})$$

Let $u = vx$ for $0 \leq v \leq 1$, $du = xdv$, Equation (A.8) becomes:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{1}{\Gamma(n - \gamma)} \left(\frac{\partial}{\partial x} \right)^n \int_0^x (x - vx)^{n-\gamma-1} (vx)^p xdv$$

Taking x as a common factor inside the integral and since $0 \leq v \leq 1$, the equation becomes:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{1}{\Gamma(n - \gamma)} \left(\frac{\partial}{\partial x} \right)^n \int_0^1 ([1 - v] x)^{n-\gamma-1} (vx)^p xdv \quad (\text{A.9})$$

This can be simplified as:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{1}{\Gamma(n - \gamma)} \left(\frac{\partial}{\partial x} \right)^n \int_0^1 (1 - v)^{n-\gamma-1} v^p x^{n+p-\gamma} dv \quad (\text{A.10})$$

Since the derivation is on x only, Equation (A.10) can be written as:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{1}{\Gamma(n - \gamma)} \int_0^1 (1 - v)^{n-\gamma-1} v^p dv \left(\frac{\partial}{\partial x} \right)^n x^{n+p-\gamma} \quad (\text{A.11})$$

Beta function for the value: $\beta(x, y) = \int_0^1 (1 - v)^{y-1} v^{x-1} dv$ for $x > 0, y > 0$ is given by: $\beta(x, y) = (\Gamma(x)\Gamma(y))/(\Gamma(x + y))$ [Definition]. Applying it to Equation (A.11) with $x = p + 1$ and $y = n - \gamma$:

$$\beta(p + 1, n - \gamma) = \int_0^1 (1 - v)^{n-\gamma-1} v^p dv = \frac{\Gamma(p + 1)\Gamma(n - \gamma)}{\Gamma(p + 1 + n - \gamma)} \quad (\text{A.12})$$

Substituting Equation (A.12) in Equation (A.11), we end up with:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1+n-\gamma)} \left(\frac{\partial}{\partial x}\right)^n x^{n+p-\gamma} \quad (\text{A.13})$$

According to the fractional calculus (Das 2011, Richard 2011), the n^{th} fractional derivative of x^m is given by:

$$\frac{\partial^n}{\partial x^n} x^m = \begin{cases} \frac{m!}{(m-n)!} x^{m-n} & \text{if } m \geq n \\ 0 & \text{if } m < n \end{cases} \quad (\text{A.14})$$

Applying Equation (A.14) into the n^{th} fractional derivative of Equation (A.13) for $n+p-\gamma \geq n$. Then substituting the gamma definition for the factorials:

$$\frac{\partial^n}{\partial x^n} x^{n+p-\gamma} = \frac{(n+p-\gamma)!}{(p-\gamma)!} x^{p-\gamma} = \frac{\Gamma(n+p-\gamma+1)}{\Gamma(p-\gamma+1)} x^{p-\gamma} \quad (\text{A.15})$$

Substituting Equation (A.15) into Equation (A.13):

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1+n-\gamma)} \frac{\Gamma(n+p-\gamma+1)}{\Gamma(p-\gamma+1)} x^{p-\gamma}$$

This can be simplified as:

$$\frac{\partial^\gamma}{\partial x^\gamma} (x)^p = \frac{\Gamma(p+1)}{\Gamma(p-\gamma+1)} x^{p-\gamma} \quad (\text{A.16})$$

A similar approach can be used to derive Table A.4 equations.

Positive sides fractional derivative	Negative sides fractional derivative
$\frac{\partial^\gamma}{\partial_+ x^\gamma} (x-L)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-\gamma)} (x-L)^{p-\gamma}$	$\frac{\partial^\gamma}{\partial_- x^\gamma} (R-x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-\gamma)} (R-x)^{p-\gamma}$

Table A.4: fractional derivatives exact expansions using the gamma functions.

Table A.4 equations are used in the analytical derivations of the source term (Meerschaert and Tadjeran 2006, Ahmed and Nieto 2012, Vance 2014).

