

Task 3.2

Title

Computational energy innovation

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Contact Simulations in Rough Fractures

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GPU-accelerated simulation of free jet deviation by rotating Pelton buckets for SmallFlex project

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Simulations of hydro-mechanical processes based on the Immersed Boundary Method

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Toward a Multifidelity method for estimating the influence of overpressure on induced seismicity

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High-performance C++ code for forecasting induced seismicity

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Adaptive Simulation Methods for Attenuation and Dispersion of Seismic Waves in fractured Media

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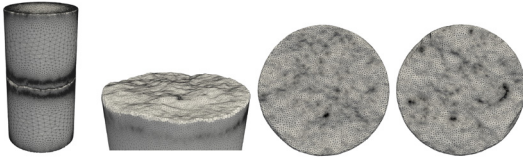
Towards Multiscale Numerical Simulations of Pelton Turbine Erosion

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Contact Simulations in Rough Fractures

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Introduction



The mechanical behavior of fractures in solids, such as rocks, has strong implications for reservoir engineering applications. Deformations, and the corresponding change in solid contact area and aperture field, impact rock fracture stiffness and permeability thus altering the reservoir properties significantly.

Simulation of contact between fractures is numerically difficult. The non-penetration constraints lead to a nonlinear problem and the surface meshes of the solid bodies on the opposing fracture sides may be non-matching. We use a parallel mortar method to resolve the contact conditions between the non-matching surfaces, a three dimensional finite element formulation of linear elasticity and linearized contact conditions.

Linear elasticity and contact

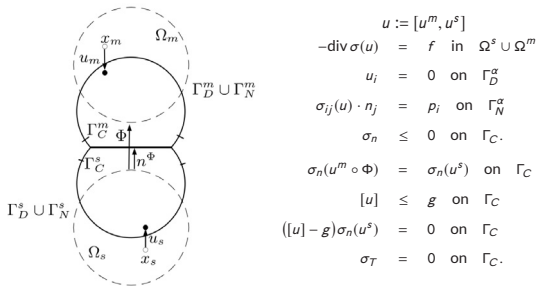


Figure: Left: Two-body contact problem. Right: Formulation of linear elasticity and frictionless contact with boundary conditions.

Mortar approach

We use a Mortar approach, in which the test space is dual to the trace space of the finite element space. The non-penetration condition is enforced in a weak sense. The resulting discretization error is local and can be reduced with local refinements.

$$\int_{\Gamma_C^s} ([u] - g)\lambda^t d\gamma \leq 0 \quad \forall \lambda^t \in L,$$

Eq: Weak non-penetration condition over the slave side of the boundary. The condition ensures that the overall jump $[u]$ of the displacements across the fracture is smaller than g , tested against a dual space L of the trace space at the slave boundary.

Enforcing the weak penetration is hard in practice. The nodes of the finite element discretization are non-matching and apart, and must be related to each other using a mortar projection. The parallel assembly of this operator has only become feasible recently with the introduction of the MOONolith library.

Implementation

We implemented the contact simulation using MOONolith, libMesh, PETSc and MOOSE. All components are open source and designed for parallel computing.

Numerical experiments

The simulations ran on 4 nodes (2 x Intel Xeon E5-2650 v3 @ 2.30GHz) with 10 CPU's each, on the cluster of the Institute of Computational Science in Lugano, Switzerland.

Validation

We first validated our method with a Hertzian contact experiment, after Hertz who derived analytical solutions for this problem class in 1881.

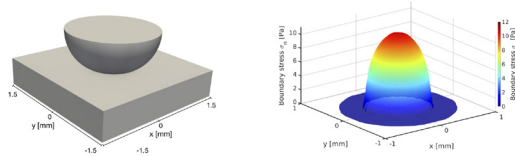


Figure: Hertzian contact; correct methods must replicate the parabolic shape of the boundary stresses σ_n as shown on the right.

Fracture closure

We meshed two rock bodies from granite specimens of the Grimsel test site in Switzerland and applied an increasing load on top of it up to 20MPa in direction of the z-axis. The aim here is to replicate the nonlinear closing behaviour of fractures and to see how our formulation gives insight to interior stresses and the change in aperture distributions.

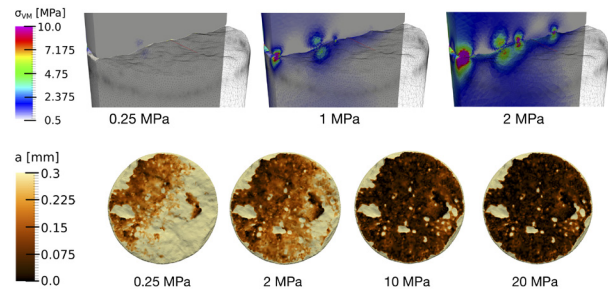


Figure: Top: Von Mises stresses developing inside the rock under increasing confining pressure. Bottom: Aperture fields under increasing normal stresses.

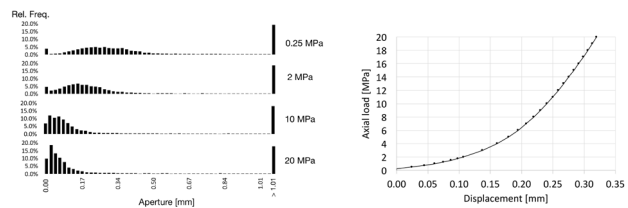


Figure: Left: distribution of aperture fields under increasing pressure. Right: nonlinear closing behavior of the fracture under increasing load.

