Book of abstracts

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Geometrically intrinsic modeling of 2D diffusive wave overland flow for coupled surface-subsurface hydrological applications

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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. Simulations on several synthetic test cases show the importance of taking into full consideration the bottom geometry even for relatively mild and slowly varying curvatures.

Effects of small-scale soil structure features on hydrological, biogeochemical, and geomorphological processes

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Terrestrial biosphere models require spatially distributed soil hydraulic properties, which are often derived from readily available soil properties (e.g., texture, bulk density, organic matter) by means of pedotransfer functions (PTFs). Present PTFs are limited due to reliance on soil sample information and only a few data sets for training. In particular, none of the PTFs consider the effects of soil structure, thus limiting their applicability in vegetated areas in which macropores are expected to significantly increase soil saturated hydraulic conductivity. Considering the strong links between vegetation and soil structure, we propose a systematic approach for incorporating structural effects on PTF-derived soil hydraulic properties. We will show that, under certain soil and climatic conditions, small-scale soil structure features prominently alter the hydrologic response emerging at larger scales and that upscaled parameterizations must explicitly consider the spatial variability of soil and vegetation attributes. Applications to both natural and managed ecosystems will be presented to highlight the role of soil structure in modulating a variety of hydrological, biogeochemical, and geomorphological processes. Progress in the representation of small-scale soil biophysical features is key for establishing more complete causal links between landscape attributes and heterogeneities in physical properties, thus providing a mechanistic strategy for model parameterization and process description across scales and a path forward for more reliable large-scale modeling under future scenarios.

Multipoint mixed finite element methods for rotation-based formulations of Stokes flow and Biot poroelasticity

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We propose a mixed finite element method for Stokes flow with one degree of freedom per element for the pressure and one per facet for the velocity on simplicial grids. The method is derived by first considering the vorticity–velocity–pressure formulation of the Stokes equations. The vorticity is then elimintated through the use of a local quadrature rule, leading to a multipoint vorticity mixed finite element method.

The discrete solution possesses several advantageous properties. First, the velocity field is pointwise divergence-free and the method is pressure robust. Second, the application of the quadrature rule leaves several properties of the solution intact. For example, the pressure is invariant to the low-order integration on the vorticity variable. We derive theoretically that the method is linearly convergent in all variables and show second order convergence in the vorticity in special cases.

Next, we remark on the similarities between the Stokes problem and Biot poroelasticity. Using an analogous approach as before, we introduce the solid rotation and fluid flux as auxiliary variables and subsequently removed from the system using a local quadrature rule. This leads to a multipoint rotation-flux mixed finite element method that employs the lowest-order Raviart-Thomas finite element space for the solid displacement and piecewise constants for the fluid pressure. Rigorous analysis shows the method to be linearly convergent and we obtain similar invariants to the quadrature rule.

For both the Stokes and the Biot problems, the analytical results concerning stability, invariants, and convergence are confirmed by numerical experiments. To benchmark the methods, we consider a lid-driven cavity flow for the multipoint vorticity MFEM and Mandel's problem for the multipoint rotation-flux MFEM.

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Stochastic Modeling of Anomalous Water Transport

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A stochastic model for anomalous water transport is considered and isotope data in precipitation and streamflow are used to verify the model. The aim is to model the movement of water particles along a slope, alternating between periods of time in which they move with a certain velocity and periods in which they remain stationary due to being trapped in the geological formation of the mountain. For this physical problem, a type of Lévy walk that takes into account the heterogeneity of the slope environment is studied and its mathematical formulation is developed. Therefore, a stochastic transport process is employed, and the transit time distribution of water is estimated using the first passage time distribution of the process for a given height.
The purpose is to validate the model of the transport process by using the concentration of stable water isotopes in precipitation and streamflow for some catchments, in order to estimate the young water fraction. This fraction represents the portion of streamflow that is younger than a specific threshold age and has recently been proposed as a reliable measure of water age in heterogeneous catchments. Stable isotopes of water naturally exist in precipitation, but their concentration varies during the hydrological cycle of water. The aim is to find a relationship between the variation in concentration of these isotopes and the model parameters for estimating the young water fraction.

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Investigating Hyghly Heterogeneous Aquifers: A Unique Experimental Approach

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Deciphering the complex processes driving water flow and mass transport in aquifers is crucial for effective water management and safeguard. Nonetheless, unraveling the principles that govern these phenomena presents significant challenges, especially in natural aquifers that exhibit considerable heterogeneity [1]. The limitations of previous studies stem from insufficient data and a lack of experimental models that could provide a solid and accurate basis for characterizing highly heterogeneous aquifers. To address these deficiencies and enhance our current comprehension, we carried out a unique experiment that examines a highly heterogeneous, laboratory-constructed, saturated aquifer, studied on an intermediate scale under radial flow conditions [2]. This significant heterogeneity was generated by randomly placing 2527 cells, over 7 layers, each filled with one of 12 different soil mixes. For each of these, the grain size distribution, porosity, and hydraulic conductivity were measured in the laboratory. We installed 37 fully penetrating piezometers, arranged radially at varying distances from the central extraction well, allowing for a comprehensive series of pumping tests to deduce the hydraulic conductivity values at each piezometer location and establish scaling laws in eight different directions. Our findings indicate that the pronounced aquifer variability led to significant vertical and directional anisotropy in hydraulic conductivity. Furthermore, we have experimentally found, for the first time, that the highly heterogeneous porous medium tends towards homogeneity when moving from the heterogeneity scale to the investigation scale, i.e., the intermediate scale. These innovative findings from a distinctly heterogeneous aquifer contribute to the scientific field and offer interesting insights for those researching water flow and mass transport. The unique dataset collected from these experiments can serve as a basis for follow-up studies and as a benchmark to confirm the findings of future research on water flow and mass transport.