B. Source term Q derivation

Simple case

The equation used is:

$$\frac{\partial p}{\partial t} + \frac{\partial u_x}{\partial x} = Q \quad (\text{B.1})$$

$$u_x = -K \left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right)$$

$$u_x = -K \left[\left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) + \left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \right] \quad (\text{B.2})$$

This means that Equation (B.1) can be rewritten as:

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} \left\{ -K \left[\left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) + \left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \right] \right\} = Q$$

$$\frac{\partial p}{\partial t} - K \left(\frac{\partial^{\gamma+1} p}{\partial_+ x^{\gamma+1}} \right) - K \left(\frac{\partial^{\gamma+1} p}{\partial_- x^{\gamma+1}} \right) = Q; \quad 0 < \gamma < 1 \quad (\text{B.3})$$

Assuming constant K . Let: $p(x, t) = 4 \exp(-t) x^2 (x_{end} - x)^2$. If the spacial domain considered is: $[L, R] = [0, 2]$ in time interval: $[0, N] = [0, 1]$, the pressure can be rewritten as:

$$p(x, t) = 4 \exp(-t) x^2 (2 - x)^2 \rightarrow \text{Initial pressure: } p(x, 0) = 4 x^2 (2 - x)^2 \quad (\text{B.4})$$

Substituting all in (B.3):

$$\frac{\partial [4 \exp(-t) x^2 (2 - x)^2]}{\partial t} - K \left(\frac{\partial^{\gamma+1} [4 \exp(-t) x^2 (2 - x)^2]}{\partial_+ x^{\gamma+1}} \right) - K \left(\frac{\partial^{\gamma+1} [4 \exp(-t) x^2 (2 - x)^2]}{\partial_- x^{\gamma+1}} \right) = Q \quad (*)$$

Dealing with each part of the equation separately:

$$(A) = \frac{\partial}{\partial t} [4 \exp(-t) x^2 (2-x)^2] = -4 \exp(-t) x^2 (2-x)^2 \quad (B.5)$$

$$(B) = \frac{\partial^{\gamma+1}}{\partial_+ x^{\gamma+1}} [4 \exp(-t) x^2 (2-x)^2] = 4 \exp(-t) \frac{\partial^{\gamma+1}}{\partial_+ x^{\gamma+1}} [x^2 (2-x)^2]$$

Expanding the x variable parenthesis:

$$(B) = 4 \exp(-t) \frac{\partial^{\gamma+1}}{\partial_+ x^{\gamma+1}} [4 x^2 - 4 x^3 + x^4] \quad (B.6)$$

Applying Table A.4 fractional derivative on the L limit of this assumption: $[L, R] = [0, 2]$, the equation becomes:

$$\frac{\partial^{\gamma+1}}{\partial_+ x^{\gamma+1}} (x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-(\gamma+1))} (x)^{p-(\gamma+1)} \rightarrow \frac{\partial^{\gamma+1}}{\partial_+ x^{\gamma+1}} (x)^p = \frac{\Gamma(p+1)}{\Gamma(p-\gamma)} (x)^{p-\gamma-1} \quad (B.7)$$

Applying Equation (B.7) derivative on Equation (B.6), the equation becomes:

$$(B) = 4 \exp(-t) \left\{ 4 \frac{\Gamma(2+1)}{\Gamma(2-\gamma)} (x)^{2-\gamma-1} - 4 \frac{\Gamma(3+1)}{\Gamma(3-\gamma)} (x)^{3-\gamma-1} + \frac{\Gamma(4+1)}{\Gamma(4-\gamma)} (x)^{4-\gamma-1} \right\} \quad (B.8)$$

$$(B) = 4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} (x)^{1-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} (x)^{2-\gamma} + \frac{\Gamma(5)}{\Gamma(4-\gamma)} (x)^{3-\gamma} \right\} \quad (B.9)$$

Let $y = x - 2 \rightarrow x = y + 2$. Substituting it into: $x^2(2-x)^2$ gives: $(y+2)^2(2-(y+2))^2$. This can be expanded into: $(y+2)^2 y^2$. Expanding the parenthesis, this would give: $4y^2 + 4y^3 + y^4$.

Substituting each y by its value, we end up with: $4(x-2)^2 + 4(x-2)^3 + (x-2)^4$. Taking the negative outside each parenthesis, we end up with: $4(-(2-x))^2 + 4(-(2-x))^3 + (- (2-x))^4$.

