Investigating the Adaptability of ALE-AMR Hydrocode for Darcy Flow and Geothermal Simulations

Alice Koniges
Information and Computer Sciences
University of Hawai'i at Mānoa
Honolulu, HI, USA
email: koniges@hawaii.edu

David Eder
Physics and Astronomy
University of Hawai'i at Mānoa
Honolulu, HI, USA
email: dceder@hawaii.edu

Jonghyun Lee
Civil & Env Eng and Water Res Center
University of Hawai'i at Mānoa
Honolulu, HI, USA
email: jonghyun.harry.lee@hawaii.edu

Jiawei Shen
Civil & Env Eng and Water Res Center
University of Hawai'i at Mānoa
Honolulu, HI, USA
email: jiaweish@hawaii.edu

Aaron Fisher
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
Livermore, CA, USA
email: fisher47@llnl.gov

Tzanio Kolev
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
Livermore, CA, USA
email: kolev1@llnl.gov

***Abstract*—The PISALE ALE-AMR hydrocode suite is an advanced computational tool that combines the Arbitrary Lagrangian-Eulerian (ALE) method with Adaptive Mesh Refinement (AMR) to simulate complex multi-physics problems involving substantial material deformation. The suite currently includes physics modules for heat conduction and radiation transport, which are handled by a finite element diffusion solver operating on a structured, adaptive mesh infrastructure provided by the SAMRAI library. This paper investigates the feasibility of extending this framework to simulate fluid flow in porous media as described by Darcy's law, a critical component for subsurface applications like geothermal energy extraction and hydrogeology. We analyze the mathematical parallels between diffusion and Darcy flow, assess the suitability of the existing solver, and consider the integration of the more general MFEM finite element library. The primary objective is to evaluate the potential of the ALE-AMR methodology for Darcy flow simulations and to outline the necessary modifications and implementation steps, including addressing challenges related to integrating different AMR and grid formulations.**

***Keywords*-ALE-AMR; Darcy flow; geothermal simulation; porous media; finite element method; MFEM; hydrocode; computational fluid dynamics.**

I. INTRODUCTION

The PISALE ALE-AMR hydrocode suite represents an advanced computational tool that combines the Arbitrary Lagrangian-Eulerian (ALE) method with Adaptive Mesh Refinement (AMR) [1]. This combination enables the simulation of physical phenomena characterized by substantial material deformation, via the Lagrangian approach, while simultaneously addressing challenges associated with mesh distortion and optimizing computational efficiency through localized mesh refinement, which are key features of AMR methodologies. Initially published as ALE-AMR, the code is more recently referred to as PISALE (Pacific Island Structured-AMR with ALE), with various specialized versions developed to model a diverse range of applications [2].

Currently, the hydrocode suite incorporates physics modules dedicated to simulating heat conduction and radiation transport, both of which are modeled using a finite element diffusion solver [3]. This solver is specifically engineered to operate on the dynamically adapting mesh structures generated by the AMR technique. The foundational support for adaptive mesh refinement within the hydrocode is provided by the SAMRAI (Structured AMR Application Infrastructure) library. Given its established infrastructure for managing complex mesh geometries and integrating various physics modules, we discuss here the potential for further expansion to simulate additional physical phenomena, including Darcy flow in subsurface applications.

Darcy's law governs the movement of fluid through a given material, and for this application, we consider flow through a porous medium [4]. This law states that the rate at which a fluid flows through a permeable material is directly proportional to the pressure gradient driving the flow and the intrinsic permeability of the material, while being inversely proportional to the viscosity of the fluid. In hydrogeology, it serves as a basis for analyzing groundwater flow; in petroleum engineering, it is used for multiphase flow modeling (e.g., the behavior of oil and gas reservoirs); and in geothermal energy, it is used for understanding the transport of both heat and fluids within the Earth's subsurface [5].

