Developing a New Three-Dimensional Finite-Difference Explicit in Time Solver Package for MODFLOW

Babak Azari

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DEVELOPING A NEW THREE-DIMENSIONAL FINITE-Difference
EXPLICIT IN TIME SOLVER PACKAGE FOR MODFLOW

by

Babak Azari

A Dissertation

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy

Major: Civil Engineering

The University of Memphis

August 2023
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Acknowledgements

I would like to express my profound gratitude to all the individuals and institutions who have been instrumental in the successful completion of my dissertation. Foremost, I want to extend my heartfelt appreciation to my primary advisor, Dr. Brian Waldron, for his unwavering support, guidance, and expertise throughout my research journey. His mentorship has greatly influenced my future path.

I am sincerely thankful to my dissertation committee members, Dr. Farhad Jazaei, Dr. Charles Camp, and Dr. Vivek Bedekar, for their valuable perspectives, constructive feedback, and scholarly contributions that have significantly enhanced the quality of my work. I am deeply grateful for the time and dedication they have devoted to my research.

The Civil Engineering Department of the University of Memphis deserves my utmost appreciation for providing a nurturing academic environment and the necessary resources for my research endeavors.

I would also like to acknowledge the invaluable collaboration and assistance provided by the Center for Applied Earth Science and Engineering Research (CAESER), which has greatly expanded the scope and impact of my work. The support and camaraderie of my colleagues and friends have been invaluable in shaping my ideas and refining my research through their encouragement, insightful discussions, and shared experiences.

Lastly, my deepest gratitude goes to my family for their unwavering love, encouragement, and understanding. Their constant support and belief in my abilities have been a constant source of motivation and strength. I would like to express a special thanks to my spouse for their exceptional support, patience, and sacrifices that have enabled me to pursue my academic aspirations.
Abstract

Integrating existing surface water (SW) and groundwater (GW) models like SWAT, MODFLOW, and HEC-RAS has been explored to simulate the complexities of SW-GW interactions. Still, challenges arise from temporal and spatial scale disparities. To tackle the temporal scale issue, this study introduces the novel explicit solver (EXP1) for MODFLOW 2005, enabling daily GW modeling similar to SWAT and HEC-RAS by reducing runtime and computational burden.

The proposed solver incorporates a stability criterion to assess the stability of the proposed solver. The study compared the EXP1 solver to the widely used Preconditioned Conjugate Gradient (PCG) solver in three scenarios: a 1D model, a 2D model, and the real-world model, which was MERAS. The results showed the efficiency and accuracy of the EXP1 solver in the 1D and 2D models, with minimal deviations in head and water budget compared to PCG and shorter runtimes. However, when applied to the complex MERAS model, some modifications were necessary to ensure stability and accuracy.

Stability analysis identified the main culprits of instability, including extremely small cell thicknesses, specific storages, and large external sources/sinks. Remarkably, unconfined cells exhibited high stability when a 1-day time step was chosen, attributed to the fact that the specific yield in unconfined aquifers is several orders of magnitude larger than that of confined cells.

While a 1-day time step was preferred and increasing cell sizes impractical, unstable cells were converted to constant heads to achieve stability. The EXP1 solver demonstrated a 57% faster speed than PCG while maintaining comparable head accuracy. A water budget comparison showed over 10% discrepancy due to many constant head cells.
To address the 1-day comparison issues, an additional assessment was conducted using a 0.01-day time step, where the EXP1 solver still performed faster and accurately in terms of GW head and water budgets.

These findings indicate that the EXP1 solver is an excellent choice for modeling unconfined aquifers, which are of great interest in SW-GW model couplings due to the characteristics of unconfined cells. Conversely, implicit solvers like PCG should be the preferred option for standalone groundwater modeling to avoid stability issues.
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Introduction

Water resources worldwide are experiencing pressure in demand because of rapid increases in world population, climate change, and economic growth (United Nations Educational, 2004). Water shortages, water quality deterioration, and flooding are among the most urgent problems that raise the necessity for effectively managing water resources (Graham et al. 2005). Numerical models benefit water management by providing alternative solutions to complex problems that assist decision-makers in making informed decisions (Abdulla & Al-Assa’d, 2006; M. Sophocleous, 2002; Wen et al. 2007). Recently, more attention has been given to the interaction between groundwater (GW) and surface water (SW) resources, as they are primarily sources for public water supply and agricultural and industrial purposes (Cao et al. 2013; Ehtiat et al. 2018; Wu et al. 2009). GW and SW are being treated less as two separate processes (Bailey et al. 2016; Kim et al. 2008a; Wang & Chen, 2021) but instead integrated as encountered in natural systems (Deb et al. 2019; Kamali & Niksokhan, 2017; Ke, 2014; Pulido-Velazquez et al. 2015; Wang & Chen, 2021).

Many numerical models that simulate GW-SW interaction are specialized in one of the processes (i.e., GW or SW). The U.S. Department of Agriculture model, SWAT (Soil and Water Assessment Tool), predicts the impacts of land-management practices (typically agricultural) on water flow, sediment transport, and nutrient mass transport at the watershed scale (Arnold et al. 1998; Neitsch et al. 2011; M. Sophocleous & Perkins, 2000). SWAT simulates runoff using the Soil Conservation Service (SCS) method and routes surface water flow to adjoining watersheds. SWAT also models groundwater for bi-directional water exchange between the unsaturated and saturated zones and accounting of water loss from the model to deep recharge (Arnold et al. 1998).
However, the SWAT model is a lumped parameter model where groundwater parameters like hydraulic conductivity are distributed parameters. Thus, SWAT cannot represent aquifer heterogeneity and spatially distributed recharge and groundwater levels (Kim et al. 2008b). Additionally, SWAT’s inclusion of GW is treated solely as a mass exchange (Jafari et al. 2021a; Neitsch et al. 2011; P. W. Gassman et al. 2007; Rumph Frederiksen & Molina-Navarro, 2021)

FEMWATER (Lin et al. 1997) and MODFLOW (Harbaugh, 2005) are primarily GW models that do include surface water exchange but without accounting for surface processes that govern runoff (Lin et al. 1997; McDonald & Harbaugh, 1984). In the context of MODFLOW, the River module (Harbaugh, 2005) is used to incorporate surface processes. However, it does not directly simulate river reach connectivity or routing. Meanwhile, the Stream module (Harbaugh, 2005) can help address some limitations of the River module (Langevin et al. 2017; Prudic et al. 2004). It serves as a rudimentary surface water simulator, but it still has inherent limitations, particularly when it comes to accounting for bank storage and variable riverbed infiltration (P. Brunner et al. 2010).

FEFLOW is a finite element groundwater model that considers surface water bodies like rivers and lakes as constant or varying head boundary conditions to simulate GW and SW interactions (DHI, 2015; Diersch, 2005)

HEC-RAS (Brunner, 1995) is a numerical modeling software primarily designed for 1D and 2D surface flow simulations. However, when it comes to modeling SW and GW interactions, HEC-RAS has limitations in comprehensively considering such dynamics. Its capability is mainly focused on incorporating the groundwater head as a boundary condition and calculating the flow into the stream using Darcy's equation (Brunner, 1995). Consequently, HEC-RAS is not equipped to comprehensively represent the intricate nature of GW and its interactions with SW.
Over the past two decades, researchers have used model coupling to take advantage of a model’s strength, whether their primary function was to simulate GW, SW, or surface processes (Guzman et al. 2015; Jafari et al. 2021b, M. A. Sophocleous et al. 1999). For example, Krause et al. (2007) developed a coupled SW-GW model called Integrated Water Balance and Nutrient Dynamics Model (IWAN), whereby surface water processes (runoff on the floodplain and open-channel flow) interact in a bi-directional fashion with MODFLOW where water movement in the unsaturated zone was modeled using WASIM-ETH-I model (Schulla & Jasper, 2007), which is a deterministic, spatially distributed hydrological model. Surface water interaction with the groundwater is modeled using the River package (RIV) (Harbaugh, 2005) in MODFLOW. Input to and outputs from WASIM-ETH-I routines are passed to MODFLOW via its Recharge package (RCH) (Harbaugh, 2005) using a non-iterative approach. Xu et al. (2012) coupled MODFLOW with the Soil-Water-Atmospheric-Plant (SWAP) model (Kroes & Van Dam, 2003). MODFLOW simulated the saturated zone, while SWAP simulated vertical water movement through the vadose zone, considering salt and heat transport to predict crop productivity. SWAP calculated recharge and evapotranspiration fluxes for input into MODFLOW. MODFLOW and SWAP iteratively converge toward approximate water table head values over multiple SWAP time steps within a single MODFLOW time step. Sophocleous et al. (1999) developed SWATMOD, which coupled SWAT and MODFLOW to evaluate long-term land management practices in the Rattlesnake Creek basin in central Kansas, USA, with moderate success. More recently, Bailey et al. (2016) coupled SWAT with MODFLOW to model SW-GW interaction in the Sprague River watershed in southern Oregon, USA. The deep percolation output from SWAT was passed to MODFLOW as recharge, and simulated GW-SW water fluxes from MODFLOW were passed to the stream channels within SWAT. In another study by Peña-Haro et al. (2012), WOFOST (Van Diepen et
al. 1989), HYDRUS-1D (Simunek et al. 1998), and MODFLOW were coupled to simulate the interaction between crop growth and unsaturated-saturated flow processes. In this coupled model, WOFOST (Van Diepen et al. 1989) calculated the Leaf Area Index (LAI) and rooting depth and sent them as input to HYDRUS-1D. HYDRUS-1D passed its estimates on evapotranspiration and recharge to WOFOST and MODFLOW, respectively. MODFLOW was used to calculate the GW heads and return them to the HYDRUS-1D (Kanda et al. 2018). Lastly, Fenske et al. (2011) successfully coupled MODFLOW and HEC-RAS using the European open interfacing language, OpenMI, which allows the two models to remain autonomous in their coding, yet co-dependent via the transfer of model parameters. This approach contrasts a fully integrated coupling of HEC-RAS and MODFLOW developed by Rodriguez et al. (2008) that uses the MODFLOW DRAIN package (DRN) (Harbaugh, 2005) as the connector between the two models.