Outlook

We have developed a parallel contact method using a mortar approach. We now have a tool to simulate contact in rough fractures, the results of which we can further use in Fluid simulations within fractures.

References

Planta, Vogler, Zulian, Saar, Krause, Solution of contact problems between rough body surfaces with non matching meshes using a parallel mortar method, 2018, submitted.

GPU-accelerated simulation of free jet deviation by rotating Pelton buckets for SmallFlex project

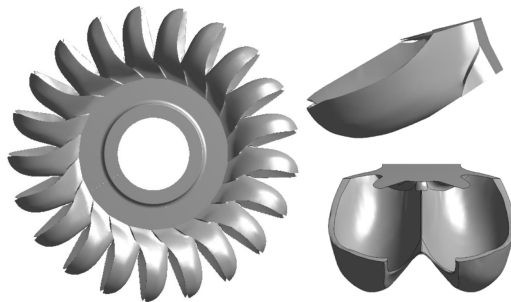
S Alimirzazadeh, E Jahanbakhsh, A Maertens, S Leguizamón, T Kumashiro, K Tani, F Avellan

GPU-SPHEROS

GPU-SPHEROS is a GPU-accelerated particle-based versatile solver based on Arbitrary Lagrangian Eulerian (ALE) Finite Volume Particle Method (FVPM) which inherits desirable features of both Smoothed Particle Hydrodynamics (SPH) and mesh-based Finite Volume Method (FVM) and is able to simulate the interaction between fluid, solid and silt [1]. With GPU-SPHEROS, the goal is to perform industrial size setup simulations of hydraulic machines.

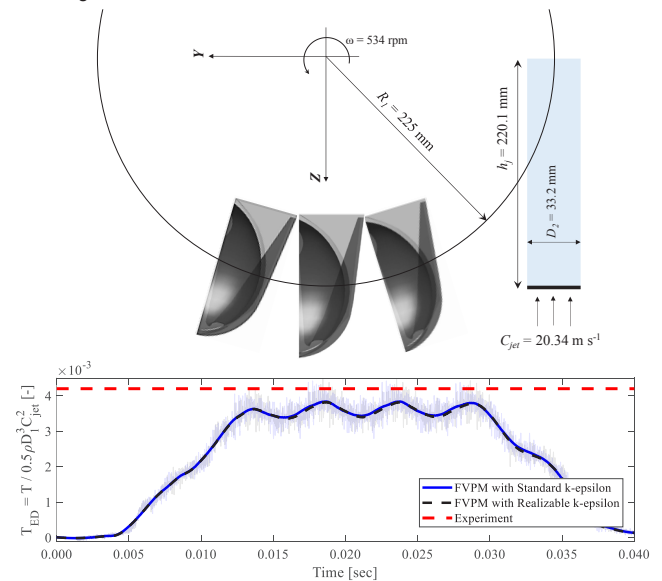
SmallFlex Project

Small hydropower plants are expected to produce a large share energy by 2050. The SmallFlex project is **demonstrator for flexible Small Hydropower Plants** (SHPs) and aimed to investigate the eco-compatible winter peak energy production by them. SmallFlex has been integrated in the activities of the SCCER-SoE [2]. A Pelton turbine is being simulated in different operating points with our in-house GPU-accelerated software, GPU-SPHEROS to predict the Pelton efficiency, torque and powerplant flexibility. Here is the geometry:



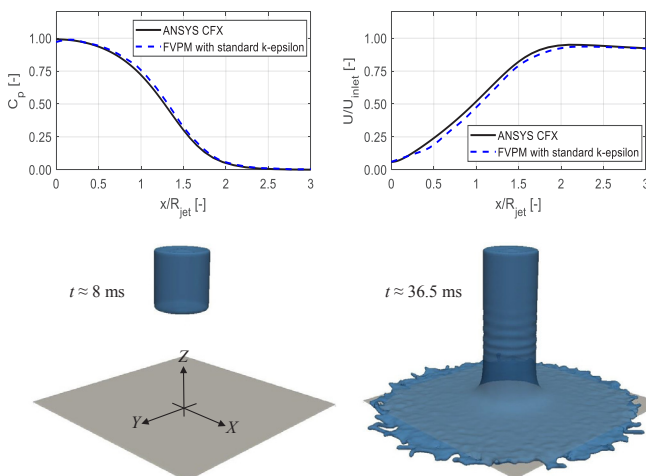
Validation for rotating Pelton turbine

- The torque generated by rotating Pelton turbine bucket has been validated by the torque measurements for a Pelton geometry with available experimental data.
- Two-equation Boussinesq-based RANS turbulence models have been integrated with FVPM as an ALE method.



