Elements: ALE-AMR Framework and the PISALE Codebase

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SUMMARY: The solution of partial differential equations (PDEs) on modern HPC platforms is essential to the continued success of research and modeling for a wide variety of areas. This project will make available software for modeling with PDEs. It will also apply the code for simulations of complex groundwater flow processes in Hawaiian islands characterized by highly heterogeneous volcanic rocks and dynamic interaction between freshwater and seawater. In Hawaii's groundwater resources, freshwater accumulates on top of the denser underlying saltwater, making it highly susceptible to anthropogenic activities and saltwater intrusion induced by possible sea water and volcanic events. The software is based on techniques of ALE (Arbitrary Lagrangian Eulerian) methods with AMR (Adaptive Mesh Refinement) to create a publicly available ALE-AMR Framework and a sustainable branch of the software known as PISALE for Pacific Island Structured-AMR with ALE. Other applications of PISALE are discussed as well as student involvement, course development, and future plans.

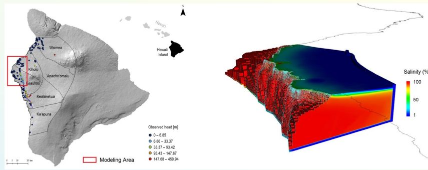
Overview, Intellectual Merit, and Impact

Overview:

- PISALE: Pacific Island Structed AMR with ALE: Software framework employing advanced mathematical techniques for the solution of partial differential equations including parallel software tools to dynamically adapt the grids
- NSF funding for simulations of complex groundwater flow processes in Hawaiian islands characterized by highly heterogenous volcanic rocks
- Applications to understand the effects of climate change via sea level rise on water resources
- Additional applications now using PISALE include hypersonics, linear accelerators, proposals for Covid-type droplet modeling

Intellectual Merit:

- Adaptive mesh implementation concentrates computation where needed and incorporates scalable high performance computing
- Lagrangian-flow methods allow for solution of equations that can reproduce sharp freshwater-seawater interfaces
- For the flow simulation, a mixed finite element method is used to provide groundwater velocity, e.g., specific discharge, to transport equation. The finite element method has an advantage in modeling complex geometries and irregular grids. Advection is coupled into the simulation with PISALE.



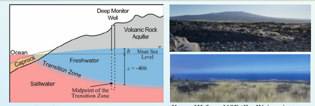
(Left) Map of the Hawai‘i island with monitoring well locations and management aquifer boundaries (Right) Preliminary USGS 3D modeling of salinity distribution
From http://files.hawaii.gov/dlnr/cwrm/submittal/2018/sb20180417C2.pdf

Impact:

- Climate change
- Water resources
- High performance computing
- Coupled Multiphysics using PDE framework
- Advanced visualization techniques
- Uncertainty quantification via experimental validation

Hawaiian Groundwater Flow Application

Motivation



Rotzoll et al., 2010 — Kona, HI from NSF ‘Ike Wai project

Groundwater is the major source for public supply in Hawai‘i. Groundwater resources exist as freshwater lens floated on top of seawater.

However, groundwater availability is limited by recharge/precipitation and seawater intrusion. Current drought conditions and future sea level rise will impact the freshwater resources in Hawai‘i.

The PISALE project will support island-scale numerical simulation of density-driven flow and transport :

1. to evaluate groundwater availability
2. to design sustainable water use planning
3. to understand the effect of climate change and sea level rise on island water resources

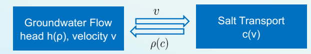
Methodology

Mathematical Model for Density-Driven Flow

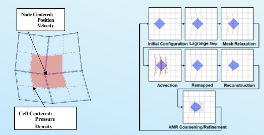
$$\nabla \cdot [K(\mathbf{x})\nabla h(\mathbf{x},t)] = S\frac{\partial h(\mathbf{x},t)}{\partial t}$$

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

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



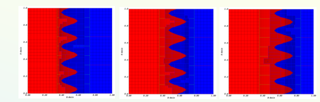
- Flow simulation using Mixed Finite Element Method
- Advection is simulated using PISALE code



1. Nodal positions and velocities are advanced in Lagrange step(s)
2. For significant plume deformation, mesh is relaxed and the flux due to relaxation is advected. Remapping/reconstruction phase followed
3. Perform mesh refinement (for plume front), if needed

