Book of abstracts

INTRUSION 2025

numerIcal aNalysis, porous media and waTer ResoUrceS: a fruItful cOntamiNation

Bari, Italy - June 30, July 2 2025

Contents

About the Conference

Reliable models for forecasting and managing water resources in an ecological transition framework ask for accurate and robust numerical methods for dealing with critical zone modeling. To this purpose, this workshop aims at bridging the gap among lexicon and contents of geosciences, hydrology, soil science, ecology, applied mathematics and numerical analysis, trying to trigger novel mathematical modeling approaches and numerical methods in these frameworks: for instance, multiphysics coupling, nonlocal models and methods, control techniques, polytopal element methods, happening over different dimensions, e.g., either through interfaces or in the bulk.

Location

Centro Polifunzionale Studenti (ex Poste), Sala "A. Leogrande", Piazza Cesare Battisti 1, Bari

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Presentations

A collision-based particle tracking algorithm for nonlinear surface reactions

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Particle tracking algorithms solve the advection-diffusion equation based on a Lagrangian picture, by discretizing solute mass into point particles. These methods mitigate numerical dispersion and do not suffer from stability issues at high Peclet number, making them ideal candidates to resolve heterogeneous reaction fronts. They are, however, less developed than their Eulerian counterparts in some respects: for example, complex boundary conditions, such as those representing nonlinear reaction processes, can be readily implemented in common Eulerian methods, but present challenges in the Lagrangian picture. Fluid-solid boundaries in porous and fractured media can include a wide range of biogeochemical processes, so that the applicability of particle tracking algorithms to perform resolved pore-scale reactive transport simulations requires handling this type of boundary condition.

In this talk, I discuss a recent approach to implement surface reactions in classical particle tracking algorithms. This approach is based on estimating the concentrations of dissolved species at the reactive interface based on particle collisions with the boundary. The algorithm can handle arbitrary numbers of reactions, with arbitrary dependencies of the surface rates on an arbitrary number of dissolved and solid-phase components. Because of its collision-based nature, this technique circumvents the need for reconstructing concentration fields from particle positions or performing multi-particle searches, so that collision-checking, local reaction rate computations, and the solution of local chemical reaction systems can be efficiently parallelized. The method is illustrated for applications to a set of nonlinear mass-action reactions under pure diffusion, and to nonlinear kinetics representing calcite dissolution in a model porous medium.

An adaptive high order finite element shallow water solver for coastal engineering applications with irregular bathymetry

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We present the first step in the development of an adaptive shallow water solver for coastal engineering applications, based on a high-order Discontinuous Galerkin method as implemented in the deal.II library. The deal.II environment provides efficient and native parallelization techniques and automatically handles non-conforming meshes to implement both static and dynamic Adaptive Mesh Refinement approaches. Within this modelling framework, we focus on a robust and accurate treatment of the bathymetry, nowadays available with higher resolution than the mesh in coastal areas. This poses a series of challenges for higher order methods that work on coarse meshes. The proposed method is automatically well-balanced and allows the use of realistic bathymetry data without any regularity assumption. We discuss some numerical implications of our approach, concerning the conservation properties of the scheme and the discretization of a passive tracer. Numerical results obtained on idealized benchmarks validate the the proposed method in presence of irregular bathymetry also with under-resolved features at the grid scale. Simulations of coastal flows using realistic and complex domain geometries and bathymetries demonstrate the effectiveness of the adaptive discretization as compared to state of the art coastal flow models and its good parallel performance.

Geometric shallow water and diffusive wave approximation for basin scale coupled surface-subsurface hydrological simulations

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Shallow water models of geophysical flows must be adapted to geometric characteristics in the presence of a general bottom topography with non-negligible slopes and curvatures, such as mountain landscapes. In this work, we derive an intrinsic formulation for the diffusive wave approximation of the shallow water equations, defined on a local reference frame anchored on the bottom surface. We then derive a numerical discretization by means of a Galerkin finite element scheme intrinsically defined on the bottom surface. We aim to analyze the differences between the diffusive wave approximation and the shallow water model, both defined within a geometrically intrinsic framework and with a focus at the basin scale. Basin scale simulations on synthetic test cases show the importance of taking into full consideration the bottom geometry even for relatively mild and slowly varying curvatures.

Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic-Numeric Computing

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Geologic porous media have played and continue to play a critical role in the energy transition, as the physical domains from which resources can be harvested, CO2 sequestered and H2 stored. Modeling and prediction of fluids and reacting species in the subsurface continues to be a major open challenge in computational physics because of the inherent multiscale nature of geologic porous media, where the relevant scales of interest can easily span 10 orders of magnitude. Despite advances in the development of multiscale models of flow and reactive transport in geologic porous media, significant challenges remain in the rigorous derivation of continuum models themselves, and their numerical implementation and verification, particularly in presence of systems of realistic complexity (e.g. tens of reacting species/minerals). The derivation and numerical implementation of macroscopic models from their fine-scale counterpart through formal upscaling techniques can take many years of concerted efforts between applied mathematicians, modelers and computational physicists to develop. These efforts can become daunting for systems of realistic complexity, such as reactive single- and multi-phase transport in geologic media. Differently from data-driven methods, recent works have shown that recursive symbolic algorithms can be used to augment and boost human deductive capabilities through the automation of rigorous (mathematical) upscaling theories, as well as to lead to scientific discoveries. Allocating to the machine time-consuming and error-prone laborious procedures allows one to speed up the time to derive upscaled equations by 5 orders of magnitude, compared to the same calculations performed by a human. Although the generated macroscopic systems of equations are accurate within estimated upscaling errors, the massive and complex differential equations are still difficult to handle for the purpose of numerical implementation and verification. To tackle this problem, we propose the first symbolic-numeric framework fully integrating automated symbolic deduction capabilities for multiscale model development and automated numerical code generation, which can be run with minimal human interaction.

Numerical Modeling of Slope-Vegetation-Atmosphere Interaction

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Deep slope movements and slope failures are often interpreted as being triggered by thermo-hydro-mechanical (THM) processes governing the slope–vegetation–atmosphere (SLVA) interaction. This is particularly the case in areas characterized by tectonically disturbed clayey lithotypes, such as flysch formations, as found in the Southern-Eastern Apennines of Italy. This study investigates the influence of SLVA interactions on slope stability through coupled hydro-mechanical (HM) numerical analysis carried out on a representative slope affected by deep-seated movements induced by SLVA processes.

The simulations incorporate real meteorological and vegetation data from 2001 to 2020, applied at the slope surface as THM boundary conditions representative of the interaction between soil, vegetation, and atmosphere. The results demonstrate that the inclusion of mechanical discontinuities enables the model to reproduce the observed timing of landslide reactivations, despite employing a simplified elasto-plastic constitutive model. This approach proved to be essential for capturing the correct stress-strain response and supports the use of such modelling procedures as valuable tools for early warning and risk mitigation in comparable geo-hydro-mechanical settings.

Bridging Theory and Applications in Explainable Scientific Machine Learning

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Scientific Machine Learning (SciML) has revolutionized computational science by bridging model-driven and data-driven approaches. A leading example of this synthesis is the development of Physics-Informed Neural Networks (PINNs), which offer a robust deep learning framework for solving complex, nonlinear partial differential equations (PDEs) across diverse scientific fields.

This presentation focuses on the emerging area of explainable SciML, with an emphasis on designing interpretable learning architectures, embedding domain-specific knowledge, and ensuring computational robustness. Special attention is devoted to strategies that enhance the transparency of neural network models, particularly those that establish a clear link between theoretical principles and practical scientific applications.

References

[1] Di Cola, V. S., Bauduin, V., Berardi, M., Notarnicola, F., and Cuomo, S. *Investigating neural networks with groundwater flow equation loss*, *Mathematics and Computers in Simulation, 230, 80-93, 2025.*

[2] Cuomo, S., Di Cola, V. S., Giampaolo, F., Rozza, G., Raissi, M., and Piccialli, F. *Scientific machine learning through physics–informed neural networks: Where we are and what's next*, *Journal of Scientific Computing, 92(3), 88, 2022.*

Riemannian Optimization on the Oblique Manifold for Solving Low-Rank models with Sparse Simplex Constraints

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This talk addresses the solution of low-rank optimization problems with sparse simplex constraints that involve variables satisfying nonnegativity, sparsity, and sum-to-one conditions.

These problems arise in various applications, as for instance Archetypal Analysis adopted to identify extreme or dominant patterns in precipitation or water levels [5, 7]; Hyperspectral Unmixing used to control water quality and construct environmental monitoring systems [8]; the construction of reduced-order models for shallow water flows, the source identification to characterize aquifer properties and hydrogeological conditions [4].

To tackle low-rank optimization problems with sparse simplex constraints efficiently, we propose a novel manifold optimization approach. This leverages the geometry of oblique rotation manifolds [1, 2, 3] to reformulate the problem and introduces a new Riemannian optimization method based on Riemannian gradient descent that strictly maintains the simplex constraints and improves optimization [6].

Preliminary experiments on synthetic datasets compared to standard Euclidean and Riemannian methods show the effectiveness of the proposed method.

References

[1] Absil, P.-A. and Gallivan, K.A *Joint Diagonalization on the Oblique Manifold for Independent Component Analysis*, 2006 IEEE International Conference on Acoustics Speed and Signal Processing Proceedings

[2] Absil, P.-A., Mahony, R. and Sepulchre, R. *Optimization On Manifolds: Methods and Applications*, Recent Advances in Optimization and its Applications in Engineering, 2010

[3] Del Buono, N. and Lopez, L. *Geometric Integration on Manifold of Square Oblique Rotation Matrices*, SIAM Journal on Matrix Analysis and Applications, 23(4), 2002

[4] Alexandrov, B.S. and Vesselinov, V. *Blind source separation for groundwater pressure analysis based on nonnegative matrix factorization*, Water Resources Research, 50, 2014

[5] Bilalova, S., Villamayor-Tomas, S. and Newig, J. *Water-related problématiques: five archetypical contexts of water governance*, Ecology and Society, 1, 2025

[6] F.Esposito, A. Ang *Riemannian Optimization on the Oblique Manifold for Sparse Simplex Constraints via Multiplicative Updates*, arXiv:2503.24075, 2025

[7] Hannachi, A. and Trendafilov, N. *Archetypal Analysis: Mining Weather and Climate Extremes* , Journal of Climate, 17, 2017

[8] Guo, Z., Min, A., Yang, B. et al., *A Sparse Oblique-Manifold Nonnegative Matrix Factorization for Hyperspectral Unmixing* , IEEE Transactions on Geoscience and Remote Sensing, 60, 2022

On the solution of elliptic PDEs through the multinode Shepard method

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The multinode Shepard method is a powerful method for interpolation of scattered data based on inverse distance weighting and local polynomial interpolants on subsets of unisolvent nearby nodes. In this talk, we discuss the ideas of the construction and implementation of the multinode Shepard method [1] and its applications to numerically solve elliptic Partial Differential Equations equipped with various conditions at the boundary of domains of different shapes [2, 3, 4, 5]. In particular, the multinode Shepard method is proposed to solve elliptic PDEs with Dirichlet and/or Neumann boundary conditions.

References

[1] F. Dell'Accio, F. Di Tommaso, F. Larosa, *The Multinode Shepard Method: MATLAB Implementation*, Journal of Approximation Software 1 (2) 2024.

[2] F. Dell'Accio, F. Di Tommaso, O. Nouisser, N. Siar, *Solving Poisson equation with Dirichlet conditions through multinode Shepard operators*, Comput. Math. Appl. 98 (2021), 254260.

[3] F. Dell'Accio, F. Di Tommaso, G. Ala, E. Francomano, *Electric Scalar Potential Estimations for Non-Invasive Brain Activity Detection Through Multinode Shepard Method*, MELECON 2022 - IEEE Mediterranean Electrotechnical Conference, Proceedings (2022), 12641268.

[4] F. Dell'Accio, F. Di Tommaso, E. Francomano, *Multinode Shepard method for two-dimensional elliptic boundary problems on different shaped domain*, J. Comput. Appl. Math., 448 (2024), 115896.

[5] F. Dell'Accio, F. Di Tommaso, E. Francomano, *The enriched multinode Shepard collocation method for solving elliptic problems with singularities*, Appl. Numer. Math. 205 (2024), pp. 87–100.

Why is fully coupled Hydro-Mechanical modelling critical in subsurface applications?

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The role of hydro-mechanical (HM) coupling in porous materials has been investigated since the beginning of the last century. On the one hand, the deformation of porous media affects pore fluid pressure and flow through the alteration of pore volume. On the other hand, pore fluid pressure controls the deformation of porous media by absorbing part of the applied loads. This two-way interaction governs numerous geological and hydrogeological processes and has been recognized as fundamental for explaining phenomena such as subsidence or reverse water level fluctuations.