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The "true" meaning of Hydrogeophysics: integration of geophysical data with hydrological modeling.

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The use of geophysical methods for the characterization of the shallow subsurface for hydrological/hydrogeological purposes has a long history. Examples go back to 1970's [1], with mixed success. In particular, the use of electrical and electromagnetic methods has found extensive application even since, even though some early ambitious goals have not (and cannot) be attained, in particular when correlation is attempted directly between geophysical and hydrological medium properties (typically, electrical conductivity and hydraulic conductivity, or, in more recent years, pore medium polarization properties with hydraulic conductivity). A major step forward, though, has been achieved since the early 1990's when a new school of thoughts has been developing and the word "hydrogeophysics" has been coined [2, 3]. The main change in the minds of the early developers was to join more closely the results of the (geo)physical measurements with the physical signal produced by hydrological processes. This, in practice means that the geophysical results shall be used, as much as possible, as data (albeit to some extent indirect) to be used to calibrate hydrological models, e.g. using data assimilation techniques, but not only. At the heart of the idea lie two main requirements: (a) that a link is established between geophysically-measured parameters (e.g. electrical resistivity) and the hydrological state variables (moisture content, water salinity etc.), rather than towards hydraulic parameters such as hydraulic conductivity; and (b) that time-lapse geophysical measurements are conducted in order to samples in time, as well as in space of course, the state variables. The approach has had tremendous impacts in understanding of complex hydrological systems, at a variety of scales, supplying hydrological models with an unprecedented amount of 4D data, that the models desperately need for a proper calibration – in this respect mimicking what is successfully done (and can be done even better) in the petroleum industry using 4D seismics. As many success stories, however, the one of "hydrogeophysics" has also some downside. In this case, the misuse of the term has been widespread. Nowadays a variety of studies that are no more than the classical, ancient, use of geophysics for the characterization of the shallow subsurface, often for hydrological purpose, call themselves "hydrogeophysical" studies, even though no attempt is made to link geophysical data with hydrological models. This contribution wishes to state a word of caution in this direction, and make a small step towards a badly needed restoration of the original goal and meaning of a still very innovative and promising approach, not always fully exploited in practice.

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A simplified numerical assessment of excessive DM growth in Self-Forming Dynamic Membrane Bioreactors (SFD MBR) for Wastewater Treatment

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Self-forming dynamic membranes for wastewater treatment are becoming increasingly popular due to the many benefits they offer over conventional technologies [1, 2]. In these systems, filtration takes place through a cake layer (Dynamic Membrane, DM) supported by a 10-200 µm filter mesh. Filtration efficiency may decrease when the DM becomes too thick or its composition changes, and this can be measured under constant flux through the increase of TMP (TransMembrane Pressure). Different DM maintenance strategies can be adopted to limit the loss of performance caused by excessive cake layer growth [3, 4]. In this study, the increase rate of the TMP over time was evaluated to analyze the cake growth on the support mesh. TMP peaks in the range 20-200 mbar and observed during 4h filtration cycles (229 minutes of filtration, 11 minutes of break) were recorded. These data were interpreted with second order interpolations and linear trends [4]. Here, the slopes of the trend lines are used to compare the performance of the different DM maintenance strategies considered. These lines provide a simplified representation of the speed at which the pressure of 200 mbar is reached, once the DM thickness starts to increase (lower TMP instability threshold of 20 mbar). These slopes allow to evaluate cake layer accumulation: the lower the slope value, the longer the time to reach the critical TMP value.

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A coupled surface-subsurface model for hydrostatic flows under saturated and variably saturated conditions

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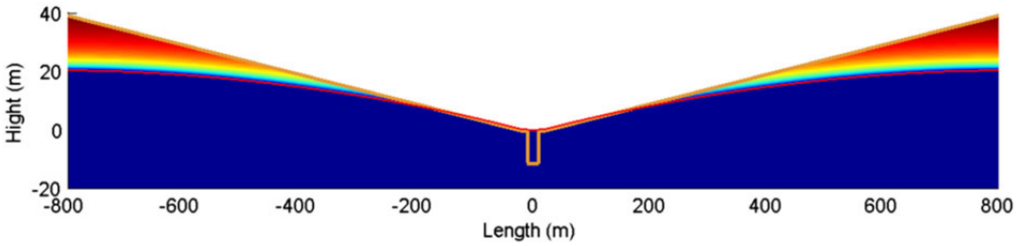
Assuming the validity of the hydrostatic approximation, coupled surface-subsurface flows governed by the Richards and by the Navier-Stokes equations are solved simultaneously by using semi-implicit finite difference equations for velocities and a finite volume approximation for the vertically integrated continuity equation. The resulting three-dimensional algorithm is relatively simple, extremely efficient, and very accurate. Stability, convergence, and exact mass conservation are assured throughout also in presence of wetting and drying, in variable saturated conditions, and during flow transition through the soil interface.



A finite difference scheme for nonlinear peridynamics

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An original numerical procedure for the nonlinear peridynamics on arbitrarily–shaped two-dimensional (2D) closed manifolds is presented. When dealing with non parameterized 2D manifolds at the discrete scale, the problem of computing geodesic distances between two non-adjacent points arise. Here, a routing procedure is implemented for computing geodesic distances by re-interpreting the triangular computational mesh as a non-oriented graph; thus returning a suitable and general method. Moreover, the time integration of the peridynamics equation is demanded to a P-(EC)^k formulation of the implicit β-Newmark scheme. The convergence of the overall proposed procedure is questioned and rigorously proved. Moreover, strength and limitations of such numerical framework are critically analyzed. The performed numerical investigations are mainly motivated by the issues related to the insurgence of singularities in the evolution problem. The obtained results return an interesting picture of the role played by the nonlocal character of the integrodifferential equation in the intricate processes leading to the spontaneous formation of singularities in real materials. This talk is based on the work with G. M. Coclite, F. Maddalena, and T. Politi [1].