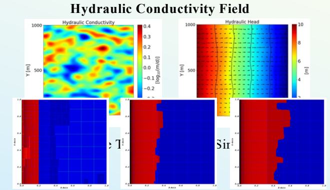
Preliminary Results

1. Salinity Transport with uniform velocity



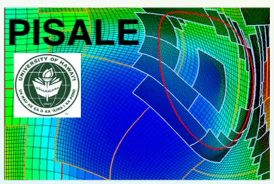
t = 0 [yr] — t = 5.75 [yr] — t = 11.5 [yr]

2. Flow and Transport with Heterogeneous Hydraulic Conductivity Field



t = 0 [yr] — t = 12.6 [yr] — t = 25.2 [yr]

Additional and Proposed PISALE Applications Seeded by NSF Funding

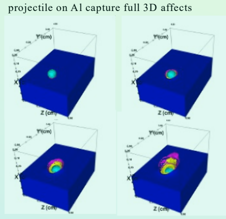


ALE (Arbitrary Lagrangian Eulerian) dynamics and structured AMR (Adaptive Mesh Refinement)

As a direct result of this NSF funded project we now have new application areas using this PISALE Framework

Some members of current PISALE core development team gather on the same island following Hawaii's lifting of Covid restrictions

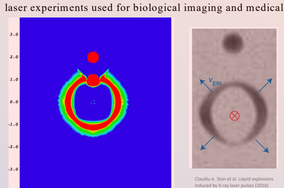
PISALE simulations of off-normal impact of steel projectile on Al capture full 3D affects



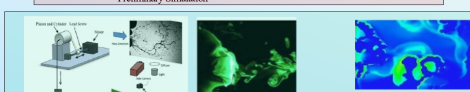
Recent Experiments by European Space Agency Highlight Importance of Hydrocode Modeling

ESA space debris studies: hypervelocity impact sample Photo Published on Twitter 12/4/21

3D PISALE simulations guide droplet spacing for x-ray free electron laser experiments used for biological imaging and medical applications



Preliminary Simulation — Experiment

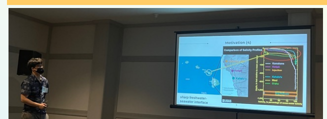


Experimental Setup Proposed by UH for testing mask efficacy

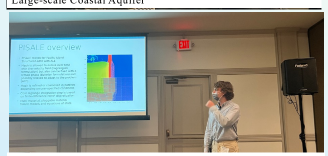
Internet photo, not our experiment

Typical PISALE simulation shows capability to capture vortex interactions and flow dynamics

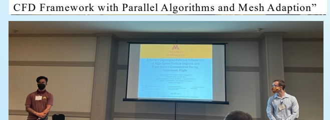
Student Involvement, Course Development, Broader Impact, and Future Plans



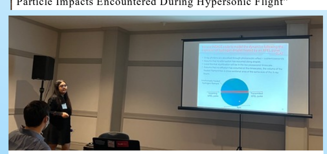
Graduate Student Young-HO Seo gives talk "Development of the PISALE Codebase for Simulating Flow and Transport in Large-scale Coastal Aquifer"



Graduate Student Jack McKee gives talk "Developing a Modern CFD Framework with Parallel Algorithms and Mesh Adaption"



Graduate Students Peter Yip and Austin Andrews give talk "Arbitrary Lagrangian Eulerian Simulations of High Speed Particle Impacts Encountered During Hypersonic Flight"



Graduate Student Claudia Parisuaña gives talk "CFD Modeling of Droplets Heated by an X-ray Free Electron Laser"

Course Development:
CEE 696-003 "Advanced Modeling in Groundwater Engineering" will be offered in Fall 2022. This course will deliver the concept and theory of ALE-AMR and demonstrate a few applications of PISALE.

Aquifer Modeling Plans:
- PISALE code will include the coupled flow and transport equations with an operator splitting method.
- We will test the accuracy and scalability for island-scale 3D freshwater-seawater interaction application in Hawaiian aquifers

Workshop Outreach

PI Koniges hosts a tiny workshop (as part of a larger CFD conference) on the use of the PISALE framework. A team attending from the Univ. of Minnesota is shown.

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