In recent years, research on fully coupled HM problems has significantly increased due to the growing interest in using the subsurface for geo-energy purposes, including deep geothermal systems, CO_2 sequestration, and the underground storage of gas, hydrogen, and heat. The need to predict the risks and efficiency of such technologies has led to the extensive development of numerical simulators for fully coupled HM modelling.

In this talk, the importance of two-way HM coupling is discussed by means of results from numerical modelling, in the context of geothermal energy and gas storage. We show that deep fluid injection activates transient poromechanical effects that play a control on fracture shear failure and induced seismicity. These effects can accelerate or delay the triggering of seismic events, and – combined with other driving mechanisms - helps explaining the observations of post-injection induced seismicity and opens the door to potential mitigation strategies.

Flow and Transport in Geological Fractures: Newtonian and non-Newtonian results and the GEONEAT approach

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The flow of non-Newtonian fluids through fractured media plays a critical role in various subsurface operations, including resource extraction, land remediation, and geothermal energy development. In these applications, complex fluids—such as polymer solutions, foams, and drilling muds—are commonly used to transport suspended nanoparticles, carry fracking proppants, and serve as heat-transfer agents in enhanced geothermal systems, as in the GEONEAT project. The interaction between the heterogeneous nature of fractured geological formations (ranging from pore scale to field scale) and the non-linear rheology of these fluids significantly affects flow localization, permeability, and transport processes. Accurately characterizing these flow and transport dynamics is essential for optimizing the efficiency, environmental sustainability, and cost-effectiveness of industrial subsurface activities.

The rough walls of geological fractures exhibit a pore-scale spatial variability that can be reproduced as an isotropic self-affine surface. The flow in between is influenced by the aperture variability which induces viscous energy losses and promote the channeling phenomenon. The non-Newtonian nature of polymer fluids plays an important role as it promotes flow localization in channels of lower apparent viscosity, mitigating energy losses and enhancing fracture-scale transmissivity through stronger flow localization up to two orders of magnitude higher than simple fluids like water; this can in turn enhance the delivery of remedial amendments.

We investigate this phenomenon implementing a lubrication-based numerical code able to generate synthetic fractures and solve the generalized Reynolds equation on a large mesh, limiting the computational cost typical of a non-linear scheme. The code is encased in a Monte Carlo framework to produce ensemble statistics through numerous flow simulations over the parameter space, providing new insight on the transition from Darcian to non-linear regime, and quantitatively characterizing transmissivity and flow characteristic length in polymer flow.

Shear-thinning rheology induces strong flow localization, with velocity fields concentrating along preferential paths that align with high-aperture zones. The apparent viscosity field reflects this structure, with low-viscosity regions coinciding with high-shear channels. Higher apparent viscosity localized in quasi-stagnant zones closed to contact zones.

Heat transport is modeled using a Time Domain Random Walk (TDRW) particle-tracking scheme based on the finite volume discretization of the ADE; particle transition (mobile) times depend on local velocities and dispersion, immobile time derived from the analytical solution of the 1D diffusion equation in a semi-infinite matrix; immobile times follow a Lévy–Smirnov distribution (heavy-tailed) captures long retention and non-Fickian exchange naturally. The scheme is physically based, handles heterogeneity efficiently, and represents anomalous transport and matrix exchange.

As to Newtonian results, a broad distribution of travel times ensues driven by strong aperture heterogeneity and high velocity contrasts across the fracture. Pronounced early breakthroughs follow due to fast preferential flow paths and channelization. Breakthrough curves exhibit long late-time thermal tails, resulting from quasi-stagnant regions, significant heat exchange with the rock matrix, and prolonged particle retention and delayed thermal release.

The non-Newtonian case adds enhanced sensitivity to fracture architecture, where flow is concentrated in high-aperture, high-transmissivity channels; it improves detection of dominant flow paths and network connectivity, highlights structures that will control heat extraction, and shows sharper breakthrough curves. This in turn improves interpretability of tracer signals and inverse modeling.

Inverse Physics-Informed Neural Networks for transport models in porous materials

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Physics-Informed Neural Networks (PINN) are a machine learning tool that can be used to solve direct and inverse problems related to models described by Partial Differential Equations by including in the cost function to minimise during training the residual of the differential operator. In this talk, based on [1], we propose an adaptive inverse PINN applied to different transport models, from diffusion to advection-diffusion-reaction, and mobile-immobile transport models for porous materials. Once a suitable PINN is established to solve the forward problem, the transport parameters are added as trainable parameters and the reference data is added to the cost function. We find that, for the inverse problem to converge to the correct solution, the different components of the loss function (data misfit, initial conditions, boundary conditions and residual of the transport equation) need to be weighted adaptively as a function of the training iteration (epoch). Similarly, gradients of trainable parameters are scaled at each epoch accordingly. Several examples are presented for different test cases to support our PINN architecture and its scalability and robustness.

References

[1] M. Berardi, FVD, M. Icardi, Inverse Physics-Informed Neural Networks for transport models in porous materials, Computer Methods in Applied Mechanics and Engineering, Volume 435, 2025, 117628. https://doi.org/10.1016/j.cma.2024.117628

Interpolation of scattered data on the sphere by multinode Shepard operators

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In this talk, we introduce a multinode Shepard operator [1, 2] for interpolating scattered data on the sphere. This method combines local polynomial interpolants with multinode Shepard functions based on geodesic distances. We analyze the operator's approximation properties and convergence behavior. Numerical experiments confirm the accuracy and efficiency of the method in various test scenarios [3, 4, 5]. Additionally, we apply it to real-world data, demonstrating its effectiveness in predicting monthly mean temperatures.

References

[1] F. Dell'Accio, F. Di Tommaso, *Rate of convergence of multinode Shepard operators*, Dolomites Research Notes on Approximation, 12: 1-6, 2019

[2] F. Dell'Accio, F. Di Tommaso, F. Larosa, *The Multinode Shepard Method: MATLAB Implementation*, Journal of Approximation Software 1, 2024.

[3] R. Cavoretto, A. De Rossi, *Fast and accurate interpolation of large scattered data sets on the sphere*, Journal of Computational and Applied Mathematics 234: 1505–1521, 2010.

[4] H. Pottmann, M. Eck, *Modified multiquadric methods for scattered data interpolation over a sphere*, Computer Aided Geometric Design 7: 313–321, 1990.

[5] P. Alfeld, M. Neamtu, L.L. Schumaker, *Fitting scattered data on sphere-like surfaces using spherical splines*, Journal of Computational and Applied Mathematics 73: 5–43, 1996.

Direct Numerical Simulation of Flow and Transport in Karst Conduits

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Karst aquifers, with their extensive and intricate conduit networks, are essential for groundwater flow and contaminant transport [1]. The complex geometry, characterized by branching conduits, varied cross-sections, and remarkable wall roughness ($k/D \simeq 10^{-1}$), add further challenges to predicting flow patterns, friction losses, and turbulence onset.

This work examines flow and transport behaviour in representative karst conduits to identify key geometrical and fluid mechanical parameters, such as average cross-sectional areas, cave centrelines, friction factors, and velocity distributions, using direct numerical simulations over a broad range of flow conditions ($Re = 1 - 10^3$). These variables are critical for upscaling methods as can be used to simulate the entire karst networks without resolving every conduit in detail. In this study a combination of finite-volume and spectral element methods has been employed: finite-volume for resolving laminar flows in more complex geometries and spectral element methods for capturing turbulent flows at higher Reynolds numbers. Conduit geometries for the simulations are reconstructed from high-resolution LiDAR scans of real karst formations, with point cloud data maintaining all features such as rough walls, branching, and variable cross-sections. An immersed boundary model [2] together with a ray-tracing algorithm allows accurate boundary representation and correct forcing of boundary conditions within these intricate geometries.

The validation of the numerical framework was first performed on classical problems, including laminar and turbulent flow in a straight circular pipe. Tests conducted in a wavy channel geometry suggest that laminar flow conditions hold in certain conduit sections, leading to smooth centerline velocities and predictable friction losses. Due to the irregularities in the conduit, the flow field is significantly disrupted, resulting in spatial variations that differ from those observed in smooth-channel conditions. Moreover, the simulations reveal that the flow transitions to turbulent regime occurs at Reynolds numbers lower than those predicted by standard empirical correlations ($Re \leq 1000$). The result suggests that the conventional friction factor estimations, often based on the Moody chart [3] and Darcy-Weisbach formulations [4], may not fully capture the effects of the complex, heterogeneous conditions typical of karst systems. The intricate geometry and roughness of karst conduits appear to significantly change the flow dynamics, causing deviations from classical behaviour. In parallel, transport simulations reveal that particles tend to accumulate in diverging sections of the conduit, where recirculation zones form. These features lead to pronounced tailing in breakthrough curves, driven by delayed particle. Together, the flow and transport results indicate that standard hydraulic approaches fail to fully characterise karst dynamics, reinforcing the need for alternative models that can incorporate the effects of roughness, branching, and localised flow separation.

References

[1] Parise M., Gunn J., (2007), Natural and anthropogenic hazards in karst areas: an introduction, *Geol. Soc., 279, pp. 1-3*

[2] Fadlun E. A., Verzicco R., Orlandi P. and Mohd-Yusof J., (2000): Combined Immersed-Boundary Finite-Difference Methods for Three-Dimensional Complex Flow Simulations, *J. Comput. Phys., 161, pp. 35-60*

[3] Moody L. F., (1944): Friction factors for pipe flow, *Transitions of the ASME, 66, pp. 671-684*

[4] White Frank M. , (2011): *Fluid Mechanics*, *Mcgraw-Hill, 7th ed.*

Adjoint-free PDE-Constrained Optimization via Variational Inference

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We propose a framework for PDE-constrained optimization based on variational inference, where the posterior distribution over unknown parameters in a finite or infinite dimension is approximated by a tractable family of probability measures. By minimizing an expected misfit functional regularized by the ν-weighted Kullback–Leibler divergence, we derive an adjoint-free algorithm that bypasses adjoint solvers. We derive explicit expressions for the variational gradients and accelerate convergence using natural gradient steps computed via the Fisher–Rao geometry of the Gaussian manifold. Our objective is to approximate the unknown parameters $\theta^\sharp$ by finding the probability measure $q(\theta)$ given a Gaussian ansatz $\mathcal{N}(\mu,\Sigma)$ such that

$$\begin{cases} \inf\limits_{\mu,\Sigma} \mathbb{E}_{q(\theta)}\left[\mathcal{J}(u_\theta;\theta)\right] + \nu\, \mathrm{D}_{\mathrm{KL}}\left(\mathcal{N}(\mu,\Sigma) \parallel \mathcal{N}(\mu_0,\Sigma_0)\right) =: \mathbb{E}_{q(\theta)}[\mathcal{F}(\mu,\Sigma,u_\theta)], \\ u_\theta \coloneqq \arg\min\limits_{v\in U} \mathcal{H}(v;\theta) \qquad \text{for } q\text{-almost every } \theta. \end{cases}$$

Here, $\mathcal{J}$ measures the misfit between predicted and observed states, and $\mathcal{H}$ defines the underlying PDE model. Thus,

$$\begin{cases} \mathrm{grad}_\mu \mathcal{F}(\mu,\Sigma,u_\theta) = \mathbb{E}_{q(\theta)}\left[\Sigma^{-1}(\theta-\mu)\mathcal{J}(u_\theta;\theta)\right] - \nu\,\Sigma_0^{-1}(\mu_0-\mu), \\ \mathrm{grad}_\Sigma \mathcal{F}(\mu,\Sigma,u_\theta) = \dfrac{1}{2}\mathbb{E}_{q(\theta)}\left[\left(\Sigma^{-1}[(\theta-\mu)\otimes(\theta-\mu)-\Sigma]\Sigma^{-1}\right)\mathcal{J}(u_\theta;\theta)\right] + \dfrac{\nu}{2}\left(\Sigma_0^{-1}-\Sigma^{-1}\right). \end{cases}$$

To respect the manifold geometry, we precondition these gradients using the Fisher–Rao metric

$$G = \begin{bmatrix} G_{\mu\mu} & 0 \\ 0 & G_{\Sigma\Sigma} \end{bmatrix} = \begin{bmatrix} \Sigma^{-1} & 0 \\ 0 & \frac{1}{2}\Sigma^{-1}\otimes\Sigma^{-1} \end{bmatrix}.$$

leading to the natural gradient directions

$$\begin{cases} \mathrm{grad}_\mu^{\mathrm{nat}} \mathcal{F} = \Sigma(\mathrm{grad}_\mu \mathcal{F}), \\ \qquad \approx \dfrac{1}{M}\displaystyle\sum_{i=1}^{M}(\theta^{(i)}-\mu)\mathcal{J}(u_{\theta^{(i)}};\theta^{(i)}) - \nu\,\Sigma\Sigma_0^{-1}(\mu_0-\mu) =: \mathrm{grad}_\mu^{\mathrm{nat}} F, \\ \mathrm{grad}_\Sigma^{\mathrm{nat}} \mathcal{F} = 2\Sigma(\mathrm{grad}_\Sigma \mathcal{F})\Sigma, \\ \qquad \approx \dfrac{1}{M}\displaystyle\sum_{i=1}^{M}\left[(\theta^{(i)}-\mu)\otimes(\theta^{(i)}-\mu)-\Sigma\right]\mathcal{J}(u_{\theta^{(i)}};\theta^{(i)}) + \dfrac{\nu}{2}\Sigma\left(\Sigma_0^{-1}-\Sigma^{-1}\right)\Sigma =: \mathrm{grad}_\Sigma^{\mathrm{nat}} F. \end{cases}$$

Then, the variational parameters are updated via stochastic gradient descent (or Adam)

$$\mu^{(k+1)} = \mu^{(k)} - \eta_\mu\, \mathrm{grad}_\mu^{\mathrm{nat}} \mathcal{F} \quad \text{and} \quad \Sigma^{(k+1)} = \Sigma^{(k)} - \eta_\Sigma\, \mathrm{grad}_\Sigma^{\mathrm{nat}} \mathcal{F},$$

where η_μ and η_Σ denote learning rates.