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Physics-Informed Neural Networks for solving Groundwater Flow Equation

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In recent years, Scientific Machine Learning (SciML) methods for solving partial differential equations (PDEs) have gained wide popularity. Within such a paradigm, Physics Informed Neural Networks (PINNs) are novel deep learning frameworks for solving forward and inverse problems with non-linear PDEs. Recently, PINNs have shown promising results in different application domains. In this paper, we approach the groundwater flow equations numerically by searching for the unknown hydraulic head. Since singular terms in differential equations are very challenging from a numerical point of view, we approximate the Dirac distribution by different regularization terms. Furthermore, from a computational point of view, this study investigate how a PINN can solve higher-dimensional flow equations. In particular, we analyze the approximation error for one and two-dimensional cases in a statistical learning framework. The numerical experiments discussed include one and two-dimensional cases of a single or multiple pumping well in an infinite aquifer, demonstrating the effectiveness of this approach in the hydrology application domain.

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Forward electromagnetic induction modelling in a multilayered half-space: An open-source software tool

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Electromagnetic induction (EMI) techniques are widely used in geophysical surveying. Their success is mainly due to their easy and fast data acquisition, but the effectiveness of data inversion is strongly influenced by the quality of sensed data, resulting from suiting the device configuration to the physical features of the survey site. Forward modelling is an essential tool to optimize this aspect and design a successful surveying campaign. In this paper, a new software tool for forward EMI modelling is introduced. It extends and complements an existing open-source package for EMI data inversion, and includes an interactive graphical user interface. Its use is explained by a theoretical introduction and demonstrated through a simulated case study. The nonlinear data inversion issue is briefly discussed and the inversion module of the package is extended by a new regularized minimal-norm algorithm.

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Non-Newtonian flow in fractured media: from deterministic to random approaches

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Non-Newtonian fluid flow in fractured media is relevant for subsurface operations aimed at resources recovery, land remediation, and geothermal exploitation. In these contexts, complex fluids (e.g., polymer solutions, foams, muds) are employed as carriers for suspended nanoparticles and fracking proppant, and potentially, as heat-exchange working fluids in enhanced geothermal systems. The interplay between the heterogeneity of fractured geological media, from the pore- to field scale, and the non-linear rheology of working fluids strongly influence flow localization, medium transmissivity, and transport phenomena across the formation. The quantitative characterization of flow and transport features is fundamental to achieve a desired performance of subsurface industrial activities to mitigate the environmental impact and increase their cost effectiveness. We present results from several of our works dealing with complex fluid flow in single fractures, from analytical conceptual models and analog experiments to numerical approaches in a stochastic framework.

In the first group of contributions, the fracture is conceptualized with the parallel plate approach and the focus is on a specific phenomenon, the backflow of fracturing fluid from fractures to wellbore in the third phase of hydraulic fracturing, after injection is ceased. We consider an Ostwald-DeWaele (power-law) or Ellis fluid, a planar or radial fracture geometry, and a time-variable aperture depending on the internal fluid pressure and the elastic relaxation of the walls. The relationship between the latter quantities may be linear, akin to a Winkler soil, or nonlinear, due to the progressive softening or stiffening of the boundary associated with the properties of the surrounding rock. The result is an integrodifferential problem that admits a closed-form similarity solution for power-law fluids, albeit implicit for some quantities; for the more realistic, three-parameter Ellis fluid, the solution is partially numerical and depends on dimensionless group N encapsulating the main problem parameters and equal to the ratio between the Cauchy number and the product of Reynolds and Ellis numbers. Results are validated in the laboratory with an original experimental device, an ad hoc replica of a rectangular or circular fracture. The match between theory and experiments is fairly good, with discrepancies of a few percent essentially due to the approximations of the theoretical model, and, for shear-thinning fluids, to the simplified constitutive equation.

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 complex 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 up to two orders of magnitude higher than simple fluids like water. We investigate this phenomenon implementing a lubrication-based numerical code able to generate synthetic fractures and solve the flow 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.

Nonnegative moment coordinates on finite element geometries

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We introduce new generalized barycentric coordinates (coined as *moment coordinates*) on nonconvex quadrilaterals and cubes with nonconvex faces. This work draws on recent advances in constructing interpolants to describe the motion of the Filippov sliding vector field in nonsmoooth dynamical systems, in which nonnegative solutions of signed matrices based on (partial) distances are studied. For a finite element with n vertices (nodes) in $\mathbb{R}^2$, the constant and linear reproducing conditions are supplemented with additional linear moment equations to set up a linear system of equations of full rank n, whose solution results in the nonnegative shape functions. On a simple (convex or nonconvex) quadrilateral, moment coordinates using signed distance are identical to mean value coordinates. For signed weights that are based on the product of distances to edges that are incident to a vertex, we recover Wachspress coordinates on a convex quadrilateral. We also present some general properties of generalized barycentric coordinates and possible extensions to finite element geometries in $\mathbb{R}^3$.

Mathematical modelling and open-source simulation of reverse-osmosis desalination

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The reverse osmosis membrane module is an integral element of a desalination system as it determines the overall performance of the desalination plant. The fraction of clean water that can be recovered via this process is often limited by salt precipitation which plays a critical role in its sustainability. In this work, we present a model to study the complex interplay between flow, transport and precipitation processes in reverse osmosis membranes, which together influence recovery and in turn process sustainability. A reactive porous interface model describes the membrane with a dynamic evolving porosity and permeability to capture the scaling of the membrane. An open-source finite-volume numerical solver is implemented within the OpenFOAM®library and numerical tests are presented here showing the effect of the various parameters of the model and the robustness of the model to describe a wide range of operating conditions.