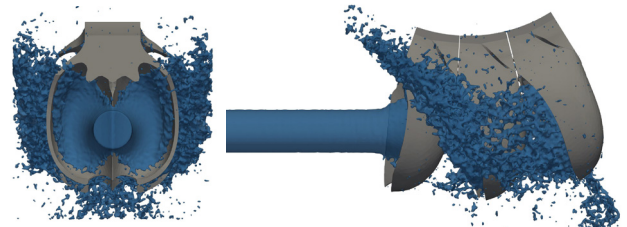
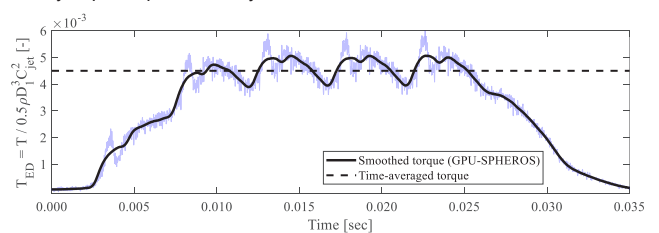
Validation for turbulent impinging jet on a flat plate

- Turbulent fluid jet impinging on a flat plate (a similar case to a jet deviation by rotating Pelton turbine buckets) has been simulated as a validation test case ($C_{jet} = 19 \text{ m}\cdot\text{s}^{-1}$ and jet inlet is located at $Z_{jet} = 4x_{D_{jet}}$ while plate is located at $X-Y$ plan).
- Both the pressure and velocity are in a good agreement with ANSYS-CFX finite volume/element solver results.
- The software has been then used to simulate of free jet deviation by SmallFlex rotating Pelton buckets.



SmallFlex Pelton turbine

- A Pelton turbine has been simulated for its best efficiency point (BEP) with GPU-SPHEROS and the torque has been predicted.
- Off-design conditions are being simulated to evaluate turbine efficiency and hydropower plant flexibility.



References

S Alimirzazadeh, E Jahanbakhsh, A Maertens, S Leguizamón, F Avellan, GPU-Accelerated 3-D finite volume particle method, *Computers & Fluids*. 171 (2018) 79–93
C Münch, P Manso, C Weber, M Staehli, M Schmid, C Nicolet, F Avellan, A Schleiss, J Derivaz, SmallFlex: Demonstrator for flexible Small Hydropower Plant, SCCER-SoE Annual Conference 2017

Simulations of hydro-mechanical processes based on the Immersed Boundary Method

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Motivation

Hydro-mechanical (HM) processes in rough fractures are highly **nonlinear** and govern productivity or associated risks in a wide range of reservoir engineering problems.

To enable high-resolution simulations of HM processes in fractures, we present an **immersed boundary method** to compute the fluid flow between rough fracture surfaces and adopt a **variational parallel transfer operator** to couple the fluid and the solid subproblem.

We simulate both the incompressible **fluid flow** and the **solid structure** in a Finite Element framework. The structural fractures are modelled as a **linear elastic material** by using **unstructured meshes** embedded into **structured fluid grids**.

The **fluid and the solid solvers are coupled by transferring fluid velocities, pressure field and surface forces** between the structured and the unstructured meshes by means of variational transfer operators.

Fictitious Domain Method

- The **solid phase** is embedded in the **Fluid phase**
- **Eulerian Formulation** (Fixed Grid) for the fluid flow
- **Lagrangian Formulation** for the solid structure

Find $(u_f, p_f; \eta_s, p_s; \lambda) \subset (V_f \times Q_f \times V_s \times Q_s \times L)$ such that

$$\int_{\Omega_f} \rho_f \frac{\partial u_f}{\partial t} \cdot v_f dV + \int_{\Omega_f} \rho_f [(u_f \cdot \nabla) u_f] \cdot v_f dV + \int_{\Omega_f} \sigma_f \cdot v_f dV - \int_{\mathcal{I}} \lambda \cdot v_f dV = 0$$

$$\int_{\Omega_f} q_f \nabla \cdot u_f dV = 0$$

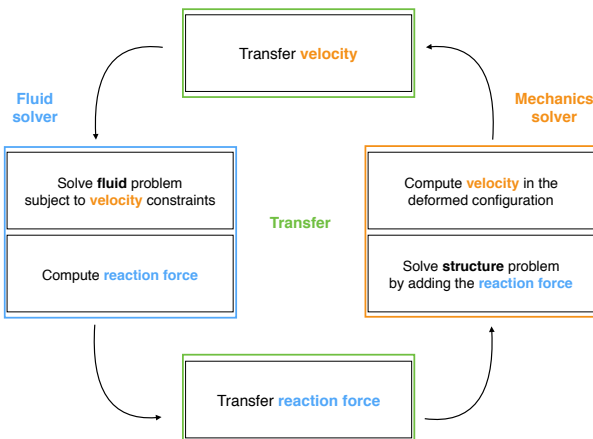
Transfer $\rightarrow \int_{\mathcal{I}} \mu \cdot \left(\frac{\partial \eta_s}{\partial t} - u_f \right) dV = 0$

$$\int_{\Omega_s} \hat{\rho}_s \frac{\partial^2 \hat{\eta}_s}{\partial t^2} \cdot \hat{v}_s + \int_{\Omega_s} \hat{P}(\hat{F}) : \nabla \hat{v}_s dV - \int_{\Omega_s} \hat{p}_s \hat{J} \hat{F}^{-T} : \nabla \hat{v}_s dV + \int_{\mathcal{I}} \lambda \cdot \hat{v}_s dV = 0$$