This paper presents an investigation into the feasibility of using the existing ALE-AMR methodology, in conjunction with its current finite element diffusion solver and/or the MFEM solver, for simulating fluid flow in porous media governed by Darcy's law. A detailed analysis examines the mathematical similarities and differences between diffusion and Darcy flow, assess the suitability of the current solver and/or replacing it with a more general finite element package, MFEM, for modeling Darcy flow. The primary objective is to evaluate the potential of ALE-AMR for Darcy flow simulations and outline the requisite steps for implementation.

The MFEM solver is a general purpose high-performance, open-source finite element library developed for solving partial differential equations. It provides a flexible and scalable framework for discretizing and solving a wide range of problems. MFEM's capabilities include support for various finite element formulations, efficient linear and nonlinear solvers, and advanced mesh management techniques. By leveraging MFEM's strengths, this investigation aims to explore its potential as a viable alternative or complement to the existing diffusion solver for Darcy flow simulations within the ALE-AMR framework. One problem with direct application of MFEM is that it has its own AMR and grid formulation which needs adaptation for PISALE. We discuss solutions to this obstacle later in the paper.

II. The ALE-AMR Hydrocode and its Finite Element Diffusion Solver

The ALE method, as implemented in ALE-AMR, provides flexibility in handling various geometries and scenarios involving large-scale deformations and multiple objects within a domain. The mathematics follows a Lagrangian description, where the mesh follows the material, and an optional and/or modified remap to an Eulerian description, where the mesh appears via the remap to remain fixed in space. The AMR capabilities integrated within ALE-AMR serve to enhance the efficiency of computations by selectively refining the mesh in regions identified as requiring higher accuracy, such as areas with sharp gradients or complex flow patterns. This localized refinement ensures that computational resources are focused where they are most needed, without incurring the overall cost of a uniformly fine mesh. This ALE-AMR framework, which was developed initially for pure gas dynamics simulations, has matured into a comprehensive multiphysics framework capable of addressing a broad spectrum of applications, including phenomena in high-energy-density physics, material impacts, and laser target modeling [2]. Some very preliminary results on the application of PISALE to groundwater flow are given elsewhere [6].

The physics modules responsible for simulating heat conduction and radiation transport within ALE-AMR are enabled by a finite element diffusion solver specifically engineered to function on the composite meshes generated by the AMR. This solver employs a nodal-based approach, where the primary variables of interest are defined at the nodes of the computational mesh. A critical feature of this solver is its utilization of transition elements to effectively manage the interfaces that arise between regions of the mesh with different levels of refinement, a direct consequence of the AMR technique. These specialized elements are designed to ensure the continuity of the solution across these coarse-fine boundaries by appropriately handling the hanging nodes, edges, and faces that are characteristic of such interfaces. For the necessary 3:1 refinement ratio (or multiples, thereof) employed by the ALE-AMR framework for consistency, a variety of transition element types are used, depending on which of the element's sides are subject to refinement.

The finite element method necessitates the use of numerical integration techniques, which are implemented through quadrature rules within the solver. For the transition elements, compound Gauss-Legendre quadrature[3] is employed to maintain a level of integration accuracy comparable to that achieved on standard elements. Additionally, mass lumping quadrature rules, which strategically place integration points at the element nodes, are utilized to produce diagonal mass matrices, a property that can be advantageous for certain time-stepping schemes. To overcome the challenge of undefined derivatives at the transition faces, which complicates the computation of the stiffness matrix, "blurred" quadrature rules are implemented. These rules work by averaging the evaluations of derivatives taken from different regions within the element, thereby ensuring the accurate assembly of the stiffness matrix.

The discretization of the diffusion equation is achieved using the standard Galerkin approach, a method where the equation is multiplied by a test function, integrated over the computational domain, and then subjected to integration by parts to derive the weak form. Both the solution being sought and the test functions used in the formulation are approximated using a basis set composed of shape functions defined on both standard and transition elements. This process culminates in a system of linear algebraic equations, typically represented in matrix form as Au = f, where A is the system/stiffness matrix, u is the vector containing the unknown nodal values of the solution, and f is the vector representing the source terms. This linear system is then solved using the HYPRE GMRES solver, an iterative algorithm particularly well-suited for handling large, sparse systems of equations, often enhanced by the use of a preconditioner to accelerate the convergence of the solution. The current finite element framework within PISALE/ALE-AMR is based on first-order H1 quadrilateral elements in two dimensions and hexahedral elements are required in three dimensions. These element types are recognized as being well-suited for the diffusion equation solvers that underpin the heat conduction and radiation diffusion modules.