The use of advanced solvers and parameters optimization software to overcome numerical errors in groundwater flow models in folded and faulted areas

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Three-dimensional (3D) numerical modeling of aquifers in folded and faulted terrains can be challenging because geological structure exerts a significant influence on the location of spring discharge locations and related groundwater flow. Reproducing such complex geometry of model layers can result in different layer thicknesses of saturated portions, which can result in drying and rewetting of cells during model iterations, leading to numerical instabilities, preventing convergence, or increasing numerical error. Otherwise, an excessive system simplification used to attain stability may lead to unsatisfactory predictive capability of the model. Recent advances have targeted such issues, including development of solvers that facilitate achieving convergence and/or reduce computational errors due to model nonlinearities [1, 2]. The aim of this research was to develop and test a procedure for the simulation of groundwater flow in a complex karst, folded, multilayer aquifer. In previous research, the complexity of the conceptual model was reproduced by progressively adding elements to the model grid, from a two-dimensional (2D) to a quasi-3D and a fully-3D model and adding layers and hydraulic conductivity zones [3]. During this process, the model response was evaluated through manual trial-and-error history matching of a steady state solution. An equivalent porous media approach was used; however, modeling identified a discrete groundwater circulation pattern, successfully simulated by adding a high permeability longitudinal strip. The fully-3D model matches the observed flow distribution at the different reaches along the river, simulating reliable flow paths and recharge partitioning into layers. The Newton-Raphson formulation of MODFLOW-2005 (MODFLOW-NWT) was required to achieve convergence and reduce model error. The steady state numerical modeling demonstrated the major impact of folded and faulted geological structures on controlling the flow dynamics in terms of flow direction, water heads, and spatial distribution of the outflows to the river and springs. A preliminary transient simulation was then performed using monthly stress periods and variable pumping simulated by MODFLOW's WEL package to test effects of withdrawals for water supply on the aquifer system. Initial runs showed a very high mass balance error (2% discrepancy over cumulative volume) and a runtime of 1 hour and 38 minutes. To reduce both mass balance error and runtime, the USGS software for the optimization of the MODFLOW-NWT solver inputs, NWTOPT [4], was used. NWTOPT identified improved solver inputs, which gave a superior tradeoff between acceptable mass balance error (-0.39%) and much reduced runtime (40 minutes and 9 seconds).

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Why diffusion-based preconditioning of Richards equation works: spectral analysis and computational experiments at very large scale.

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We consider here a cell-centered finite difference approximation of the Richards equation in three dimensions [1],

$$\rho\,\phi\frac{\partial s(p)}{\partial t} - \nabla\cdot K(p)\nabla p - \frac{\partial K(p)}{\partial z} = f,$$

where $p(t)$ is the pressure head at time t, $s(p)$ is water saturation at pressure head p, ρ is water density, ϕ is the porosity of the medium, $K(p)$ the hydraulic conductivity, f represents any water source terms and z is elevation. The discretization uses averages at the interface values for the hydraulic conductivity $K = K(p)$, a highly nonlinear function, by arithmetic, upstream and harmonic means. The nonlinearities in the equation can lead to changes in soil conductivity over several orders of magnitude and discretizations with respect to space variables often produce stiff systems of differential equations.

A fully implicit time discretization is provided by *backward Euler* one-step formula; the resulting nonlinear algebraic system is solved by an inexact Newton Armijo-Goldstein algorithm, requiring the solution of a sequence of linear systems involving Jacobian matrices.

We prove some new results concerning the distribution of the Jacobians eigenvalues and the explicit expression of their entries. Moreover, we explore some connections between the saturation of the soil and the ill conditioning of the Jacobians. The information on eigenvalues justifies the effectiveness of some preconditioner approaches which are widely used in the solution of Richards equation.

We also propose a new software framework [2, 3] to experiment with scalable and robust preconditioners suitable for efficient parallel simulations at very large scales. Performance results on a literature test case show that our framework is very promising in the advance towards realistic simulations at extreme scale.

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Network inpainting via Optimal Transport

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The precise digital reconstruction of natural networks such as plant roots or rivers is crucial to ensure the quality of simulation-driven predictions. However, the identification of these structures may be an extremely challenging problem, due to noise, resolution limits and/or usage of noninvasive techniques. This leads to artifacts that compromise the reliability of the data and the derived simulations.

Variational image processing methods can reconstruct corrupted networks as the result of a minimization problem that involves a discrepancy measure and penalization terms, in a process known as inpainting. In this talk we will show how the optimal transport theory can provide the proper mathematical tool to address the reconstruction of natural networks. We will present some preliminary experiments where these ideas are tested.

Evaluation of concrete quality through estimation of absorbed water and water penetration depth using electromagnetic wave radar

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Most of the deteriorations of concrete structures are caused by the excessive amount of water which penetrates the porous concrete. In this study, the applicability of the Electromagnetic Wave Radar as a Non-Destructive Test tool in the assessment of concrete quality related with penetrated water is investigated experimentally and numerically for various water-cement ratios of concrete which uses Finite Difference Time Domain (FDTD). As an output, the index calculated from the area difference of reflected electromagnetic waveform between the different saturated conditions of water could be used to evaluate the clear effects on the varying amount of water absorbed by the concrete and depth of water penetrated depending on the concrete quality related with water cement ratio. This experimental and Numerical study discussed the utilization of the results of electromagnetic wave radar as a non-destructive tool for the evaluation of quality of concrete and construction joints depending on the water absorption ratio. First many specimens with different water-cement ratios, construction joint, and repair material were prepared. Then, water absorption tests were conducted for each specimen and the electromagnetic reflection wave was measured from dry and wet surfaces of the concrete by using electromagnetic wave radar. An index calculated from the reflection wave was applied to evaluate the relationship between the quality of concrete and construction joint. It was understood that the applied index was useful to evaluate concrete and construction quality by using electromagnetic wave radar.

keyword: Non-destructive testing, water penetration depth, water absorption, concrete quality.