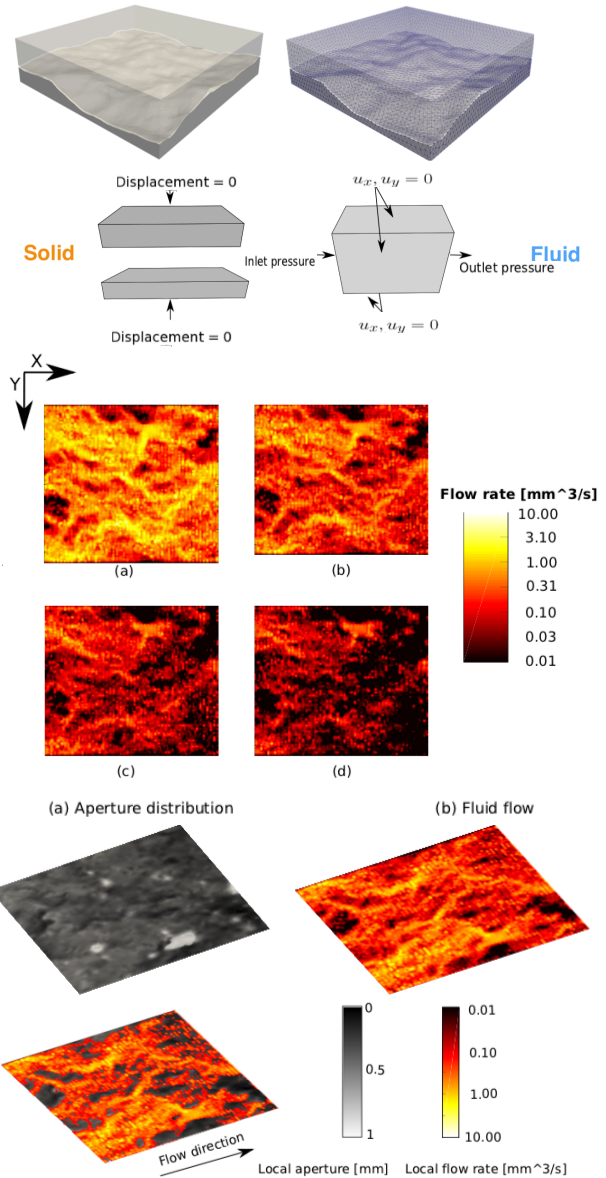
$$\int_{\Omega_s} (\hat{J} - 1) q_s dV = 0$$

for all $(v_f, q_f; v_s, q_s; \mu) \subset (V_f \times Q_f \times V_s \times Q_s \times L)$, where $\mathcal{I} = \Omega_s \cap \Omega_f$

Fixed point iteration



Results



Discussion

The numerical experiments with real fracture geometries show that the approach is able to resolve the boundary of the rough fracture surface into the fluid and also to simulate the change of the fluid flow paths within the fractures under increasing normal loads.

References

An immersed boundary method based on the L2-projection approach. Maria Giuseppina Chiara Nestola, Barna Becsek, Hadi Zolfaghari, Patrick Zulian, Dominik Obrist, and Rolf Krause. Proceedings of the 24th International Conference on Domain Decomposition Methods, 2018.

A Parallel Approach to the Variational Transfer of Discrete Fields between Arbitrarily Distributed Unstructured Finite Element Meshes. Rolf Krause and Patrick Zulian. SIAM Journal on Scientific Computing, 2016.

Toward a Multifidelity Method for Estimating the Influence of Overpressure on Induced Seismicity

Alessio Quaglini, Marco Favino, Dimitrios Karvounis, Claudio Tomasi, Stefan Wiemer, Thomas Driesner, Rolf Krause

Motivation: the FASTER project

Induced seismicity hazard from Enhanced Geothermal Systems (EGS) needs to be reliably forecasted. The Swiss Seismological Service (SED) has developed a hybrid 3D-2D model that forecasts induced seismicity in EGS. The fracture distribution in the subsurface is only known in a stochastic sense, hence to evaluate the seismic hazard, in terms of the seismic events number and magnitude, several fracture distributions have to be simulated with a Monte Carlo approach. While fast solution methods are necessary to solve each single sample, Multifidelity and Multilevel Monte Carlo methods are necessary for accelerating the convergence of the expectation of the number of seismic events. The idea behind these methods is to employ surrogate models which are computationally cheaper but also well-correlated with the detailed one. The project FASTER arises from a strong collaboration between SED, ETH Zurich, USI-Lugano, and the Swiss National Supercomputing Center (CSCS), in order to improve the simulated model, the solution algorithms, and their software implementation.

Models and Methods

Balance of mass leads to a set of diffusion equations

$$c \frac{\partial p}{\partial t} = \nabla \cdot K \nabla p + q \quad \text{background}$$

$$c \frac{\partial p_i}{\partial t} = \nabla \cdot K_i \nabla p_i + q_i, \quad i \in A \quad \text{Triggered fractures}$$

$$q = \sum q_i$$

Diffusion equation in a fracture is solved only when the fracture has been triggered: pressure in its hypocenter exceeds a "sliding condition".

- Discretization is based on
- finite volume method;
 - semi-implicit Euler schemes.