Our approach is applicable in high dimensions and extends naturally to infinite-dimensional Hilbert spaces. It enables efficient posterior exploration and uncertainty quantification in inverse problems, with applications in physics-based machine learning, control, and model calibration.

Multi-physics and multi-domain simulations of coupled processes in porous media

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The simulation of multiple physical processes in porous media, such as fluid flow, poromechanics, fault activation, thermal flow, and chemical reactions, that can take place simultaneously with multiple time and space scales, play a crucial role for a proper management of underground resources. The present communication focusses on the development of GReS [1], a novel open-source modular platform specifically designed with the aim at contributing to the design and testing of numerical algorithms for fully coupled multi-physics multi-domain poromechanical applications. The idea is to partition the overall computational domain into possibly non-conforming subdomains where different physics and discretization schemes can be used. The code is based on a high-level programming platform (MATLAB) that should lower the entry barrier for new users and developers, as well as the effort for implementing and testing innovative numerical algorithms. Moreover, the modular structure of the code encourages contributions from different developers at variable levels, from the implementation of new physics and discretization schemes to specific algorithms to accelerate the linear and non-linear solver.

In the present communication, we will introduce the GReS concept and its current development state, including advances to the mortar algorithm used to transfer the information among non-conforming subdomains with independent meshes [2]. Basic benchmarks will be presented to show the current code's potentials, along with the projects for future developments.

References

[1] M. Ferronato, A. Franceschini, D. Moretto. *Advances in multi-physics and multi-domain simulations of coupled poromechanics*, in "Large Scale Scientific Computations", Lecture Notes in Computer Science, Springer, 2025..

[2] D. Moretto, A. Franceschini, M. Ferronato, *A novel mortar method integration using Radial Basis Functions*, arXiv:2409.11735, math.NA, 2024.

PORE SCALE CFD SIMULATION TO INVESTIGATE TRANSPORT PHENOMENA IN MULTIPHASE CATALYTIC PACKED-BED REACTORS

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In chemical engineering many innovative processes are based on heterogeneous catalysis: one of the most common configurations for this kind of reactive systems is the packed-bed reactor, whose performance is strongly dependent on the mass transfer of reagents. Indeed, it is possible to improve reactor productivity by optimizing the catalytic pellets geometry to obtain better pore-scale transport phenomena.

To better capture the interplay of transport and reaction, computational fluid dynamics (CFD) at the pore scale enable simulation of actual geometries. A practical application is aqueous phase reforming (APR), which generates hydrogen from wastewater at moderate temperatures (220–270 °C) and employs a fixed-bed reactor containing catalytic particles. The goal of this work is to use CFD to investigate how catalyst geometry influences reactive transport and reactor performance.

A 3D representation of the catalyst packing was created using Blender, based on real catalyst fragments. Initial simulations focused on the dispersion of an inert species in a single-phase flow to highlight geometry-induced flow anomalies such as bypasses and stagnant zones. OpenFOAM was used to solve the mean age transport, that represents residence time in the domain.

Subsequently, experimental tests were carried out in a perfectly mixed batch system, where the absence of transport resistance is ensured. From this data, a kinetic model for glycerol APR was developed by fitting the experimental data as shown in Figure 1 a).

The kinetic model thus developed was implemented in OpenFOAM to simulate, through reactive pore scale CFD, the performance of a packed-bed reactor as shown in Figure 1 b) and c). The reactions were implemented as a boundary condition in the catalytic external surface, and fluid flow is considered only outside the catalyst. This methodology was then also compared to a more accurate model that resolves also the species transport inside the catalyst, increasing the accuracy of the simulation, at the cost of increasing computational expense and numerical instability.

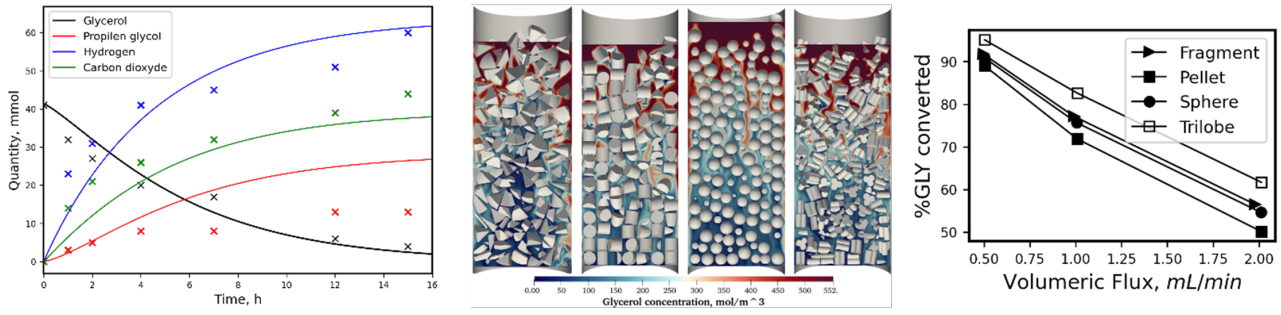

Figure 1: a) Experimental fitting to obtain the kinetic model. b) Contour plot of the glycerol concentration. c) Glycerol conversion at different condition

Acknowledgments: PNRR M4C2, Investimento 1.4 - Avviso n. 3138 del 16/12/2021 - CN00000013 National Centre for HPC, Big Data and Quantum Computing (HPC) - CUP E13C22000990001

Development of a hydromechanical model for peat

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In recent years several approaches have been developed to model the complex hydrological and ecological processes involved in peatland development. In recent works, these models have been coupled with a poro-elastic mechanical model, encapsulating the complex interactions between solid deformation and fluid flow which occur throughout peat development. In the current work, a new formulation is proposed, which aims to improve the mathematical rigour of the approach. Here, the layered model is replaced with a continuum description of the peat properties. To accommodate this, the ecological, hydrological, and mechanical models are re-worked to describe the rate of change of key peatland properties over short timesteps. The improved mathematical rigour of this approach will enable the new formulation to model the influence of extreme, short-timescale, events – such as droughts or wildfires – on peatland development. Such advancements will be key in modelling the effect of increasingly severe weather patterns induced by worsening climate change.

Integrating Irrigation Water Demand in a Hydrological Digital Twin: Insights from the COACH-WAT Project

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Irrigation is the deliberate application of water to crops when natural precipitation is insufficient to meet their water requirements [1]. It plays a critical role in global food production, enabling intensified agricultural output and stability across climate-vulnerable regions [3]. However, irrigation is increasingly constrained by climate change-induced reductions in freshwater availability [4], making it essential to accurately quantify irrigation practices and their hydrological implications [2]. In this context the COACH-WAT PRIN project aims to develop a multidisciplinary and innovative conceptual framework for realistically quantifying water resources in human-influenced river basins. This will be achieved by integrating the latest Earth observation data with novel hydrological models. A key focus of COACH-WAT is the explicit representation of irrigation water use and groundwater abstraction, which are dynamically linked to other hydrological components. Ground-based measurements and high-resolution satellite observations (e.g., snow depth, soil moisture, irrigation volumes) will be assimilated to produce accurate estimates of the current hydrological state. In this study, a novel irrigation modeling component has been developed for integration into a hydrological digital twin using the open-source modeling framework GEOframe. The model estimates irrigation water demand based on soil moisture and evapotranspiration, while accounting for crop- specific water requirements. Irrigation is triggered when soil moisture drops below a defined activation threshold. The flexibility of the hydrological digital twin framework allows for the evaluation of how varying soil moisture activation thresholds impact irrigation estimates and, consequently, the overall water balance. Two water availability scenarios are considered: (1) limited, where water is drawn from other model components (e.g., river discharge), and (2) unlimited, with unrestricted water access. The model also incorporates daily irrigation limits and irrigation efficiency. Results are presented for a case study in the Adige River basin (11,000 km^2) in northeastern Italy. The implementation operates at high temporal (daily) and spatial (1 km) resolution, allowing for a detailed assessment of irrigation practices and their impacts on hydrological processes and the overall water budget across the study area.

References

[1] Dieter, C. A., Linsey, K. S., Caldwell, R. R., Harris, M. A., Ivahnenko, T. I., Lovelace, J. K., ... , and Barber N.L., *Estimated use of water in the United States county-level data for 2015. US Geological Survey data release, 10, 2018.*

[2] Döll, P. and Siebert, S. *Global modeling of irrigation water requirements. Water resources research,38(4), 8-1, 2002.*

[3] Kukal, M. S., Irmak, S. and Sharma, K. *Development and application of a performance and operational feasibility guide to facilitate adoption of soil moisture sensors. Sustainability, 12(1), 321, 2019.*

[4] Mastrotheodoros, T., Pappas, C., Molnar, P., Burlando, P., Manoli, G., Parajka, J., ..., and Fatichi, S. *More green and less blue water in the Alps during warmer summers. Nature Climate Change, 10(2), 155-161, 2020.*

Modelling metal growth through PDEs on Evolving Surfaces

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Metal growth is a necessary process for batteries to work. However, battery performance and duration is strongly affected by the way electrodes grow inside of it. For short times, metal grows in the form of Turing patterns (spots, holes, stripes, labyrinths, spirals, etc.). Over the last decade, the so-called DIB model, a reaction-diffusion system in two space variables, was proven to successfully model short-time metal growth in batteries. For longer times, however, the deposited metal can branch and self-intersect, thereby forming sponge-like structures known as dendrites, which can no longer be modelled as Turing patterns. In this talk, we introduce a novel extension of the DIB model where the spatial domain is an evolving surface. In the new model, the metal profile is modelled by the surface itself, rather than the graph of a space-time dependent function defined on a stationary surface. Numerical simulations demonstrate that the model can exhibit various behaviours depending on the reaction parameters. The comparison between simulations and electronic microscope observations validates the model qualitatively.

Model Reduction Techniques for Faulted Poroelastic Media

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Subsurface resource exploitation, including CO2 storage, necessitates computationally intensive simulations to evaluate fluid transport and fault stability, often requiring coupled modeling of porous media flow and geomechanics. To reduce these computational demands, we employ deep learning-based reduced-order modeling (DL-ROM), leveraging autoencoders to identify low-dimensional representations from high-fidelity simulation data. The framework accounts for uncertainties such as Young's modulus, permeability, fault transmissibility, and operational controls like CO2 injection rates.

We apply DL-ROM to synthetic $CO2$ storage scenarios involving sloping, potentially unstable faults. High-fidelity simulations integrate commercial finite volume software for flow modeling and finite element or PorePy-based methods for mechanical deformation. The resulting surrogate model maintains high accuracy while significantly enhancing computational efficiency, successfully reproducing fault stress states and enabling rapid multi-query analyses for probabilistic fault stability assessment-marking a novel application of DL-ROMs in this domain.

Extending the DL-ROM framework to two-phase flow, we first address the added complexity introduced by fractures and faults, along with gravity- and pressure-driven counter-current flows. To mitigate computational costs, we adopt a mixed-dimensional formulation, while hybrid upwinding schemes enhance the stability and convergence of the nonlinear solver. Tested across diverse flow regimes and geometries, this strategy substantially improves solver performance, particularly by reducing the number of Newton iterations.