Model Reduction and Operator Learning for Environmental Flows

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High-fidelity numerical simulation plays an important role in addressing complex scientific and engineering problems in environmental fluid dynamics. Despite the progress in computational resources and methodologies over the last two decades, high-fidelity models remain computationally expensive and require substantial expertise. Non-intrusive reduced order modeling techniques have become increasingly popular as a way to address these computational challenges because they offer an alternative by leveraging available data and observations without explicit access to the underlying governing equations. Here, we will consider several non-intrusive techniques based on linear and nonlinear dimension reduction as well as recently introduced operator learning frameworks. We will evaluate their performance for riverine, estuarine, and near-shore systems, with an eye to both fast prediction and parameter inference.

Numerical models for frictional contact mechanics and flow in fractured porous media

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The simultaneous simulation of frictional contact mechanics and fluid flow in fractured geological media is a tightly coupled physical processes and a key component in the design of sustainable technologies for several subsurface applications, such as geothermal energy production, CO2 sequestration and underground gas storage. Typically, the aperture and slippage between the contact surfaces drive the fluid flow in the fractures, while the pressure variation perturbs the stress state in the surrounding medium and influences the contact mechanics itself. This usually produces a stiff non-linear problem associated with a series of generalized saddle-point linear systems, whose solution is often hard to obtain efficiently. In this work, we focus on a blended finite element/finite volume method, where the porous medium is discretized by low-order continuous finite elements with nodal unknowns, cell centered Lagrange multipliers with a stabilization are used to prescribe the contact constraints, and the fluid flow in the fractures is described by a classical two-point flux approximation scheme. A class of scalable preconditioning strategies based on the physically-informed block partitioning of the unknowns and state-of-the-art multigrid techniques is developed for the robust and efficient solution to the resulting sequence of linear systems with the Jacobian matrix. A set of numerical results concerning fractured porous media applications illustrate the robustness of the proposed approach, its algorithmic scalability, and the computational performance on large-size realistic problems.

A Semi-Conservative Depth Integrated Material Point Method For Run-Out of Flow-like Landslides and Mudflows

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Landslides are one of the most problematic natural occurrences for the safety of people, not only because of their intrinsic unpredictability but also because of their potentially catastrophic consequences in terms of human and economic losses [1, 2]. It is essential to continuously monitor locations that are prone to landslides. Despite satellite surveys can offer extensive topography and elevation information of the study area, and *in-situ* detection equipment like piezometers and strain gauges allow accurate analysis of internal pressures, these kind of empirical monitoring is often insufficient, expecially for preventive purposes [3, 4]. The great economic cost, as well as very limited practicality in carrying out real experiments, have made the development of numerical techniques capable of simulating landslide phenomena increasingly necessary. In this work we present a two dimensional time-adapted particle numerical method to modeling flow-like landslides, developing a semi-conservative variant of the Depth-Averaged Material Point Method (DAMPM) [5]. The mathematical model is given by the Shallow Waters equations, derived from depth-integrating the Navier-Stokes equations. Both bed friction and the rheology are considered in the presented framework, following the Voellmy model and the depth integrated Bingham visco-plastic stress model respectively [6, 7]. After verifying the performances of the numerical method through different benchmarks and idealized settings, it has been tested on a realistic scenario.

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A bulk-surface reaction-diffusion model for electrodeposition and novel numerical solvers

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We present a novel Bulk-Surface Reaction-Diffusion System (BSRDS) for the simulation of electrodeposition processes taking place in batteries, called BSDIB model. As the name suggests, the model is composed of two surface PDEs that model metal growth on the electrodes, coupled with two bulk PDEs that model concentrations in the electrolyte. The BSDIB model extends the so-called DIB model previously introduced in [1], where the bulk PDEs were not present and the electrolyte concentrations were assumed to be spatially uniform for simplicity. The novel BSDIB model instead accounts for the space-time dependence of the electrolyte concentrations in a more realistic fashion.

Novel numerical methods for BSRDS of our own, such as the Bulk-Surface Virtual Element Method (BSVEM) [2] and the Matrix-Oriented Finite Element Method (MOFEM) [3] are used to solve the BSDIB model. Our numerical simulations are backed up experimentally through lab tests.

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A machine learning approach that ensure local mass conservation for single-phase flow in fractured porous media

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Constructing fast solution schemes often involves deciding which errors are acceptable and which approximations can be made for the sake of computational efficiency. Herein, we consider a mixed formulation of Darcy flow and take the perspective that the physical law of mass conservation is significantly more important than the constitutive relationship, i.e. Darcy's law. Within this point of view, we propose a three-step solution technique that guarantees local mass conservation. In the first step, an initial flux field is obtained by using a locally conservative method, such as the TPFA Finite Volume Method. Although this scheme is computationally efficient, it lacks consistency and therefore requires a suitable correction. Since this correction is divergence-free, the Helmholtz decomposition ensures that it is given by the curl of a potential field. The second step therefore employs an H(curl)-conforming discretization to compute the correction potential and update the flux field. The pressure field is computed in the final step by using the same TPFA system from the first step.

The procedure guarantees local mass conservation regardless of the quality of the computed correction. Thus, we relax this computation using tools from reduced order modeling. We introduce a reduced basis method that is capable of rapidly producing a potential field for given permeability fields. By applying the curl to this field, we ensure that the correction is divergence-free and mass conservation is not impacted.

Finally, we extend the method to solving Darcy flow in fractured porous media. We rewrite the equations in terms of mixed-dimensional differential operators and identify the problem as a mixed-dimensional Darcy flow system. In turn, the proposed three-step solution procedure directly applies using the mixed-dimensional curl to ensure local mass conservation.