UQ problem

Interested in **number of seismic events** and **maximum magnitude**

Example 3D:

- Monte Carlo with 250 samples
- In particular, magnitude > 3.5
- 75 simulations out of 250 (30%)
- With ~250 samples, RMSE is 1% of the mean

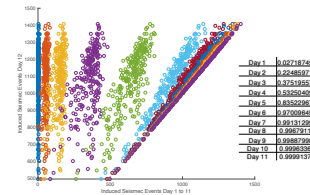
Can we reach the same accuracy with less effort?

Multifidelity Monte Carlo

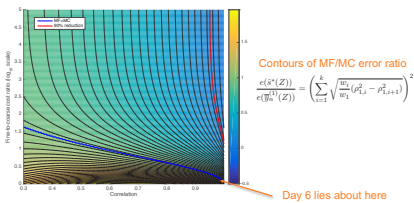
	Single-fidelity	Multi-fidelity [Peherstorfer15]
(Co)Variance	$\sigma_z^2 = \text{Var}[f^{(1)}(Z)]$	$\rho_{i,j} = \frac{\text{Cov}[f^{(i)}(Z), f^{(j)}(Z)]}{\sigma_i \sigma_j}$
Estimator	$\bar{y}_m^{(1)} = \frac{1}{m} \sum_{j=1}^m f^{(1)}(z_j)$	$\hat{s} = \frac{1}{m_1} + \sum_{i=2}^k \alpha_i \left(\frac{1}{m_i} - \frac{1}{m_{i-1}} \right)$
Cost	$c(\bar{y}_m^{(1)}(Z)) = w_1 m$	$c(\hat{s}(Z)) = \sum_{i=1}^k w_i m_i = w^T m$
MSE	$e(\bar{y}_m^{(1)}(Z)) = \frac{\sigma_z^2}{m}$	$\frac{\sigma_z^2}{m_1} + \sum_{i=2}^k \left(\frac{1}{m_{i-1}} - \frac{1}{m_i} \right) (\alpha_i^2 \sigma_i^2 - 2\alpha_i \rho_{i,i-1} \sigma_i \sigma_{i-1})$
Optimal allocation of budget p	$m = p/w_1$	Minimize MSE w.r.t. m and α at fixed cost p

Surrogate models

1) Shorter final time



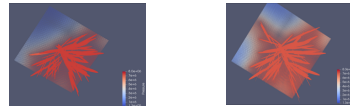
Despite the good correlation, the error is **higher** than standard MC



2) Space-time coarsening

Correlation between high- and all low-fidelity models

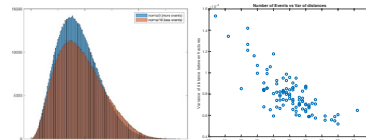
- $\rho_{12} = 0.8654$ (1 level of coarsening) – cost 1/4
- $\rho_{13} = 0.8433$ (2 levels of coarsening) – cost 1/16
- $\rho_{14} = 0.7496$ (3 levels of coarsening) – cost 1/64



3) 0D model

correlation between distances of hypocenters and seismic events

- $\rho_{15} = 0.7574$ (0D model) – cost negligible



Best combination of 2 models

- High-fidelity + 0D = error reduced to 43%

Best combination of 3 models

- High-fidelity + 2 levels of coarsening + 0D = error to 40%

Conclusions

- more statistical analysis on the fracture networks may lead to better surrogates
- extension to 3d is under development
- better solver to achieved desired mesh resolution

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High-performance C++ code for forecasting induced seismicity

Dimitrios Karvounis, Marco Favino, Patrick Zulian, Andreas Fink, Nur A. Fadel, Stefan Wiemer, Rolf Krause, Thomas Driesner

FASTER project

For the safe implementation of the Energy Strategy 2050, induced seismicity hazard from Enhanced Geothermal Systems (EGS) needs to be reliably forecasted and the electricity produced needs to be maximized for the affordable hazard. To this end, the Swiss Seismological Service (SED) has developed a 3D hybrid model, which consists of a stochastic and a deterministic part, and forecasts both induced seismicity and produced electricity in EGS. Main aim of the FASTER project is these forecasts to be concluded in almost real time. The project started approximately one year ago, it will last three years, it is funded by the Platform for Scientific Computing (PASC), and it brings together researchers from ETH Zurich, SED, USI university, and the Swiss National Supercomputing Center (CSCS). A speedup of approximately 670 times has been achieved up to now from optimizing the coding and employing more efficient algorithms.

Forecasting induced seismicity with the 3D hybrid model

The hybrid model consists of HFR-Sim and of the so-called "Seed model". HFR-Sim is the in-house EGS simulator of ETH Zurich that can deterministically model flow and heat transport in a fractured reservoir. The "Seed model" is a stochastic modelling approach for seismicity, where a large number of fractures and of potential seismic events along these fractures is sampled for each simulation of the MC integration, and the pore-pressure value that triggers each of the events is computed ("Seed setup"). At each time step of the hybrid simulation are called:

1. The Solver: HFR-Sim approximates the solution of pore-pressure diffusion inside the fractures, the well and the matrix surrounding the fractures. Necessary input the considered injection strategy.
2. Seed Update: The stochastic model locates the seeds triggered with the current deterministic solution and updates the HFR-Sim model accordingly.