With high-fidelity two-phase flow simulations available, we further integrate DL-ROM within the mixed-dimensional setting, incorporating both rock and fluid properties. This enables efficient execution of tasks such as sensitivity analysis and inverse modeling, delivering strong performance in terms of both accuracy and computational speed for complex, fractured systems.

HydroCAL: a novel computationally efficient ISSHM developed through the Cellular Automata paradigm

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This study introduces HydroCAL (Hydrological Cellular Automata Layer) [1], a novel spatially distributed Integrated Surface-Subsurface Hydrological Model (ISSHM). The model is fully developed within the Cellular Automata (CA) framework, leveraging the latest release of the OpenCAL software library [2]. HydroCAL is designed to tackle the computational challenges commonly faced by ISSHMs, which are essential for accurately capturing the complex interplay between surface and subsurface hydrological processes.

The CA approach provides significant benefits, especially in minimizing computational costs through parallel processing and advanced optimization. A standout feature is its asynchronous update mechanism [3], which allows the model to selectively update only the areas of interest at specific time steps, thereby reducing computational costs while preserving numerical precision.

This note introduces an updated version of HydroCAL, restructured to be compatible with the latest version of OpenCAL, called OOpenCal (Object-oriented Open Computing Abstraction Layer). This enhancement enables capabilities for transparently transforming the implemented serial version into a CUDA API version, allowing users to fully exploit the power of General-Purpose Graphics Processing Units (GPGPUs).

HydroCAL has been validated using well-established benchmark cases from the literature [4], confirming its robustness in reproducing key hydrological processes. It has also been applied to real-world events in a small headwater catchment (7 km^2), where it accurately replicated streamflow dynamics, achieving high evaluation metrics performance. Furthermore, HydroCAL performance has also been compared with a Rain-on-Grid (RoG) model to highlight the specific features of the two different numerical modelling approaches.

HydroCAL delivers fully spatially distributed outputs for various surface and subsurface hydrological variables, offering in-depth insights into watershed behavior. Its implementation in the new computing environment enables highly efficient simulations, with performance gains reaching up to hundreds of times faster compared to traditional serial CPU-based execution.

References

[1] L. Furnari, A. De Rango, A. Senatore and G. Mendicino *HydroCAL: A novel integrated surface– subsurface hydrological model based on the Cellular Automata paradigm* Adv. in Wat Res., 185, 104623 (2024).

[2] D. D'Ambrosio, A. De Rango, M. Oliverio, D. Spataro, W. Spataro, R. Rongo, G. Mendicino and A. Senatore *The Open Computing Abstraction Layer for Parallel Complex Systems Modeling on Many-Core Systems* J. of Parallel and Distributed Computing, 121, 53-70 (2018).

[3] L. Furnari, A. Senatore, A. de Rango, M. De Biase, S. Straface and G. Mendicino *Asynchronous cellular automata subsurface flow simulations in two- and three-dimensional heterogeneous soils*, Adv. in Wat Res., 153, 103952 (2021)

[4] Maxwell, R. M., et al. *Surface-subsurface model intercomparison: A first set of benchmark results to diagnose integrated hydrology and feedbacks*, Water Resour. Res., 50, 1531–1549 (2014)

FLOWS: a web-based physically-based model for one-dimensional water flow and solute transport simulations in heterogeneous agricultural and environmental systems

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Several well-known issues related to environmental and water quality require the accurate simulation of water flow and solute transport in the vadose zone. Agrohydrological models can be a powerful tool to carry out these simulations. FLOWS is a physically-based agrohydrological models capable of simulating the one-dimensional water flow and solute transport in the soil. Water flow is simulated by solving the 1-D form of Richards Equation, RE, while accounting for root water uptake and water fluxes to subsurface drains. Runoff is calculated as either a Hortonian or a Dunnian mechanism runoff. Solute transport is simulated by solving the 1-D form of the Advection-Dispersion Equation, ADE. Solute decay, sorption, volatilization, uptake by plant roots and losses to drainage are simulated. The FLOWS model simulates fertilizer additions in the form of organic matter (such as manure and crop residue) and mineral fertilizers. It requires an input parameter for incorporation depth, assuming uniform distribution within that depth. The model supports two simulation modes: (1) full simulation of organic matter decomposition and the transport and transformation of carbon, nitrogen, and phosphorus, which is governed by organic matter dynamics and C:N and C:P ratios; and (2) nitrogen-only transport simulation, where nitrogen mineralization is modeled independently of organic matter decomposition using an empirical decay approach, without considering the C:N ratio. Root water uptake is calculated according to the potential evapotranspiration, root density distribution and water and salinity stresses. FLOWS can simulate soil temperature distribution. It can also optimize irrigation fluxes and scheduling according to user-defined criteria on critical soil water pressure head and irrigation intervals. FLOWS can also be used to simulate a single soil profile (single site simulations) or multiple soil profiles (multi-site simulations). The latter can be applied in a stochastic environment, allowing for estimating the uncertainty connected to simulation outputs. To make FLOWS more useful, a system organized according to a client-server architecture was developed, which allows the user to use the model without having to carry out any configuration in their work area but only by entering the system through their own access credentials. To showcase its potential in simulating different water flow and nutrient transport and processes, FLOWS was applied to a real complex agrohydrological case study.

Basset-type fractional models for heterogeneous porous media

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Fractional time-derivative operators have been increasingly used to model anomalous advection-diffusion-reaction phenomena in porous media, where classical models often fail to capture the observed non-local and memory effects. Many fractional models in the literature are derived heuristically, lacking a rigorous connection to the underlying physical processes. In this work, we present a novel approach by deriving a fractional advection-diffusion-reaction model directly from a micro-macro scale framework for transport in a heterogeneous porous medium (i.e., a medium with micro-scale inclusions). The resulting fractional model is described by a Basset-type time-fractional advection-diffusion-reaction differential equation of order $1/3 < \alpha < 1$, with the limiting case of one-dimensional semi-infinite inclusions leading to $\alpha = 1/2$.

We perform a qualitative analysis of the model, focusing on the early- and late-time asymptotic behaviour for a general fractional exponent $0 < \alpha < 1$. Our results highlight the loss of regularity in the solution, a characteristic phenomenon of fractional-order models and a source of significant numerical challenges. To address these, we propose a first-order product-integration method tailored to the fractional model, combining temporal discretisation with spatial finite-difference schemes, together with a special treatment of the boundary conditions to allow the problem to be rewritten as a standard vectorial Basset equation.

Numerical results for an application-relevant scenario are proposed, demonstrating numerically the early and late-time behaviour and the robustness of the approach. We show that at late times the solution tends to be self-similar to the principal eigenfunction of the (advection-diffusion-reaction) transport operator, which we compute analytically and numerically.

This work bridges theoretical derivations, numerical analysis, and practical applications, offering an overview for applied mathematicians interested in anomalous and fractional transport phenomena in porous media and addressing challenges at the interface of fractional calculus, porous media science, and numerical methods

Flow in fractured porous media: mathematical analysis, numerical methods and large scale simulations

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Subsurface rocks are naturally porous and may contain numerous fractures that intersect in complex configurations. Fractures are, in general, permeable pathways and are responsible for most of the flow. They are classically modeled as structures of co-dimension one in the surrounding rock [1]. Due to the porosity of the rock, a 3D flow also occurs in the rock, and this flow is coupled to the 2D flow in the fractures. In this talk, we formulate and analyze the mathematical formulation of this coupled system, study its discretization by mixed-hybrid finite element methods and discuss its efficient simulation by means of a domain decomposition preconditioner.

The mathematical analysis rests on a mixed formulation, where the function spaces need to be carefully specified in order to take into account the mixed-dimension geometry of the problem. Existence and uniqueness is proved through the Babuska-Brezzi conditions. Next, a finite dimensional approximation by the lowest order Raviart-Thomas-Nédélec finite element is studied, and a first order a priori error estimate is obtained. The method is validated on analytical solution as well as on a benchmark problem.

The mesh of the fracture network is performed using a dedicated surface mesher MODFRAC, and the 3D domain using the efficient volume mesher GHS3D. The mixed hybrid finite element (MHFEM) is convenient for discretizing this coupled flow problem, as the face unknowns ease the coupling between the 2D (in the fractures) and 3D (in the rock) flows. In addition, the MHFEM leads to a symmetric positive definite linear system with traces of hydraulic head as unknowns, the velocity then being calculated locally, in a post-processing step.

The resulting linear system is large and very poorly conditioned due to the permeability contrasts between rock and fractures, as well as the low-quality elements present in the mesh. We show how this system can be solved efficiently by using the domain decomposition HPDDM library [2], implemented in PETSc, as a preconditioner. We present several examples demonstrating the excellent performance obtained with HPDDM on highly heterogeneous and large-scale fractured porous media, containing up to 700k fractures (242M of unknowns) [3].

References

[1] V. Martin, J. Jaffré, and J. E. Roberts, *Modeling Fractures and Barriers as Interfaces for Flow in Porous Media*, SIAM J. Sci. Comp., 26 (5), 2005. https://doi.org/10.1137/S1064827503429363.

[2] P. Jolivet, J. Roman, and S. Zampini. *KSPHPDDM and PCHPDDM: extending PETSc with advanced Krylov methods and robust multilevel overlapping Schwarz preconditioners*, Comp. Math, Apps, 84:277–295, 2021. https://doi.org/10.1016/j.camwa.2021.01.003.

[3] P. Jolivet, M. Kern, F. Nataf, G. Pichot, and D. Zegarra Vasquez. *Domain decomposition preconditioners for efficient parallel simulations of single-phase flow in three-dimensional fractured porous media with a very large number of fractures,* Preprint, 2025. https://inria.hal.science/hal-05029676

Modelling peatland - unanswered questions and physical complexity

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Peat accumulates slowly over 1000s years due to an imbalance between production and decay of plant matter. This imbalance is a consequence of water saturation that inhibits the supply of oxygen. Typical accumulations being on the order of 4-7m over 10 kyrs. Resulting peat soils contain a third of global soil carbon, a quantity equivalent to the carbon in the atmosphere. Peat is typically 95% water with a dual porosity and the physical properties of an elastomers. As decay progresses, residual plant matter weakens and the hydration of the decayed organic matter produces a gel. This gel swells while simultaneously the macroscopic pore structure collapses.

To understand peat requires modelling, primarily due to the long timeframes of accumulation, however this modelling is dominated by the fields of ecology and hydrology with little consideration of material properties and underlying physics and little application of advanced mathematical modelling. Many problems and questions associated with peat remain unresolved. For example: Patterning of peatland surfaces is widespread, distinct and spatially variable yet no eco-hydrological models can account of its presence, absence or variability. Mechanical limits to peatland growth are unknown. Lateral creep of peat a process with potentially profound consequences for peat science has been observed but is not understood. Advances in the mathematics and physics soft poro-elastic matter now make tackling peat deformation a tractable forefront problem. Peat creep models have been formulated in 1-D and fully coupled 2D ecohydrological poro-elastic continuum models of peat have recently been developed. The time is now right to quantitatively tackle the physics and mechanics of peatland processes.

Multi-Level Monte Carlo for Monitoring Salinity Transport in Uncertain Groundwater Systems

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We investigate a Henry-type intrusion problem that models the mixing of saline and freshwater in a coastal aquifer, where fluid flow is driven by density variations. A key objective is to predict the earliest time at which the salt mass fraction exceeds a specified threshold. Due to uncertainty in model parameters, the solution exhibits stochastic behavior. These uncertainties are represented through a combination of random variables, stochastic processes, and spatially distributed random fields.

In our formulation, the primary uncertain parameters include porosity, permeability, recharge rate, and fracture aperture. For each realization of these parameters, the evolution of the salt concentration is governed by a coupled system of nonlinear, time-dependent partial differential equations (PDEs). The resulting deterministic PDEs are solved efficiently using a parallel geometric multigrid method.

To quantify uncertainty and estimate relevant statistics of the solution, we employ the Multi-Level Monte Carlo (MLMC) method. Our numerical experiments demonstrate that MLMC achieves significant computational savings compared to classical Monte Carlo sampling, without compromising accuracy.

The findings of this study support the development of efficient and reliable tools for monitoring groundwater quality, tracking pollutant transport, and managing freshwater resources—especially in vulnerable coastal and agricultural regions where groundwater extraction is prevalent.

References

[1] D. Logashenko, A. Litvinenko, R. Tempone, G. Wittum, *Estimation of uncertainties in the density driven flow in fractured porous media using MLMC.*, Engineering with Computers (2024), https://doi.org/10.1007/s00366-024-02089-6

[2] D. Logashenko, A. Litvinenko, R. Tempone, E. Vasilyeva, G. Wittum, *Uncertainty quantification in the Henry problem using the multilevel Monte Carlo method*, Journal of Computational Physics, Volume 503, 2024, 112854, ISSN 0021-9991, https://doi.org/10.1016/j.jcp.2024.112854.