Modeling Water Stress in Root Water Uptake

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In this talk we will present a novel way to mathematically frame the concept of ecological memory of plant water stress in the context of root water uptake in unsaturated flow equations. We will discuss the results obtained in [1]; here, inspired by recent eco-hydrological papers, we modeled the water content dynamics in a soil plant system by Richards' equation with a non-local root water absorption term. In order to account for this memory term, an integral equation is defined, and sufficient conditions are provided for ensuring existence and uniqueness of its solution. We will also show numerical simulations in order to compare the solution to our non-local equation with the solution to classical models studied in the literature.

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Optimal irrigation strategies in a Richards' framework

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We introduce an optimal control approach to Richards' equations in an irrigation framework, aimed at minimizing water consumption while maximizing root water uptake. We first describe the physics of the nonlinear model under consideration, and then develop the first-order necessary optimality conditions of the associated boundary control problem. We show that our model provides a promising framework to support optimized irrigation strategies, thus facing water scarcity in irrigation. The characterization of the optimal control in terms of a suitable relation with the adjoint state of the optimality conditions is then used to develop numerical simulations on different hydrological settings, that supports the analytical findings of the paper.

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Analysing the role of soil and vegetation spatial variability in modelling hydrological processes for irrigation optimisation at large scale

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The main purpose of this study was to analyse the effect of spatial variability of soil hydraulic properties (HP) and vegetation parameters (VP) (e.g., leaf-area index, LAI, and crop coefficient, Kc) on modelling agro-hydrological processes and optimising irrigation volumes at large scale. Based on this analysis, the effect of partly overlooking the spatial variability of soil HP and/or VP inputs was verified on a 140-ha irrigation sector in "Sinistra Ofanto" irrigation system in Apulia Region, Southern Italy. Five soil profiles were excavated and the HP were measured in all the soil horizons. Additionally, measurements of soil HP were taken in the surface soil layer in ninety sites distributed over the whole irrigation sector. All the HP measurements were carried out by using tension infiltrometer. Remote sensing applications were used to obtain LAI and Kc using European Space Agency's (ESA) Sentinel-2 images with 10-meter resolutions. Firstly, distributed (on ninety polygons with an average area of about 1.5 ha) optimal irrigation volumes and related deep percolation volumes at a depth of 80 cm, were computed using the physically-based agro-hydrological model FLOWS and accounting for the actual observed variability of soil HP and VP inputs. The sector scale irrigation and deep percolation volumes were obtained by aggregating the distributed irrigation volumes. This was considered as the reference scenario (hereafter DVS – Detailed Variability Scenario). Then, reduced variability scenarios (hereafter RVS – Reduced Variability Scenario) were considered, where the information on the actual spatial variability of the soil HP and VP was gradually overlooked to find the minimum data set needed to still have sector scale irrigation volumes and related deep percolation volumes comparable to those obtained under the DVS. Results showed that overlooking VP (RVS-VP) variability did not significantly change the optimal irrigation volumes and the deep percolation fluxes. By contrast, neglecting the HP variability (RVS-HP) showed significant effects on both the irrigation and percolation volumes compared to the DVS. The main practical finding was that, at least for the area investigated in this study, hydraulic characterization of one soil profile in an area of approximately 30 ha provides sector scale irrigation volumes and percolation fluxes comparable to those obtained under the DVS, thus by accounting for all the observed local variability.

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HIgh order Projection-based HOMogenisation for advection diffusion reaction problems

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We propose a new method to reduce the complexity of multiscale scalar transport problems with a dominant axial dynamic. Our approach combines the Hierarchical Model (HiMod) reduction and a two-scale asymptotic homogenisation technique. First, we extend the two-scale asymptotic expansion to any desired order. Then, we utilise high-order correctors to define the HiMod modal basis, which approximates the transverse dynamics of the flow. We use finite element discretisation to model the leading stream. We name this method HiPhomϵ (High-order Projection-based Homogenisation). We have successfully tested HiPhomϵ on both steady and unsteady advection-diffusion-reaction scenarios. The numerical results demonstrate that HiPhomϵ outperforms HiMod in terms of accuracy and convergence rate. Additionally, it extends the reliability of standard homogenised solutions to transient and pre-asymptotic regimes. This method has applications in various fields such as hydraulics, and haemodynamic. A reformulation of the method to derive closed high-order homogenised models for general porous media applications will be also discussed.

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Uncertainty quantification in coastal aquifers using the multilevel Monte Carlo method

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We consider the problem of salinisation of coastal aquifers. In particular, the Henry saltwater intrusion problem with uncertain porosity, permeability and recharge parameters is used as a test case. This problem is non-linear and time-dependent. The solution is the salt mass fraction, which is uncertain and changes with time. Uncertainties in porosity, permeability, recharge and mass fraction are modelled using random fields. This work investigates the applicability of the well-known multilevel Monte Carlo (MLMC) method to such problems. The MLMC method can reduce the overall computational and storage costs. In addition, the MLMC method runs multiple scenarios on different spatial and temporal grids and then estimates the mean value of the mass fraction. The parallelization is performed in both physical and stochastic space. To solve each deterministic scenario, we run the parallel multigrid solver ug4 in a black-box fashion.

An accurate estimation of the output uncertainties can facilitate a better understanding of the problem, better decisions, and improved control and design of the experiment. The following questions can be answered:

1. How long can a particular drinking water source be used (i.e. when does the mass fraction of salt exceed a critical threshold)?
2. Which regions have particularly high uncertainty?
3. What is the probability that the salt concentration will exceed a threshold value at a given place and time?
4. What is the average scenario (and its variations)?
5. What are the extreme scenarios?
6. How do the uncertainties change with time?

