Eleventh International Conference on Computational Fluid Dynamics (ICCFD11), Maui, Hawaii, July 11-15, 2022

ICCFD11-2022-1502

Development of the PISALE Codebase for Simulating Flow and Transport in Large-scale Coastal Aquifer

Young-Ho Seo[*,**], Jonghyun Lee[*,**], Alice Koniges[***], Aaron Fisher[****]
Corresponding author: jonghyun.harry.lee@hawaii.edu

[*] Civil and Environmental Engineering, University of Hawai‘i at Manōa, USA.
[**] Water Resources Research Center, University of Hawai‘i at Manōa USA.
[***] Information and Computer Sciences, University of Hawai‘i at Manōa, USA.
[****] Information Technology Sciences, University of Hawai‘i at Manōa, USA.

Abstract: The solution of partial differential equations (PDEs) on modern high performance computing (HPC) platforms is essential to the continued success of groundwater flow and transport modeling in Pacific islands where complex regional groundwater flow is governed by highly heterogeneous volcanic rocks and dynamic interaction between freshwater and seawater. For accurate simulations of complex groundwater flow processes in the Hawaiian islands, the PISALE (Pacific Island Structured-AMR with ALE) software has been developed to offer an innovative combination of advanced mathematical techniques such as arbitrary Lagrangian-Eulerian method (ALE) and Adaptive Mesh Refinement (AMR). The software uses parallel programming models to accelerate the time to solution and dynamically adapt the grids using AMR. This allows for the solution of equations that can reproduce the sharp freshwater-seawater interface in large-scale coast aquifers. In this work, we summarize our ongoing efforts to create a publicly available sustainable branch of the software focused on the groundwater problem. The island-scale numerical groundwater flow modeling will play an important role in predicting the sustainable yields and potential contaminant transport for the volcanic aquifer systems and planning groundwater resources management.

Keywords: Flow in Porous Media, Adaptive Mesh Refinement, Arbitrary Lagrangian Eulerian, PISALE.

1 Introduction

Accurate simulation of density-driven flow and transport in coastal aquifers is crucial for evaluation of fresh groundwater sustainability and reliable water supply design amid climate change and associated sea level rise [1]. The numerical simulation of the density-driven flow process becomes more challenging for the prediction of the groundwater resources in Hawaii where complex groundwater flow processes governed by highly heterogeneous volcanic rocks and dynamic interaction between freshwater and seawater. We use the PISALE (Pacific Island Structured-AMR with ALE) code developed by the University of Hawai‘i [2] (see also https://pisale.bitbucket.io/). The project discussed here has developed a software toolkit aiming for accurate and scalable simulations of groundwater flow in the Hawaiian islands. This PISALE project combines advanced mathematical techniques for the solution of partial different equations (PDEs), including parallel software tools to dynamically adapt the grids and special Lagrangian-flow methods that allow for the solution of equations that can reproduce the sharp freshwater-seawater interface observed in seawater monitoring locations in Hawai‘i [3]. The PISALE software is based on the techniques of Arbitrary Lagrangian Eulerian (ALE) [4] methods with Adaptive Mesh Refinement (AMR) [5] to create a publicly available sustainable branch of the software. It is well known that the flow and salinity transport should be locally mass conservative to avoid unphysically spurious dispersion or oscillation especially when the flow is coupled with the transport system. The ALE-AMR method is formulated to ensure the local conservation of mass while preserving the sharp interface between freshwater and seawater.

2 Method Description

Complex groundwater flow process in coastal aquifers considers the interaction between freshwater and seawater. Especially in the Pacific islands, the simulation of groundwater flow and salt transport becomes more complex due to highly heterogeneous volcanic porous media and requires coupling the governing equations which are the groundwater flow equation and advection-dispersion equation for the so-called density-driven flow simulation. In this case, the hydraulic head will be dependent on the (salt) concentration, thus two-way coupling of transient flow and transport equations are needed to simulate fresh water lens.