[3] A. Litvinenko, D. Logashenko, R. Tempone, G. Wittum, *Solution of the 3D density-driven groundwater flow problem with uncertain porosity and permeability.* Int J Geomath 11, 10 (2020). https://doi.org/10.1007/s13137-020-0147-1

[4] A. Litvinenko, D. Logashenko, R. Tempone, G. Wittum, D. Keyes, (2021), *Propagation of Uncertainties in Density-Driven Flow.* In: Bungartz, HJ., Garcke, J., Pflüger, D. (eds) Sparse Grids and Applications - Munich 2018. Lecture Notes in Computational Science and Engineering, vol 144. Springer, Cham. https://doi.org/10.1007/978-3-030-81362-8_5

Towards Gradient-Enhanced Surrogate Modeling for Groundwater Flow Problems

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In this contribution, we present our ongoing research into developing surrogate models for Uncertainty Quantification (UQ) in groundwater flow simulations. The physical problem is governed by Darcy's law, which describes fluid flow in a porous medium. More specifically, we consider the free-boundary formulation of the Darcy problem, in which the shape of the saturated zone is unknown a priori and is determined through a shape optimization process. To account for the inherent uncertainty in the soil composition, we introduce a parametrized family of permeability fields, and consider the values of the parameters as uncertain.

In this work, we explore the possibility of employing a novel gradient-enhanced sparse grid technique to construct an efficient surrogate model for quantities of interest (QoI) of the problem, specifically the total flux across a surface. The idea is to integrate the information about the derivatives of the QoI with respect to the uncertain parameters at the evaluation points, since it should be possible to obtain the gradients of the QoI - which only require solving a linearized problem - at a lower computational cost than adding further evaluation points for the QoI. However, linearizing a free-surface problem is tricky, and we will therefore discuss several approaches to this end, with different trade-offs between accuracy and computational costs.

Modeling carbon sequestration in coastal wetlands with moisture dynamics

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Coastal wetlands are highly functional ecosystems at the interface between land and sea, offering a wide spectrum of services including carbon sequestration, flood mitigation, water purification, and biodiversity support [1]. Their capacity to regulate biogeochemical cycles, particularly the carbon cycle, is intimately governed by hydrological processes that shape sediment saturation, redox gradients, and microbial activity across depth profiles.

Building on the recent development of a fractional order RothC model [2], we present the study detailed in [3], which integrates this fractional formulation with the Richards equation to simulate the vertical dynamics of soil organic carbon (SOC) in coastal wetland sediments. The model couples the fractional RothC formulation with the Richards equation, thereby capturing the interactions between moisture transport, temperature, and substrate availability that regulate carbon turnover. This approach allows for the estimation of both CO_2 and CH_4 emissions across saturated and unsaturated zones, as microbial respiration and decomposition rates respond dynamically to evolving hydrological conditions. Numerical simulations under different water regimes, including seasonal flooding and persistent saturation, highlight the role of hydrological control in shaping SOC retention and its vertical distribution within the sediment column.

As a further line of development, we aim to explore the economic implications of the modeled hydrological interventions, with particular attention to the quantification of co-benefits such as potential revenues from carbon markets, improvements in water quality, and the promotion of nature-based economic activities [4]. In this perspective, the proposed model could be extended to serve as a decision-support tool for the design of integrated water and carbon management strategies in wetland restoration, taking into account both environmental and socio-economic constraints.

Acknowledgment: This work has been carried out within the project HORIZON RESTORE4Cs "Modelling RESTORation of wEtlands for Carbon pathways, Climate Change mitigation and adaptation, ecosystem services, and biodiversity, Co-benefits", Grant Agreement No. 101056782.

References

[1] W.R. Moomaw, G. Chmura, G.T. Davies, et al., *Wetlands in a changing climate: Science, policy and management*, Wetlands, 38(2), 183–205, 2018.

[2] V. Bohaienko, F. Diele, C. Marangi, C. Tamborrino, S. Aleksandrowicz, E. Woźniak, *A novel fractional-order RothC model*, Mathematics, 11(7), 1677, 2023.

[3] V. Bohaienko, F. Diele, F.V. Difonzo, C. Marangi, A. Martiradonna, A. Provenzale, *Vertical modeling of carbon sequestration in coastal wetlands using fractional-order derivatives and moisture dynamics*, Mathematics and Computers in Simulation, 233, 369–388, 2025.

[4] D. Russi, P. ten Brink, A. Farmer, T. Badura, et al., *The Economics of Ecosystems and Biodiversity for Water and Wetlands*, IEEP, Ramsar Secretariat, 2021.

VEM fully discrete discretisation of frictional contact mechanics with application to fluid induced fault reactivation

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The simulation of poro-mechanical models in fractured (or faulted) porous rocks plays an important role in many subsurface applications such as fault reactivation by fluid injection in geological storages or the hydraulic fracture stimulation in deep geothermal systems. One of the key difficulty to simulate such models is the discretization of the contact-mechanical model which must be adapted to geological typically polytopal meshes and to the complex geometry of fracture/fault networks including tips, corners and intersections. In this talk, we will discuss the application of the first order nodal Virtual Element Method (VEM) combined with a mixed formulation based on facewise constant Lagrange multipliers for contact mechanics with Coulomb friction at matrix-fracture interfaces. The scheme uses vertex unknowns complemented by "bubble"-like degree of freedom, designed to ensure the inf-sup condition of the displacement jumps with the space of Lagrange multipliers [2]. This fully discrete scheme is equivalent to a Virtual Element scheme. We prove the inf-sup condition, as well as the convergence of the scheme in the case of Tresca friction [1]. It will be applied to a fluid induced fault reactivation test case in a simplified CO2 injection scenario [3].

References

[1] J. Droniou, A. Haidar, R. Masson *Analysis of a VEM-fully discrete polytopal scheme with bubble stabilisation for contact mechanics with Tresca friction*, M2AN, 2025

[2] J. Droniou, E. Guillaume, I. Faille, A. Haidar, R. Masson *A bubble VEM–fully discrete polytopal scheme for mixed-dimensional poromechanics with frictional contact at matrix-fracture interfaces*, CMAME, 422, 2024

[3] M. Laaziri, R. Masson *VEM fully discrete Nitsche's discretization of Coulomb frictional contact-mechanics for mixed-dimensional poromechanical models*, Preprint 2025 https://hal.science/hal-05019674

A PolydG discretization for low-frequency poroelasticity coupled to unsteady Stokes flow

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This work presents a comprehensive numerical analysis of a polygonal discontinuous Galerkin (PolydG) method designed to simulate fluid exchange between a deformable, saturated poroelastic medium and an adjacent free-flow channel. The model accounts for wave propagation phenomena in the poroelastic region using the low-frequency Biot equations, coupled with the unsteady Stokes equations governing fluid flow in the open channel, which may represent either an isolated cavity or a connected fracture network. Interface conditions based on conservation laws are employed to ensure consistent coupling between the two domains. The spatial discretization is built upon a weak formulation of the two-displacement poroelastic system and a mixed stress-based formulation of the Stokes equations, where symmetry is imposed in a weak sense. A rigorous stability analysis of the resulting semi-discrete system is conducted, and a priori hp-error estimates are derived, demonstrating the robustness and accuracy of the proposed approach.

Degenerate & singular mixed dimensional diffusion systems: A journey from modelling, and numerical methods, to well-posedness

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Nonlinear, degenerate, and coupled (mixed-dimensionally) systems arise in various applications of societal relevance such as biofilm growth, reactive transport in fractured porous media, and cellular biology. For such problems, the biomass or the main-substrate is restricted to a lower-dimensional manifold embedded in a domain in d-dimensional space, and the evolution of the biomass density/substrate concentration exhibits degenerate and singular diffusion behaviour. The other equations (for nutrients/reagents) are defined on the bulk, and are of linear advection-reaction-diffusion type.

In our analysis, we propose a backward Euler time-discretisation of the problem where the reactive terms coupling the equations are estimated semi-implicitly. Thus, the equations are dimensionally decoupled and can be solved sequentially. A bulk-surface finite element method is used to discretise the system in space. Then, an iterative linearisation algorithm is proposed to solve the fully-discrete nonlinear problem on the discretised interface. It is proven that the iterations converge unconditionally even for degenerate/singular cases and for curved interfaces, thus, showing the existence of solution of the fully-discrete nonlinear problem. Then, for flat interface, the convergence of the fully-discrete solutions to the time-discrete solution is shown, and order of convergence with respect to mesh-size is estimated. Properties such as well-posedness, boundedness, and positivity of the time-discrete solutions are proven, and the existence of the time-continuous solutions is shown by passing the time-step size to zero. Numerical results validate the theoretical predictions. They demonstrate that the iterative solver and the discretization are extremely robust and efficient compared to existing alternatives.

Mathematical and numerical modeling for seasonal vegetation gaps

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Modeling spatial vegetation patterns is a key research topic with important implications for understanding and preserving fragile ecosystems. In this talk, we focus on the derivation of a new reaction-diffusion model based on Partial Differential Equations (PDEs) specifically designed to reproduce seasonal vegetation gaps observed in semi-arid regions of Kenya, and on its efficient solution using adapted numerical methods. The mentioned patterns involve the coexistence of two plant species: a perennial species, which persists all year round, and a seasonal species, which emerges only during the rainy season.

This model extends the classical framework where the annual precipitation rate is considered to be constant (e.g. in the Klausmeier model) by explicitly accounting for seasonal rainfall. Furthermore, it is calibrated using real data, enabling realistic simulations that reflect observed spatial patterns in the field. The numerical solution of the system of PDEs is performed by means of tailored numerical techniques, including nonstandard finite differences, in such a way as to ensure accurate and efficient simulations.

Acknowledgements: this work is supported by the PRIN PNRR 2022 project MatForPat (A multidisciplinary approach to evaluate ecosystems resilience under climate change).

References

[1] D. Conte, G. Pagano, and B. Paternoster. *Nonstandard finite differences numerical methods for a vegetation reaction-diffusion model*, J. Comput. Appl. Math., 419:Paper No. 114790, 17, 2023.

[2] L. Eigentler and J. A. Sherratt. *Metastability as a coexistence mechanism in a model for dryland vegetation patterns*, Bull. Math. Biol., 81:2290–2322, 2019.

[3] A. Marasco, A. Iuorio, F. Cartenì, G. Bonanomi, D. M. Tartakovsky, S. Mazzoleni, and F. Giannino. *Vegetation Pattern Formation Due to Interactions Between Water Availability and Toxicity in Plant–Soil Feedback*, Bull. Math. Biol., 76(11):2866–2883, 2014.

A Non-Parametric Analytical Tool for Modeling Infiltration and Retention in Plio-Quaternary Calacarenites

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Understanding infiltration mechanisms in the vadose zone is essential for characterizing the spatial and temporal distribution of hydrogeological cycle components, particularly for estimating groundwater recharge. In Southern Italy (Apulia and Basilicata), outcrops of Plio-Quaternary calcarenites-specifically the Calcarenite di Gravina Formation - represent a key hydrogeological unit. These deposits exhibit highly variable depositional and diagenetic features, which significantly influence their hydraulic behavior. This study presents a practical analytical tool developed through an integrated methodological approach to investigate the infiltration dynamics and water retention capacity of calcarenites. Non-parametric constitutive relationships were derived from a conceptual model of infiltration pathways, based on pore distribution data obtained through combined microporosimetry techniques, including mercury intrusion porosimetry and image analysis. Conventional and non-conventional laboratory procedures for petrophysical characterization were performed, along with falling-head infiltration tests at bench scale, using calcarenite blocks sampled from a quarry site in the "Tufarelle" district near Canosa di Puglia. An analytical-numerical tool was developed, incorporating the pore bundle model framework and an advection–diffusion form of Richards' equation [1], to simulate infiltration and retention behavior. Experimental results demonstrated that the bimodal nature of the pore size distribution plays a critical role in accurately predicting infiltration mechanisms and water content distribution. In contrast, simple models assuming unimodal pore size distributions, such as the Brooks and Corey model [2], fail to capture the observed hydraulic behavior - despite providing good fits to estimated non-parametric functions. These findings offer valuable insights for geo-engineering and environmental applications involving multilayered systems where infiltration processes are of primary concern.