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Conceptual Models of Flow and Transport in Fracture-Dominated Aquifers

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Flow and transport mathematical models in fracture-dominated aquifers are characterized by impermeable rock matrix and should consider the simultaneous occurrence of laminar, non-laminar, and turbulent fluxes in the fractures rather than the laminar flow by the cubic law that has been widely applied in the scientific literature. Some simulations show overestimations up to 75Model simulations in these aquifers typically present uncertainties owing to the impossibility of determining the exact input data, such as fractures' spatial positions, orientation and deep angles, lengths, apertures, and fracture densities and intersections. Available data from field reliefs of outcrops or tunnel advancement fronts represent only a fraction of the fracture network properties of an entire geological rock formation of aquifer. Furthermore, the heterogeneities related to the spatial variation of the fracture network properties cannot be "averaged" using equivalent porous models or random analytical solutions. Among numerous existing conceptual models of a fracture-dominated aquifer, the possible simplest conceptualizations in layered fractured models, tube models and backbones of three-dimensional fracture networks, have been presented. Then we show the mathematical model equations to approximate the pollutant and pathogen flow and transport affected by fast and slow flow pathways in fracture-dominated aquifers.

A space-time discontinuous Galerkin method for wave propagation problems in coupled poroelastic-elastic domains

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We present a space-time finite element discontinuous Galerkin method on polytopal meshes (XT-PolydG) for the numerical discretization of wave propagation in coupled poroelastic-elastic media. We consider the low-frequency Biot's equations in the poroelastic medium and the elastodynamics equation for the elastic one. To realize the coupling, suitable transmission conditions on the interface between the two domains are (weakly) embedded in the formulation. The proposed PolydG discretization in space is then coupled with a dG time integration scheme, resulting in a full space-time dG discretization. We present the stability analysis for both the continuous and the semidiscrete formulations, and we derive error estimates for the semidiscrete formulation in a suitable energy norm. The method is applied to a wide set of numerical test cases to verify the theoretical bounds. Examples of physical interest are also presented to investigate the capability of the proposed method in relevant geophysical scenarios.

Problem oriented discretizations for a vegetation model

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The use of functional equations represents the most common strategy for modeling real phenomena. In particular, we are interested in the numerical solution of models of Partial Differential Equations (PDEs) coming from applications in real contexts, such as corrosion [3, 7], sustainability [8], vegetation [6]. The numerical treatment of these problems is not trivial, since they are often characterized by high stiffness, which requires the use of very dense spatial and temporal discretizations. This obviously leads to unacceptable computing times. Furthermore, a numerical method is not always able to exploit a-priori known properties of the problem, such as any positivity or oscillating trend of the solution, the asymptotic stability, and so on.

In this talk, we focus on a reaction-diffusion vegetation model that has been introduced to investigate the coexistence of two different plant species in arid environments, characterized by scarce presence of water [6]. The considered system of PDEs is an extension of the well-known Klausmeier model. The latter investigates the growth of a single type of plant with varying water availability. The first, on the other hand, constitutes a generalization of the Klausmeier model, as it considers the competition of two different species of plants, which must somehow try to survive by sharing the same limiting resource.

The model under investigation has high stiffness, and is characterized by positivity and oscillating behavior in space. We therefore show numerical techniques capable of dealing with the stiffness of the problem, and also of preserving the a-priori known properties of the exact solution for each choice of the spatial and temporal discretization steps [4]. In particular, to preserve positivity, we extend non-standard finite differences using exponential integrators and TASE operators, which have been recently introduced to stabilize explicit Runge-Kutta methods [1]. This also helps to deal with the stiffness of the problem. Furthermore, to preserve the spatial oscillations of the solution, we integrate the exponential fitting framework within the non-standard discretizations. To further improve the efficiency of the proposed approaches, we show the use of adapted parallel peer methods for the considered vegetation problem [2, 5]. Finally, numerical tests are shown to confirm the effectiveness of the proposed techniques.

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A Spectral Method for a Nonlocal Richards' Equation

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We present a nonlocal, derivative free model for transient flow in unsaturated, heterogeneous, and anisotropic soils based on the peridynamic formulation of continuum mechanics. In the proposed model, we consider a Chebyshev collocation method based on the implementation of the Fast Fourier Transform (FFT) algorithm to approximate numerically the solution of the model. We show the convergence of the method and present several simulations to study the properties of the solutions.

Non-standard models for flow in porous media

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Mathematical models that are commonly used for porous media flows assume that quantities like saturation, phase pressure differences, or relative permeability are related by monotone, algebraic relationships. Under such assumptions, the solutions of the resulting mathematical models satisfy the maximum principle. On the other hand, phenomena like saturation overshoot, or the formation of finger profiles have been observed in experiments. Such results are ruled out by standard models. Moreover, the relationships determined experimentally for the same type of medium differ, depending on the context (e.g. drainage or imbibition) or the dynamics of the flow.

This motivated the development of non-standard models, where dynamic or hysteretic effects are included in the above-mentioned relationships. The resulting models are nonlinear evolution systems of (pseudo-)parabolic and possibly degenerate equations, involving differential inclusions. Here we present briefly aspects related to the existence and uniqueness of weak solutions to such models. We then discuss different numerical schemes, including aspects like the rigorous convergence of the discretization, domain decomposition, and solving the emerging nonlinear time-discrete or fully discrete problems.

This is joint work with X. Cao (Toronto), C.J. van Duijn (Eindhoven), S. Karpinski (Munich), S. Lunowa (Hasselt), K. Mitra (Paris), F.A. Radu (Bergen)

Moisture fluctuations in soil biogeochemical cycles: from the emblematic case of iron-redox cycles to current challenges

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Infiltration of unpredictable rainfall inputs determine complex space time variability in soils, which in turn drives pulsing dynamics of biogeochemical processes and ultimately controls plant productivity and ecosystem carbon storage. After briefly discussing the moisture controls on the variety of soil biogeochemical processes going from aerobic to anaerobic conditions, we focus on the emblematic case of iron-redox 'cycles', whereby the alternation of dry and wet conditions promotes the cycling between ferrous oxide reduction during oxic conditions and the biologically mediated ferric oxidation in anoxic conditions. The statistical analysis of soil moisture level crossing, coupled to simplified dynamical system analysis of biogeochemical cycling, unveils the presence of optimal ecohydrologic conditions leading to maximal rates of iron redox cycling, with implication for plant growth and organic matter decomposition. We close by highlighting some important challenges and open questions, especially in relation to the random spatial variability of such processes, which are important for their upscaling.