The PISALE diffusion solver serves as the foundation for modeling heat conduction through the dynamic diffusion equation, which accounts for the temporal evolution of temperature and the flow of heat within the material. This equation incorporates parameters such as specific heat, thermal conductivity, and the absorptivity of the medium. Similarly, radiation transport can be modeled using the diffusion approximation, a simplification of the more complex radiative transfer equations that is applicable under certain conditions, such as in optically thick media. This approach involves formulating equations for both the energy density of radiation and the temperature of the material, with coupling terms that describe the absorption and emission of radiation. A significant hurdle in integrating these physics modules with the ALE-AMR framework arises from the inherent difference in how physical variables like temperature and energy are represented within the code. Specifically, the finite element method uses nodal representations, while PISALE uses cell-centered values for certain variables. To bridge this gap, we employ projection integrals as a means of mapping variables between the nodes and the cell centers, a technique that ensures the conservation of energy during the transfer process. This mapping involves calculating the differences in cell temperatures after the hydrodynamic step, using the specific heat capacity to determine the corresponding energy and specific heat differences at the nodes, updating the nodal temperatures based on these differences, and then transferring these changes back to the cells to update their internal energy.

III. Darcy's Law and Flow in Porous Media

In its most fundamental form, Darcy's law describes the rate of fluid flow (Q) through a porous medium as being directly proportional to the cross-sectional area (A) of the flow path and the pressure difference (ΔP) over a given length (L), and inversely proportional to the viscosity (μ) of the fluid. Mathematically, this relationship is expressed as $Q = -(kA/\mu)(\Delta P/L)$, where k represents the permeability of the porous medium. The negative sign in the equation signifies that the direction of flow is from regions of higher pressure to regions of lower pressure. Permeability (k) is an intrinsic property of the porous medium that quantifies its capacity to transmit fluids. This property is influenced by the grain size, shape, and interconnectedness of the pores within the material. Permeability can be uniform in all directions, in which case it is termed isotropic, or it can vary with direction, in which case it is termed anisotropic and is mathematically represented as a tensor. The differential form of Darcy's law relates the Darcy velocity (v), which is the volumetric flow rate per unit cross-sectional area, to the gradient of the pressure (∇p) and is given by $v = -(k/\mu)\nabla p$. The ratio k/μ multiplied by the specific weight (ρg) is often referred to as the hydraulic conductivity (K), particularly when considering the flow of a specific fluid with a known viscosity. Hydraulic conductivity can also incorporate the effect of gravity when the flow is described in terms of hydraulic head ($h = p/\rho g + z$), leading to the form $v = -K\nabla h$ [4].

For a steady-state flow of an incompressible fluid through a porous medium, the principle of mass conservation, expressed by the continuity equation, dictates that the divergence of the velocity field must be zero ($\nabla \cdot v = 0$). By combining this with the differential form of Darcy's law ($v = -(k/\mu)\nabla p$), we arrive at the governing equation for the pressure distribution within the medium: $\nabla \cdot (-(k/\mu)\nabla p) = 0$ when there is no source/sink to the system. In scenarios where the permeability (k) and the fluid viscosity (μ) are spatially uniform, this equation simplifies to Laplace's equation: $\nabla^2 p = 0$. However, in heterogeneous media where these properties vary from one point to another, the equation retains its more general elliptic partial differential form [7]. This mathematical similarity in form between the governing equation for pressure in Darcy flow and the steady-state diffusion equation ($\nabla \cdot (D\nabla u) = 0$), where D corresponds to k/μ and u to p, is a significant factor in considering the potential for adapting the existing diffusion solver.