There are also fully integrated models like MIKE SHE (Refshaard & Storm, 1995) that incorporates many hydrologic processes into its simulation (Graham et al. 2005; Refshaard & Storm, 1995) and CATHY (Niu et al. 2014), which targets catchment scale simulation and is capable of three-dimensional GW and one-dimensional SW modeling (Dean et al. 2016; Niu et al. 2014). However, the most significant disadvantage of MIKE SHE and CATHY is that they are physically based, distributed parameter models that need vast amounts of data and numerous parameters which can be challenging to obtain in many real-world cases (Graham et al. 2005; M. Sophocleous & Perkins, 2000; Wang & Chen, 2021; Yan et al. 2004).

The concept of coupled models can be divided into "loosely coupled" and "fully coupled" (Guevara-Ochoa et al. 2020). Loosely coupled models are the traditional approach to model coupling (Dangol et al. 2022; Panday & Huyakorn, 2004), where outputs of one model are transferred into the next model as an input without a cyclic return of information back to the initial
model for correction or reconsideration. Fully coupled models follow a dynamic process governing the exchange of information between the models, whereby data exchange continues between the models until they reach convergence before moving to the next time step (Aliyari et al. 2019a). Regarding fully coupled hydrological models, Dehghanipour et al. (2019) coupled WEAP (Sieber, 2006), a water resource planning software, and MODFLOW fully coupled to simulate SW-GW interaction in irrigated plains. Vincendon et al. (2010) developed a fully coupled model by combining ISBA (Noilhan & Planton, 1989) with TOPMODEL (Beven & Freer, 2001), which are land-surface and hydrological models, respectively, to simulate soil water content inputs for forecasting the intensity and time of flood peaks. Tian et al. (2015) combined GSFLOW, a coupled GW and SW model developed by the USGS (Markstrom et al. 2012), and the EPA SWMM (Gironás et al. 2010), an urban runoff quality and quantity model, to simulate agricultural water use impacts.

Coupled models reveal two key complications: matching temporal and spatial scales (Bailey et al. 2016; Chunn et al. 2019). Surface processes change on a daily scale (e.g., river discharge, runoff, plant uptake) and manifest themselves as linear or area features that do not match slower processes (e.g., GW flow) that change monthly to yearly and are represented over large space domains (e.g., finite difference cells or finite elements). For example, SWAT’s surface processes act on a daily scale in hydrologic representative units (Arnold et al. 1998; Bailey et al. 2016), HEC-RAS models open channel flow at one-day time steps capable of simulating flow on a detailed terrain (1-m resolution) (Furman, 2008; Gassman et al. 2007; Rodriguez et al. 2008), and MODFLOW simulates GW flow often at large time scales (monthly or yearly) and any range of cell sizes (especially MODFLOW 6 with an unstructured grid) (Harbaugh, 2005; Langevin et al. 2017). Hence, the idea of coupling surface processes (SWAT) with HEC-RAS (runoff and stream flow)
and MODFLOW (GW flow) would be complicated due to the mismatch in spatial and temporal elements. This raises the question of if MODFLOW could use one-day time steps to simulate stress periods, similar to the popular SWAT and HEC-RAS models.

Under MODFLOW’s current structure, the code breaks down the partial differential equation for GW flow using an implicit time step method due to its proved stability (Psilovikos, 2017); however, this requires an inversion of the solution matrix. Matching the temporal structure of SWAT and HEC-RAS, using one-day stress periods in MODFLOW, may prove burdensome for large, complex models that would only be exacerbated in a fully-coupled model architecture owing to the iterative dual passage of information. However, the MODFLOW formulation could be solved explicitly at one-day stress periods, thereby not requiring matrix inversion and possibly outperforming the implicit solvers. If this was the case, in our example, SWAT, HEC-RAS, and MODFLOW could be fully coupled, and the temporal challenge would be eliminated, thereby reducing the key complications to only one (i.e., spatial). Additionally, despite stability issues, solving a set of governing equations explicitly in time could increase the accuracy of the results depending on the technique used (Aly et al. 2018; Bailey et al. 2016; Chunn et al. 2019; Dehghan, 2006; Roberts & Selim, 1984).

The review of model coupling efforts in groundwater research indicates that the majority of researchers have utilized either MODFLOW 2005 or MODFLOW NWT (Abbas et al. 2022; Aliyari et al. 2019a; Bezabih & Alemayehu, 2022; Dehghanipour et al. 2019; Francés & Lubczynski, 2023; Gao et al. 2019; Hou et al. 2020; Jafari et al. 2021a; Jaxa-Rozen et al. 2019; Molina-Navarro et al. 2019; Niswonger et al. 2011; Ware et al. 2023). MODFLOW NWT (Niswonger et al. 2011) is a standalone version of MODFLOW, built on the same structure as MODFLOW 2005. It features its own flow and solver packages, designed to improve stability in
groundwater modeling problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation where other solvers within MODFLOW 2005 may struggle to converge (Niswonger et al. 2011).

Therefore, MODFLOW 2005 was chosen as the platform to develop the new solver primarily because of its widespread usage (standalone or serving as another model’s base) in research involving model coupling. MODFLOW 2005 has been standard code for GW modeling and extensively employed in various studies related to the coupling of groundwater models with other disciplines, such as surface water modeling, hydrological modeling, and environmental impact (Aliyari et al. 2019b; Gao et al. 2019; Hou et al. 2020; Jaxa-Rozen et al. 2019; Molina-Navarro et al. 2019; Wang & Chen, 2021). Its robustness, flexibility, and compatibility with different modeling approaches make it a popular choice for researchers investigating the interactions between groundwater and other environmental components. Utilizing MODFLOW 2005 as the foundation for developing the new solver ensures compatibility with existing modeling frameworks and facilitates seamless integration with other simulation components in coupled modeling studies. Hence, this paper explores the development of an explicit solver for MODFLOW 2005 that attempts to stabilize convergence to a one-day stress period to match those time steps of the more common surface process models HEC-RAS and SWAT.
Methods

MODFLOW implicit formulation

MODFLOW 2005 uses the diseized GW partial differential equation (PDE) using the Finite difference method and implicit in time scheme. Using an implicit time-step approach, Equation (1) shows MODFLOW’s FDM discretization of GW flow in an anisotropic and heterogeneous aquifer. A full description of how the equation had been driven can be found in Harbaugh (2005).

\[ CR_{i,j-\frac{1}{2},k} h_{i,j-1,k}^{t+1} + CR_{i,j+\frac{1}{2},k} h_{i,j+1,k}^{t+1} + CC_{i-\frac{1}{2},j,k} h_{i-1,j,k}^{t+1} + CC_{i+\frac{1}{2},j,k} h_{i+1,j,k}^{t+1} + CV_{i,j,k-\frac{1}{2}} h_{i,j,k-1}^{t+1} + CV_{i,j,k+\frac{1}{2}} h_{i,j,k+1}^{t+1} - \left( CR_{i,j-\frac{1}{2},k} + CR_{i,j+\frac{1}{2},k} CC_{i-\frac{1}{2},j,k} + CC_{i+\frac{1}{2},j,k} + CV_{i,j,k-\frac{1}{2}} + CV_{i,j,k+\frac{1}{2}} + HCOFi,j,k \right) h_{i,j,k}^{t+1} = RHS_{i,j,k} \]

Where:

\[ HCOFi,j,k = P_{i,j,k} \frac{SS_{i,j,k} \Delta r \Delta c \Delta v_k}{\Delta t} \]

\[ RHS_{i,j,k} = -Q_{i,j,k} - SS_{i,j,k} (\Delta r \Delta c \Delta v_k) \frac{h_{i,j,k}^{t}}{\Delta t} \]

In reference to cell \( i, j, k \), \( CR, CC \), and \( CV \) are the row, column, and vertical conductance from six adjacent cells, respectively; \( P_{i,j,k} \) is the coefficient for head-dependent external source/sink; \( SS_{i,j,k} \) is the storage coefficient; \( \Delta r, \Delta c \) and \( \Delta v_k \) are cell dimensions along the row, column, and vertical direction, respectively; \( \Delta t \) is the current time step size, \( Q_{i,j,k} \) is head independent external source/sink; and \( h_{i,j,k}^{t} \) and \( h_{i,j,k}^{t+1} \) are the heads in the previous (\( t \)) and current time (\( t + 1 \)) steps, respectively. The only known head in Equation (8) is \( h_{i,j,k}^{t} \) and all other heads in time \( t + 1 \) are unknown.

So, assume that there are \( n \) cells within a model, which means \( n \) unknown heads at time step \( t + 1 \) and \( n \) equations to be solved. Therefore, to obtain heads at time step \( t + 1 \), it is required to solve
a system of \( n \) equations simultaneously. The matrix form of a system of equations for an implicit in-time approach is shown in Equation (2):

\[
[A]{h} = \{\text{RHS}\}
\]  

(2)

Where: \([A]\) is the matrix of the coefficients of the heads from the left side of Equation (1) for all active nodes in the grid; \{\(h\)\} is the vector of head values at the end of time step \( t+1 \) for all nodes in the grid (i.e., unknown heads); \{\text{RHS}\} is a vector of the known terms for all grid nodes. To solve the above system of equations, \([A]\) needs to be inverted and multiplied by \{\text{RHS}\}, as seen in Equation (3), to obtain heads at the current time step.

\[
\{h\} = [A]^{-1} \times \{\text{RHS}\}
\]  

(3)

Due to their typically large dimensions, inverting the \([A]\) in MODFLOW can be computationally expensive and time-consuming. The choice of solver in MODFLOW determines how matrix inversion is performed. It can be done directly using a Direct Solver package or iteratively using solvers like Preconditioned Conjugate-Gradient (Harbaugh, 1995; Hill, 1990).

**Groundwater Flow Explicit Formulation**

The implicit scheme in groundwater modeling offers advantages in terms of stability and error propagation control between time steps. However, it comes with the drawback of requiring matrix inversion, resulting in extensive computational efforts and longer runtimes. This method becomes particularly burdensome in large models, especially when fully coupling them with models like SWAT and HEC-RAS while aiming for 1-day simulations.
To address this challenge, this research aims to introduce a new explicit solver that can significantly reduce runtime, allowing for faster groundwater flow simulations. The computational burden associated with matrix inversion can be alleviated by successfully implementing the explicit solver, facilitating efficient and accurate simulations within a shorter time frame. This advancement would enable seamless integration and synchronization between different models, enhancing the capabilities of integrated groundwater-surface water modeling systems.