References

[1] L.A. Richards *Capillary conduction of liquids through porous media*, Physics, 1 (1931), pp. 318-333

[2] R.H. Brooks, A.T. Corey *Hydraulic properties of porous media*, Hydrol. Pap., 3, Colorado State Univ., Fort Collins (1964)

Inverse PINNs for the analysis of the micromodulus function in bond-based peridynamics and its applications

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In the framework of continuum mechanics, the bond-based peridynamic theory is a nonlocal approach to study homogeneous deformations in microelastic materials. The principal physical characteristic of such material model is that it accounts for the effects of long-range forces and as a consequence its solutions profile shows dispersive effects. In particular, the stiffness of the material in the presence of long-range forces is incorporated in the micromodulus function. The analytical assumptions of such a function establish the physical properties of the body under consideration. In particular, a suitable choice of micromodulus functions allow the description of desiccation cracks in unsaturated soils.

An important issue in this setting consists in deriving the shape of such a function as it measures the non locality of the model. Deep learning is a powerful tool for solving data driven differential problems and has come out to have successful applications in solving direct and inverse problems described by PDEs, even in presence of integral terms. In this context, we propose to apply radial basis functions (RBFs) as activation functions in suitably designed Physics Informed Neural Networks (PINNs) to solve the inverse problem of computing the perydinamic kernel and the associated horizon in the nonlocal formulation of classical wave equation. We show that the selection of a RBF is necessary to achieve meaningful solutions and that, with classical choices, non admissible solutions are provided. We support our results with numerical examples and experiments, comparing the solution obtained with the proposed RBF-PINN to the exact solutions.

Diffusion in fractured networks

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We study the behavior of diffusion processes in fractured networks. These processes are relevant in scenarios involving underground hydrogen and carbon dioxide storage, where gases may diffuse and react in fractured caprock. We first consider the diffusion-limited reactions at the fracture scale to compute simple reaction kinetics such as absorption and degradation rates that later serve as input for studying the diffusion dynamics at network level. The reaction efficiency is measured in terms of the survival probability and the effective reaction rate is determined by the derivative of the logarithm of the survival time distribution. We find that the effective reaction rates evolve in time towards an asymptotic value that depends on the characteristic diffusion time scale. The characterisation of fractured network mainly relies on the distribution of fracture length and aperture observed in literature to generate fractured domain with a high degree of realism. Effective diffusion values are estimated by fitting the analytical solution of the transient diffusion equation integrated in time to numerical breakthrough curves. The study of fractures at network scale is conducted both, in 2 and 3D. Depending on the number of dimensions two different approaches are followed. 2D simulations leverage on the coupling of a Python algorithm for the generation of fractured networks with a pore-throat simulation software for solving the transient diffusion equation while 3D simulations are performed using dfnWorks. The findings from this study offer valuable insights into solute behavior in fractured media and provide a foundation for improving predictive models in subsurface applications.

Stable linear iterative schemes for nonlinear, doubly-degenerate diffusion equations

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Doubly degenerate parabolic equations appear as mathematical models for various real-life processes. Prominent examples are the unsaturated flow and the biofilm growth in porous media (e.g. in the subsurface). The main feature of such problems is that the diffusion may vanish or blow up, or even become multi-valued for certain values of the solution. As a consequence, the equation may change its type from parabolic to hyperbolic or elliptic, in time-space sub-domains that are not known a priori.

Motivated by stability reasons and by the lacking regularity of the solution, the backward Euler method is often used as a time stepping method for such types of problems. The outcome is a sequence of time-discrete, nonlinear and possibly degenerate elliptic equations. For approximating their solutions, linear iterative schemes are needed. Widely used is the Newton scheme, which converges quadratically, but under severe constraints for the initial guess. In the present context, the initial guess is the solution at the previous time step, so having a sufficiently good initial guess induces a severe restriction on the time step. This restriction may even depend on the chosen spatial discretization, and can become more severe as the mesh is refined. Alternatively, the L-scheme has a robust, but only linear convergence behaviour. A modified variant of it (the M-scheme) combines the features of the two schemes mentioned before, leading to a robust, yet linear convergence behaviour, but with an improved convergence rate. It can be seen as an interpolation between the two schemes, as, depending on a parameter, the scheme is closer to either the L-scheme, or to Newton.
In this presentation we discuss these schemes when applied to the Euler-implicit time discretisation of doubly-degenerate parabolic equations. These schemes build on a reformulation in terms of a new unknown, which reduces the complexity of the nonlinearities involved and leads to a formulation that is more suitable for dealing with the degeneracies. Also, a splitting approach is used, in which the nonlinear dependencies are written as algebraic equations, leaving the original equation linear. For these systems, the convergence of the Newton scheme, the L-scheme, and the M-scheme is proved. Using an a posteriori estimator, an adaptive algorithm is proposed to select the optimal parameters for the M-scheme, which accelerates its convergence.

Numerical results are presented, showing that the M-scheme and its adaptive variant are more stable than the Newton scheme, as they converge irrespective of the mesh. This makes them relevant also for adaptive mesh refinement, and for problems involving multiple scales. Moreover, the adaptive scheme consistently out-competes the Newton scheme, showing a quadratic convergence behaviour.

Modelling contaminant transport under (many) uncertainties

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Contaminant transport in soil and aquifers is subject to diverse types of uncertainties related to diverse sources. In this talk we will go through the types of uncertainties that can affect the modelling chain, taking transport of contaminants such as pesticides and pharmaceuticals as case studies. The discussion will encompass approaches and data to constrain uncertainties to obtain reliable estimation of contaminant concentrations. The talk will address the characterization of contaminant sources, as well as of physical, chemical, biological characterization of subsurface porous systems, such as soils and aquifers. As part of this revision of uncertainty sources we will present a recently published dataset providing spatial maps of pesticides application rates, complemented by the associated uncertainty. We then explore available techniques to link forward uncertainty quantification, sensitivity analysis and inverse modelling frameworks. Notably, we discuss the application of machine learning algorithms to the simulation of solute transport under parametric uncertainty, presenting a strategy that can leverage Physics Informed Neural Networks (PINNs) in addressing this challenge.

Water resilience strategy in the Apulian region: old challenges and new opportunities

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The Apulia region is a peninsula of about 20,000 km^2, and may be considered a typical example of groundwater overexploitation due to the limited availability of surface water resources (concentrated in the north-western part of the region) contrasting with valuable groundwater bodies extending from the carbonate ridge to the sea shoreline. Less extensive, but yet important, aquifers of the region are located in the clastic sediments of Quaternary age outcropping in the Capitanata plain, in the Brindisi plain facing the Adriatic Sea and in the plain surrounding the western limit on the Ionian gulf. Water scarcity has always been a major constraint to the social and economic development of the region, due to climatic conditions and the low water supply capacity of surface water bodies. To overcome this problem, huge water systems were built between 1906 and 1982 to transfer water from the bordering regions on the Apennines, mainly to drinking water supplies but also for uses in agriculture. Besides the critical dependency on these external water resources, the available water supply was not enough to satisfy the entire demand for water. During the last three decades, there has been a continuous increase in groundwater withdrawal by farmers (as single farm and as irrigation consortia) without appropriate legislation for sustainable resource management, resulting in lowering of groundwater levels in many places. With the aim of reducing groundwater overexploitation the regional policy to increase water resilience has been strongly addressed towards non-conventional water resources such as treated wastewater and desalination. Although such resilience strategy is recognized to achieve multiple environmental and socio-economic benefits, a few challenges still exist along the route for its full implementation.

Pore Scale Modelling of Soil Carbon and Nitrogen Turnover on Dynamic Geometries

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Carbon storage and its turnover in soils depend on the interplay of soil architecture, microbial activities, organic C and nitrogen (N) dynamics. For a fundamental understanding of the mechanisms that drive these processes, not only the exploitation of advanced experimental techniques down to the nanoscale is necessary but also spatially explicit and dynamic image-based modeling at the pore scale. We present a modeling approach that resolves processes on the pore scale, but also transfers microscale information to simulations at the profile scale. We consider a model for CO2 transport across soil profiles (macroscale), which is informed by a pore-scale (microscale) model for coupled, microbially mediated C and N turnover. It allows for the dynamic, self-organized re-arrangement of solid building units, aggregates and particulate organic matter (POM) based on surface interactions, realized by a cellular automaton method, and explicitly takes spatial effects on POM turnover such as occlusion into account. We further include the macroscopic environmental conditions water saturation, POM content, and oxygen concentration. The coupled simulations of macroscopic transport and pore-scale carbon and aggregate turnover reveal the complex, nonlinear interplay of the underlying processes. Limitations by diffusive transport, oxygen availability, texture-dependent occlusion and turnover of OM drive CO2 production and carbon storage. This emphasizes the need for such micro–macro models exchanging information on different scales to investigate and quantify the effects of structural changes, variations in environmental conditions, or degradation processes on carbon turnover.

Robust and efficient splitting schemes for poromechanics

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We will present splitting schemes for poromechanics, i.e. flow in deformable porous media. There are many practical applications of poromechanics, e.g. geothermal energy extraction, biomedical research or CO2 storage. The typical mathematical models behind poromechanics are based on the Biot theory and are consisting on coupled, linear or nonlinear partial differential equations. We will first briefly review the main existing results for the fixed-stress scheme for the quasi-static Biot model [3] and then discuss some generalisations. In particular we will look at a fixed-stress type scheme for a nonlinear Biot model [1]. Finally, a new family of splitting schemes based on approximate Schur complement will be presented [2].

References

[1] J. Kraus, K. Kumar, M. Lymberly, F.A. Radu (2024). *A fixed-stress splitting method for nonlinear poroelasticity*. Engineering with Computers, 1-12.

[2] R. Nuca, E. Storvik, F.A. Radu, M. Icardi (2024). *Splitting schemes for coupled differential equations: block Schur-based approaches and partial Jacobi approximation*, Computers & Mathematics with Applications 161, 190–201.

[3] E. Storvik, J. W. Both, K. Kumar, J.M. Nordbotten, F.A. Radu (2019). *On the optimization of the fixed-stress splitting for Biot's equations*. IJNME 120, 179–194.

Fault reactivation: numerical simulation using VEM

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A safe exploitation of the subsurface is key for the development of green energy sources such as geothermal energy, and to reduce greenhouse gas emissions via long term carbon dioxide storage. However, the recent increase in seismicity caused by such human activities demands for a deeper understanding of the processes involved [3].

The goal of project Freya, funded in the scope of PRIN2022 and involving researchers from Politecnico di Milano, Università degli studi Milano Bicocca, Politecnico di Torino and Univerità di Bari, is to study the phenomena leading to fault slip, taking into account the two-ways coupled poroelastic problem applying advanced numerical methods.

In particular, since we are interested in domains crossed by faults, we develop algorithms to generate hybrid grids composed of a majority of tetrahedral elements and some polyhedral elements to fit geometrical constraints with fewer elements, and apply the Virtual Element Methods to deal with such general grids. We consider the mixed-mixed VEM formulation of the poroelastic problem [1], which has the advantage of i) producing good approximation of stresses and Darcy velocity and ii) enforcing the stress tensor symmetry directly in the discrete space without resorting to Lagrange multipliers. Finally, we tackle the frictional contact condition on the fault [2]: the nonlinearity is solved iteratively using an Uzawa algorithm to compute fault slip if the Coulomb condition is violated.

References

[1] Botti M., Prada D., Scotti A., Visinoni M. *Fully-Mixed Virtual Element Method for the Biot Problem* , arXiv:2504.17729

[2] Cerroni, D., Formaggia, L., Scotti, A. *A control problem approach to Coulomb's friction* , Journal of computational and applied mathematics, vol 385 (2021)

[3] Vadacca, L., Rossi, D., Scotti, A., Buttinelli, M. *Slip tendency analysis, fault reactivation potential and induced seismicity in the Val d'Agri oilfield (Italy)*, Journal of geophysical research. Solid Earth, vol. 126 (2020)

Pattern Formation and Numerical Simulations for a New Fractional Vegetation-Water Model in Arid and Semi-Arid Environments

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In arid and semi-arid sloped environments, the vegetation migrates upward and aligns in bands due to a downward-oriented water flow. One of the simplest and most commonly used models for studying vegetation patterns in sloped domains is the Klausmeier model (KL) [3], a system of two partial differential reaction-diffusion-advection equations that describes the dynamics of water and plant biomass in arid and semi-arid environments. The Gray-Scott model (GS) [2] is a reformulated version of the Klausmeier model, where the water advection term is replaced by a diffusion term, describing plant growth on flat lands.