In this work, groundwater flow modeling part has been implemented and tested in the Eulerian framework with AMR capability. The developed flow module is integrated into the advecton module already implemented in PISALE for density-driven flow in coastal aquifers. Flow models are developed and tested using MFEM [6], a free, lightweight, scalable C++ library for finite element methods. The Eulerian step in flow simulation will be projected onto the Lagrangian mesh of advection through operator splitting to solve coupled governing equations in the PISALE framework. Previously, a nodal finite element based diffusion model was implemented into an ALE-AMR method to simulate heat conduction and radiation transport [7]. Such implementations lay the ground work for these new models.

2.1 Mathematical Model for Density-Driven Groundwater Flow

The governing equation in groundwater flow in porous media is given by the conservation law in the domain $\Omega \in \mathcal{R}^3$ with the boundary $\partial\Omega$:

$$\nabla \cdot \mathbf{q} = f \qquad \text{in} \quad \Omega \tag{1}$$

where $\mathbf{q}$ and f are the Darcy velocity and source/sink term $[L/T]$, respectively. The velocity is defined as

$$\mathbf{q} = -\mathbf{K}\nabla h = -\mathbf{K}\left(\nabla p + \rho(c) g \nabla z\right) \qquad \text{in} \quad \Omega \tag{2}$$

where $\mathbf{K}$ is hydraulic conductivity $[L/T]$, h is hydraulic head $[L]$, p is pressure head $[L]$, ρ is the fluid density $[M/L^3]$. For density-driven groundwater flow models, the density is generally assumed as a linear function of salinity c:

$$\rho(c) = \rho_f + \frac{\partial \rho}{\partial c}(c - c_0) \approx \rho_f + (\rho_s - \rho_f)\, c \tag{3}$$

The transport of groundwater is described as:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\mathbf{v} c) + R \tag{4}$$

where D is the diffusivity $[L/T^2]$, $\mathbf{v}$ is the velocity of groundwater $[L/T]$ obtained from $\mathbf{q}$ with the material porosity, and R is the sink/source term.

2.2 Mixed Finite Element Method for Flow Simulation

For the flow simulation, a mixed finite element method [8, 9] is used to provide groundwater velocity, e.g., specific discharge, to transport equation as in Equations 1 and 2. The finite element method has an advantage in modeling complex geometries and irregular grids and the mixed finite element method provides an accurate, continuous groundwater velocity that the tracer transport model for density-driven flow requires. Equation 5 derives a weak formulation from Equation 2 by multiplying a test function by τ and integrating it over the domain Ω:

$$
\begin{aligned}
\int_{\Omega} (\mathbf{q}\cdot\tau + \mathbf{K}\nabla h\tau)\,\mathrm{d}x = 0 \qquad \forall\tau\in\Sigma \\
\int_{\Omega} (\mathbf{q}\cdot\tau - \mathbf{K}h\nabla\cdot\tau + \nabla\cdot(\mathbf{K}h\tau))\,dx = 0 \\
\int_{\Omega} (\mathbf{q}\cdot\tau - \mathbf{K}h\nabla\cdot\tau)\,\mathrm{d}x = -\int_{\partial\Omega} \mathbf{K}h\tau\cdot n \quad \mathrm{d}s
\end{aligned} \tag{5}
$$

where τ is vector test function and Σ is its function space. Equation 6 represents the weak formulation of the mass conservation in Equation 1 multiplying a test function by v and integrating it over the domain on both sides.

$$
\int_{\Omega} \nabla\cdot\mathbf{q}v\mathrm{d}x = -\int_{\Omega} fv\mathrm{d}x \qquad \forall v\in V \tag{6}
$$

where v is test function and V is function space. Equation 7 represents the weak formulation expressed as the general form. The variational form of a and L for the mass matrix and a right hand side vector are defined as in Equations 8 and 9, respectively and assembled into a linear system for the solution of the groundwater flow problem.

$$
a((\mathbf{q},h),(\tau,v)) = L((\tau,v)) \qquad \forall(\tau,v)\in(\Sigma_0,V) \tag{7}
$$

$$
a((\mathbf{q},h),(\tau,v)) = \int_{\Omega} (\mathbf{q}\cdot\tau - \mathbf{K}h\nabla\cdot\tau + \nabla\cdot\mathbf{q}v)\,\mathrm{d}x \tag{8}
$$

$$
L((\tau,v)) = -\int_{\Omega_D} fv\mathrm{d}x - \int_{\partial\Omega} \mathbf{K}h_0\tau\cdot n \quad \mathrm{d}s \tag{9}
$$