The development of an explicit solver for MODFLOW-2005 followed the code’s modular functionality whereby the solver would be chosen by the user and act as a subroutine call within the code (Harbaugh, 2005). In determining the explicit form of the MODFLOW three-dimensional explicit FDM formulation, head-dependent external stresses (e.g., river/stream, evapotranspiration) were simultaneously solved with the variable heads at the current time step. The explicit formulation for the GW flow equation in an anisotropic, heterogenous medium is shown in Equation (4):

\[
\begin{align*}
CR_{i,j,k} & \frac{1}{2} h_{i,j,k}^t + CR_{i,j,k} h_{i,j,k}^t + CC_{i,j,k} h_{i,j,k}^t + CC_{i,j,k} h_{i,j,k}^t + CV_{i,j,k} h_{i,j,k}^t \quad (4) \\
+ CV_{i,j,k} h_{i,j,k}^t
\end{align*}
\]

\[
\begin{align*}
&+ \left(-CR_{i,j,k} h_{i,j,k}^t - CR_{i,j,k} h_{i,j,k}^t - CC_{i,j,k} h_{i,j,k}^t - CC_{i,j,k} h_{i,j,k}^t - CV_{i,j,k} h_{i,j,k}^t - CV_{i,j,k} h_{i,j,k}^t \right) \\
&+ \left(\frac{SS_{i,j,k}(\Delta r_i \Delta c_i \Delta v_k)}{\Delta t}\right) h_{i,j,k}^t
\end{align*}
\]

\[
= -Q_{i,j,k} + \left(\frac{SS_{i,j,k}(\Delta r_i \Delta c_i \Delta v_k)}{\Delta t}\right) - P_{i,j,k} h_{i,j,k}^{t+1}
\]

where: \(i, j, \text{ and } k\) represent the cell’s position by column, row, and layer, respectively; \(CR, CC, \text{ and } CV\) are the row, column, and vertical conductance from six adjacent cells; \(P_{i,j,k}\) is the coefficient
for head-dependent external source/sink; $SS_{i,j,k}$ is the specific storage; $\Delta r_j$, $\Delta c_i$ and $\Delta v_k$ are cell dimensions along the row, column, and vertical direction, respectively; $t$ is the previous time and $\Delta t$ is the current time step size; $Q_{i,j,k}$ is head independent external source/sink; and $h_{i,j,k}^t$ and $h_{i,j,k}^{t+1}$ are the heads in the previous time ($t$) and current time ($t + 1$) steps, respectively.

Since the head in cell $i,j,k$ at time $t + 1$ ($h_{i,j,k}^{t+1}$) is the only unknown inversion of the coefficient matrix, $[A]$ (see Equation 2), as performed if implicit in time, reverts to a direct matrix multiplied against $\{h\}$ (i.e., heads at the end of the time step, $t$); thereby resulting in an inexpensive and fast procedure to determine heads at the current time step. Therefore, Equation (5) could solve to obtain the heads at the current time step, which are stored in $\{\text{RHS}\}$:

$$[A] \times \{h\} = \{\text{RHS}\} \quad (5)$$

However, it is important to note that the increased speed of the explicit scheme comes at the cost of conditional stability. By implementing appropriate stability criteria and selecting optimal parameter values such as cell and time step sizes, the accuracy of the explicit scheme can be effectively maintained while benefiting from its faster computational performance.

**Stability Criteria**

The explicit solver is anticipated to significantly reduce the computational burden in large problems with strong non-linearity (Jachimavičiené et al. 2014). However, as mentioned before its stability must be addressed. The Von Neumann method (Von Neumann & Richtmyer, 1950) was applied, following others who have used it successfully (Chan, 1984; Li et al. 1994; Miga et al. 1998; Psilovikos, 2017; Tuzikiewicz & Duda, 2015).
In this method $h(x, y, z, t)$ and $\bar{h}(x, y, z, t)$ are the analytical and numerical solutions of Equation (4), respectively. Therefore, the error is written as in Equation (6):

$$h(x, y, z, t) = \bar{h}(x, y, z, t) + \varepsilon_{i,j,k}^t$$

(6)

where: $\varepsilon_{i,j,k}^t$ is the summation of error at node $x$, $y$ and $z$ at time step $t$. The error term is defined using the Fourier series in Equation (7):

$$\varepsilon_{i,j,k}^t = \gamma^t \exp\left(I(s_1x_i + s_2y_j + s_3z_k)\right), I = \sqrt{-1}$$

(7)

where: $\gamma$ is the amplification factor and $s_1$, $s_2$ and $s_3$ are the wavenumbers. Von Neumann’s method requires the amplification factor to be less than unity to call the method stable ($\gamma < 1$) (Psilovikos, 2017). Therefore, by substitution of the $\varepsilon_{i,j,k}^t$ into Equation (4), one can determine the cases for which the explicit solver is stable. The stability criteria resulting from the Von Neumann method for explicit finite different discretization is shown in Equation (8).

$$\Delta t < \frac{SS_{i,j,k}(\Delta r \Delta c \Delta v_k)}{P_{i,j,k} + CR_{i,j-1/2,k} + CR_{i,j+1/2,k} + CC_{i-1/2,j,k} + CC_{i+1/2,j,k} + CV_{i,j,k-1/2} + CV_{i,j,k+1/2}}$$

(8)

The inequality (8) will guarantee the stability of the scheme. Appendix S1 discusses the derivation of Equation (8) in detail. Importantly, the stability criteria demonstrate the stability of individual cells based on their specific characteristics, rather than indicating the overall stability of the model. Therefore, to assess the stability of a model, it is necessary to consider the stability of each active cell within the model. Consequently, the biggest $\Delta t$ that ensures stable modeling is determined by the minimum value among the maximum $\Delta ts$ of all the active cells.
**EXP 1 Solver development**

The explicit scheme solver was developed using Fortran 90 to match the code of MODFLOW-2005. Figure 1 shows the flow of information within the MODFLOW and the explicit solver, called EXP1.

![MODFLOW and EXP1 solver flow chart and information flow (Adopted from Harbaugh (2005))](image-url)
Following the sequencing shown in Figure 1, MODFLOW’s native modules perform the memory allocation and reading of the input files. The stress period loops are created, and variables such as storage coefficients, hydraulic conductivity, and time step sizes are allocated for each stress period. The EXP1 package calculates the stability criteria for each cell and compares them with the time step specified by the user. If the specified time step is smaller than the computed stability criteria, the EXP1 solver formulates the solution. Otherwise, the user will be notified that the selected time step size does not satisfy the stability conditions and shows the biggest required time step size. In this case, the user should update the time step size in model inputs.

The EXP1 solver then formulates the groundwater flow equation and creates the coefficient matrix ([A]) based on Equation (4), and solves it. MODFLOW will iterate through all the stress periods before deallocating memory and terminating the solutions. The significant difference between EXP1 and MODFLOW’s current implicit solvers is the absence of an “iteration loop” since the EXP1 solver handles non-linear problems without Picard’s or any other iterative method, and there is no need to check the convergence of the results in each time step.
Performance and Results

Tests were conducted to compare the developed EXP1 solver against MODFLOW 2005 results to gauge the accuracy and processing time. Tests included 1-Dimensional (1D), 2-Dimensional (2D), and vast real-world 3-Dimensional (3D) models.

The results of EXP1 in terms of accuracy and computational time could have been compared to the MODFLOW 2005 Preconditioned Conjugate-Gradient (PCG) solver, which is one of the most used solvers among modelers, or MODFLOW-NWT’s Newton-Raphson’s formulation. However, due to the generation of asymmetric matrices, MODFLOW-NWT requires additional computations compared to other solvers in MODFLOW-2005. While other solvers take advantage of symmetry by storing only one-half of the off-diagonal non-zero elements in the coefficient matrix, the NWT solver must store all non-zero elements (Niswonger et al. 2011). Consequently, MODFLOW-NWT may be slower than other MODFLOW-2005 solvers, such as PCG. The extra computations necessary to solve asymmetric matrices are justified if MODFLOW-NWT can successfully provide solutions for problems that fail to converge. However, without representation of convergence problems in a simulation, NWT’s choice over other MODFLOW 2005 solvers seems unwarranted. As the primary goal of this research was to improve computational time in groundwater modeling using a 1-day time step, the EXP1 solver was specifically compared to the PCG solver, which is generally faster than the NWT.

The PCG solver's results were the benchmark for evaluating the accuracy of the EXP1 solver's outcomes. Errors were determined by calculating the differences in hydraulic heads between the EXP1 and PCG solvers and the water budget outputs. All tests were conducted on an Intel Core i7 9700 CPU with 16 GB of physical memory.
Test 1 - 1D Model

The 1D test model was built to only extend along the X-axis. As can be seen from Figure 2, the 1D test model contains 50 cells with boundary conditions set to constant heads for both sides. The recharge package (RCH) (Harbaugh et al. 2000) was added to the model to add complexity and check the EXP1 solver's capabilities. The model was built in MODFLOW-2005 using the pre and post-processing software GMS (Groundwater Modeling System, v.10.6) developed by Aquaveo (Aquaveo, 2022). However, the model simulation was conducted using the original MODFLOW executable file and a modified version that included the EXP1 package in the command line. Figure 2 and Table 1 show the schematic and details of the 1D model.

![Figure 2: Schematic of the 1D test model cross-section (Aquifer thickness is vertically exaggerated for better visualization).](image)

The 1D test model was run for a simulation period of 50 days, with a time step size of 1 day using EXP1 and PCG solver. Figure 3 compares the EXP1 and PCG solvers' results, where both solvers resulted in the same head values. The maximum error value between the results was 0.27%, and the EXP1 solver captured all the abrupt head changes accurately, such as the cells with a well.
Figure 3  1D test model results at Day 50 for PCG and EXP1 solvers.