Simulating Darcy flow typically involves the application of specific boundary conditions that define the state of the flow at the edges of the computational domain. These commonly include: (i) Prescribed Pressure (Dirichlet boundary condition), where the pressure is set to a known value on certain boundaries, such as at the interface with a large fluid reservoir; (ii) Prescribed Flow Rate (Neumann boundary condition), where the rate at which fluid enters or leaves the porous medium across a boundary is specified such as no-flux boundary representing impermeable conditions; (iii) and Mixed Boundary Conditions, which involve applying different types of conditions on different segments of the domain's boundary. These are often used to model injection or production from wells. Well injection/extraction are typically dealt as source/sink conditions (non-zero RHS in the mass conservation equation). The ALE-AMR framework would need to be capable of implementing these types of boundary conditions, which might differ from those typically used in simulations of heat conduction and radiation transport.

One important point to note about the ALE-AMR framework however is the fact that because of the AMR refinement levels, one can often make the computational domain so large that the boundary conditions play little role in determining the early time behavior of the system. This is particularly beneficial for field-site applications since the modelers often make the domain large enough to minimize the effect of uncertain boundary conditions estimated in the field using geophysics or sparse field data sets. One can wrap the problem in a largely non-participatory airmesh for certain dynamical situations and effectively remove the boundary effects for the problem at hand.

Darcy's law and the associated governing equations are used extensively in modeling a wide variety of phenomena. These include the flow of groundwater in aquifers, encompassing scenarios such as flow towards extraction wells for freshwater supply, the regional movement of groundwater for contaminant remediation, and the interaction between groundwater and surface water bodies for flooding and drought risk mitigation. Notably, ALE methods have been successfully applied to simulate groundwater flow in situations involving free surfaces, which are characterized by moving boundaries [8]. In the field of petroleum engineering, Darcy's law is fundamental for simulating the flow of hydrocarbons (oil and gas) and water within subsurface reservoirs, enabling the prediction of production rates and the design of effective recovery strategies. The extraction of geothermal energy from the Earth's internal heat relies on the flow of fluids through porous rock formations, a process that can be modeled using Darcy's law, often in conjunction with equations governing heat transfer. Beyond these primary applications, Darcy's law is also utilized in modeling flow through various types of filters, membranes, and porous electrodes in devices like fuel cells.

While Darcy's law is a powerful tool, it is predicated on certain assumptions that limit its applicability to specific flow regimes and porous media characteristics. A fundamental assumption is that the flow is laminar, a condition typically met at low flow velocities and within media having small pore sizes, resulting in low Reynolds numbers (generally below

1 to 10). At higher velocities, inertial forces become non-negligible, and the flow transitions to turbulence, a regime where Darcy's law in its basic form is no longer accurate. In such cases, modifications like the Forchheimer equation, which incorporates a term proportional to the square of the velocity, are employed to account for these inertial effects. Furthermore, Darcy's law typically assumes a homogeneous and isotropic porous medium, meaning that the properties of the medium (like permeability) are uniform throughout and are the same in all directions. In reality, many geological formations and engineered materials exhibit heterogeneity, where properties vary spatially, and anisotropy, where permeability differs depending on the direction of flow. While the tensorial form of Darcy's law can accommodate anisotropy, significant heterogeneity might necessitate finer spatial discretization with more advanced modeling techniques. In very low permeability media under extremely small pressure gradients, deviations from the linear relationship described by Darcy's law have been observed, a phenomenon known as pre-Darcy flow. This behavior is thought to be due to factors such as the presence of immobile fluid layers at the pore walls. Lastly, the basic formulation of Darcy's law is for single-phase flow, where only one fluid is present in the porous medium. For scenarios involving multiple immiscible fluids (like oil and water in a reservoir), generalized forms of Darcy's law are used, which introduce the concept of relative permeabilities for each fluid phase. The dependence of fluid/rock density and permeability on the temperature, pressure, and displacement further complicate the modeling effort. We first consider what is involved in adapting the ALE-AMR code for Darcy flow based on its current diffusion solver for simulating laminar, single-phase flow in porous media. Modeling more complex flow regimes or multiphase scenarios would require additional developments.