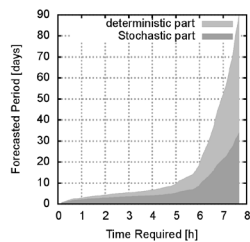
Final outputs of the hybrid model are a synthetic catalogue of induced seismicity, as well as a network of discrete fractures. With the latter as necessary input, the expected power generated due to the considered injection strategy can be estimated and the stimulation of an EGS can be optimized.

Accelerating the stochastic part

Significant speedup, which reaches up to two orders of magnitude, is achieved by pre-processing the sampled Seeds during their setup and not repeating time-costly searches over the set of all seeds for each new time step. During setup, the sampled seeds are divided into subsets according to their location. The subsets, where induced seismicity is possible, are located at each time step, and only the seeds of these subsets are updated. Triggered seeds are collected and are sorted by the order with which they were sampled, before the HFR-Sim model is updated. The latter sorting is necessary only for comparing the new optimized code with its initial version; i.e. the sorting ensures identical outputs between the two codes.

Further acceleration has been achieved by:

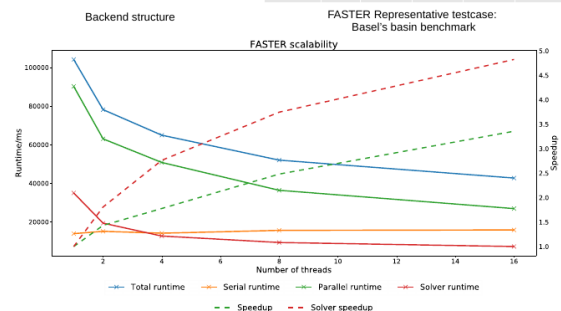
1. coupling the code with the Eigen library.
2. Employing features introduced with c++11 (e.g. enumerators)
3. Resolving computational bottlenecks during the updating of the HFR-Sim mesh.
4. Employing the Counter-Based Random123 Number Generators, instead of the sprng library.



preFASTER representative testcase: Basel's basin benchmark

Accelerating the deterministic part

	Serial	2 Threads	8 Threads	16 Threads	Original
Total (s)	104	78	52	43	29112 (8h)
Solver	55	34	20	16	15762 (>4h)
Seed Setup	7	8	8	8	51
Seed Update	35	29	17	10	12725 (3.5h)
Output	4	4	4	4	10
Speedup	1x	1.33x	2.00x	2.41x	670x

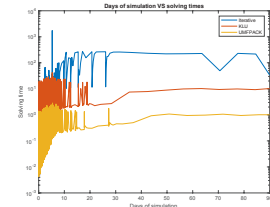


Comparison of performance of solution methods

Due to the structure of the stiffness matrices, naïve application of efficient solution methods, such as algebraic multigrid (AMG), is not trivial. While good convergence rates of AMG have been obtained in the early times of simulation, performances degraded when fractures were added, resulting in a total solution time of more than 4 hours.

- Given the relative small size of the linear system, direct solution methods have also been tested, in particular:
- KLU (direct solver of Trilinos) and
 - UMFPACK, which implements an Unsymmetric MultiFrontal method.

The first one allowed to reduce the solution time to approx. 2 hours, while the latter to 8.8 minutes.



	ML	KLU	UMFPACK
Mean solving time per time step	24.44 s	7.84 s	0.71 s
Total time for numerical solving	4.3 h	1.63 h	8.84 m (530.6 s)
Mean residual per time step	5.4207e-05	1.7455e-10	6.2338e-10

Discussion

FASTER is about to complete its first year and almost three orders of magnitude speedup is achieved in forecasting induced seismicity. Current run times allow the integration of the software in the Adaptive Traffic Light System (ATLS) of SED, where ATLS plans to assist in real time the operators of EGS to safely achieve the targets of Energy 2050. Due to the improved runtime, finer scenarios can be studied and fundamental research on induced seismicity can be performed at length scales that were previously prohibitive.

Possible next steps in this agile project include accelerating the convergence of the non-symmetric linear system solvers, improving accuracy with adaptive mesh refinement approaches, employing Multi Level Monte Carlo approaches for uncertainty quantification, the Phase Field Method for modeling microseismicity, and validating the analytical model of the code with real experimental data.

Adaptive Simulation Methods for Attenuation and Dispersion of Seismic Waves in fractured Media

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Motivation

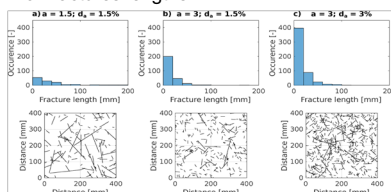
Numerical simulations of seismic waves in fractured rocks can result in significant advances for the indirect characterization of such environments. In fact, attenuation and modulus dispersion are due to fluid flow induced by pressure differences between regions of different compressibilities. Understanding these mechanisms in fractured rocks may provide information not only on fracture density but also on fracture connectivity. The main bottlenecks for these kinds of simulations are:

- mesh generation: the creation of computational grids which resolve numerous and complex interfaces still remains a tedious and time-consuming task, which requires a highly degree of human interaction.
- solution of the Finite Element (FE) system due to its complicated structure, the large jumps in the material parameters, the complex nature of the variables in the frequency domain.