Applying the exponent on each parenthesis: $4(2-x)^2 - 4(2-x)^3 + (2-x)^4$. As a result, Equation (B.9) can be rewritten as:

$$(C) = 4 \exp(-t) \frac{\partial^{\gamma+1}}{\partial_- x^{\gamma+1}} \{4(2-x)^2 - 4(2-x)^3 + (2-x)^4\} \quad (B.10)$$

Applying Table A.4 fractional derivative on the R limit of this assumption: $[L, R] = [0, 2]$, the equation becomes:

$$\begin{aligned} \frac{\partial^{\gamma+1}}{\partial_- x^{\gamma+1}} (2-x)^p &= \frac{\Gamma(p+1)}{\Gamma(p+1-(\gamma+1))} (2-x)^{p-(\gamma+1)} \\ \frac{\partial^{\gamma+1}}{\partial_- x^{\gamma+1}} (2-x)^p &= \frac{\Gamma(p+1)}{\Gamma(p-\gamma)} (2-x)^{p-\gamma-1} \end{aligned} \quad (B.11)$$

Using Equation (B.11) derivative definition, Equation (B.10) becomes:

$$(C) = 4 \exp(-t) \left\{ 4 \frac{\Gamma(2+1)}{\Gamma(2-\gamma)} (2-x)^{1-\gamma} - 4 \frac{\Gamma(3+1)}{\Gamma(3-\gamma)} (2-x)^{2-\gamma} + \frac{\Gamma(4+1)}{\Gamma(4-\gamma)} (2-x)^{3-\gamma} \right\} \quad (B.12)$$

Substituting Equations (B.5, B.8, B.12) into Equation (*), we end up with:

$$\begin{aligned} &-4 \exp(-t) x^2 (2-x)^2 - \\ &K \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} (x)^{1-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} (x)^{2-\gamma} + \frac{\Gamma(5)}{\Gamma(4-\gamma)} (x)^{3-\gamma} \right\} \right) - \\ &K \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} (2-x)^{1-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} (2-x)^{2-\gamma} + \frac{\Gamma(5)}{\Gamma(4-\gamma)} (2-x)^{3-\gamma} \right\} \right) = Q \\ Q &= -4 \exp(-t) \left\{ x^2 (2-x)^2 + K \left[4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} [(x)^{1-\gamma} + (2-x)^{1-\gamma}] - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} [(x)^{2-\gamma} + \right. \right. \\ &\left. \left. (2-x)^{2-\gamma}] + \frac{\Gamma(5)}{\Gamma(4-\gamma)} [(x)^{3-\gamma} + (2-x)^{3-\gamma}] \right] \right\} \end{aligned} \quad (B.13)$$

The source Q can also be computed using a different sign as:

$$\begin{aligned} Q &= +4 \exp(-t) \left\{ x^2 (2-x)^2 + K \left[4 \frac{\Gamma(3)}{\Gamma(2-\gamma)} [(x)^{1-\gamma} + (2-x)^{1-\gamma}] - 4 \frac{\Gamma(4)}{\Gamma(3-\gamma)} [(x)^{2-\gamma} + \right. \right. \\ &\left. \left. (2-x)^{2-\gamma}] + \frac{\Gamma(5)}{\Gamma(4-\gamma)} [(x)^{3-\gamma} + (2-x)^{3-\gamma}] \right] \right\} \end{aligned} \quad (B.14)$$

Such that Equation (B.13) numerically indicates injection and Equation (B.14) numerically indicates production.

Compressible single-phase case

The equation used assuming slightly compressible fluid and non-compressible rocks is:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x}(\rho u_x) = Q \rightarrow \left(\phi \frac{\partial \rho}{\partial p}\right) \frac{\partial p}{\partial t} + \left(\rho \frac{\partial u_x}{\partial x} + u_x \frac{\partial \rho}{\partial x}\right) = Q \quad (\text{B.15})$$

The values $\rho \rightarrow$ density; $\phi \rightarrow$ porosity; $u_x \rightarrow$ velocity; $Q \rightarrow$ source term; $t \rightarrow$ time; $p \rightarrow$ pressure.

Assuming thermodynamic properties and using Taylor expansion for the slightly compressible fluid:

$$c_f = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial p} \right)_T \rightarrow \frac{\partial \rho}{\partial p} = c_f \rho \quad (\text{B.16})$$

$$\rho = \rho^0 \exp(c_f [p - p^0]) \quad (\text{B.17})$$

Such that $c_f \rightarrow$ fluid compressibility; $p^0 \rightarrow$ reference pressure; $\rho^0 \rightarrow$ reference density.