IV. Mathematical Parallels and Divergences: Diffusion vs. Darcy Flow

The general form of the diffusion equation is given by $\partial u/\partial t = \nabla \cdot (D\nabla u) + S$, where u represents the quantity undergoing diffusion (such as temperature or concentration), D is the diffusion coefficient (e.g., thermal diffusivity or mass diffusivity), and S denotes any sources or sinks of the quantity u. In a steady-state scenario, where the conditions do not change with time, the time derivative becomes zero, resulting in the equation $\nabla \cdot (D\nabla u) + S = 0$. If, in addition, there are no sources or sinks within the domain, the equation further simplifies to $\nabla \cdot (D\nabla u) = 0$. In the special case where the diffusion coefficient D is also constant throughout the domain, the equation reduces to Laplace's equation, $\nabla^2 u = 0$. Within the ALE-AMR hydrocode, for the simulation of heat conduction, u corresponds to the temperature (T), and D is related to the thermal conductivity of the material. The source term S in this context can represent the generation or absorption of heat. For the modeling of radiation transport using the diffusion approximation, the equations involve the radiation energy density (E_R) and the material temperature (T), with the "diffusion coefficient" being a function of radiation-specific properties such as opacities and the speed of light. Thus, the diffusion equation fundamentally describes the transport of a scalar quantity driven by its own spatial gradient.

As previously discussed, the steady-state flow of an incompressible fluid in a heterogeneous porous medium under Darcy's law is governed by the equation $\nabla \cdot (-(k/\mu)\nabla p) = 0$, where p is the pressure, k is the permeability tensor of the medium, and μ is the viscosity of the fluid.

Despite their different physical contexts, both the steady-state diffusion equation and the governing equation for Darcy flow with homogeneous medium share significant mathematical similarities. First, they are both second-order partial differential equations of the elliptic type. This classification implies that the solution at any given point within the domain is influenced by the conditions imposed at all the boundaries of the domain. Second, both equations describe a flux—be it heat flux or radiation flux in the case of diffusion, or Darcy velocity in the case of Darcy flow—that is directly proportional to the gradient of a scalar potential. For diffusion, this potential is temperature or radiation energy density, while for Darcy flow, it is pressure or hydraulic head. The constant of proportionality is a transport property, which is the diffusion coefficient in the diffusion equation and the permeability (divided by viscosity) in Darcy's law. Third, both types of equations are amenable to solution using similar numerical techniques, most notably the finite element method. This method involves discretizing the continuous domain into a mesh of smaller elements and then approximating the solution within each element using a set of basis functions. This suggests that the numerical methodologies already in place within the ALE-AMR diffusion solver could be adapted to address problems involving Darcy flow.

However, there are also key differences between these two types of physical processes and their mathematical representations. A primary divergence lies in the nature of the primary variable and the desired output. The diffusion solver in ALE-AMR is designed to solve for a scalar quantity, such as temperature or energy, which is also the main result of the simulation. In contrast, while the governing equation for Darcy flow is often solved for pressure, which is a scalar, the quantity of principal interest is frequently the Darcy velocity, which is a vector quantity representing the rate and direction of fluid flow [9]. To obtain this velocity, Darcy's law itself must be applied to the computed pressure gradient, either as a post-processing step or through a different formulation. Another significant difference pertains to the physical properties involved. The diffusion equation utilizes properties like thermal conductivity or radiation opacities, which are typically scalar quantities, although they can exhibit anisotropic behavior in some materials. Darcy flow, however, is characterized by permeability, which in anisotropic porous media is inherently a tensor, reflecting the fact that fluid flow can be more or less restricted depending on the direction. Another more complicated issue is spatial variability. One may need to discretize the domain with finer resolution, for example, the number of the cells with different permeability in the domain can be 100 x 100 x 100

