Task 4.3

Task Title

Modeling Facility: Mathematical Modeling and Numerical Simulation in Hydro- and Geo-Sciences

Research Partners

École polytechnique fédérale de Lausanne (EPFL), Swiss Federal Institute of Technology in Zurich (ETHZ), Lucerne University of Applied Sciences and Arts (HSLU), University of Lausanne, Goethe Center for Scientific Computing (G-CSC) of the Goethe University Frankfurt, Karlsruhe Institute of Technology (KIT), University of Siegen, University of Leeds, RWTH Aachen University

Current Projects (presented on the following pages)

Discretization and Multigrid Methods for Modeling permeability and stimulation for deep heat mining

C. v. Planta, R. Alessandro, T. Driesner, R. Krause

A new software for modeling seismic velocity dispersion and attenuation in realistically fractured media

M. Favino, J. Hunziker, E. Caspari, B. Quintal, K. Holliger, R. Krause

Task Objectives

- The modeling facility in Task 4.3 provides state of the art knowledge and techniques from numerical analysis, computational science, HPC, and scientific software engineering. In cooperation with partners from other tasks, the modeling facility aims at improving existing or providing new simulation tools for hydro and geo science, which combine robustness and efficiency with HPC capabilities.

Interaction Between the Partners – Synthesis

- Task 4.3 is interacting with the tasks of work package 1 and 3. Interaction in the different projects is mostly connected to questions in numeric / scientific computing or on the knowledge exchange between geo / hydro science and the modeling facility.

Highlights 2016

- PhD Product version of our transfer library Moonolith for variational transfer between arbitrarily distributed meshes
- Semi-geometric multigrid for vracture problems
- Good scaling version of software libraries (UTOPIA, PASSO and moonolith) for the numerical simulation of coupled multiphysics problems

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Nonlinear Multigrid Methods
for
Modeling permeability and stimulation for deep heat mining

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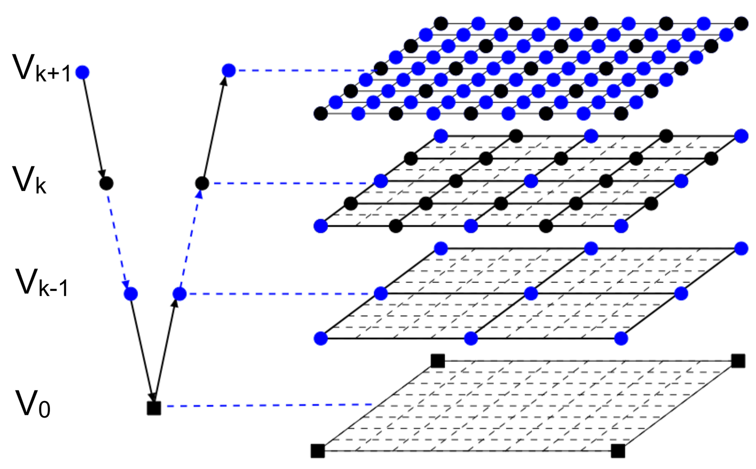
Introduction

Numerical simulations play a key role for a better understanding of the hydraulic stimulation mechanisms. Numerically these simulations relate to frictional contact problems. Using our experience in simulating this problem class we aim to improve accuracy, robustness and speed of hydraulic stimulation simulations.

Our strategy is based on bringing the efficiency of the well-known Multigrid algorithm from linear to non-linear problems using L^2 - projections based on biorthogonal basis elements, non-linear block Gauss-seidel smoother and truncated basis functions.

Multigrid Algorithm



Multigrid Algorithm $MG(y, k, y_0)$:

k: level, y: current value, y_0: starting value, GS: Gauss-Seidel step

1: Presmoothing: $x_{n+1} = x_n + GS(I, b - A * x_n)$
2: Project residual from level k to $k-1$: $\tilde{r}_{n+1} = P_k^{k-1} * (b - A * x_{n+1})$
3: Recursive call to MG: $\tilde{u} = MG(\tilde{r}_{n+1}, k-1, 0)$
4: Interpolate solution back from level $k-1$ to k: $u = I_{k-1}^k * \tilde{u}$
5: Postsmoothing: $x_{n+2} = x_{n+1} + GS(I, b - A * (x_{n+1} + u))$

The multigrid algorithm is an iterative solver which uses several representations of the problem from fine to coarse. Simply put, every level is suitable for a specific wavelength of the solution and multigrid makes use of that by projecting the non-resolved part of the solution to a suitable level. It is one of the most efficient linear solver for elliptic problems such as linear elasticity.