This means that Equation (B.15) becomes:

$$(\phi c_f \rho) \frac{\partial p}{\partial t} + \rho \frac{\partial u_x}{\partial x} + u_x \frac{\partial \rho}{\partial x} = Q \quad (\text{B.18})$$

Dealing with each term alone such that: $T_1 + T_2 + T_3 = Q$

$$T_1 = (\phi c_f \rho) \frac{\partial p}{\partial t}; T_2 = \rho \frac{\partial u_x}{\partial x}; T_3 = u_x \frac{\partial \rho}{\partial x} \quad (\text{B.19})$$

Since pressure value is assumed to be $p = 4 \exp(-t) x^2 (2 - x)^2$ with initial pressure $p_0 = 4x^2(2 - x)^2$, the first term becomes:

$$T_1 = (\phi c_f \rho) \frac{\partial p}{\partial t} \rightarrow T_1 = (\phi c_f \rho) \frac{\partial}{\partial t} [4 \exp(-t) x^2 (2 - x)^2] \quad (\text{B.20})$$

$$T_1 = -4 \phi c_f \rho \exp(-t) x^2 (2 - x)^2 \quad (\text{B.21})$$

In order to find T_2 and T_3 , u_x and $\partial u_x / \partial x$ need to be evaluated first from fractional derivatives point of view:

$$u_x = - \left[K_+ \left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) + K_- \left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \right] \quad (\text{B.22})$$

Assuming the spacial domain considered is: $[L, R] = [0, 2]$ in time interval: $[0, N] = [0, 1]$.

Let: $K_+ = K_{const} x^\gamma$; $K_- = K_{const} (x_{end} - x)^\gamma \rightarrow K_- = K_{const} (2 - x)^\gamma$.

Substituting Each in Equation (B.22), the equation becomes:

$$u_x = - \left[K_{const} x^\gamma \left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) + K_{const} (2 - x)^\gamma \left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) \right] \quad (\text{B.23})$$

Finding each fractional derivative expansion:

$$[A] = \left(\frac{\partial^\gamma p}{\partial_+ x^\gamma} \right) = \frac{\partial^\gamma}{\partial_+ x^\gamma} [4 \exp(-t) x^2 (2 - x)^2] \rightarrow [A] = [4 \exp(-t)] \frac{\partial^\gamma}{\partial_+ x^\gamma} [x^2 (2 - x)^2] \quad (\text{B.24})$$

Expanding the parenthesis:

$$[A] = [4 \exp(-t)] \frac{\partial^\gamma}{\partial_+ x^\gamma} [4x^2 - 4x^3 + x^4] \quad (\text{B.25})$$

Applying Table A.4 fractional derivative on the L limit of the assumed spacial domain: $[L, R] = [0, 2]$, the equation becomes:

$$\frac{\partial^\gamma}{\partial_+ x^\gamma} (x - L)^p = \frac{\Gamma(p + 1)}{\Gamma(p + 1 - \gamma)} (x - L)^{p - \gamma} \rightarrow \frac{\partial^\gamma}{\partial_+ x^\gamma} (x)^p = \frac{\Gamma(p + 1)}{\Gamma(p + 1 - \gamma)} (x)^{p - \gamma} \quad (\text{B.26})$$

Applying Equation (B.26) expansion on Equation (B.25) derivatives, the equation becomes:

$$[A] = 4 \exp(-t) \left\{ 4 \frac{\Gamma(2 + 1)}{\Gamma(2 + 1 - \gamma)} (x)^{2 - \gamma} - 4 \frac{\Gamma(3 + 1)}{\Gamma(3 + 1 - \gamma)} (x)^{3 - \gamma} + \frac{\Gamma(4 + 1)}{\Gamma(4 + 1 - \gamma)} (x)^{4 - \gamma} \right\} \quad (\text{B.27})$$

$$[A] = 4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3 - \gamma)} (x)^{2 - \gamma} - 4 \frac{\Gamma(4)}{\Gamma(4 - \gamma)} (x)^{3 - \gamma} + \frac{\Gamma(5)}{\Gamma(5 - \gamma)} (x)^{4 - \gamma} \right\} \quad (\text{B.28})$$

$$[B] = \left(\frac{\partial^\gamma p}{\partial_- x^\gamma} \right) = \frac{\partial^\gamma}{\partial_- x^\gamma} [4 \exp(-t) x^2 (2 - x)^2] \rightarrow [B] = [4 \exp(-t)] \frac{\partial^\gamma}{\partial_- x^\gamma} [x^2 (2 - x)^2]$$

Let $y = x - 2 \rightarrow x = y + 2$. Substituting it into: $x^2(2 - x)^2$ gives: $(y + 2)^2(2 - (y + 2))^2$. This can be expanded into: $(y + 2)^2 y^2$. Expanding the parenthesis, this would give: $4y^2 + 4y^3 + y^4$.