2.3 Arbitrary Lagrangian-Eulerian Method with Adaptive Mesh Refinement for Tracer Transport

The velocity of groundwater is calculated from the previously explained groundwater model and fed to the transport model to update the salinity c over time. In turn, the salinity $c(t)$ computed from the transport model changes the head distribution and groundwater velocity. In this work, we assume dispersion coefficients to be zero indicating that the sharp interface exists between freshwater and seawater often observed in a regional aquifer in Hawaii [3]. Furthermore, the velocity is decoupled to the flow equation, thus does not change over the time, *i.e.*, conservative tracer simulation:

$$
\frac{\partial c}{\partial t} + \nabla\cdot(\mathbf{v}c) = 0 \tag{10}
$$

This advection-dominant configuration is intended to illustrate the effectiveness and efficiency of our proposed PISALE framework.

In general, the numerical simulation of transport with discontinuities is computationally challenging due to numerical difficulties in preserving sharp boundary conditions and associated fine space/time mesh discretization in the widely used Eulerian framework. To address these issues in a computationally efficient manner, mixed Eulerian and Lagrangian methods [10, 11] have been proposed with the method of characteristics (MOC) and particle tracking when solving the contaminant transport in groundwater flow. However, various boundary conditions for realistic groundwater transport simulations may not be implemented suitably in MOC and particle tracking may require a number of memory-intensive particle transport simulations to ensure the local mass conservation. The ALE-AMR approach implemented in PISALE can offer a systematic treatment for accurate advection-dominated simulations in a computationally scalable manner. The ALE formulation takes advantage of the Lagrangian and Eulerian descriptions in solving the advection problems without additional artificial dispersion to reduce spurious oscillations. For more accurate solution without extensive computation an adaptive mesh is introduced within the context of the ALE formulation. The Adaptive Mesh Refinement(AMR) framework SAMRAI [5] is used to automate mesh relaxation and adaptation in a highly parallel fashion optimized for High Performance Computing (HPC) platforms. SAMRAI is included in PISALE as an underlying library. Coupled density-driven flow examples will be demonstrated elsewhere.

3 Examples

Examples for one way coupling of flow and transport simulations, e.g., velocity computed from groundwater flow simulation fed to salt tracer transport simulation, are illustrated here. The 2D square domains with two different hydraulic conductivity fields are tested to update pressure and velocity fields followed by the conservative transport simulation. The numerical simulations were performed on a computational node with 48 Intel Xeon 6240R 2.4GHz cores in the University of Hawaii HPC cluster Mana.

3.1 Groundwater flow model simulation

For the accurate continuous groundwater velocity simulation, the mixed finite element method through the MFEM library is used to simulate both the hydraulic head and velocity field. Figure **??** represents the domain $\Omega = (0, 1000\,\mathrm{m})^2$ of the groundwater flow model which consists of a 50 by 50 triangular mesh grid. The left and right boundaries are set to 10 m and 0 m of hydraulic heads, respectively and the upper and lower boundaries have a constant head decreasing from 10 m to 0 m linearly.

To illustrate, we generate isotropic homogeneous and heterogeneous hydraulic conductivity (K) fields as shown in Figures 1 (b) and 2 for the groundwater flow model coefficients, i.e., hydraulic conductivity K in Equation 2. The heterogeneous K field is generated from a log-normal distribution with a variance of 0.01 with an anisotropy ratio of 4 to 1 assigned to the spatial correlation during the random field generation.

Figures 1 (b) and 2 (b) represent the hydraulic head distribution from homogeneous and heterogeneous hydraulic conductivity fields respectively. The contour maps for both cases depict equipotential lines of hydraulic heads varying from 10 to 0 m at 2 m intervals. The quiver plots depict the groundwater velocity as arrow sizes and directions. In the homogeneous case, the hydraulic head changes linearly in which contour lines appear in a straight line and the velocity field is uniform. Figure 2 (b) shows the results affected by the heterogeneous hydraulic conductivity field (Figure 2 (a)) in which the equipotential lines of the head follow meandering lines and the velocity vector varies depending on the hydraulic conductivity and the gradient of hydraulic head.