 ISBN: 978-1-68558-289-0

or 1000 x 1000 x 1000 for 3D. In many cases, modelers assign only horizontal and vertical permeability in a cell instead of full tensor values. The full tensor is typically needed for coarse-scale discretization to simulate directional flow. With finer discretization, it can handle directional flow with small-scale horizontal/vertical permeability. The ALE-AMR solver would need to be capable of handling such tensorial properties for permeability. Additionally, the viscosity (μ) of the fluid is a critical parameter in Darcy's law, whereas it does not explicitly appear in the standard heat or radiation diffusion equations. While both types of equations can include source terms, their physical interpretations differ. Sources in diffusion problems represent the generation or absorption of the diffusing quantity (heat or energy), whereas in Darcy flow, sources typically correspond to the injection or extraction of fluid from the porous medium. Finally, the boundary conditions commonly encountered in Darcy flow simulations, such as prescribed flow rates or impermeable boundaries, might not have direct analogs in heat conduction or radiation transport problems, necessitating the implementation of new types of boundary conditions within the ALE-AMR framework.

V. Adaptability of the Finite Element Diffusion Solver for Darcy Flow

The current finite element diffusion solver within ALE-AMR employs a standard Galerkin method using first-order H1 elements. This choice of numerical method and element type is also prevalent in the solution of Darcy's equation, particularly when the primary variable being solved for is pressure. The solver's inherent capability to manage complex meshes arising from AMR, including the use of transition elements and specialized quadrature rules, presents a considerable advantage for potentially simulating fluid flow in porous media that exhibit geometric complexity or heterogeneity requiring localized mesh refinement. Furthermore, the utilization of an implicit solver (GMRES with a preconditioner) within the ALE-AMR framework suggests its suitability for handling elliptic partial differential equations, such as the steady-state form of the Darcy flow equation.

However, several potential challenges need to be addressed to adapt the existing diffusion solver for Darcy flow simulations. The solver would need to be modified to correctly interpret the "diffusion coefficient" in the governing equation as the permeability tensor of the porous medium divided by the viscosity of the fluid (k/μ). This adaptation would likely involve changes to the process of assembling the element stiffness matrix, particularly if the permeability is anisotropic, requiring the solver to handle tensor properties. The current diffusion solver is designed to output a scalar field (temperature or energy). For Darcy flow, the Darcy velocity vector is a key quantity that needs to be determined. This could be achieved through a post-processing step, where the gradient of the computed pressure field is calculated at the nodes or element centers, and then Darcy's law is applied to derive the velocity [9]. Alternatively, more significant modifications could involve exploring the implementation of mixed finite element methods, which are formulated to solve for both pressure and velocity simultaneously, potentially offering a more direct and accurate way to obtain the velocity field [7]. The ALE-AMR framework would also require the implementation of boundary conditions that are specific to Darcy flow, such as the ability to prescribe flow rates at boundaries, which would necessitate adding new functionalities to both the solver and the overall framework. Finally, the way in which the pressure and velocity fields interact with the ALE mesh movement and remapping processes would need to be carefully designed and implemented, drawing upon the existing strategies used for coupling temperature and energy with the hydrodynamics.

VI. Potential Modifications and Additions to the ALE-AMR Framework

To enable the simulation of Darcy flow within the ALE-AMR hydrocode, several modifications and additions to the existing framework would be necessary. A dedicated physics module for Darcy flow should be developed to encapsulate the governing equations and the specific parameters associated with fluid flow in porous media [7]. This module would be responsible for handling the input of spatially varying permeability (which could be a scalar or a tensor field), the viscosity of the fluid, and potentially porosity if more complex scenarios such as transient or compressible flow are to be considered. It would also manage the definition of source and sink terms that represent the injection or extraction of fluid from the porous medium.