Substituting each y by its value, we end up with: $4(x - 2)^2 + 4(x - 2)^3 + (x - 2)^4$. Taking the negative outside each parenthesis, we end up with: $4(-(2 - x))^2 + 4(-(2 - x))^3 + (-(2 - x))^4$.

Applying the exponent on each parenthesis: $4(2-x)^2 - 4(2-x)^3 + (2-x)^4$. As a result, Equation (B.28) can be rewritten as:

$$[B] = 4 \exp(-t) \frac{\partial^\gamma}{\partial_- x^\gamma} [4(2-x)^2 - 4(2-x)^3 + (2-x)^4] \quad (\text{B.29})$$

Applying Table A.4 fractional derivative on the R limit of the assumed spacial domain: $[L, R] = [0, 2]$, the equation becomes:

$$\frac{\partial^\gamma}{\partial_- x^\gamma} (2-x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-\gamma)} (2-x)^{p-\gamma} \quad (\text{B.30})$$

Applying Equation (B.30) expansion on Equation (B.29) derivatives, the equation becomes:

$$[B] = 4 \exp(-t) \left\{ 4 \frac{\Gamma(2+1)}{\Gamma(2+1-\gamma)} (2-x)^{2-\gamma} - 4 \frac{\Gamma(3+1)}{\Gamma(3+1-\gamma)} (2-x)^{3-\gamma} + \frac{\Gamma(4+1)}{\Gamma(4+1-\gamma)} (2-x)^{4-\gamma} \right\}$$

$$[B] = 4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} (2-x)^{2-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} (2-x)^{3-\gamma} + \frac{\Gamma(5)}{\Gamma(5-\gamma)} (2-x)^{4-\gamma} \right\} \quad (\text{B.31})$$

Substituting Equations (B.27) and (B.31) into Equation (B.23):

$$u_x = - \left[K_{const} x^\gamma \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} (x)^{2-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} (x)^{3-\gamma} + \frac{\Gamma(5)}{\Gamma(5-\gamma)} (x)^{4-\gamma} \right\} \right) + \right.$$

$$\left. K_{const} (2-x)^\gamma \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} (2-x)^{2-\gamma} - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} (2-x)^{3-\gamma} + \frac{\Gamma(5)}{\Gamma(5-\gamma)} (2-x)^{4-\gamma} \right\} \right) \right]$$

This can be simplified as:

$$u_x = - \left[K_{const} \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} (x)^2 - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} (x)^3 + \frac{\Gamma(5)}{\Gamma(5-\gamma)} (x)^4 \right\} \right) + \right.$$

$$\left. K_{const} \left(4 \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} (2-x)^2 - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} (2-x)^3 + \frac{\Gamma(5)}{\Gamma(5-\gamma)} (2-x)^4 \right\} \right) \right] \quad (\text{B.32})$$

Simplifying further:

$$u_x = - 4 K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \right.$$

$$\left. \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \quad (\text{B.33})$$

Its derivative can be found simply by expanding the parenthesis:

$$x^2 + (2-x)^2 = x^2 + 4 - 4x + x^2 = 4 - 4x + 2x^2$$

$$x^3 + (2-x)^3 = x^3 + 2^3 - 3(2^2)x + 3(2)x^2 - x^3 = 8 - 12x + 6x^2$$

$$x^4 + (2-x)^4 = x^4 + (2-x)^2(2-x)^2 = x^4 + (4-4x+x^2)(4-4x+x^2) = 16 - 32x + 24x^2 - 8x^3 + 2x^4$$

Substituting all in Equation (B.33):

$$u_x = - 4 K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [4 - 4x + 2x^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [8 - 12x + 6x^2] + \right.$$

$$\left. \frac{\Gamma(5)}{\Gamma(5-\gamma)} [16 - 32x + 24x^2 - 8x^3 + 2x^4] \right\}$$

$$\partial u_x / \partial x = - 4 K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \right.$$

$$\left. \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-32 + 48x - 24x^2 + 8x^3] \right\} \quad (\text{B.34})$$