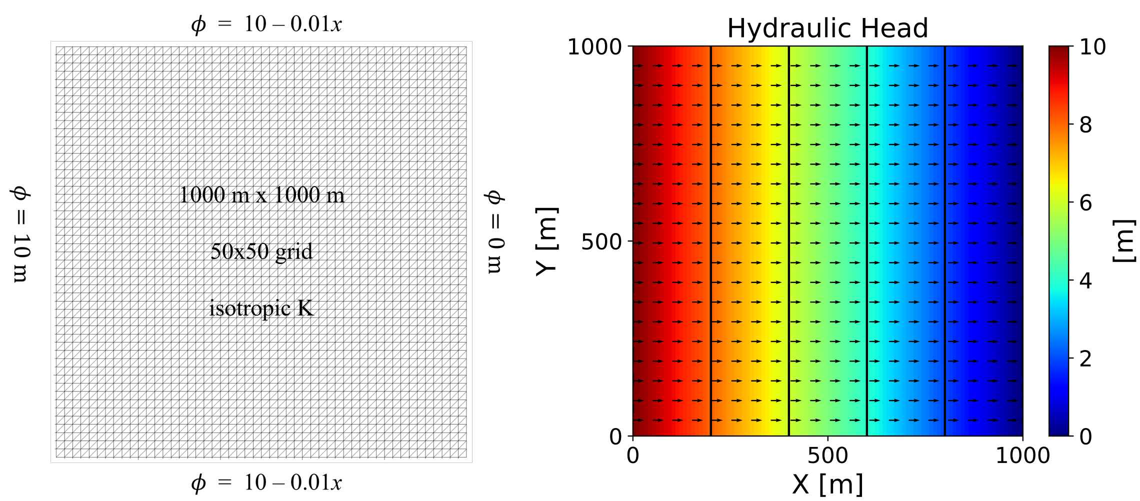

Figure 1: (a) model domain and Finite Element mesh used in the flow simulation (b) simulated hydraulic head and flow velocity of the Homogeneous Test Case