Table 1  1D test model details

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td></td>
</tr>
<tr>
<td>Length in X (m)</td>
<td>50,000</td>
</tr>
<tr>
<td>Length in Y (m)</td>
<td>1</td>
</tr>
<tr>
<td>Length in Z (m)</td>
<td>100</td>
</tr>
<tr>
<td>Number of cells in X</td>
<td>50</td>
</tr>
<tr>
<td>Number of cells in Y</td>
<td>1</td>
</tr>
<tr>
<td>Number of cells in Z</td>
<td>1</td>
</tr>
<tr>
<td>Time</td>
<td></td>
</tr>
<tr>
<td>Stress period count</td>
<td>1</td>
</tr>
<tr>
<td>Stress period length (day)</td>
<td>50</td>
</tr>
<tr>
<td>Time step size (day)</td>
<td>1</td>
</tr>
<tr>
<td>Wells</td>
<td></td>
</tr>
<tr>
<td>Wells pumping rate (m$^3$/day)</td>
<td>60,000</td>
</tr>
<tr>
<td>Well package</td>
<td>WEL</td>
</tr>
<tr>
<td>Recharge</td>
<td></td>
</tr>
<tr>
<td>Recharge rate (m/day)</td>
<td>0.0075</td>
</tr>
<tr>
<td>Recharge package</td>
<td>RCH</td>
</tr>
<tr>
<td>Aquifer parameters</td>
<td></td>
</tr>
<tr>
<td>Hydraulic conductivity K (m/day)</td>
<td>1</td>
</tr>
<tr>
<td>Specific storage Ss (m$^{-1}$)</td>
<td>0.01</td>
</tr>
<tr>
<td>Specific yield Sy</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 2 compares the runtime for EXP1 and PCG solvers. While results showed that the EXP1 solver was slightly faster than PCG, due to the small model size and low computational burden, runtime comparison between solvers was inconclusive.
Table 2  Runtimes of PCG and EXP for 1-day time step simulation in 1D test model

<table>
<thead>
<tr>
<th>Simulation Length (day)</th>
<th>Time Step size (day)</th>
<th>PCG runtime (sec)</th>
<th>1Day EXP runtime (sec)</th>
<th>% improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>1</td>
<td>0.123</td>
<td>0.113</td>
<td>8.13%</td>
</tr>
</tbody>
</table>

Another comparison that can be made is to compare the water budget between two solvers. In MODFLOW 2005, water budgets are provided for each time step, as well as cumulative values. This feature allows for comparing the water and total budgets at a specific time step. The discrepancy between the total inflow and outflow is one of the factors that can indicate the validity of the model. In this case, the discrepancies for both the PCG and EXP solvers were negligible, with values less than 1%. This result indicates the validity of the model. Table 3 illustrates the differences in water budget outputs between the EXP1 and PCG solvers. Total inflow and outflow from the model at the last time step and cumulative water budget of EXP1 and PCG were very close, and the highest difference was observed in total flow out of the model at the last time step where EXP1 showed a 0.20% difference. As can be seen from the table, EXP1 accuracy is again proved with the results.

Table 3  Water budget output difference between EXP1 and PCG solver in the 1D test model

<table>
<thead>
<tr>
<th></th>
<th>Total Flow In Difference</th>
<th>Total Flow out Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Last Time Step Water Budget</td>
<td>0.14%</td>
<td>0.20%</td>
</tr>
<tr>
<td>Cumulative Water Budget</td>
<td>0.12%</td>
<td>0.19%</td>
</tr>
</tbody>
</table>

Test 2 - 2D Model

The 2D model contained multiple rows and columns but only one layer. This model was built to test how the solver handles cell-to-cell flow in row and column directions. The 2D model includes
2,500 cells, Streamflow routing (SFR) package (Prudic et al. 2004), Multi-Node Wells (MNW) (Konikow et al. 2009), Time-variant specified head (CHD), and specified head cells. The left boundary condition was set to CHD, experiencing a head drop from 110 m to 80 m during four stress periods. During the simulation, the right boundary conditions were set to constant head (specified head cells). Figure 4 and Table 4 show the model details. The 2D test model was run for a simulation period of 200 days with a time step size of 1 day using EXP1 and PCG solvers.

Figure 4  2D test model’s schematic

Figure 5 shows the results of the PCG and EXP1 solvers at the final time step (i.e., day 200) and day 100. Figure 5 illustrates a close match between both solvers' results. At the time step of 100 days, the maximum difference between EXP1 and PCG solver was only 0.185%, and that of day 200 was 0.184%, and it can be seen that the maximum difference between the PCG and EXP1 solver results decreased from day 100 to day 200. The average difference increased from 0.017%
to 0.02% from day 100 to day 200. However, the standard deviation decreased from 0.009 to 0.0082.

The results showed that although the average difference slightly increased from day 100 to day 200, the maximum difference and standard deviation decreased. It is important to note that the differences were not consistently higher or lower for either solver, indicating the absence of error propagation. The cells near the wells and streams exhibited the highest differences, while the differences were negligible. In addition to the complexity of having a 2D problem, these results proved the EXP1’s capability to handle SFR, MNW, CHD, and specified head packages.

Table 4  2D test model details

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td></td>
</tr>
<tr>
<td>Length in X (m)</td>
<td>10,000</td>
</tr>
<tr>
<td>Length in Y (m)</td>
<td>10,000</td>
</tr>
<tr>
<td>Length in Z (m)</td>
<td>150</td>
</tr>
<tr>
<td>Number of cells in X</td>
<td>50</td>
</tr>
<tr>
<td>Number of cells in Y</td>
<td>50</td>
</tr>
<tr>
<td>Number of cells in Z</td>
<td>1</td>
</tr>
<tr>
<td>Time</td>
<td></td>
</tr>
<tr>
<td>Stress period count</td>
<td>4</td>
</tr>
<tr>
<td>Stress period length (day)</td>
<td>50</td>
</tr>
<tr>
<td>Time step size (day)</td>
<td>1</td>
</tr>
<tr>
<td>Packages</td>
<td></td>
</tr>
<tr>
<td>MNW well discharge</td>
<td>-6000 (m³/day)</td>
</tr>
<tr>
<td>SFR conductance</td>
<td>2 m/day</td>
</tr>
<tr>
<td>Aquifer parameters</td>
<td></td>
</tr>
<tr>
<td>Hydraulic conductivity K (m/day)</td>
<td>1</td>
</tr>
<tr>
<td>Specific storage Ss (m⁻¹)</td>
<td>0.01</td>
</tr>
<tr>
<td>Specific yield Sy</td>
<td>0.1</td>
</tr>
</tbody>
</table>

According to Table 5, EXP1 demonstrated a 33.77% shorter runtime compared to the PCG solver. However, once again, the small size of the model and short runtime prevent these results from being considered conclusive.
Table 5  Runtimes of PCG and EXP for 1-day time step simulation in 2D test model

<table>
<thead>
<tr>
<th>Simulation Length (day)</th>
<th>Time Step size (day)</th>
<th>PCG runtime (sec)</th>
<th>1Day EXP runtime (sec)</th>
<th>% improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1</td>
<td>0.647</td>
<td>0.977</td>
<td>33.77%</td>
</tr>
</tbody>
</table>

Comparing the water budget for the 2D model further reinforces EXP1’s capability. Table 6 compares the water budget between the EXP1 and PCG solvers at day 100 and day 200 and the cumulative water budgets. In the 2D test, the discrepancy in the water budget remained well below 1%, confirming the validity of the test model. This result indicates that both solvers effectively simulated the flow dynamics and accurately captured the inflows and outflows within the system.

Table 6  Water budget output difference between EXP1 and PCG solver in the 1D test model

<table>
<thead>
<tr>
<th></th>
<th>Total Flow In Difference</th>
<th>Total Flow Out Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Day 100 Water</td>
<td>0.20%</td>
<td>0.14%</td>
</tr>
<tr>
<td>Budget</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Day 200 Water</td>
<td>0.07%</td>
<td>0.23%</td>
</tr>
<tr>
<td>Budget</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cumulative Water</td>
<td>0.04%</td>
<td>0.23%</td>
</tr>
<tr>
<td>Budget</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Based on Table 6, it is evident that the differences in both time steps and cumulative water budgets were minimal. Specifically, the total inflow difference decreased from day 100 to day 200, while the total outflow experienced a slight increase. Additionally, the cumulative inflow and outflow also exhibited very small differences. These findings suggest that the EXP1 solver effectively handled the test model and utilized the associated packages, demonstrating its capability and validity.
Test 3 - USGS-MERAS Model

A vast real-world model was used to further test the capabilities of the proposed EXP1 solver. The Mississippi Embayment Regional Aquifer Study (MERAS) model is a complex real-world transient model developed by the United States Geological Survey (USGS) as part of the Groundwater Resources Program’s assessment of the nation’s groundwater availability (Clark et al. 2013). MERAS encompasses portions of eight states (i.e., Arkansas, Tennessee, Mississippi, Alabama, Louisiana, Kentucky, Missouri, and Illinois) with a total area of approximately 202,000 $km^2$, including roughly 11,200 km of stream, 70,000 well locations, and ten hydrological units with various hydraulic properties to include aquifers and their aquitards. The modeled system in MERAS was heterogeneous and anisotropic. The calibrated model covers 137 years, from January 1, 1870 to April 1, 2007, discretized into 69 stress periods with variable lengths (Clark et al. 2013; Clark & Hart, 2009). The model time step sizes vary between years (initial stress periods) and
months (later stress periods). This model contains 919,485 active cells in 13 layers. Figure 6 illustrates the extent of MERAS.

MERAS was built in MODFLOW-2005, and packages such as Multi-Node Well (MNW), recharge (RCH), Horizontal flow barrier (HFB) (Harbaugh, 2005), and stream flow routing (SFR) were implemented to simulate stressors and boundaries. Except for the RCH layer, these layers can be seen in Figure 7. However, RCH is only applied to layer 1, and since it represents areal properties, it was not included in this figure to avoid cluttering the visualization.

![Figure 6](image)

**Figure 6** Location of MERAS model study area (Clark et al. 2011)

**MERAS Simulation with 1 Day Time Step**

Preliminary execution of MERAS using the EXPI1 solver showed that extremely short time steps, as low as $6 \times 10^{-8}$ days were required to maintain stability, while the desired time step was 1 day.
Further investigation indicated that almost 54% of the cells within the model would be unstable if a 1-day time step was used, making it impossible to run MERAS without any modification.

**Figure 7**
Schematic of MERAS model’s layers
Further investigation was conducted into the reason(s) for such an extreme time step. Firstly, the cells’ thickness was taken into account. Analysis of the unstable cells revealed that 13% had thicknesses less than 1 m, which is a small value even for shallow aquifers. Some cells had extremely small thicknesses, as low as $6 \times 10^{-5}$ m. These cells were not limited to the edges but could be found throughout the model domain. Moreover, approximately 40% of the cells had thicknesses less than 10 m. The presence of such short vertical cell dimensions necessitated using shorter than 1-day time steps to remain stable.

