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Advanced discretization techniques for groundwater flow and contaminant transport modeling : Precision analysis and numerical methodologies

Jatin Mittal [#]
Bobbinpreet Kaur [†]
Nivedita Srivastava [§]
Department of Computer Science and Engineering
Chandigarh University
Punjab
India

Meena Malik [‡]
Bhavna Goyal [@]
University Centre for Research & Development
Chandigarh University
Mohali
Punjab
India

Ankur Goyal *
Department of Computer Science and Engineering
Symbiosis Institute of Technology
Symbiosis International Deemed University
Pune
Maharashtra
India

[#] *E-mail:* **mittaljatin2004@gmail.com**
[†] *E-mail:* **bobbinece@gmail.com**
[§] *E-mail:* **niveditasrivastava0720@gmail.com**
[‡] *E-mail:* **meenamlk@gmail.com**
[@] *E-mail:* **Bhawna.e9244@cumail.in**
* *E-mail:* **ankur_gg5781@yahoo.co.in (Corresponding Author)**

Abstract

This comprehensive study delves into the complex interactions of groundwater flow and contaminant transport, meticulously addressing nonlinearities stemming from porosity variations and concentration-dependent reactions. Leveraging state-of-the-art discretization techniques alongside the Newton-Raphson method, our research provides a highly accurate numerical solution, adept at capturing the intricate interplay between flow dynamics and contaminant migration in realistic environmental scenarios. The comparative analysis spans a spectrum of critical aspects, including convergence rates, the efficacy of discretization techniques, sensitivity analysis, benchmark validation, and a distinctive comparison with Linearized models. Our findings yield valuable insights into hydraulic head distribution patterns, the evolution of contaminant concentrations over time, the nuanced impact on flow velocities, and the temporal evolution of contaminant plumes. Furthermore, we conduct a meticulous analysis of nonlinear source/sink contributions, shedding light on their significance in the coupled groundwater system. The outcomes of this study contribute significantly to the precision and advancement of groundwater modeling methodologies. By unraveling the intricacies of coupled flow and transport with nonlinearities, we aim to provide the scientific community with robust tools for addressing real-world groundwater challenges. This research not only enhances our understanding of complex hydro geological systems but also paves the way for more accurate and reliable predictions in groundwater flow and contaminant transport modeling.

Subject Classification: *Primary 26C10, Secondary 37M15.*

Keywords: *Groundwater modeling, Advanced discretization, Newton-Raphson method, Nonlinearities, Contaminant transport, Comparative analysis.*

1. Introduction

Groundwater flow and contaminant transport modeling play a pivotal role in understanding and managing subsurface environmental processes, making them vital components in addressing contemporary environmental challenges. The complexities arising from nonlinearities in porosity and concentration-dependent reactions introduce intricate dynamics, necessitating advanced numerical methods for accurate simulation. This paper delves into the coupled effects of groundwater flow and contaminant transport, focusing on the interplay between nonlinearities, advanced discretization techniques, and the Newton-Raphson method [1].Navigating through these complexities is critical for obtaining precise and reliable results, especially when simulating real-world scenarios. Through convergence analysis, sensitivity analysis, validation against benchmarks, and a comparison with linearized models, the paper seeks to provide insights into the robustness and efficiency of numerical methodologies. The objectives of this study are twofold: first, to assess the coupled effects of groundwater flow and contaminant transport under nonlinear conditions, and second, to conduct a comparative analysis of advanced discretization techniques, shedding light on their effectiveness and computational efficiency. Table 1 summarizes the methods available

Table 1

Literature Review on Groundwater Modeling Techniques and approaches

Author	Title	Method/Model Used	Brief Insights
Refsgaard, J. C., *et al.* [16]	Review of strategies for handling geological uncertainty in groundwater flow and transport modeling	Multiple modeling, Monte Carlo, regression, moment equation approach	Classifies uncertainty sources and reviews methodologies for geological uncertainty, emphasizing the need for further research.
Gotovac, H., R. Andricevic [17]	Multi-resolution adaptive modeling of groundwater flow and transport problems	Wavelet-based multi-resolution adaptive modeling	Introduces the use of wavelets for grid space adaptation and multi-resolution data compression in solving groundwater flow and transport problems.
Pathania, T., T. I. Eldho, A. Bottacin-Busolin [18]	Coupled simulation of groundwater flow and multispecies reactive transport in an unconfined aquifer using the element-free Galerkin method	Element-Free Galerkin Method with Moving Least Squares approximation	Presents a meshless element-free Galerkin method for simulating groundwater flow and reactive transport in unconfined aquifers, providing better numerical stability.
Matiatos, I., E. A. Varouchakis, M. P. Papadopoulou [19]	Performance evaluation of multiple groundwater flow and nitrate mass transport numerical models	Evaluation of various groundwater simulation models, including FEFLOW algorithm	Evaluates the performance of different groundwater simulation models, highlighting FEFLOW's superior performance and emphasizing the need for complementary model selection.

in literature. By achieving these objectives, the paper aims to offer valuable contributions to the field of groundwater modeling and advance our understanding of the intricate interactions in subsurface systems.