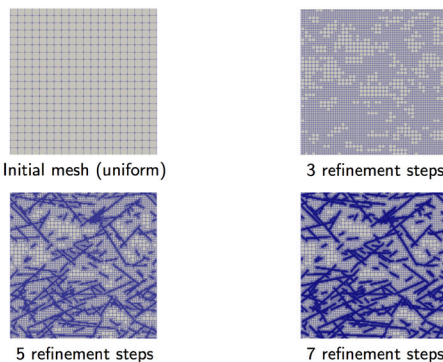
Methods

To enable a fast and easy meshing procedure of complex fracture networks, we developed a novel strategy based on adaptive mesh refinement (AMR) (Favino et al., 2018). The strategy has been implemented in MOOSE. In particular, the new app Parrot has been developed to simulate Biot's equations (Biot, 1941) in the time-frequency domain and to study attenuation and modulus dispersion of seismic waves caused by fluid pressure diffusion in heterogenous materials. MOOSE has also been extended in order to work with complex variables and hence to speed-up the solution process when parallel direct solvers are employed. The strategy comprises the following steps:

1. Generation of a natural fracture networks, e.g. using a power-law distribution for fractures lengths



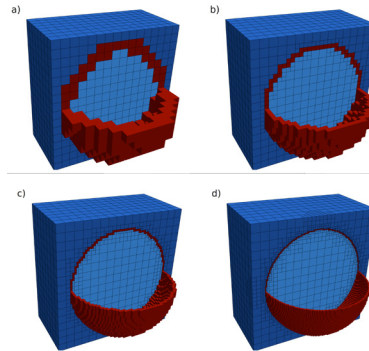
2. Adaptive mesh refinement (AMR) starting from a uniform coarse mesh



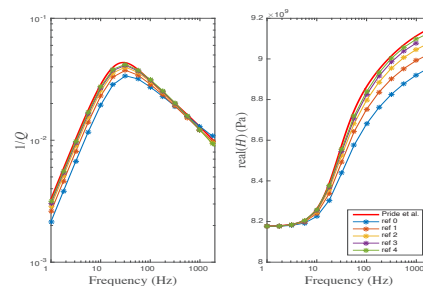
3. Solution of the linear system: the generated mesh is used to solve Biot's equations. The different levels can be employed in a multigrid solution process. The library MOONLith allows for the parallel transfer between arbitrarily distributed meshes.

Validation

To show the effectiveness of our approach, we consider the problem of a spherically shaped inclusion. For this problem, an analytical solution has been provided by Pride et al. (2004). Starting from a coarse mesh 16x16x16, we applied 6 AMR steps.



Convergence



Discussion

The AMR approach allowed to reproduce the predicted attenuation and dispersion curves with a moderate number of unknowns compared to a uniform refinement strategy (3M vs 135M). In particular, it confirmed the importance of refining meshes at the interfaces where numerical inaccuracies are concentrated. The discretization of Biot's equations with complex FE allowed to reduce the computational cost by a factor of 4 with respect to a real FE implementation, employing a parallel direct solver (MUMPS). The simulation time is about 3-4 minutes per simulated frequency.

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 Marco Favino, Jürg Hunziker, Eva Caspari, Beatriz Quintal, Klaus Holliger, Rolf Krause, Fully-Automated Adaptive Mesh Refinement for the Simulation of Fluid Pressure Diffusion in Strongly Heterogeneous Poroelastic Media, *Journal of Computational Physics* (2018, under review).
 Pride, Berriman, Harris, Seismic attenuation due to wave-induced flow, *Journal of Geophysical Research*, (2004), vol. 109.

Towards Multiscale Numerical Simulations of Pelton Turbine Erosion

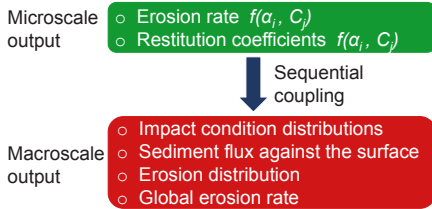
Sebastián Leguizamón, Ebrahim Jahanbakhsh, Audrey Maertens, Siamak Alimirzazadeh, François Avellan

Motivation and Problem Description

The hydro-abrasive erosion of turbomachines is a **significant problem** worldwide. In the context of the Energy Strategy 2050, it is a problem which will become **more severe in the future** due to the retreat of glaciers and permafrost caused by **climate change**. Our objective is to provide the **capability of simulating** the erosion process using the Finite Volume Particle Method [1]. Such simulations will become **advantageous** for the **design** and the **operation** of the machines. The erosion of hydraulic turbomachines is an **inherently multiscale process**, so its simulation is complicated. It demands a multiscale modeling approach.

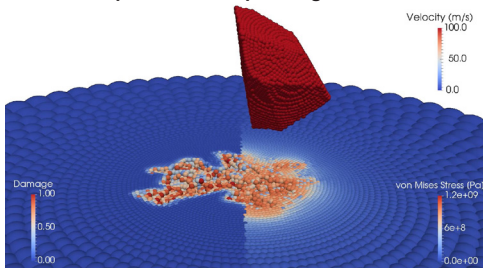
Multiscale Coupling and Validation

A multiscale model has been formulated and then validated [1]. It encompasses two submodels to tackle the multiscale character of the problem.