The existing finite element solver would require several adaptations. Firstly, it needs to be capable of accepting the permeability tensor (divided by the fluid viscosity) as the transport property in the governing equation, instead of the thermal conductivity or radiation-related parameters it currently uses. This would likely necessitate modifications to the process by which the element stiffness matrix is assembled. Secondly, the solver should be configured to solve for pressure (or hydraulic head) as the primary unknown variable at the mesh nodes. Thirdly, a post-processing function should be incorporated to calculate the Darcy velocity vector at each node or within each element, based on the computed pressure gradient and Darcy's law. For potential future extensions to model transient Darcy flow, which would be relevant for applications such as groundwater flow with time-varying boundary conditions or sources, e.g., extraction in wells, the solver would need to include a time-stepping scheme. Furthermore, consideration should be given to exploring the implementation of mixed finite element methods, which employ different basis functions for pressure and velocity and solve for both simultaneously. This approach can often yield more accurate velocity fields directly, which is particularly important for problems where flow is coupled with transport processes. Various finite element methods, including continuous Galerkin (CG), discontinuous Galerkin (DG), weak Galerkin (WG), and mixed finite element methods (MFEM), are used for Darcy flow simulations, and the choice would depend on the desired accuracy and computational cost.

The ALE-AMR framework must also be extended to support boundary conditions that are specific to fluid flow in porous media. This involves implementing: the ability to prescribe flow rates at selected boundaries; the option to define impermeable boundaries where no flow occurs; and ensuring that these new boundary condition types can be applied and handled correctly by the finite element solver, while also being compatible with the ALE and AMR features of the code.

The mechanisms for mapping data between the nodal finite element representation and the cell-centered representation used in the ALE hydrodynamics need to be adapted to handle pressure and velocity fields. This is crucial for scenarios where Darcy flow might be coupled with other physical processes already modeled in ALE-AMR, such as thermal effects in geothermal reservoirs, or where the flow interacts with the moving mesh in ALE simulations. For example, changes in fluid pressure might induce deformation of the porous medium that in turn affect the rock permeability, or the movement of the computational mesh could affect the flow domain.

Finally, a rigorous program of verification and validation is essential. This includes developing a comprehensive suite of unit tests to ensure the correct implementation of the Darcy flow physics module and the modifications made to the finite element solver. Additionally, the adapted code should be thoroughly validated against analytical solutions for standard Darcy flow problems, such as flow in simple geometries or radial flow towards a well, and against established benchmark problems reported in the literature to confirm the accuracy and reliability of the new simulation capabilities.

VII. Suitability Assessment and Recommendations

To simulate Darcy flow within the framework of the ALE-AMR hydrocode, a series of key steps would be necessary. The most critical of these would be the development of a dedicated Darcy flow physics module. This module would be responsible for managing the input of parameters specific to porous media flow, such as permeability and fluid viscosity, as well as defining the source and sink terms relevant to fluid flow. The existing finite element solver would need to be modified to correctly interpret these parameters, to solve for pressure (or hydraulic head) as the primary variable, and to provide the Darcy velocity as a key output, either directly or through a post-processing calculation. Furthermore, the solver would need to be enhanced to handle permeability as a tensor to accurately model anisotropic porous media. The implementation of boundary conditions specific to fluid flow in porous media, such as prescribed flow rates and impermeable boundaries, would also be a necessary addition to the framework. Careful design and implementation of the coupling mechanisms between the new Darcy flow module and the existing ALE hydrodynamics would be crucial, drawing upon the experience gained from coupling heat conduction and radiation transport. Finally, a thorough and rigorous program of verification and validation, using both (semi-)analytical solutions and established benchmark problems from the literature, would be essential to ensure the accuracy and reliability of the newly implemented Darcy flow simulation capabilities.

In summary, we believe that extending the PISALE ALE-AMR framework to simulate Darcy flow is not only feasible but also holds significant promise for advancing subsurface models for geothermal applications. As high-performance computing increasingly relies on GPU architectures for acceleration, adapting a proven, fully parallel AMR-capable hydrocode like PISALE is a critical step toward next-generation modeling. We give details here of a direct path to building simulation tools that can exploit modern HPC architectures and software, and thus enable discovery of critical new important details in geothermal reservoir modeling.

VIII. Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy (DOE) by the University of Hawai'i at Mānoa and by Lawrence Livermore National Laboratory supported by DOE Science Foundations for the Energy Earthshots Award Number DE-SC0024728. 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. Work at LLNL also supported by Contract DE-AC52-07NA27344. LLNL-CONF-2008557

References

[1] A. Koniges *et al.*, "Multi-material ale with amr for modeling hot plasmas and cold fragmenting materials," Plasma Sci. and Technol., vol. 17, pp. 117–128, 2015.