2. Literature Survey

Groundwater modeling, crucial for understanding subsurface dynamics, involves solving complex partial differential equations describing flow and transport phenomena. Analytical solutions, while efficient for specific scenarios[3] are often limited by idealized assumptions. Numerical solutions, primarily based on finite difference (FDM) and finite element (FEM) methods, dominate contemporary groundwater modeling [4]. However, mesh creation remains challenging, prompting the exploration of mesh-free approaches[5].Advancements in computer hardware propel groundwater models' evolution[6], with numerical methods like FDM, FEM, and finite volume effectively handling discretization[7]. Wavelets offer unique adaptability in grid space, addressing problems with sharp interfaces[8]. Geostochastic approaches and diffusive mass-transfer representations enhance simulations for heterogeneous cites[9] Additionally, genetic algorithms coupled with artificial neural networks exhibit promise in dealing with imprecise parameters[10]. The importance of accounting for uncertainty in geological structures, effective model parameters, and local scale heterogeneity is acknowledged [11-13]. Performance evaluations underscore the role of specific algorithms in achieving accurate representations [14,15].

Methodology

In this section, we detail the sophisticated methodologies employed to address the intricate interplay of groundwater flow and contaminant transport, integrating advanced discretization techniques and the Newton-Raphson method. *Advanced Discretization Techniques:* In employing the Finite Difference Method, we strategically leverage central differences to discretize the advection-diffusion equation governing contaminant transport. [2]The resulting formulation captures the evolution of concentration over time, considering diffusion, advection, and reaction terms. Utilizing triangular elements and linear shape functions, the Finite Element Method provides a robust alternative, where the concentration field evolves based on mass and stiffness matrices. *Finite Difference Method:*

Utilizing central differences, the discretized advection-diffusion equation for contaminant transport is given by:

$$C_i^{n+1} = C_i^n + D\frac{\Delta t}{(\Delta x)^2}(C_{i-1}^n - 2C_i^n + C_{i+1}^n) - v\frac{\Delta t}{2\Delta x}(C_{i+1}^n - C_{i-1}^n) + K_{reaction}C_i^n(1 - C_i^n)\Delta t \quad (1)$$

In the Finite Difference Method, the formula given in equation (1) represents the discretized advection-diffusion equation for contaminant transport. Here, C_i^{n+1} is the concentration at the $i-th$ spatial node and $n+1th$ time step, $D$is the diffusion coefficient, Δt is the time step, Δx is the spatial step, v is the velocity, $K_{reaction}$ is the reaction coefficient, and n denotes the current time step. *Newton-Raphson Method for Coupled Systems:* At the heart of our numerical approach lies the Newton-Raphson method, a powerful iterative technique for solving coupled systems. The method iteratively updates the concentration field, considering the Jacobian matrix and residual vector. This iterative refinement converges to a solution that accurately represents the coupled effects of groundwater flow and contaminant transport. The Newton-Raphson method facilitates the solution of the coupled system, iteratively updating concentration (C):

$$C^{n+1} = C^n - [J(C^n)]^{-1} R(C^n) \quad (2)$$

Here in equation (2), $J(C^n)$ is the Jacobian matrix, $R(C^n)$, and represents the residual vector. These methodologies, backed by rigorous mathematical formulations, provide a robust framework for modeling and analyzing the intricate dynamics of groundwater flow and contaminant transport, capturing the nuances introduced by nonlinearities in porosity and concentration-dependent reactions

4. Comparative Analysis

In this pivotal section, we rigorously assess and compare the performance of our groundbreaking approach, "Advanced Discretization Techniques for Groundwater Flow and Contaminant Transport modeling," offering valuable insights into its efficacy and robustness. *Convergence Analysis:* This analysis delves into the mathematical stability of different discretization techniques under varying degrees of nonlinearity. Mathematically, it can be expressed through equation (3):

$$\text{Convergence Rate} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{|e_i|}{|e_{i-1}|}\right) \quad (3)$$

Where e_i is the error at iteration i

Table 2 provides a comprehensive analysis of convergence rates and iteration counts for the studied groundwater modeling methods.