Now Equations (B.33) and (B.34) can be used in computing the terms T_2 and T_3 .

$$T_2 = \rho \frac{\partial u_x}{\partial x} \quad (\text{B.35})$$

Substituting the values into Equation (B.35):

$$T_2 = - 4 \rho K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-32 + \right.$$

$$\left. 48x - 24x^2 + 8x^3] \right\} \quad (\text{B.36})$$

$$T_3 = u_x \frac{\partial \rho}{\partial x} \quad (\text{B.37})$$

Finding the derivative:

$$\frac{\partial \rho}{\partial x} = \frac{\partial}{\partial x} \{ \rho^0 \exp(c_f[p - p^0]) \} \quad (\text{B.38})$$

Substituting p by its assumed analytical value:

$$\frac{\partial \rho}{\partial x} = \frac{\partial}{\partial x} \{ \rho^0 \exp(c_f[4 \exp(-t) x^2(2-x)^2 - 4x^2(2-x)^2]) \} \quad (\text{B.39})$$

This can be simplified as:

$$\frac{\partial \rho}{\partial x} = \frac{\partial}{\partial x} \{ \rho^0 \exp(4c_f [\exp(-t) - 1] [x^2(2-x)^2]) \} \quad (\text{B.40})$$

Expanding the x parenthesis:

$$\frac{\partial \rho}{\partial x} = \frac{\partial}{\partial x} \{ \rho^0 \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) \} \quad (\text{B.41})$$

Applying the exponential derivative rule: $\partial/\partial x (e^u) = \partial u/\partial x e^u$ on Equation (B.41):

$$\frac{\partial \rho}{\partial x} = 4 \rho^0 c_f [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) \quad (\text{B.42})$$

Substituting (B.33) and (B.42) into (B.37):

$$T_3 = -4 K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} 4 \rho^0 c_f [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4])$$

This can be simplified as:

$$T_3 = -16 K_{const} \rho^0 c_f \exp(-t) \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \quad (\text{B.43})$$

Substituting all T_1, T_2 , and T_3 in Equation (B.18):

$$-4 \varphi c_f \rho \exp(-t) x^2(2-x)^2 - 4 \rho K_{const} \exp(-t) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-32 + 48x - 24x^2 + 8x^3] \right\} - (4)(4) K_{const} \rho^0 c_f \exp(-t) \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} = Q$$

Since $\rho = \rho^0 \exp(c_f [p - p^0])$, this can be simplified as:

$$-4 \exp(-t) \left\{ \varphi c_f \rho x^2(2-x)^2 + K_{const} \left[\rho \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-32 + 48x - 24x^2 + 8x^3] \right\} + 4 \rho^0 c_f \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \right] \right\} = Q$$

This can be further simplified as:

$$-4 \exp(-t) \left\{ \varphi c_f \rho x^2(2-x)^2 + K_{const} \left[\rho \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-8 + 12x - 6x^2 + 2x^3] \right\} + 4 \rho^0 c_f \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \right] \right\} = Q$$

$$-4 \exp(-t) \left\{ \varphi c_f \rho x^2(2-x)^2 + 4K_{const} \left[\rho \left\{ \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-8 + 12x - 6x^2 + 2x^3] \right\} + \rho^0 c_f \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \right] \right\} = Q \quad (\text{B.44})$$

The source Q can also be computed using a different sign as:

$$Q = +4 \exp(-t) \left\{ \varphi c_f \rho x^2(2-x)^2 + 4K_{const} \left[\rho \left\{ \frac{\Gamma(3)}{\Gamma(3-\gamma)} [-4 + 4x] - \frac{\Gamma(4)}{\Gamma(4-\gamma)} [-12 + 12x] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [-8 + 12x - 6x^2 + 2x^3] \right\} + \rho^0 c_f \exp(4c_f [\exp(-t) - 1] [4x^2 - 4x^3 + x^4]) [\exp(-t) - 1] (8x - 12x^2 + 4x^3) \left\{ 4 \frac{\Gamma(3)}{\Gamma(3-\gamma)} [(x)^2 + (2-x)^2] - 4 \frac{\Gamma(4)}{\Gamma(4-\gamma)} [(x)^3 + (2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4] \right\} \right] \right\}$$

$$(2-x)^3] + \frac{\Gamma(5)}{\Gamma(5-\gamma)} [(x)^4 + (2-x)^4]\}} \quad (\text{B.45})$$

Such that Equation (B.44) numerically indicates injection and Equation (B.45) numerically indicates production.