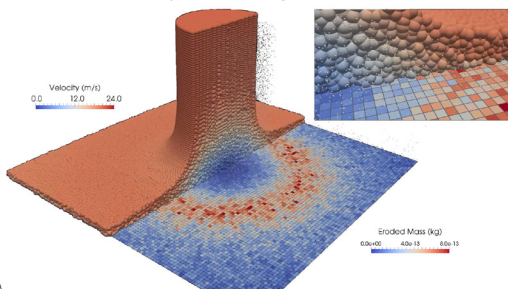
In the **Microscale Model** we perform detailed impact simulations that take into consideration all the important physical effects. This results in the **erosion rate** for each impact condition.

Sharp Sediment Impacts against Solid



In the **Macroscale Model** the turbulent sediment transport is computed. Each time a sediment impact is detected, the results of the microscale model are used, resulting in the macroscopic **erosion accumulation**.

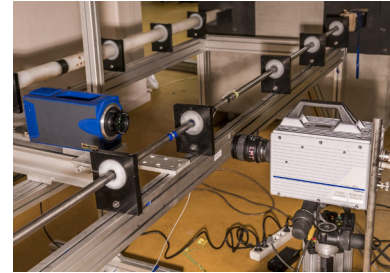
Slurry Jet Eroding a Flat Plate



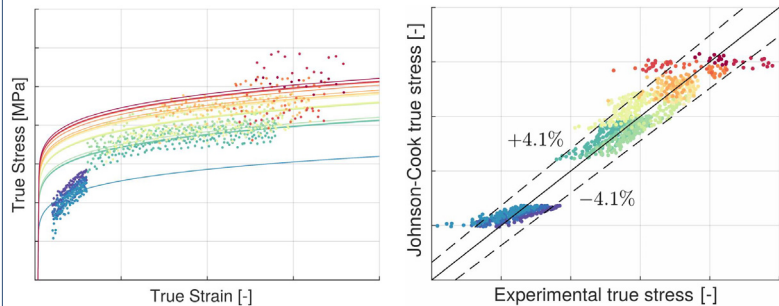
Material Characterization

To perform realistic multiscale simulations of the erosion of turbines it is necessary to perform a characterization of the material: **stainless steel 13Cr-4Ni**. A combination of quasi-static tension tests and split-Hopkinson tension bar tests is used to find the parameters of the **Johnson-Cook Model** that best describe the material behavior. A **genetic algorithm** was programmed to find the optimum set of model parameters that fit the experimental data obtained.

Split-Hopkinson Bar Experiment

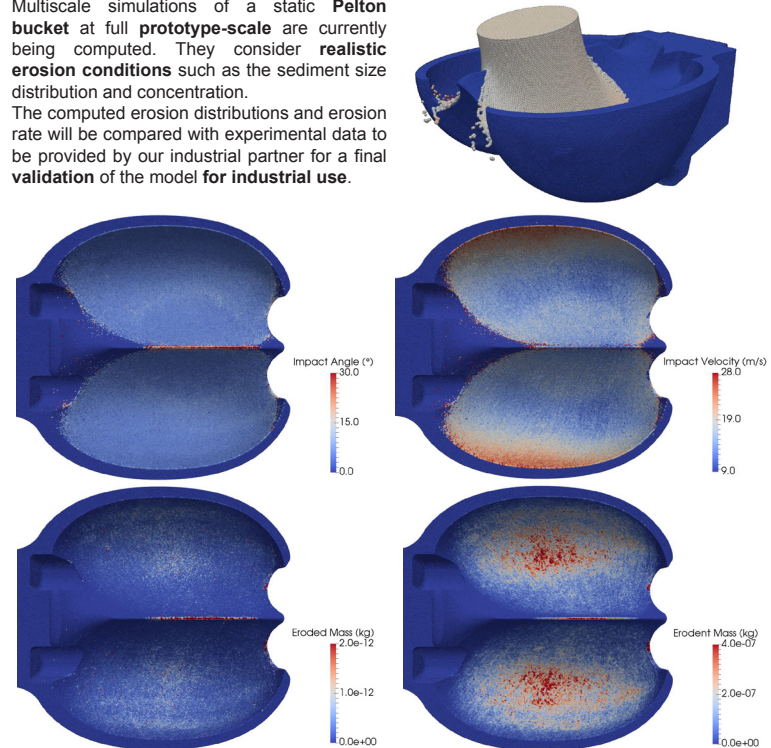


High Strain-Rate Material Response and Johnson-Cook Model Fit



Multiscale Erosion Simulation of a Pelton Bucket

Multiscale simulations of a static **Pelton bucket** at full **prototype-scale** are currently being computed. They consider **realistic erosion conditions** such as the sediment size distribution and concentration. The computed erosion distributions and erosion rate will be compared with experimental data to be provided by our industrial partner for a final **validation of the model for industrial use**.



References

[1] S. Leguizamón, E. Jahanbakhsh, A. Maertens, S. Alimirzazadeh and F. Avellan, A multiscale model for sediment impact erosion simulation using the finite volume particle method, *Wear* 392-393 (2017).