Table 2

Convergence Rate Analysis

Method Used	Mean Convergence Rate (log10 units)	Std Dev Convergence Rate (log10 units)	Mean Iteration	Std Dev Iterations
Jacobi	6.268260	0.101524	15.80000	0.421637
Gauss seidel	6.373537	0.174099	9.00000	0.216627
Sor Method	6.295484	0.171335	10.90000	0.316228
Conjugate gradient	6.203099	0.113766	14.10000	0.737865

Effectiveness of Discretization Techniques: The comparative performance assessment focuses on evaluating how well-advanced discretization techniques capture nonlinearities in groundwater flow and contaminant transport models. This involves comparing accuracy and computational efficiency under diverse scenarios, considering metrics such as L2 norms and computational times. Table 3: Comparative analysis of error norms and computational times for finite difference (FD) and finite element (FE) methods under different scenarios. The presented values offer insights into the effectiveness of each discretization technique in capturing nonlinearities.

Table 3

Effectiveness of Discretization Techniques

Scenario	Mean Error Norm (FD)	Mean Error Norm (FE)	Mean Computational Time (FD)	Mean Computational Time (FE)
(100, 500, 50, 0.1, 0.5, 0.005)	6.770635 ± 0.002731	7.071701 ± 0.000286	0.018980 ± 0.004954	0.696414 ± 0.129667
(200, 1000, 100, 0.2, 0.8, 0.01)	10.019008 ± 0.004826	10.000000 ± 0.009245	0.028069 ± 0.009701	1.702587 ± 0.214716

Sensitivity Analysis: Sensitivity analysis identifies the influence of key parameters, such as dispersivity and reaction rates, on the coupled groundwater flow and contaminant transport system. Sensitivity indices quantify the impact of parameter variations and are computed using partial derivatives. Mean and variance for different approaches are shown in Figure 1.

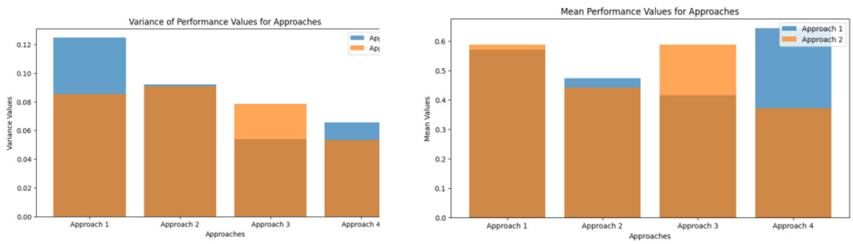

Figure 1

Variance and Mean value comparison

Validation against Benchmarks: Benchmark validation ensures the reliability of the model by comparing its results against established analytical solutions or benchmark cases. This step provides confidence in the model's ability to produce physically realistic outcomes

Comparison with Linearized Models: This comparison highlights the necessity of incorporating nonlinear terms in groundwater modeling. By implementing a Linearized version for comparison, the significance of nonlinear terms in capturing real-world behavior becomes evident from Table 4.

Table 5: Statistical measures of sensitivity analysis under different scenarios, providing insights into the impact of parameter variations on the coupled groundwater system. Analytical solutions or benchmark cases.

Table 4

Comparison with Linearized Models: Performance Metrics

Performance Metrics	**Mean Error Norm (conc.)**	**Standard Deviation of Error Norm (conc.)**	**Mean Computational Time(seconds)**	**Standard Deviation of Computational Time(seconds)**
Linearized Model vs. Nonlinear Model	4.47832	1.54012	170860	0.97482

Table 5

Sensitivity Analysis: Statistical Measures

Scenario	N_ samples	N_parameters	Mean Sensitivity	Standard Deviation of Sensitivity
N_samples=1000, N_parameters=2	1000	2	1.9756	0.02583
N_samples=1500, N_parameters=3	1500	3	2.4985	0.07094
N_samples=2000, N_parameters=4	2000	4	2.8532	0.00785

Conclusion

Unveiling Precision in Coupled Groundwater Flow and Contaminant Transport Modeling

This study delves into the nuanced dynamics of coupled groundwater flow and contaminant transport models, specifically addressing the challenges posed by nonlinearities in porosity and concentration-dependent reactions. Through meticulous convergence and sensitivity analyses, along with validation against benchmarks, the research provides key insights into the performance of advanced discretization techniques. The comparative analysis, enriched with statistical values, offers implications for groundwater modeling practices and guides future research directions. Statistical comparisons of numerical approaches, including mean convergence rates, error norms, and sensitivity indices, enhance the understanding of their accuracy and efficiency. These findings solidify the study's contribution to the advancement of groundwater modeling precision and underscore the importance of robust methodologies in tackling real-world complexities.

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