Efficient solvers for Richards' equation

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Richards' equation is modelling flow in variably saturated porous media. It is a highly nonlinear, degenerate elliptic-parabolic equation, which is known to be very challenging to solve. In this talk we discuss different solution strategies for Richards' equation, with the main focus on linearization methods. The Newton method and the L-scheme (a stabilized Picard method) will be considered, as well as a combination of the two. The combined scheme, which is both robust and efficient, is based on an adaptive switching between the two linearization methods. The theoretical properties of the scheme will be discussed. Illustrative numerical examples will be shown.

Nanoscale investigation and Stochastic assessment of calcite dissolution

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We investigate the main traits of the spatial heterogeneity of dissolution rates that are directly observed through Atomic Force Microscopy on the surface of a millimeter-scale calcite sample in contact with deionized water. Our analyses are framed within a stochastic approach and are motivated from the observation that detailed characterizations of mineral dissolution/precipitation rates is critical in the context of a variety of applications including, e.g., aquifer contamination assessment, geologic carbon sequestration, or hydraulic fracturing of hydrocarbon reservoirs. Experimental evidences based on Atomic Force Microscopy (AFM) enable direct observations of the mechanisms taking place across the mineral surface during the reaction and constitute a key information basis for interpretive modeling efforts. In this context, the dissolution process is evidenced to be strongly affected by several sources of variability at the local (i.e., micro-scale) mineral-fluid interface and a marked spatial heterogeneity in the dissolution rate is documented. In this general framework, we collect datasets of surface topography at several observation times from which reaction rate maps are evaluated. The study is aimed at (1) characterizing the statistical behavior of dissolution rates and their spatial increments within a unique and consistent theoretical framework; (2) identifying an appropriate interpretive model for such statistics; and (3) evaluating quantitatively, through observed trends of model parameters, the temporal evolution of the spatial heterogeneity of the dissolution reaction.

Flow and transport in a doublet-type flow configuration

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Transport takes place between an injecting well and a pumping one through to a porous formation. The controlling parameter is the conductivity which, unlike the classical approach, here is regarded, in line with field findings, as spatially variable. This renders the problem at stake extremely difficult to solve. However, a simple solution is achieved by adopting a few simplifying assumptions, which nevertheless resemble most of the existing aquifers, and therefore it is applicable to numerous real world situations. It is shown that the proposed solution finds application in the identification of the aquifer's parameters as well as the quantification of efficiency of decontamination procedures. Finally, the theoretical framework is applied to a couple of transport experiments, in order to illustrate (and to quantify) how dispersion process develops in the zone delimited by the two wells.

A virtual element scheme for the Brinkman model of porous media flow

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In this talk we develop a C^1-conforming virtual element method to solve the Brinkman equations in stream-function formulation. We establish optimal a priori error estimates for the stream-function and we present some numerical experiments supporting our theoretical results on different families of polygonal meshes.

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ModelFreeFFC: A Versatile Tool for Fitting NMRRelaxation Dispersion Curves in Porous Media andMolecular Dynamics Studies

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In this contribution, we introduce the *ModelFreeFFC* tool, a software developed at the University of Bologna (Bologna, Italy) for fitting Nuclear Magnetic Relaxation Dispersion curves obtained from Fast Field Cycling (FFC) Nuclear Magnetic Resonance (NMR) Relaxometry measurements. FFC-NMR relaxometry is a non-destructive technique to investigate molecular dynamics [1]. It has emerged as a crucial tool for analyzing porous media structures and their interactions with hydrogenous fluids in various contexts, including biological systems and hydrocarbon-bearing sedimentary rocks [2].

The ModelFreeFFC tool employs a regularized inversion algorithm grounded in the Model Free approach [3], modelling the parameters identification problem as a constrained L_1-regularized non-linear least squares problem. Following the strategy proposed in [3], the non-linear least squares term enforces data consistency by decomposing the acquired relaxation profiles into relaxation contributions related to $^1H - {}^1H$ and $^1H - {}^{14}N$ dipole-dipole interactions. The data fitting and L_1-based regularization terms are balanced using the regularization parameter [4]. The software is equipped with a graphical user interface (GUI) for Windows and Linux operating systems and is available at https://site.unibo.it/softwaredicam/en/modelfree. This contribution aims to showcase the ModelFreeFFC tool and the underlying mathematical modeland present some results from porous media measurements.

Figure 1 illustrates the two main components of the ModelFreeFFC GUI: the data input and inversion parameters are displayed in the left window, while the output quantities and plots are presented on the right.

Figure 1: ModelFreeFFC tool GUI.

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Wetlands deserve specific modelling tools for the effective management of their ecosystem services

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Wetlands, once regarded as unhealthy environments and often reclaimed for dry land, have gained global recognition for their crucial role in climate change adaptation and their provision of multiple ecosystem services (ES) such as groundwater recharge, flood mitigation, biodiversity enhancement, nutrient recovery, and water reclamation [1]. To effectively manage natural and constructed wetlands within local hydrological contexts, where water resources are shared among various users and treated wastewater is discharged, the integration of modeling tools for water management is essential [2]. While well-established modeling tools exist for river and groundwater systems, the same cannot be said for wetland ecosystems [3].

This paper reviews the existing approaches found in the literature and presents a comprehensive conceptual framework for wetland management. Furthermore, this framework will be integrated into a system dynamics model for water management in wetland ecosystems aimed to optimize their ES [4]. The Doñana National Park (Spain) will be used as case study to develop and test the proposed model.

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