The materials' storage coefficient was another significant factor in the cells' instability. The studies revealed that 58% of the cells had storage coefficients of less than $1 \times 10^{-6}$ m$^{-1}$ among them,
46% had storage coefficients as low as $1 \times 10^{-8} m^{-1}$. According to the stability criteria (Equation (8)), $SS$ appears in the fraction numerator, so its low values necessitate larger cell dimensions to produce stable results for a one-day simulation. Although the value of $SS$ is not the sole factor affecting stability, low values can force the modeler to either reduce the time step size or significantly increase the cell sizes to maintain stability for large time steps.

Investigating the effects of storage coefficients on stability revealed that unconfined cells are generally less susceptible to instability. The stability of the unconfined cells can be attributed to using specific yield ($Sy$), which is generally several orders of magnitude larger than the specific storage ($SS$) of confined layers. For example, Layer 1 in MERAS primarily consisted of unconfined cells, with only 9% of cells exhibiting instability issues using a 1-day time step. The unstable cells were predominantly confined, but some unconfined cells displayed instability. Unconfined cell instability was attributed solely to cell thickness (vertical cell dimension, not saturated thickness) and not the storage term, and all of them had abnormal thicknesses, measuring less than 0.8 meters.

Another critical factor to consider is $P$ (the head-dependent source/sink coefficient). $P$ is inherently a negative value. Depending on its magnitude and those of the conductance terms in the denominator, the denominator of Equation 8 can become a negative number; therefore, unconditionally unstable. In MERAS, specific STREAM cells were experiencing this instability, particularly those situated at the model's edges or in regions where no active cells were directly above or below them. These instances occurred when one or more conductivity values in specific directions were zero. Such circumstances led to an unstable cell and, ultimately, to an unstable
model. The cells experiencing instability caused by external stressors accounted for only 3% of the cells with head-dependent source/sink.

Furthermore, these unstable cells represented less than 0.2% of the total active cells in the model. Thus, this kind of instability was relatively limited and affected only a tiny fraction of the overall cell population and would not require broad modification of the model. However, determining this was not part of this investigation.

There are several options available to stabilize these unstable cells. One option is to increase the cell size. However, increasing cell sizes may result in a loss of hydrogeological detail and precision in the simulation. Therefore, careful consideration and analysis are necessary to determine the optimal balance between stability and model accuracy.

Employing the proposed stability criteria makes it possible to assess the stability of the model for different cell sizes. The cell size used in MERAS was approximately 1.5 km × 15 km. Stability was assessed by increasing cell sizes by factors of 2, 3, 5, and 10. The objective was to determine the percentage of stable cells for a 1-day time step. Table 7 presents the results of the stability analysis:

<table>
<thead>
<tr>
<th>Cell size (km)</th>
<th>% of the stable cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5 x 1.5</td>
<td>46%</td>
</tr>
<tr>
<td>3 x 3</td>
<td>71%</td>
</tr>
<tr>
<td>4.5 x 4.5</td>
<td>77%</td>
</tr>
<tr>
<td>7.5 x 7.5</td>
<td>90%</td>
</tr>
<tr>
<td>15 x 15</td>
<td>95%</td>
</tr>
</tbody>
</table>
Table 7 demonstrates the positive impact of increasing cell sizes to achieve stability for a 1-day step. At the largest square cell dimension (15 km), only 5% of cells showed instability, where 85% of them were cells with a vertical dimension of less than 10 m. The remaining unstable cells were influenced by a combination of low specific storage (SS) and high head-dependent source/sink coefficient (P). These findings emphasize the significance of considering cell size and other factors when considering stability at larger $\Delta t$. However, enforcing large cell sizes is not usually conducive to accurately modeling heads in heterogenous material and where detail near stressors (e.g., wells, streams, drains) is desired. Therefore, for MERAS, altering cell sizes was not a feasible option.

Another option to address instability was to reduce the time step to less than one day. As mentioned prior, due to extremely small vertical cell dimensions (i.e., $< 10^{-5}$ m), $\Delta t$ would need to be $6 \times 10^{-8}$ days. Knowing that such small cell sizes are errant and to still use MERAS for testing EXP1 against PCG, a decision was made to convert unstable cells to constant head cells. Unfortunately, just over half (54%) of the cells had to be converted, greatly reducing the model's effectiveness. However, considering that only 9% of the cells in Layer 1 required alteration and that in the model coupling, it is often the shallow, unconfined aquifer that mostly interacts with surface processes, we still considered conducting a comparison.

One more modification was made to MERAS to its early stress periods (2, 3, and 4) that fell from 1 January 1870 to 1 January 1920. This time span constituted 36.5% of the total model period yet represented less than 3% of the pumping (the major stress in the model simulation). These three early stress periods were reduced to 100 days each to reduce model runtimes from many days to just a few. After these modifications, the MERAS model was run using the EXP1 and PCG solvers
with a 1-day time step. EXP1 and PCG solved the same modified MERAS model, and results were
compared based on runtimes and accuracy.

Table 8 compares the results of EXP1 and PCG solver using a 1-day time step. Comparison of
resulting heads in the final time step of the model (i.e., 1 April 2007) showed that 99.87% of EXP1
results had less than 5% difference with PCG, while an error value of less than 10% is considered
reasonable for most groundwater modeling applications (Anderson et al. 2015). This threshold is
a commonly used criterion for evaluating the accuracy and reliability of groundwater models (US
Environmental Protection Agency, 2002).

Table 8 Differences in head values between EXP1 and PCG solvers across layers, for
MERAS 1-day time step simulation.

<table>
<thead>
<tr>
<th>Layers</th>
<th>Less than 5%</th>
<th>Between 5% and 10%</th>
<th>Between 10% to 25%</th>
<th>Between 25% to 50%</th>
<th>More than 50%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>99.11%</td>
<td>0.38%</td>
<td>0.40%</td>
<td>0.05%</td>
<td>0.06%</td>
</tr>
<tr>
<td>2</td>
<td>100.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>3</td>
<td>100.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>4</td>
<td>100.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>5</td>
<td>100.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>6</td>
<td>99.20%</td>
<td>0.44%</td>
<td>0.29%</td>
<td>0.03%</td>
<td>0.05%</td>
</tr>
<tr>
<td>7</td>
<td>99.84%</td>
<td>0.09%</td>
<td>0.05%</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>8</td>
<td>99.96%</td>
<td>0.03%</td>
<td>0.01%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>9</td>
<td>99.99%</td>
<td>0.01%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>10</td>
<td>99.92%</td>
<td>0.04%</td>
<td>0.03%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>11</td>
<td>99.89%</td>
<td>0.05%</td>
<td>0.04%</td>
<td>0.02%</td>
<td>0.00%</td>
</tr>
<tr>
<td>12</td>
<td>99.91%</td>
<td>0.04%</td>
<td>0.04%</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>13</td>
<td>99.97%</td>
<td>0.02%</td>
<td>0.01%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>All Layers considered</td>
<td>99.87%</td>
<td>0.07%</td>
<td>0.05%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

Note: The table represents the percentage of cells in each layer (and overall) where the head differences
between the EXP1 and PCG solvers fall within specific difference ranges. For example, in row 1, 99.11% of
the cells showed less than 5% head difference between the EXP1 and PCG solvers and so on.
In terms of water balance, both the EXP1 and PCG solvers resulted in a water budget discrepancy below 1%, confirming their validity. Table 9 compares the modified MERAS model's water budget output for EXP1 and PCG solver. However, upon comparing the water budgets for both solvers, it is observed that the differences are slightly over 10%, with the main contributing factor being slightly higher flows in and out of constant head cells in both solvers. Constant head cells can remove or add unlimited water from or to the model. As this model unquestionably has enumerable constant head cells, any small head differences in adjacent variable head cells between PCG and EXP1 will be summative, leading to larger discrepancies in the water budget. Therefore, the water budget difference in this model is higher than in the 1D and 2D test models. However, it was expected that reducing the number of constant head cells would resolve this issue.

Table 9  Water budget output difference between EXP1 and PCG solver in MERAS 1-day simulation

<table>
<thead>
<tr>
<th></th>
<th>Total Flow in Difference</th>
<th>Total Flow Out Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Last Time Step Water Budget</td>
<td>12.1%</td>
<td>12.1%</td>
</tr>
<tr>
<td>Cumulative Water Budget</td>
<td>11.5%</td>
<td>11.4%</td>
</tr>
</tbody>
</table>

The most important comparison was determining how the EXP1 solver improved the computational burden and run time. Results showed that the EXP1 solver improved the runtime significantly. Table 10 shows the time it took for EXP1 and PCG to solve the MERAS model using 1 day time steps. EXP1 processing time is less than half of the time of the PCG solver, resulting in a 57.06% improvement.
**MERAS Simulation with 0.01 Day Time Step**

The main disadvantage of the 1-day simulation comparison was the number of cells that had to be deactivated to keep the model stable. To avoid deactivating a large number of cells during the simulation, a 0.01-day time step was also selected to have an additional comparison in which MERAS experienced minimal changes. In this case, only 9% of the cells had to be changed to constant head, making the results more realistic.

<table>
<thead>
<tr>
<th>Simulation Length (day)</th>
<th>Time Step size (day)</th>
<th>1Day PCG runtime (min)</th>
<th>1Day EXP runtime (min)</th>
<th>% improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50130</td>
<td>1</td>
<td>177</td>
<td>76</td>
<td>57.06%</td>
</tr>
</tbody>
</table>

In Figure 8, a comparison is presented between the results obtained from the EXP1 and PCG solvers for different layers of the MERAS model at the final time step during a 0.01-day simulation. The differences between the solvers are expressed as percentages, indicating the closeness of the EXP1 solver's heads to those of the PCG solver. A zero difference signifies identical head values obtained from both solvers. Overall, the results demonstrate a strong agreement between the solvers, with only minor areas exhibiting noticeable discrepancies.