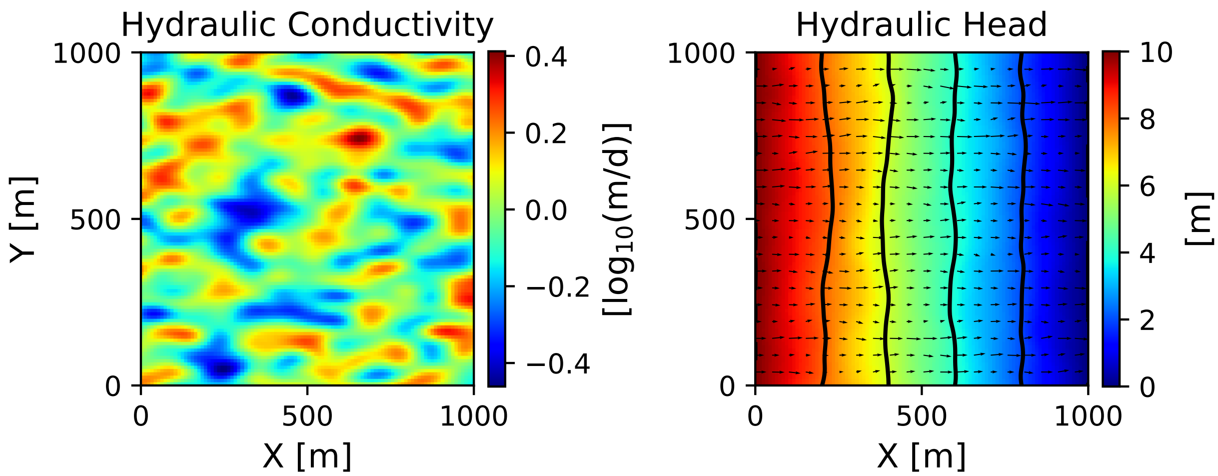

Figure 2: Hydraulic head and flow velocity of the Heterogeneous Test Case

3.2 Conservative Tracer Transport Simulation

With the velocity fields computed from the flow simulation, our PISALE framework is used to simulate the conservative tracer (i.e., salt) transport. This simulation assumes that convective seawater intrusion in the 1000 m by 1000 m square model domain. The red and blue areas represent seawater and freshwater, respectively. Figure 3 shows the convective tracer transport with the homogeneous K field. The initial concentration distribution of tracer is set to a sine function at $x = 400\,\text{m}$ as shown in the Figure 3 (left). It is illustrated that the tracer moved to $x = 470\,\text{m}$ and 540 m without change in the tracer distribution, it takes 5.75 years and 11.5 years respectively. Figure 4 represents the convective tracer transport with the heterogeneous K field. The initial distribution of the tracer starts from the uniform at $x = 200\,\text{m}$ as shown in the 4 (left). The tracer moves to $x = 350\,\text{m}$ and 500 m (Figure 4 center and right, respectively), it takes 12.6 year to travel 150 m on average. The uniform distribution of the trace has been changed as it is transported. The changes are propagated due to the heterogeneous K and corresponding velocity fields. For both cases, PISALE successfully adapt the mesh following the flow velocity field and preserve the freshwater-seawater interface.

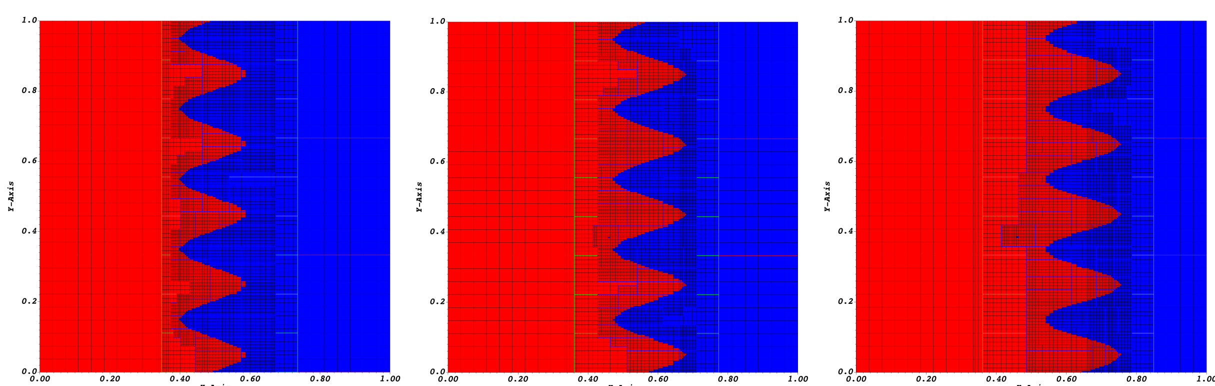

Figure 3: Conservative tracer transport with homogeneous K field at t = 0 yr (left), 5.75 yrs (center) and 11.5 yrs (right)

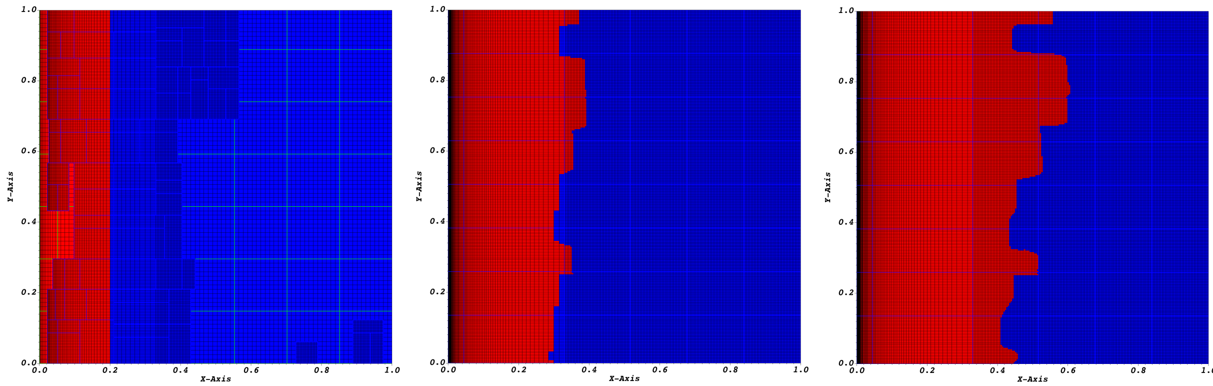

Figure 4: Conservative tracer transport with heterogeneous K field at t = 0 yr (left), 12.6 yrs (center) and 25.2 yrs (right)