In this paper, we propose a new fractional mathematical model describing the dynamics and the interaction of plants and water on flat and no-flat domains by using the fractional Caputo operator [1]. The new fractional model allows to get the periodic solutions, which ensure the vegetation pattern formation by varying the value of the fractional parameter, assumed to be linked to the slope of the domain, so that the new proposed fractional model represents a connection between the KL and the GS ones. An analytical study on the stability of the Hopf bifurcation demonstrates that the migration speed results to be a function of the fractional parameter, confirming the connection between the fractional parameter and the slope of the domain. The reported numerical results validate the analytical ones, the reliability and efficiency of the fractional formulation of the considered model, showing the vegetation pattern formation in sloped and no-sloped environments.

References

[1] K. Diethelm. *The Analysis of Fractional Differential Equations.* Springer-Verlag, Berlin (2004).

[2] P. Gray, S.K. Scott. *Autocatalytic reactions in the isothermal continuous stirred tank reactor: isolas and other forms of multistability* Chem. Eng. Sci., 38 (1): 29–43, (1983).

[3] C.A. Klausmeier. *Regular and irregular patterns in semiarid vegetation.* Science, 284: 1826–1828 (1999).

[4] A. Jannelli, M.P. Speciale, *Fractional Vegetation-Water Model in Arid and Semi-Arid Environments: Pattern Formation and Numerical Simulations.* Submitted (2025).

From systems of particles to continuous fields: a space-time upscaling

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Discrete systems of particles with piece-wise analytical trajectories are described macroscopically by almost everywhere continuous fields. The macroscopic description is achieved through space-time averages on d-dimensional cubes and symmetric time intervals of a kinematic description available at the discrete level. The latter consists of piece-wise analytic time functions modeling physical properties of the particles. The fields defined by these averages verify unclosed relations having the structure of the hydrodynamic balance equations. One obtains in this way a versatile tool which enables, for instance, derivations of the Liouville and Schrödinger equations, verifications of material laws for granular materials, hydrodynamic analysis of financial time-series, continuous modeling of lipid bilayers, with applications in cell biology. A practical application that will be presented in more detail is the space-time upscaling of the reactive transport in variably saturated porous media. The kinematic description is provided by an ensemble of as many random walkers as molecules involved in chemical reactions. The space-time scales of the averaging procedure may be chosen as representative of the macroscopic observations and experimental measurements.

Multi-Index Stochastic Collocation for PDEs with Imperfect Solvers

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This talk considers the construction of surrogate models (response surfaces) for parametric PDEs using multi-fidelity collocation methods, namely Multi-Index Stochastic Collocation (MISC). In some scenarios, in addition to "standard" discretization errors, the PDE approximations used to build a MISC response surface are affected by "noise" (e.g. due to iterative method tolerances, pre-asymptotic meshes, time-stepping). This noise is particularly problematic in low fidelity models; it might be parameter-dependent and hard to estimate and control a priori. Noise is interpolated by MISC and corrupts the approximated response surface (loss of monotonicity, spurious high-frequency oscillations), spoiling any subsequent UQ analysis. We propose an improved version of MISC that can detect such phenomena. Within our updated adaptive algorithm, at each iteration, we inspect the spectral content of the response surface and consequently stop exploring fidelities once the decay of their spectral coefficients stagnates due to such noise. Numerical experiments show the effectiveness of our approach in preventing the MISC approximation from becoming corrupted.

Posters

Control-Based Irrigation Optimization in Richards' Equation

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Here we present the results published in the paper "State Dependent Riccati for dynamic boundary control to optimize irrigation in Richards' equation framework", published on Mathematics and Computers in Simulation in 2025. We present an approach for the optimization of irrigation in a Richards' equation framework. We introduce a proper cost functional, aimed at minimizing the amount of water provided by irrigation, at the same time maximizing the root water uptake, which is modeled by a sink term in the continuity equation. The control is acting on the boundary of the dynamics and due to the nature of the mathematical problem we use a State Dependent Riccati approach which provides suboptimal control in feedback form, applied to the system of ODEs resulting from the Richards' equation semidiscretization in space. The problem is tested with existing hydraulic parameters, also considering proper root water uptake functions. The numerical simulations also consider the presence of noise in the model to further validate the use of a feedback control approach.

Optimized Soil-Water Dynamics Prediction with CRNS, Hydrus-1D, and Machine Learning Integration

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The vadose zone-particularly its root zone—forms a pivotal link between the atmosphere, vegetation, soil, and groundwater. By mediating energy and water exchanges, it governs infiltration, evapotranspiration, runoff, and soil-moisture dynamics, which in turn control aquifer recharge, microbial activity, plant physiology, and pollutant transport. Thorough characterization of this uppermost soil layer is therefore essential for efficient agricultural and irrigation management. Modern monitoring tools support this goal: cosmic-ray neutron probes (CRNPs) provide area-averaged (up to 240 m radius) estimates of root-zone "effective" moisture content by counting fast neutrons generated when cosmic rays collide with atmospheric nuclei. Because these neutrons are slowed chiefly by hydrogen in soil water, the measured flux decreases as volumetric moisture increases. The value of CRNPs can be further amplified by integrating their data into hybrid physically-based–machine-learning models. Such coupling offsets the neural network's large data requirements and lack of physical constraints, thereby improving the reliability of soil-process predictions.

As a proof of concept, we generated synthetic time series that mimic soil properties, atmo- spheric forcings, the leaf-area index (LAI) of a cornfield, and neutron-flux measurements. These inputs were processed in the HYDRUS-1D COSMIC module [1] to calibrate a physically-based model and produce a long-term, dense spatio-temporal dataset for the synthetic field. The same atmospheric forcings—temperature and precipitation—along with the resulting neutron- flux and soil-moisture series were then used to train a Long Short-Term Memory (LSTM) neural network, a recurrent architecture designed to model sequential data and capture long- term dependencies. Our aim was to determine whether an LSTM trained on the outputs of the physically-based model could directly predict soil moisture and irrigation water demand using only atmospheric variables as inputs.

The results show that the neural network reproduces neutron-flux and soil-moisture dynamics with accuracy comparable to the physically-based model, underscoring the promise of this synergistic approach. Future work will focus on training with real-world data and exploring alternative network architectures to further enhance predictive accuracy and enable direct estimation of irrigation requirements using only atmospheric observations.

References

[1] Brunetti, G., Šimůnek, J., Bogena, H., Baatz, R., Huisman, J. A., Dahlke, H., and Vereecken, H., *On the information content of cosmic-ray neutrons in Bayesian optimization of soil hydraulic properties. Vadose Zone Journal, 18:1–24, 2019.* https://doi.org/10.2136/vzj2018.06.0123

Time-Series Analysis and Learning Approaches for Soil Moisture Prediction in Precision Irrigation

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Soil water content is a key element for managing precision irrigation in crops, especially in agricultural contexts where water stress and soil salinity pose significant challenges, thus motivating the interest in deepening the forecast of this variable. This study examines high-frequency monitoring data collected from an experimental agricultural site in Gallipoli, Italy. The dataset includes time series of i) soil water content measurements at different depths, ii) atmospheric data (mainly precipitation and temperature), iii) irrigation data, with different temporal resolution.

To address the diverse forecasting needs, we compare a range of data-driven models. For univariate forecasting, we adopt Chronos, a neural network architecture specifically designed for time-series data, which adapts the Transformer mechanisms originally developed for natural language processing (such as GPT models) to capture temporal dependencies.

For multivariate forecasting, we employ machine learning techniques such as Random Forest and Gradient Boosting Regression. Both methods are based on ensembles of decision trees, but differ in their learning strategies: Random Forest builds multiple trees in parallel and averages their predictions, thus reducing variance and improving generalization, while Gradient Boosting builds trees sequentially, where each new tree corrects the errors of the previous ones, allowing the model to better capture complex, nonlinear interactions between features.

To enhance the models' ability to capture the real dynamics of soil water content, we integrate external variables, particularly irrigation data, precipitation, and weather conditions. By comparing univariate and multivariate approaches, we demonstrate that incorporating such external data allows multivariate models to achieve more accurate and reliable short-term predictions. The integration of data from different platforms makes our methodology a practical tool for forecasting soil water content, optimizing water use, and promoting sustainable agricultural management.

Participatory System Dynamics Modelling for Water-Ecosystem-Food Nexus management

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The security of natural resources is increasingly under threat from a combination of climate change impacts and socio-economic dynamics, which necessitates coordinated action from multiple practitioners and policymakers. The concept of the Nexus, which aims to ensure natural resource security in a holistic and integrated way, has attracted significant attention in recent scientific literature. Despite this, its practical application remains limited. This study introduces the use of Participatory System Dynamics Modelling (PSDM) techniques to improve the understanding, analysis, and management of Water-Ecosystem-Food (WEF) Nexus systems [1]. By utilizing Stock and Flow Diagrams (SFDs), this modelling approach provides a clearer representation of the complex interactions and interdependencies among sectors, facilitating the evaluation of various interventions. The integration of Sensitivity Analysis and Scenario Analysis within the SFD framework enables the assessment of potential impacts under different future conditions, helping to inform decision-making processes. The active involvement of stakeholders throughout the modelling phases, ranging from the design of the model structure to the selection and analysis of scenarios, ensures the incorporation of local knowledge and perspectives, which enhances the relevance and ownership of the results.

The approach is demonstrated through two Mediterranean case studies. These areas, characterized by typical Mediterranean socio-environmental conditions, face common challenges related to water resource management, agricultural practices, and ecosystem preservation. Through the use of SFDs, the study identifies key variables and processes that affect the sustainability of the WEF Nexus. The analysis highlights the importance of managing water availability, irrigation demands, and the health of ecosystems to ensure long-term resource security. Scenario Analysis is employed to explore different future pathways under climate change scenarios, evaluating the impacts of various management strategies, including water conservation measures, Nature-Based Solutions such as riparian forest restoration, and the optimization of agricultural practices. The results show how these interventions can mitigate the negative effects of climate change, reduce pressures on local ecosystems, and improve the sustainability of agricultural systems. By presenting various interventions and assessing their long-term implications, this study provides valuable insights for decision- makers looking to manage interconnected resource systems in a way that promotes sustainability and resilience.

References

[1] Pagano, A., Coletta, V.R., Portoghese, I., Panagopoulos, A., Pisinaras, V., Chatzi, A., Malamataris, D., Babakos, K., Lilli, M.A., Nikolaidis, N.P., Giordano, R. *On the use of Participatory System Dynamics Modelling for WEF Nexus management: Hints from two case studies in the Mediterranean region. Environmental Impact Assessment Review, 115, 108012, 2025.*

Transport of pathogens in saturated porous rocks under variable flow and salinity

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The transport of pathogens through rocks is often regarded as negligible unless there are fractures in the medium. However, sedimentary rocks may have a porosity that allows the migration of pathogens even when they are unfractured. In this work, we investigated the transport behavior of several pathogens (namely Escherichia coli and Enterococci faecalis) through a sedimentary porous rock made of 98.5 wt.% of calcite ($CaCO_3$), hydraulic conductivity $6 \cdot 10 - 6$ m/s, and porosity 0.43. After ensuring full saturation of the samples, the flow and pathogen concentration were monitored. After an initial stabilization of the core, a suspension containing a known concentration of pathogens was superimposed onto the sample and allowed to drain through. Upon complete suspension drainage, several cycles of sterile saline solution (0.9 vol.%) were performed until the pathogen concentration at the outlet became negligible.

A reactive transport model through saturated porous media was developed and implemented to describe the tests. The model couples conservation laws for flow and transport under variable head conditions with constitutive equations of straining and attachment/detachment. The data show significant retention of pathogens within the core during suspension drainage and rapid mobilization during distilled water infiltration in the case of E.coli. This behavior is well captured by the model and shows that rocks can act as bioreactors for selected pathogens favoring accumulation and growth during loading and mobilization during flooding with low-salinity water.

This may suggest that porous rock deposits may exacerbate contamination of the underlying aquifers under intermittent conditions of accumulation/growth and release rather than protecting underground water resources, as generally assumed.

This topic is the objective of DY.MI.CR.ON. project “Predictive dynamics of microbiological contamination of groundwater in the earth critical zone and impact on human health (DY.MI.CR.ON Project)” funded by the European Union – Next Generation EU, mission 4 component 1, CUP I53D23000500001.

Preliminary Flood Hazard Assessment for the Trento Municipality Using a Semi-Implicit, Subgrid, Hyper-Resolution Hydrodynamic Model

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Floods are among the most devastating natural hazards, with growing societal and economic impacts worldwide (e.g. [4]). Flood hazard assessment, as a non-structural strategy for flood mitigation, plays a crucial role alongside structural interventions in raising risk awareness and reducing potential damages.