In Figure 8, regions with relatively higher differences (more than 25%) are shown by blue and red arrows, helping pinpoint their origin. Blue arrows indicate areas in layers 2, 3, and 4 which are cells around the streams. Maximum head differences in layers 2, 3, and 4 are 87%, 86.5%, and 57.7%, respectively. On the other hand, red arrows show the high differences areas on layers 6, 7, 8, and 9. These regions are around horizontal flow barriers (HFB) and wells. Maximum head differences in these regions are 77.18%, 99.03%, 88.77%, 23.09%, and 21.03% for layers 6, 7, 8, 9, and 10, respectively, while the average difference in all the mentioned layers was below 0.20%.
Stream, HFB, and MNW cell distribution within the model region were random and not limited only to areas that experienced high differences in head. For example, in Layer 7, HFB and MNW cells were present in various parts of the layer, as shown in Figure 9. However, significant differences were observed primarily in the indicated region, whereas the differences were relatively low in other areas where HFB and MNW cells appeared.

Figure 8  Percent differences in MERAS results for 13 layers at the final time step (Blue arrows show the areas with the highest differences around stream cells, and red arrows show high difference areas around wells).
Figure 8     Percent differences in MERAS results for 13 layers at the final time step (Blue arrows show the areas with the highest differences around stream cells, and red arrows show high difference areas around wells). (Continued).
Figure 8  Colormap for the percent differences in MERAS results for 13 layers at final time step (Blue arrow show areas with highest differences around stream cells, red arrows show high difference areas around wells)  (*Continued*).

The exact reasons for these differences are unclear but could be attributed to the model structure and the modifications made. Before this, 1D and 2D test models had already demonstrated the compatibility of the EXPI solver with the SFR and MNW packages. A model was constructed and analyzed to ensure the compatibility of the proposed solver with the HFB package. The results of the HFB test model, along with the model setup and findings, are provided in Appendix S2, confirming that the Explicit solver can fully simulate models incorporating the HFB package.
Figure 9   MERAS model layer 7 distributions of HFB and well cells. The blue circle shows a high difference region.

Table 11 shows how EXP1 and PCG solvers’ results match. The results from the comparison between the EXP1 and PCG solvers indicate that the majority of the results (98.50%) exhibited differences of less than 5%. Only a small portion of the results (1.5%) showed differences higher than 5%, with approximately 0.23% exhibiting differences exceeding 25%. Notably, cells with more significant differences in head values exceeding 50% constituted less than 0.04% of the total model cells. These findings provide confidence in the reliability and suitability of the EXP1 solver for complex and extensive models like MERAS. The overall high agreement and the small proportion of cells with larger differences highlight the effectiveness of the EXP1 solver in simulating groundwater flow in such models.

As indicated in Table 11, when comparing the results of the 0.01-day time step simulation to the 1-day time step analysis, there was a decrease in overall accuracy by approximately 1.3%. This reduction in accuracy can be attributed to the differences in the number of active cells available for comparison. In the 1-day time step analysis, around 54% of the cells were deactivated and converted to constant cells, making fewer cells available for evaluation. Conversely, the 0.01-day
simulation included a larger number of active cells considered for comparison. This increase in the number of cells used for comparison likely contributed to the slight drop within the 5% accuracy metric. Despite this decrease in accuracy, a finer time step allowed for a more detailed analysis and a larger sample size of active cells.

Table 11 Differences in head values between EXP1 and PCG solvers across layers, for MERAS 0.01-day time step simulation

<table>
<thead>
<tr>
<th>Layers</th>
<th>Less than 5%</th>
<th>Between 5% and 10%</th>
<th>Between 10% to 25%</th>
<th>Between 25% to 50%</th>
<th>More than 50%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>98.85%</td>
<td>0.93%</td>
<td>0.18%</td>
<td>0.04%</td>
<td>0.00%</td>
</tr>
<tr>
<td>2</td>
<td>94.44%</td>
<td>2.24%</td>
<td>2.08%</td>
<td>0.97%</td>
<td>0.27%</td>
</tr>
<tr>
<td>3</td>
<td>95.41%</td>
<td>2.12%</td>
<td>1.46%</td>
<td>0.81%</td>
<td>0.20%</td>
</tr>
<tr>
<td>4</td>
<td>97.28%</td>
<td>1.33%</td>
<td>1.23%</td>
<td>0.16%</td>
<td>0.00%</td>
</tr>
<tr>
<td>5</td>
<td>99.72%</td>
<td>0.27%</td>
<td>0.01%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>6</td>
<td>98.54%</td>
<td>0.83%</td>
<td>0.58%</td>
<td>0.04%</td>
<td>0.01%</td>
</tr>
<tr>
<td>7</td>
<td>97.69%</td>
<td>1.04%</td>
<td>0.75%</td>
<td>0.45%</td>
<td>0.07%</td>
</tr>
<tr>
<td>8</td>
<td>98.20%</td>
<td>0.85%</td>
<td>0.76%</td>
<td>0.16%</td>
<td>0.03%</td>
</tr>
<tr>
<td>9</td>
<td>99.42%</td>
<td>0.52%</td>
<td>0.05%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>10</td>
<td>99.92%</td>
<td>0.08%</td>
<td>0.01%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>11</td>
<td>99.96%</td>
<td>0.04%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>12</td>
<td>99.97%</td>
<td>0.03%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>13</td>
<td>99.97%</td>
<td>0.03%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>All Layers considered</td>
<td>98.50%</td>
<td>0.74%</td>
<td>0.53%</td>
<td>0.19%</td>
<td>0.04%</td>
</tr>
</tbody>
</table>

Note: The table represents the percentage of cells in each layer (and overall) where the head differences between the EXP1 and PCG solvers fall within specific difference ranges. For example, in row 1, 98.85% of the cells showed less than 5% head difference between the EXP1 and PCG solvers and so on.

Upon comparing the water budget outputs from both solvers, a notable decrease in differences was observed compared to the 1-day simulation. As previously discussed, when using a time step of 1-day for the comparison, a large number of constant head cells were present, which primarily caused the observed discrepancy in water budgets. It should be noted that having an extremely large number of constant head cells, as seen in the 1-day MERAS simulation, was not a typical scenario, and it was predicted that reducing the count of constant head cells would resolve the significant
difference between water budgets. As expected, this test confirmed the water budget results exhibited an excellent match between the EXP1 and PCG solvers when there are fewer constant head cells. Table 12 illustrates the differences in water budget between the EXP1 and PCG solvers with the highest % - a difference of 2.81% for cumulative total flow in and all other percent differences below 1%.

Table 12  Water budget output difference between the EXP1 and PCG solvers in MERAS 0.01-day simulation

<table>
<thead>
<tr>
<th></th>
<th>Total Flow in Difference</th>
<th>Total Flow out Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Last Time Step Water Budget</td>
<td>0.64%</td>
<td>0.70%</td>
</tr>
<tr>
<td>Cumulative Water Budget</td>
<td>2.81%</td>
<td>0.83%</td>
</tr>
</tbody>
</table>

Table 13 shows the details of the runtime for each solver. The EXP1 solver significantly reduced the time needed for the MERAS model simulation by 32.02% and relatively resulted in the same groundwater head values.

Table 13  Runtimes for the PCG and EXP solvers for 0.01-day time step simulation

<table>
<thead>
<tr>
<th>Simulation Length (day)</th>
<th>Time Step size (day)</th>
<th>PCG runtime (Hours)</th>
<th>EXP runtime (Hours)</th>
<th>% Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>50130</td>
<td>0.01</td>
<td>236.68</td>
<td>160.90</td>
<td>32.02%</td>
</tr>
</tbody>
</table>

While EXP1 has been shown to accurately simulate various groundwater scenarios with reduced runtimes compared to PCG, there are important considerations to consider when utilizing this solver. It is crucial to carefully consider cell sizes and time steps before creating the model, as modifying cell sizes post-construction can be a complex, time-consuming process. Hence, the stability checker function within the EXP1 solver allows for assessing the stability of the model before running it and can adjust the time step accordingly to ensure stability. However, as done in
this research, the checker can also ascertain reasons for undesired small-time steps (e.g., extremely small cell sizes, storage terms, and points of unconditional instability).
Effective water resource management is of utmost importance in the face of increasing global population, climate change, and economic growth. Groundwater and surface water are interconnected parts of the hydrological cycle and play a significant role in water availability, water quality, ecosystem support, and water management. It is, therefore, crucial to develop simulation platforms that accurately represent water exchanges and interactions between surface water and groundwater resources. Traditional numerical tools such as SWAT, MODFLOW, and HEC-RAS cannot fully capture the complexity of surface water and groundwater interactions. All these numerical tools are primarily designed to simulate either groundwater or surface water processes individually, which can lead to oversimplification and inaccurate representation of the coupled system.

Model coupling has become increasingly popular to overcome these limitations, aiming to integrate the strengths of individual tools and develop more comprehensive groundwater-surface water coupling frameworks. Coupled models enable a more holistic understanding of the complex spatial and temporal interactions, allowing for the analysis of feedback mechanisms, water exchanges, and dynamic changes within the coupled system. By leveraging the capabilities of different models, coupled models can provide a more accurate representation of the hydrological processes occurring at the interface of groundwater and surface processes. Nevertheless, fully coupling these models and appropriately exchanging data with each other is challenging. Related to groundwater and surface processes, one of the challenges faced by fully coupled models is the disparity in temporal and spatial scales. Surface processes, such as rainfall, evaporation, and stream level fluctuations, exhibit daily variations, while groundwater flow operates over longer time frames, such as weeks or months. As a result of this spatial and temporal discrepancy, individual
groundwater and surface models could not be effectively coupled. This study developed an explicit solver (EXP1) for MODFLOW 2005 to address the issue. EXP1 offers a potential solution to reduce runtime and computational burden in groundwater modeling by directly solving the equations at each time step without requiring iterative matrix inversions. By incorporating EXP1 into the coupled model framework, we aimed to bridge the gap between the different temporal scales of surface water and groundwater processes. The stability analyzer was also developed using stability criteria to ensure the stability of the model and notify modelers of any unstable cells within the constructed model.

The introduction of the EXP1 solver can potentially improve the efficiency of coupled models by streamlining the computational processes. EXP1 allows groundwater modelers to choose finer temporal resolutions (i.e., 1 day) to match that of surface flow models. Such short time scales are possible with MODFLOW 2005 and its PCG solver; however, it is ineffective because matrix inversion is computationally intensive and, in a fully coupled setting (i.e., bi-directional iteration), this burden greatly increases. The additional computational load of PCG solver in a fully coupled setting stems from the need for multiple iterations to solve groundwater head for each time step. This iterative process extends the simulation runtimes, particularly when coupled with the reduced time step size (i.e., 1 day) required to match the finer temporal resolutions of surface flow models. Reducing the time step size increases the number of time steps that need to be simulated, contributing further to the computational burden. As the model size and complexity increase, this burden becomes more pronounced and can significantly impact the overall efficiency of the coupled modeling process.