4 Concluding Remarks

In this work, we present our ongoing efforts in density-driven flow simulation in Pacific island aquifers. The groundwater flow equation is solved using the mixed finite element method and the saltwater transport is simulated using an ALE with AMR methodology. As an ongoing project, we will couple the flow and transport codes with an operator splitting method within the full PISALE codebase. The accuracy and computational scalability will be tested for island-scale 3D freshwater-seawater interaction applications.

5 Acknowledgements

We would like to thank many additional members of the PISALE team for their expertise and assistance throughout all aspects of our study and for their help in writing this manuscript. The PISALE code is supported by the National Science Foundation, under Office of Advanced Cyber Infrastructure Award Number 2005259, the U. S. Department of Energy, Office of Science, under Fusion Energy Sciences Research Division Award Number DE-SC0021374, and the Office of Naval Research, under ONR MURI Award Number N00014- 20-1-2682. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC awards ERCAP0020882 and ERCAP0020890.

The technical support and advanced computing resources from University of Hawaii Information Technology Services – Cyberinfrastructure, funded in part by the National Science Foundation MRI award # 1920304, are gratefully acknowledged.

References

[1] Peter K Kang, Jonghyun Lee, Xiaojing Fu, Seunghak Lee, Peter K Kitanidis, and Ruben Juanes. Improved characterization of heterogeneous permeability in saline aquifers from transient pressure data during freshwater injection. *Water Resources Research*, 53(5):4444–4458, 2017.

[2] Alice Koniges, Nathan Masters, Aaron Fisher, David Eder, Wangyi Liu, Robert Anderson, David Benson, and Andrea Bertozzi. Multi-material ale with amr for modeling hot plasmas and cold fragmenting materials. *Plasma Science and Technology*, 17(2):117, 2015.

[3] D. S. Oki. Modeling the groundwater flow system of the keauhou area, hawaii, Apr 2018.

[4] Jean Donea, Antonio Huerta, J.-Ph. Ponthot, and A. Rodríguez-Ferran. *Arbitrary Lagrangian–Eulerian Methods*, chapter 14. John Wiley & Sons, Ltd, 2004.

[5] Richard D Hornung and Scott R Kohn. Managing application complexity in the samrai object-oriented framework. *Concurrency and computation: practice and experience*, 14(5):347–368, 2002.

[6] R. Anderson, J. Andrej, A. Barker, J. Bramwell, J.-S. Camier, J. Cerveny V. Dobrev, Y. Dudouit, A. Fisher, Tz. Kolev, W. Pazner, M. Stowell, V. Tomov, I. Akkerman, J. Dahm, D. Medina, and S. Zampini. MFEM: A modular finite element methods library. *Computers & Mathematics with Applications*, 81:42–74, 2021.

[7] A. C. Fisher, D. S. Bailey, T. B. Kaiser, D. C. Eder, B. T. N. Gunney, N. D. Masters, A. E. Koniges, and R. W. Anderson. An AMR capable finite element diffusion solver for ALE hydrocodes. *Plasma Science and Technology*, 17(2):109–116, feb 2015.

[8] Douglas N Arnold and Franco Brezzi. Mixed and nonconforming finite element methods: implementation, postprocessing and error estimates. *ESAIM: Mathematical Modelling and Numerical Analysis*, 19(1):7–32, 1985.

[9] G Chavent and JE Roberts. A unified physical presentation of mixed, mixed-hybrid finite elements and standard finite difference approximations for the determination of velocities in waterflow problems. *Advances in Water Resources*, 14(6):329–348, 1991.

[10] Shaul Sorek. Two-dimensional adaptive eulerian-lagrangian method for mass transport with spatial velocity distribution. *Transport in porous media*, 3(5):473–489, 1988.

[11] Chunmiao Zheng, P Patrick Wang, et al. Mt3dms: a modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems; documentation and user's guide. 1999.