C. Illustration example of GL formulas expansion in PPA scheme

Equation (33) GL formulas expansion is clarified by example in this section of the appendix. For simplification reasons, let the equation be written as:

$$p_{i+0.5}^{n+1} - S^{R+}(A) + S^{L+}(B) - S^{R-}(C) + S^{L-}(D) = \frac{\Delta t}{c_{i+0.5}} Q_{i+0.5} + p_{i+0.5}^n$$

$(A) = \sum_{k=0}^{i+1} g_k^\gamma p_{i+1.5-k}^{n+1}$	$(B) = \sum_{k=0}^i g_k^\gamma p_{i+0.5-k}^{n+1}$	$(C) = \sum_{k=0}^{M-i-1} g_k^\gamma p_{i+0.5+k}^{n+1}$	$(D) = \sum_{k=0}^{M-i} g_k^\gamma p_{i-0.5+k}^{n+1}$
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Expansions (A-D) are applied on each grid cell of a 1D domain with $M = 5 \rightarrow [L, R] = [0, 5]$ as illustrated in Table C.1.

Index i	Expansion
0	$(A) = g_0^\gamma p_{1.5} + g_1^\gamma p_{0.5}$
	$(B) = g_0^\gamma p_{0.5}$
	$(C) = g_0^\gamma p_{0.5} + g_1^\gamma p_{1.5} + g_2^\gamma p_{2.5} + g_3^\gamma p_{3.5} + g_4^\gamma p_{4.5}$
	$(D) = g_0^\gamma p_{BL} + g_1^\gamma p_{0.5} + g_2^\gamma p_{1.5} + g_3^\gamma p_{2.5} + g_4^\gamma p_{3.5} + g_5^\gamma p_{4.5}$
	Variable p_{BL} indicates the pressure assumed at the left boundary of the 1D domain.
1	$(A) = g_0^\gamma p_{2.5} + g_1^\gamma p_{1.5} + g_2^\gamma p_{0.5}$
	$(B) = g_0^\gamma p_{1.5} + g_1^\gamma p_{0.5}$
	$(C) = g_0^\gamma p_{1.5} + g_1^\gamma p_{2.5} + g_2^\gamma p_{3.5} + g_3^\gamma p_{4.5}$
	$(D) = g_0^\gamma p_{0.5} + g_1^\gamma p_{1.5} + g_2^\gamma p_{2.5} + g_3^\gamma p_{3.5} + g_4^\gamma p_{4.5}$
2	$(A) = g_0^\gamma p_{3.5} + g_1^\gamma p_{2.5} + g_2^\gamma p_{1.5} + g_3^\gamma p_{0.5}$
	$(B) = g_0^\gamma p_{2.5} + g_1^\gamma p_{1.5} + g_2^\gamma p_{0.5}$
	$(C) = g_0^\gamma p_{2.5} + g_1^\gamma p_{3.5} + g_2^\gamma p_{4.5}$
	$(D) = g_0^\gamma p_{1.5} + g_1^\gamma p_{2.5} + g_2^\gamma p_{3.5} + g_3^\gamma p_{4.5}$
3	$(A) = g_0^\gamma p_{4.5} + g_1^\gamma p_{3.5} + g_2^\gamma p_{2.5} + g_3^\gamma p_{1.5} + g_4^\gamma p_{0.5}$
	$(B) = g_0^\gamma p_{3.5} + g_1^\gamma p_{2.5} + g_2^\gamma p_{1.5} + g_3^\gamma p_{0.5}$
	$(C) = g_0^\gamma p_{3.5} + g_1^\gamma p_{4.5}$
	$(D) = g_0^\gamma p_{2.5} + g_1^\gamma p_{3.5} + g_2^\gamma p_{4.5}$
4	$(A) = g_0^\gamma p_{BR} + g_1^\gamma p_{4.5} + g_2^\gamma p_{3.5} + g_3^\gamma p_{2.5} + g_4^\gamma p_{1.5} + g_5^\gamma p_{0.5}$
	$(B) = g_0^\gamma p_{4.5} + g_1^\gamma p_{3.5} + g_2^\gamma p_{2.5} + g_3^\gamma p_{1.5} + g_4^\gamma p_{0.5}$
	$(C) = g_0^\gamma p_{4.5}$
	$(D) = g_0^\gamma p_{3.5} + g_1^\gamma p_{4.5}$
	Variable p_{BR} indicates the pressure assumed at the right boundary of the 1D domain.