By eliminating the need for iterative matrix inversions, the EXP1 reduces the computational time of solving large-scale groundwater flow equations for small steps. Hence, an explicit formulation
of groundwater flow for MODFLOW 2005 was developed using FORTRAN 90 and its stability criteria were derived.

To assess the effectiveness of the the EXP1 solver, it was compared with the commonly utilized PCG solver across four distinct model scenarios: a 1D model, a 2D model, and the real-world MERAS model at a 1-day and 0.01-day time step. Therefore, given the goal of improving computational efficiency, the focus was primarily on comparing the EXP1 solver with the faster and widely used PCG solver. The NWT solver, another widely used implicit solver for model coupling purposes in MODFLOW, is known to be less computationally efficient and slower compared to other solvers like the PCG. Consequently, the NWT solver was not considered for this specific study.

In the 1D test model with two pumping wells, the EXP1 and PCG solvers had close agreement on resulting heads with a maximum error of 0.27%. In this case, EXP1 solver resulted in 8.13% shorter runtime compared to PCG solver but the results were inconclusive due to the model's small size and extremely short runtime (i.e. < 1 second). The water budget comparison also showed a close match between the two solvers, demonstrating EXP1’s capability to accurately simulate groundwater flow dynamics for simple 1D simulations.

The 2D model simulated well pumping and groundwater-surface water interaction using a recharge package and a 1-day time step. Head differences, checked at two time periods (100 days and 200 days), showed close agreements at 0.185% and 0.184%, respectively. The observed slight increase in average head difference over time was accompanied by a decrease in maximum difference and standard deviation, indicating the absence of error propagation. A water balance comparison showed differences of less than 0.25. EXP1 simulated the 2D model 33.77% faster than PCG. However, due to the small size of the model and very short runtimes (i.e., less than 1 second), the
runtime comparison was inconclusive. The successful utilization of different packages, such as specified head cells, Streamflow Routing (SFR), Multi-Node Wells (MNW), and Time-variant specified head (CHD), showcases the versatility of the EXP1 solver in groundwater modeling applications and its capability to include different MODFLOW packages.

In the 2D test model, the specified head cells package allowed for the accurate representation of fixed head boundaries in the model, the Streamflow Routing (SFR) package was employed to simulate the movement of water in streams and rivers, the Multi-Node Wells (MNW) package enabled the modeling of complex well systems and lastly, the Time-variant specified head (CHD) package was used to represent time-varying head boundaries.

The last two tests used MERAS, a large-scale, real-world model spanning portions of eight states and simulating 137 years. Preliminary investigation of MERAS revealed instability when using the EXP1 solver with a 1-day time step due to cells with a minimal vertical thickness (as low as $6 \times 10^{-5}$ m). Low values of specific storage coefficients ($10^{-6}$ to $10^{-8}$ m$^{-1}$) also created instability when using EXP1 at this time step size. However, to the benefit of potential model coupling MODFLOW to surface process models, often such a surface process interacts with a shallow, unconfined aquifer whose storage term is specific yield, a larger value than specific storage. Layer 1 of the MERAS model, which consisted mostly of unconfined cells, had only 9% of its cells exhibit instability. Here, the primary cause of instability in these cells was their extremely small thickness, with values as low as 0.8 meters. This finding supports the observation that unconfined cells are seemingly more stable than confined cells.

The instability of MERAS in the EXP1 solver was also influenced by the head-dependent source/sink coefficient. In some cases, when the coefficient (P) value was large (inherently negative), it caused the entire denominator of the stability criteria to be negative, which resulted
in unconditional instability. This result emphasizes the importance of considering the magnitude of the head-dependent source/sink coefficient and its impact on stability during groundwater flow simulations. Careful evaluation and adjustment of this coefficient are necessary to ensure the stability of the model. However, selecting slightly larger cell sizes can often resolve instability issues caused by source/sink coefficients.

Although increasing cell sizes could increase the time step, doing so was undesirable. Hence, for comparative purposes only and to use a complex, large model like MERAS, a time step of 1 day was chosen, which resulted in approximately 54% of the cells being converted to constant head. The comparison was considered well-matched with 99.87% of the EXP1 results having less than a 5% difference compared to the PCG results. Upon comparison of water budgets, there were higher differences between the two solvers of upwards of 12%. This high differences in water budgets resulting from EXP1 and PCG can be attributed to the large number of constant head cells within the modified MERAS model. These constant head cells could considerably alter the water budget, even with minor differences in hydraulic head values between the EXP1 and PCG solvers. Consequently, the substantial impact of constant head cells on the water budget explains the observed variations between the two solvers.

Though running MERAS with a 1-day time step was nonideal, the EXP1 solver exhibited a remarkable improvement in runtime, reducing the time needed to simulate the model by 57.06% compared to the PCG solver. This reduction in runtime highlights the efficiency of the EXP1 solver in simulating complex groundwater models within a shorter timeframe. (comments)

The final test attempted to use MERAS as close to its original structure by determining that at a 0.01-day time step, only 9% percent of the MERAS cells would need to be converted to constant
head cells. With this new modified version of MERAS, the EXP1 solver continued to exhibit high accuracy, where 98.5% of the EXP1 head values differed less than 5% from the PCG solver.

Among the remaining 1.5% of the cells with more than 5% difference, some cells had more than 50% difference; however, these high error cells only represented 0.04% of total model cells. The presence of cells with high errors, particularly around streams, Multi-Node Wells (MNW), and Horizontal Flow Barriers (HFBs) prompted further investigation. While these features were distributed throughout the model domain, it was observed that the high errors were confined to specific locations. Having not tested HFB in the 1D and 2D tests, a quick test model was built using the HFB package. The results of this dedicated test model did confirm the applicability of the EXP1 solver to accurately solve heads using the HFB package. Comparison of water budgets improved over the 1-day time step MERAS simulation and model modification with cumulative water budget errors below 3%. This reduction in discrepancy illustrates the enhanced capability of the EXP1 solver to capture and simulate the water budget dynamics accurately. Moreover, the EXP1 solver demonstrated its convergence efficiency by completing the simulation 32.02% faster than the PCG solver. This significant reduction in runtime further emphasizes the computational advantages of the EXP1 solver for groundwater modeling applications, especially when considering coupled model bi-directional iteration.

In conclusion, this investigation highlights the effectiveness of the proposed EXP1 solver in simulating groundwater flow using MODFLOW 2005. When the solver operates in a stable model, it significantly reduces computational time while maintaining relative accuracy compared to the more common PCG solver, utilizing the same time step size. However, it is important to acknowledge the limitations of the explicit scheme when extremely thin cells, very low specific storage, large sink/source terms or a combination of them can result in short, undesirable time
steps, here less than 1 day, to maintain the stability. Model stability determination is possible with the stability criteria and code developed herein. Therefore, analyzing the stability and striking a balance between increasing the cell size and reducing the time step size is essential to achieve modeling goals effectively. It is acknowledged that cells representing unconfined conditions, with dimensions that are not extremely small, can be stably simulated for 1-day time steps using EXP1 solver. This is particularly suitable when considering interactions of GW with SW, which predominantly occur in unconfined aquifers. Hence, with the appropriate parameters in place, the EXP1 solver's speed make it a valuable tool for GW-SW model coupling applications, providing faster solutions for water resource management and decision-making processes. Still, further investigation of the EXP1 solver for differing model scenarios is warranted.

On the other hand, traditional implicit solvers are preferable for standalone groundwater modeling or confined aquifers to avoid stability issues. Generally, when small time steps are not required, implicit solvers could be more suitable since they are not sensitive to cell or time step sizes, enabling the choice of larger time steps, even up to months, to achieve modeling goals effectively.
References


Dehghan, M. (2006). Finite difference procedures for solving a problem arising in modeling and


Appendix 1: Stability Criteria Derivation

This appendix discusses the derivation of stability criteria using the Von Neuman method. In this method, $h(x, y, z, t)$ and $\bar{h}(x, y, z, t)$ were defined as the analytical and numerical solutions of Equation (4), respectively. Therefore, the error is written as (9):

$$h(x, y, z, t) = \bar{h}(x, y, z, t) + e^t_{i,j,k}$$  \hspace{1cm} (9)

where: $e^t_{i,j,k}$ is the summation of error at node $x, y$ and $z$ at time step $t$. The error term is defined using the Fourier series:

$$e^t_{i,j,k} = \gamma^t \exp \left( I \left( s_1 x_i + s_2 y_j + s_3 z_k \right) \right), \quad I = \sqrt{-1}  \hspace{1cm} (10)$$

where: $\gamma$ is the amplification factor and $s_1$, $s_2$ and $s_3$ are the wavenumbers. Von Neumann’s method requires the amplification factor to be less than unity to call the method stable ($\gamma < 1$).