Traditional numerical methods for flood hazard mapping can yield high-fidelity results; however, they are often computationally expensive, especially when high accuracy is required over large areas. To address these limitations, subgrid modeling has been introduced. The core idea behind subgrid models is to incorporate high-resolution digital elevation data at the subgrid level while performing computations on a coarser grid, thereby improving efficiency without compromising detail. Casulli [1] and Casulli & Stelling [2] proposed an algorithm that ensures precise mass balance in areas experiencing wetting and drying. This approach guarantees strict mass conservation and non- negative water depths for any time step size, significantly enhancing both accuracy and computational efficiency.

We tested the algorithm, implemented in the UnTRIM hydrodynamic model by Casulli [1], for the Adige River, focusing on the study area within the Trento municipality (covering an area of approximately 60km^2). The potential of the proposed methodology was explored with particular attention to: i) generating flood hazard maps at hyper-resolution with low computational costs, and ii) accurately representing man-made structures that influence flood behavior and risk quantification Casiulli [3], such as levees, backwater effects, and pressurized pipes.

Preliminary results show good agreement with existing high-resolution flood hazard maps developed by local authorities, with noticeable improvements in specific areas of the municipality, thanks to the enhanced spatial resolution used in this study.

References

[1] Casulli, V. *A high-resolution wetting and drying algorithm for free-surface hydrodynamics. Int. J. Numer. Method Fluids 60:391-408. 2009.*

[2] Casulli, V. and Stelling, G.S. *Semi-implicit subgrid modelling of three-dimensional free-surface flows. Int. J. Numer. Method Fluids 67:441-449 2010.*

[3] Casulli, V. *Computational grid, sub-grid and pixels. Int. J. Numer. Method Fluids 90: 140-155, 2019.*

[4] Jongman, B. *The fraction of the global population at risk of floods is growing. 2021.*

A nonconforming extended virtual element method for Stokes interface problems

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In this paper, we propose a nonconforming extended virtual element method, which combines the extended finite element method with the nonconforming virtual element method, for solving Stokes interface problems with the unfitted- interface mesh. By introducing some stabilization terms and penalty terms, as well as some special terms defined on non-cut edges of interface elements in the discrete bilinear form, we prove the discrete inf-sup condition and obtain optimal error estimates. It is shown that all results are not only independent of the mesh size and the viscosity coefficient, but also the interface position. Numerical experiments are performed to verify theoretical results.

Using treated wastewater in agriculture: reducing environmental pressure on intermittent streams

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Temporary river systems are the most common waterways in the Mediterranean Region. These rivers, characterized by extremely low streamflow or dry conditions in summer, are essential for supporting diverse ecosystems. Anthropogenic activities such as agriculture and treated wastewater discharges into these fragile environments may threaten their hydrological and ecological status. In addition, changes in the rainfall regime, combined with temperature increases (evaporative demands), increase the need for irrigation and exacerbate the natural degree of intermittency of the river systems. Going beyond a case study, the Triolo catchment (Apulia, Italy), this paper aims to define a methodology for analysing the environmental impact of agriculture and point sources (WWTPs) on surface waters and to evaluate the treated wastewater as a potential resource of water and nutrients for use in agriculture. The ecohydrological model "Soil and Water Assessment Tool" (SWAT), combined with field data, was used to simulate hydrology and water quality. Under the current anthropogenic pressures (agriculture and WWTP), monitoring and modeling results showed that the TP and NO3 concentrations are above desirable values for good ecological status in surface waters. The dry season was critical for TP pollution, and the WWTP discharge caused the main pressure on surface waters. The rainy season was key to NO3 pollution, and agriculture was the main pressure. The results of this study demonstrated that treated wastewater could represent an important resource of water and nutrients capable of satisfying the seasonal irrigation requirements for approximately 1600 ha of olive grove (2000 m3 ha-1), providing approximately 25 kg ha-1 of TN and 8 kg ha-1 of TP.

A Physics-Informed Approach to Slow Landslides: The Pianello Hillslope Case Study

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Slow-moving landslides pose significant threats to infrastructure and communities, with their behavior intrinsically linked to subsurface hydrological processes. The complex relationship between rainfall infiltration and pore water pressure dynamics exhibits distinctive piezometric patterns described by Richards' equation for unsaturated flow in porous media.

This study presents a novel computational approach using Physics-Informed Neural Networks (PINNs) to model subsurface water dynamics in landslide-prone areas. Under the approximation of constant diffusion coefficient, Richards' equation reduces to a diffusion equation for volumetric water content.

The methodology is applied to the two-dimensional domain of the Pianello hillslope in Bovino (FG), Italy, characterized by active slow-landslide phenomena. The subsurface is approximated as a single homogeneous clay layer, consistent with the dominant soil type and observed landslide mechanisms.

Boundary conditions are defined using both synthetic and real precipitation data spanning 2007-2024. The 17-year dataset encompasses multiple hydrological cycles, with real data exhibiting pronounced seasonal variability. These seasonal patterns are reproduced in synthetic datasets for consistency and parametric studies.

The objective is to develop a PINN-based solution able to capture the oscillatory piezometric behavior measured by field instruments at various depths, potentially improving predictive capabilities compared to other traditional numerical methods. Expected outcomes include validation of the PINN approach for hydrological modeling in landslide contexts, improved understanding of subsurface dynamics at the Pianello site, and development of a framework extensible to other slow-landslide systems. This work advances machine learning applications in geotechnical engineering and natural hazard assessment.

Enhancing sustainable water resources use in irrigation systems: the ERASMUS approach

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The concept of Nexus represents an evolution of the Integrated Water Resources Management (IWRM) paradigm, with an explicit focus on interconnections among different sectors (typically Water-Energy-Food-Ecosystems, WEFE). Nexus approaches have therefore increasingly been used in science and policy context, to identify sustainable development pathways for complex environmental systems where a multiplicity of sectors and agents need to be taken into account. The concept of Nexus has become particularly critical in the analysis of irrigated agro-ecosystems, considering the multiplicity of natural resources involved/impacted (e.g., surface water or groundwater for irrigation, land for agriculture, energy) and the multiplicity of drivers to be considered (e.g., climate change, socio-economic conditions, environmental impacts of agricultural practices, etc.). However, despite the increasing attention received, a gap still exists in the identification of suitable modelling approaches for putting Nexus into practice. The present work details some of the modelling approaches proposed as part of the ERASMUS project (Funded by the European Union—Next-Generation EU—National Recovery and Resilience Plan NRRP —MISSION 4 COMPONENT C2, INVESTIMENT N. 1.1, CALL PRIN 2022 D.D. 104 02-02-2022, Project 2022WLW9X8, Equality and Resilience of Agroecosystems through Smart water Management and Use—ERASMUS CUP N. B53D23006510006), which aims at providing tools for an improved understanding of the WEFE Nexus in irrigated agroecosystems, while supporting its implementation exploring the role that innovative technologies might have.

More specifically. ERASMUS exploits the potential of numerical modelling approaches, based on well-established codes (such as EPANET and COPAM) to simulate the behavior of irrigation networks under a multiplicity of operating scenarios. The focus of the analysis is on the identification of extreme conditions that might affect system resilience and reliability such as pressure deficit or excess pressure. The analysis facilitates the selection of resilience-enhancing measures that range from changes in network structure, to modifications in network operating conditions, to the adoption of technologies and tools (e.g., the OAS, a smart valve developed by Politecnico di Milano) that can improve network management and control under a multiplicity of conditions. Based on numerical simulations, a set of indicators has been identified and calculated to describe key system properties such as water distribution equity, pressure deficit or excess, and water/energy use efficiency. Indicators have been selected with the aim of providing a broad overview of the impacts that technologies and strategies might have on the system, therefore accounting for a multiplicity of aspects that impact the Nexus as a whole. The use of System Dynamics Modelling tools, mainly in the form of Causal Loop Diagrams, will ultimately help aggregating indicators, better understanding their interdependencies and implications. The proposed approaches will jointly provide a comprehensive overview of the state of irrigated systems and their potential evolution under multiple scenarios. The approach is being tested in two case studies in Southern Italy, namely in the Capitanata area and in the Ufita area, but can be replicated in other contexts.

Coupled Physics-Informed Neural Networks for Spatiotemporal Estimation, Monitoring and Prediction of Soil Moisture/volumetric water content via Richards' Equation and Electromagnetic/Electrical methods of Exploration Geophysics

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Monitoring the dynamics of soil moisture in the vadose zone is essential for understanding hydrological processes, managing irrigation, and assessing environmental risks. We propose a hybrid modeling framework based on Coupled Physics-Informed Neural Networks (cPINNs) that integrates variably saturated flow modeled by Richards' equation with electromagnetic and electrical geophysical measurements, including Electrical Resistivity Tomography (ERT), Time Domain Electromagnetics (TDEM), Ground Penetrating Radar (GPR), and Time-Domain Reflectometry (TDR).

Our approach fuses physical laws and observational data by embedding both the Richards' equation and geophysical forward models into the training of neural networks. This enables the inversion of spatially and temporally varying volumetric water content (θ) and soil hydraulic parameters. The methodology is currently being demonstrated on synthetic benchmarks and would be extended to real soil moisture datasets acquired from controlled field experiments, where sensor-based θ measurements and geophysical observations shall be jointly used to constrain the model. Thus, the model learns both the hydrology and the geophysics principles simultaneously. The main advantages of this approach are, much more physically consistent inversion, Shared information between hydrology and geophysics reduces ambiguity (non-uniqueness) and this opens up possibilities of integrating sparse hydro data and dense geo data (or vice versa).

Initial results show that the proposed cPINN framework accurately captures the spatiotemporal evolution of soil moisture profiles in 3D, even in the presence of noise, irregular topography & acquisition configuration, and limited data coverage. Compared to traditional inversion methods, our model offers better generalization, interpretable parameter recovery, and enhanced robustness to data sparsity.

This research underscores the potential of physics-informed machine learning for non-invasive, time-resolved hydrological monitoring and prediction in heterogeneous and complex subsurface environments, combining the physical principles of Fluid-Dynamics and Exploration-Geophysics.

Recurrent Neural Network models for Soil Moisture Forecasting and Smart Irrigation Scheduling

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The increasing demand for scalable, cost-effective solutions in precision agriculture has highlighted the need to reduce reliance on physical sensing infrastructure. While deep learning methods have shown promise in various agrotechnical applications, there remains a notable lack of research focused on predicting both soil moisture content and irrigation demand using neural networks—particularly in the context of limited input data. To address this gap, this study presents an evaluation of recurrent deep learning models for the joint prediction of soil moisture and irrigation. Central to this analysis is the introduction of IRRMAP, a synthetic dataset specifically designed to support data-driven decision-making in agriculture. Spanning 5000 days of simulated yet seasonally coherent agronomic and climatic data, IRRMAP replicates conditions typical of South European environments. A total of 18 network configurations were tested, combining convolutional, recurrent (LSTM and BiLSTM), and fully connected layers. The best-performing architecture-consisting of a BiLSTM layer followed by 10 dense layers—achieved RMSE values of 1.702 for soil moisture and 1.652 for irrigation. Notably, the model maintained high predictive accuracy even when trained on a reduced set of input features, indicating its potential for deployment in sensor-constrained farming systems.

Algebraic Multigrid Methods for Uncertainty Quantification in Stochastic Groundwater Flow: A Computational Framework for Singular Source Problems

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Predicting groundwater flow in heterogeneous aquifers poses considerable computational difficulties, particularly when hydraulic conductivity displays spatial variability and flow is influenced by discrete sources. This study shows a numerical framework that integrates algebraic multigrid (AMG) solvers with Monte Carlo uncertainty quantification to tackle these challenges, illustrating the beneficial intersection of computational mathematics and hydrogeology.

Hydraulic conductivity is modeled as a log-normal random field characterized by exponential spatial correlation. The resulting stochastic Poisson equation with Dirac delta sources is solved using finite volume discretization. The mathematical challenge involves addressing the singular characteristics of point sources alongside the significant coefficient variations. This study compares seven AMG configurations, including classical, aggregation, and F-cycle variants, in conjunction with Krylov accelerators (FGMRES, GMRES, PCG) to determine optimal solver strategies.

Benchmarking against analytical Green's functions for homogeneous cases demonstrates that AMG-CLASSICAL-PMIS and Chebyshev-based smoothers exhibit better convergence. In heterogeneous Monte Carlo simulations, statistical convergence patterns exhibit significant variation based on problem parameters: low-variance cases achieve stabilization within 100 realizations, whereas high-variance scenarios necessitate over 800 realizations to attain higher-order moments.

The GPU-accelerated implementation (FiPy + AMGx + GSTools) facilitates uncertainty quantification workflows that were previously computationally prohibitive, allowing for the completion of full statistical analyses in less than one hour. The framework extends beyond immediate hydrogeological applications, addressing the broader challenge of solving stochastic PDEs with singular sources, a problem prevalent in various geoscience domains, including seismic wave propagation and contaminant transport.