[2] A. Koniges *et al.*, "A survey of recent applications of the pisale code and pde framework," ADVCOMP 2023 : The Seventeenth International Conference on Advanced Engineering Computing and Applications in Sciences, pp. 20–25, 2023.

[3] A. Fisher *et al.*, "An amr capable finite element diffusion solver for ale hydrocodes," Plasma Science and Technology, vol. 17, no. 2, p. 109, 2015.

[4] G. Brown, "Henry darcy and the making of a law," Water Resources Research, vol. 38, no. 7, pp. 11–1, 2002.

[5] Z. Chen and R. E. Ewing, Fluid Flow and Transport in Porous Media, Mathematical and Numerical Treatment: Proceedings of an AMS-IMS-SIAM Joint Summer Research Conference on Fluid Flow and Transport in Porous Media, Mathematical and Numerical Treatment, June 17-21, 2001, Mount Holyoke College, South Hadley, Massachusetts. American Mathematical Soc., 2002, vol. 295.

[6] Y. Seo, J. Lee, A. Koniges, and A. Fisher, "Development of the pisale codebase for simulating flow and transport in large-scale coastal aquifer," Eleventh International Conference on Computational Fluid Dynamics (ICCFD11), 2022, Paper 1502.

[7] J. Liu, L. Mu, and X. Ye, "A comparative study of locally conservative numerical methods for darcy's flows," Procedia Computer Science, vol. 4, pp. 974–983, 2011.

[8] Y. Jin, E. Holzbecher, and M. Sauter, "A novel modeling approach using arbitrary lagrangian–eulerian (ale) method for the flow simulation in unconfined aquifers," Computers & Geosciences, vol. 62, pp. 88–94, 2014.

[9] R. W. Zimmerman, The Imperial College Lectures in Petroleum Engineering: Volume 5: Fluid Flow in Porous Media. World Scientific, 2018.

TABLE I. COMPARISON OF DIFFUSION AND DARCY FLOW EQUATIONS

Feature	Diffusion Equation	Darcy Flow Equation
Governing Equation	$\partial u/\partial t = \nabla \cdot (D\nabla u) + S$ (General)	$\nabla \cdot (-(k/\mu)\nabla p) = S$ (Steady-State)
Primary Unknown	Temperature (T), Energy (E_R)	Pressure (p), Hydraulic Head (h)
Key Properties	Conductivity, Diffusivity, Opacities	Permeability (k), Viscosity (μ)
Applications in ALE-AMR	Heat Conduction, Radiation Transport	Groundwater, Petroleum, Geothermal

TABLE II. SUMMARY OF REQUIRED MODIFICATIONS FOR DARCY FLOW IMPLEMENTATION

Category	Specific Action Required	Purpose	Potential Challenges
New Physics Module	Develop a dedicated Darcy flow module.	Organize parameters (permeability, viscosity) and equations.	Seamless integration with ALE-AMR architecture.
Solver Adaptations	Modify solver for permeability (tensor) and viscosity; solve for pressure; post-process for velocity. Consider mixed FEM.	Accurately represent Darcy's law; provide velocity output; handle anisotropy and transient flow.	Handling tensor properties; ensuring velocity accuracy; significant code changes for mixed FEM.
Boundary Conditions	Implement prescribed flow rate and impermeable boundaries.	Model physical conditions at domain edges; ensure compatibility with ALE/AMR.	Correctly imposing conditions on AMR meshes with hanging nodes.
Data Mapping	Define pressure/velocity interaction with ALE hydrodynamics and evolving media properties.	Enable coupling with other physics (thermal, structural); ensure consistent data transfer.	Designing robust and conservative mapping strategies.
Verification	Develop unit tests and benchmark problems. Validate against analytical solutions.	Ensure correctness and accuracy of the new simulation capabilities.	Identifying appropriate validation cases and benchmark problems.

 ISBN: 978-1-68558-289-0