Hence, $e^t_{i,j,k}$ is substituted in Equation (4) with the following simplifications:

a) $R_1 = CR_{i,j-\frac{1}{2},k}$

b) $R_2 = CR_{i,j+\frac{1}{2},k}$

c) $C_1 = CC_{i-\frac{1}{2},j,k}$

d) $C_2 = CC_{i+\frac{1}{2},j,k}$

e) $V_1 = CV_{i,j,k-\frac{1}{2}}$

f) $V_2 = CV_{i,j,k+\frac{1}{2}}$

g) $L = -CR_{i,j-\frac{1}{2},k} - CR_{i,j+\frac{1}{2},k} - CC_{i-\frac{1}{2},j,k} - CC_{i+\frac{1}{2},j,k} - CV_{i,j,k-\frac{1}{2}} - CV_{i,j,k+\frac{1}{2}} + \frac{SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)}{\Delta t}$

h) $Q = Q_{i,j,k}$

i) $RHS_{i,j,k} = \frac{SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)}{\Delta t} - p_{i,j,k}$

Substituting into Equation (4), we get:
\[ C_1 \gamma^t \exp \left( I(s_1 x_i + s_2 y_{j-1} + s_3 z_k) \right) + C_2 \gamma^t \exp \left( I(s_1 x_i + s_2 y_{j+1} + s_3 z_k) \right) + R_1 \gamma^t \exp \left( I(s_1 x_{i-1} + s_2 y_j + s_3 z_k) \right) + R_2 \gamma^t \exp \left( I(s_1 x_{i+1} + s_2 y_j + s_3 z_k) \right) + V_1 \gamma^t \exp \left( I(s_1 x_i + s_2 y_j + s_3 z_{k-1}) \right) + V_2 \gamma^t \exp \left( I(s_1 x_i + s_2 y_j + s_3 z_{k+1}) \right) + L \gamma^t \exp \left( I(s_1 x_i + s_2 y_j + s_3 z_k) \right) = \text{RHS} \gamma^{t+1} \exp \left( I(s_1 x_i + s_2 y_j + s_3 z_k) \right) \]

Dividing both sides of Equation (12) by \( \gamma^t \exp \left( I(s_1 x_i + s_2 y_j + s_3 z_k) \right) \) results in:

\[ R_1 \exp(-Is_1 \Delta r) + R_2 \exp(Is_1 \Delta r) + C_1 \exp(-Is_2 \Delta c) + C_2 \exp(Is_2 \Delta c) + V_1 \exp(-Is_3 \Delta v) + V_2 \exp(Is_3 \Delta v) + L = \text{RHS} \gamma \]

Using the Euler formulas, one can obtain:

\[ (C_1 + C_2) \cos(s_1 \Delta c) + (C_1 - C_2)I \sin(s_1 \Delta c) + (R_1 + R_2) \cos(s_2 \Delta r) + (R_1 - R_2)I \sin(s_2 \Delta r) + (V_1 + V_2) \cos(s_3 \Delta v) + (V_1 - V_2)I \sin(s_3 \Delta v) + L = \text{RHS} \gamma \]

Or

\[ \text{(15)} \]
\[ I \left( (C_1 - C_2) \sin(s_1 \Delta c) + (R_1 - R_2) I \sin(s_2 \Delta r) + (V_1 - V_2) I \sin(s_3 \Delta v) \right) \frac{RHS}{RHS} = \gamma \]

Here in Equation (15) \( \gamma \) is a complex number and its magnitude should be less than one; otherwise, the scheme will be unstable. Therefore:

\[
\left( \frac{(C_1 + C_2) \cos(s_1 \Delta c) + (R_1 + R_2) \cos(s_2 \Delta r) + (V_1 + V_2) \cos(s_3 \Delta v) + L}{RHS} \right)^2 + \\
\left( \frac{(C_1 - C_2) \sin(s_1 \Delta c) + (R_1 - R_2) \sin(s_2 \Delta r) + (V_1 - V_2) \sin(s_3 \Delta v)}{RHS} \right)^2 < 1
\]

Choosing the worst-case depends on the sign of \( L \). Assuming \( L > 0 \):

\[
-CR_{i,j-\frac{1}{2},k} - CR_{i,j+\frac{1}{2},k} - CC_{i-\frac{1}{2},j,k} - CC_{i+\frac{1}{2},j,k} - CV_{i,j,k-\frac{1}{2}} - CV_{i,j,k+\frac{1}{2}} \\
+ SS_{i,j,k} \left( \frac{\Delta r_i \Delta c_j \Delta v_k}{\Delta t} \right) < 0
\]

Then \( \Delta t \) should satisfy (18):

\[
\Delta t < \frac{SS_{i,j,k} \left( \frac{\Delta r_i \Delta c_j \Delta v_k}{\Delta t} \right)}{CR_{i,j-\frac{1}{2},k} + CR_{i,j+\frac{1}{2},k} + CC_{i-\frac{1}{2},j,k} + CC_{i+\frac{1}{2},j,k} + CV_{i,j,k-\frac{1}{2}} + CV_{i,j,k+\frac{1}{2}}}
\]

Then, the worst case for Equation (16) will happen if all the cosines in the nominator are equal to +1. Consequently, the sines will be zero resulting in Equation (19):

\[
\left( \frac{C_1 + C_2 + R_1 + R_2 + V_1 + V_2 + L}{RHS} \right)^2 < 1
\]

or
−1 < \frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{\Delta t} < 1
\quad \text{(20)}

\frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{\Delta t} - P_{i,j,k}

P_{i,j,k} is always a negative number, so the denominator of (20) is always a positive number; therefore, the left side of (20) is always true. Hence,

\frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{\Delta t} > 1
\quad \text{(21)}

or

\frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{\Delta t} - P_{i,j,k} > \frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{\Delta t}
\quad \text{(22)}

This means the scheme will be stable if (18) is true. The next step is to investigate when \( L < 0 \).

Hence,

\Delta t > \frac{SS_{i,j,k}(\Delta r \Delta c_i \Delta v_k)}{CR_{i,j-\frac{1}{2},k} + CR_{i,j+\frac{1}{2},k} + CC_{i-\frac{1}{2},j,k} + CC_{i+\frac{1}{2},j,k} + CV_{i,j,k-\frac{1}{2}} + CV_{i,j,k+\frac{1}{2}}}
\quad \text{(23)}

Then the worst-case for (16) happens if all the cosines in the nominator will be -1. Consequently, the sinuses will be zero. Then one can obtain the following:

\left(\frac{-C_1 - C_2 - R_1 - R_2 - V_1 - V_2 + L}{RHS}\right)^2 < 1
\quad \text{(24)}

or
\[-1 < -\frac{2CR_{i,j,\frac{1}{2}k} - 2CR_{i,j+\frac{1}{2}k} - 2CC_{i-\frac{1}{2},j,k} - 2CC_{i+\frac{1}{2},j,k} - 2CV_{i,j,k-\frac{1}{2}} - 2CV_{i,j,k+\frac{1}{2}} + \frac{SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k)}{\Delta t}}{SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k) - P_{i,j,k}} < 1 \] (25)

Knowing that the sign of the nominator is negative and the denominator is positive, the right-hand side of (25) is always true. So then, considering the left-hand side of (26), one can obtain the following:

\[-\frac{SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k)}{\Delta t} + P_{i,j,k} < -2CR_{i,j,\frac{1}{2}k} - 2CR_{i,j+\frac{1}{2}k} - 2CC_{i-\frac{1}{2},j,k} - 2CC_{i+\frac{1}{2},j,k} - 2CV_{i,j,k-\frac{1}{2}} - 2CV_{i,j,k+\frac{1}{2}} \]

\[+ \frac{SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k)}{\Delta t} \] (26)

or

\[-\frac{2 * SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k)}{\Delta t} < -P_{i,j,k} - 2CR_{i,j,\frac{1}{2}k} - 2CR_{i,j+\frac{1}{2}k} - 2CC_{i-\frac{1}{2},j,k} - 2CC_{i+\frac{1}{2},j,k} - 2CV_{i,j,k-\frac{1}{2}} - 2CV_{i,j,k+\frac{1}{2}} \] (27)

Using mathematical manipulations:

\[\Delta t \]

\[< \frac{2 * SS_{i,j,k}(\Delta \tau \Delta c_i \Delta v_k)}{P_{i,j,k} + 2CR_{i,j,\frac{1}{2}k} + 2CR_{i,j+\frac{1}{2}k} + 2CC_{i-\frac{1}{2},j,k} + 2CC_{i+\frac{1}{2},j,k} + 2CV_{i,j,k-\frac{1}{2}} + 2CV_{i,j,k+\frac{1}{2}}} \] (28)

The intersection of (18), (23), and (28) should be determined to obtain the stability criteria, which will result in the following stability criterion leading to inequality (29).
\[
\Delta t < \frac{SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)}{P_{i,j,k} + CR_{i,j - \frac{1}{2}k} + CR_{i,j + \frac{1}{2}k} + CC_{i - \frac{1}{2}j,k} + CC_{i + \frac{1}{2}j,k} + CV_{i,j,k - \frac{1}{2}} + CV_{i,j,k + \frac{1}{2}}} \tag{29}
\]

The (29) inequality will guarantee the stability of the scheme. It should be considered that if the value of \( P_{i,j,k} \), which is inherently a negative number is more significant than \( R_{i,j - \frac{1}{2}k} + CR_{i,j + \frac{1}{2}k} + CC_{i - \frac{1}{2}j,k} + CC_{i + \frac{1}{2}j,k} + CV_{i,j,k - \frac{1}{2}} + CV_{i,j,k + \frac{1}{2}} \) then the scheme will be unstable. In fact, Equation (29) shows that the maximum allowable time step for an explicit scheme is directly proportional to the storage term \( SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k) \) and inversely proportional to the conductance terms \( P_{i,j,k} + CR_{i,j - \frac{1}{2}k} + CR_{i,j + \frac{1}{2}k} + CC_{i - \frac{1}{2}j,k} + CC_{i + \frac{1}{2}j,k} + CV_{i,j,k - \frac{1}{2}} + CV_{i,j,k + \frac{1}{2}} \).

One of the results of this stability criteria is that in some extreme cases where the thickness is extremely small (generally when \( \Delta v_k \ll 1 \)) and the vertical hydraulic conductivity is exceptionally high, increasing the cell’s dimensions \((\Delta r_j \text{ and } \Delta c_i)\) may result in a reduction of maximum \( \Delta t \). In this cases, increasing the cell dimension could significantly increase the value of \( CV_{i,j,k - \frac{1}{2}} \) and \( CV_{i,j,k + \frac{1}{2}} \) in the denominator due to small amounts of \( \Delta v_k \) (See (Harbaugh, 2005)) which could result in a reduction in maximum \( \Delta t \). However, this cases are extremely unlikely in real world problems.
Appendix 2: HFB Package Modeling Using EXP1

A transient model was created to conduct the tests to investigate the compatibility of the EXP1 solver with the HFB package. This model used HFB cells in different positions and patterns to simulate possible scenarios. Figure 10 shows the model’s top view and HFB’s locations and situations.

Figure 10  Top view of test model for HFB package

The right-hand side boundary conditions in the model were defined using the Time-Variant Specific Head package. The head values were initially set to 15 m and gradually decreased to 5 m over 25 days. In contrast, the left-hand side boundary conditions were set as constant head with a value of 15 m. Figure 11 shows EXP1 and PCG solver results for the HFB model.
As seen in Figure 11, both solvers resulted in the same head values, which showed that EXP1 could fully include the HFB package in a model. Head differences between the EXP1 and PCG solver ranged from 0 to 0.95%.