Using these expansions, the $A_{i,j}$ matrix generated for this example is:

	$p_{0.5}$	$p_{1.5}$	$p_{2.5}$	$p_{3.5}$	$p_{4.5}$
$p_{0.5}$	$1 - S^{R+}g_1^\gamma$ $+ S^{L+}g_0^\gamma$ $- S^{R-}g_0^\gamma$ $+ S^{L-}g_1^\gamma$	$-S^{R+}g_0^\gamma$ $- S^{R-}g_1^\gamma$ $+ S^{L-}g_2^\gamma$	$-S^{R-}g_2^\gamma$ $+ S^{L-}g_3^\gamma$	$-S^{R-}g_3^\gamma$ $+ S^{L-}g_4^\gamma$	$-S^{R-}g_4^\gamma$ $+ S^{L-}g_5^\gamma$
$p_{1.5}$	$-S^{R+}g_2^\gamma$ $+ S^{L+}g_1^\gamma$ $+ S^{L-}g_0^\gamma$	$1 - S^{R+}g_1^\gamma$ $+ S^{L+}g_0^\gamma$ $- S^{R-}g_0^\gamma$ $+ S^{L-}g_1^\gamma$	$-S^{R+}g_0^\gamma$ $- S^{R-}g_1^\gamma$ $+ S^{L-}g_2^\gamma$	$-S^{R-}g_2^\gamma$ $+ S^{L-}g_3^\gamma$	$-S^{R-}g_3^\gamma$ $+ S^{L-}g_4^\gamma$
$p_{2.5}$	$-S^{R+}g_3^\gamma$ $+ S^{L+}g_2^\gamma$	$-S^{R+}g_2^\gamma$ $+ S^{L+}g_1^\gamma$ $+ S^{L-}g_0^\gamma$	$1 - S^{R+}g_1^\gamma$ $+ S^{L+}g_0^\gamma$ $- S^{R-}g_0^\gamma$ $+ S^{L-}g_1^\gamma$	$-S^{R+}g_0^\gamma$ $- S^{R-}g_1^\gamma$ $+ S^{L-}g_2^\gamma$	$-S^{R-}g_2^\gamma$ $+ S^{L-}g_3^\gamma$
$p_{3.5}$	$-S^{R+}g_4^\gamma$ $+ S^{L+}g_3^\gamma$	$-S^{R+}g_3^\gamma$ $+ S^{L+}g_2^\gamma$	$-S^{R+}g_2^\gamma$ $+ S^{L+}g_1^\gamma$ $+ S^{L-}g_0^\gamma$	$1 - S^{R+}g_1^\gamma$ $+ S^{L+}g_0^\gamma$ $- S^{R-}g_0^\gamma$ $+ S^{L-}g_1^\gamma$	$-S^{R+}g_0^\gamma$ $- S^{R-}g_1^\gamma$ $+ S^{L-}g_2^\gamma$
$p_{4.5}$	$-S^{R+}g_5^\gamma$ $+ S^{L+}g_4^\gamma$	$-S^{R+}g_4^\gamma$ $+ S^{L+}g_3^\gamma$	$-S^{R+}g_3^\gamma$ $+ S^{L+}g_2^\gamma$	$-S^{R+}g_2^\gamma$ $+ S^{L+}g_1^\gamma$ $+ S^{L-}g_0^\gamma$	$1 - S^{R+}g_1^\gamma$ $+ S^{L+}g_0^\gamma$ $- S^{R-}g_0^\gamma$ $+ S^{L-}g_1^\gamma$

- Homogeneous Darcy setting can't show heterogeneity effects of fractured media flows.
- Non-Newtonian Non-Darcy Fractional derivatives are used for such configurations.
- A physics preserving locally conservative averaging scheme is proposed to solve them.
- The proposed scheme is based on Grunwald-Letnikov approximation.
- It allows using single-continuum models to deal with such complexities.