L^2- Projection

The efficient computation of the interpolation operators between the different grids is crucial. We use L^2 projections which define the Projection P_k^{k+1} using the weak form (or L^2-norm):

$$\int_{V_k} (v - P_k^{k-1}(v))\mu d\mathbf{x} \overset{w := P_k^{k-1}(v)}{=} \int_{V_k} (v - w)\mu d\mathbf{x} = 0, \quad v \in V_k, \forall \mu \in V_{k-1}$$

Using the finite element discretization one gets:

$$\sum_{i=0}^{dim(V_k)} v_i \int_{V_k} \phi_i \psi_n d\mathbf{x} = \sum_{j=0}^{dim(V_{k-1})} \int_{V_k} \theta_j \psi_n d\mathbf{x}, \qquad n = 1, ..., dim(V_{k-1})$$

Thus the product of basis functions of the spaces V_k and V_{k-1} defines the matrices D, B and at last the discrete form T of the projection Operator P_k^{k+1}:

$$\mathbf{Bv} = \mathbf{Dw} \Rightarrow \mathbf{w} = \mathbf{D}^{-1}\mathbf{Bv} = \mathbf{Tv}$$

Biorthogonal basis functions

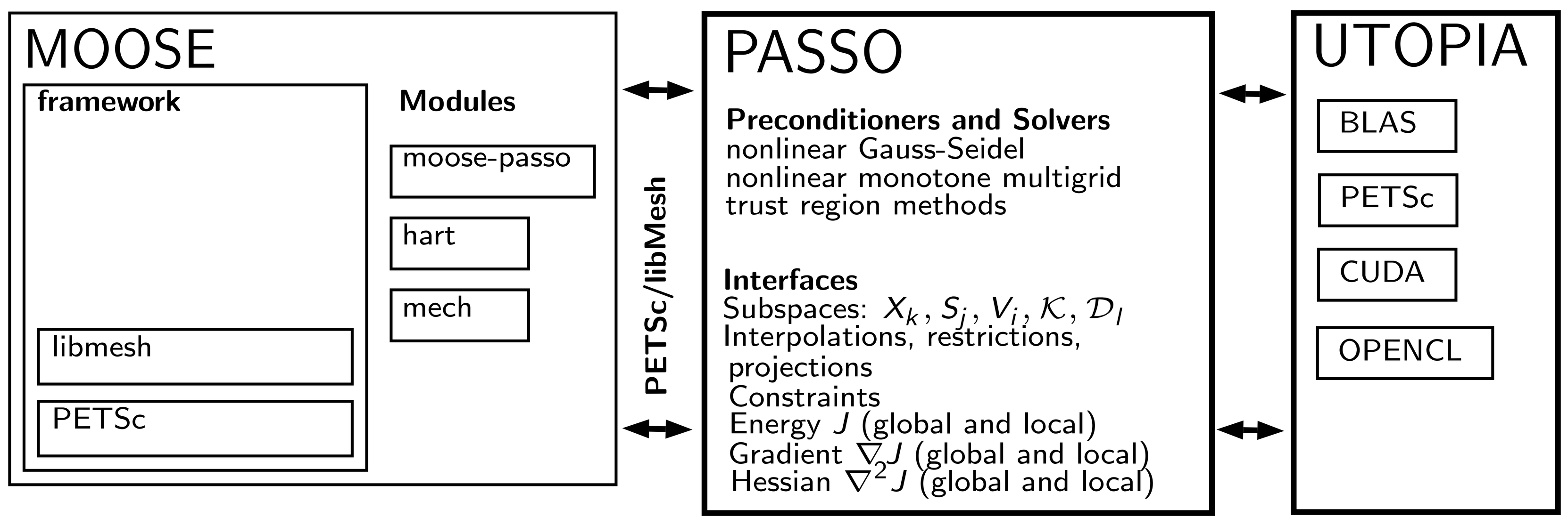
Since solving a linear system to obtain **w** is in general too expensive, we replace the original approximation space with one that is spanned by a family of biorthogonal functions:

$$\int_{V_k} \psi_n \lambda_j d\mathbf{x} = \delta_{j,n} \int_{V_k} \lambda_j, \qquad \forall j, n \in 1, ..., dim(V_{k-1})$$

Thus **D** above becomes a diagonal matrix and is easily invertible.

Implementation

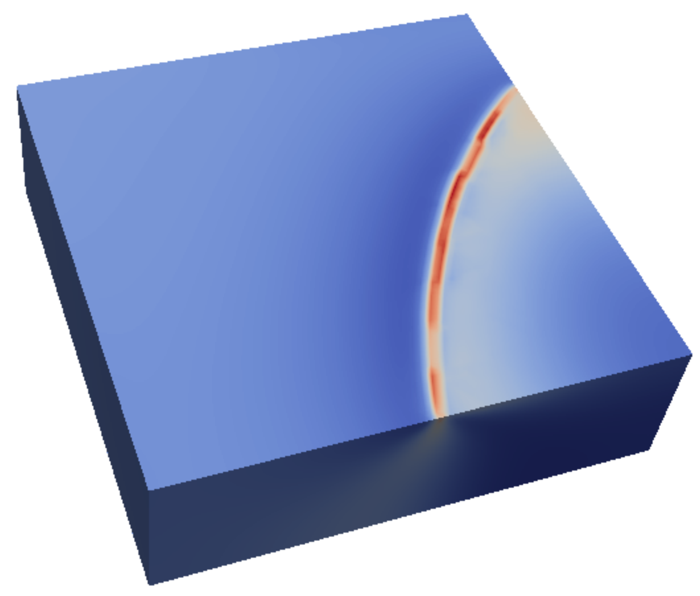
We use MOOSE for the finite element discretization. Our Framework, the parallel subspace solver and optimization library "PASSO" uses the PETSC SNES and libMesh to interface to MOOSE on on side. On the other side PASSO interfaces to UTOPIA which serves as wrapper for linear algebra backends suited for CPUs and GPUs.



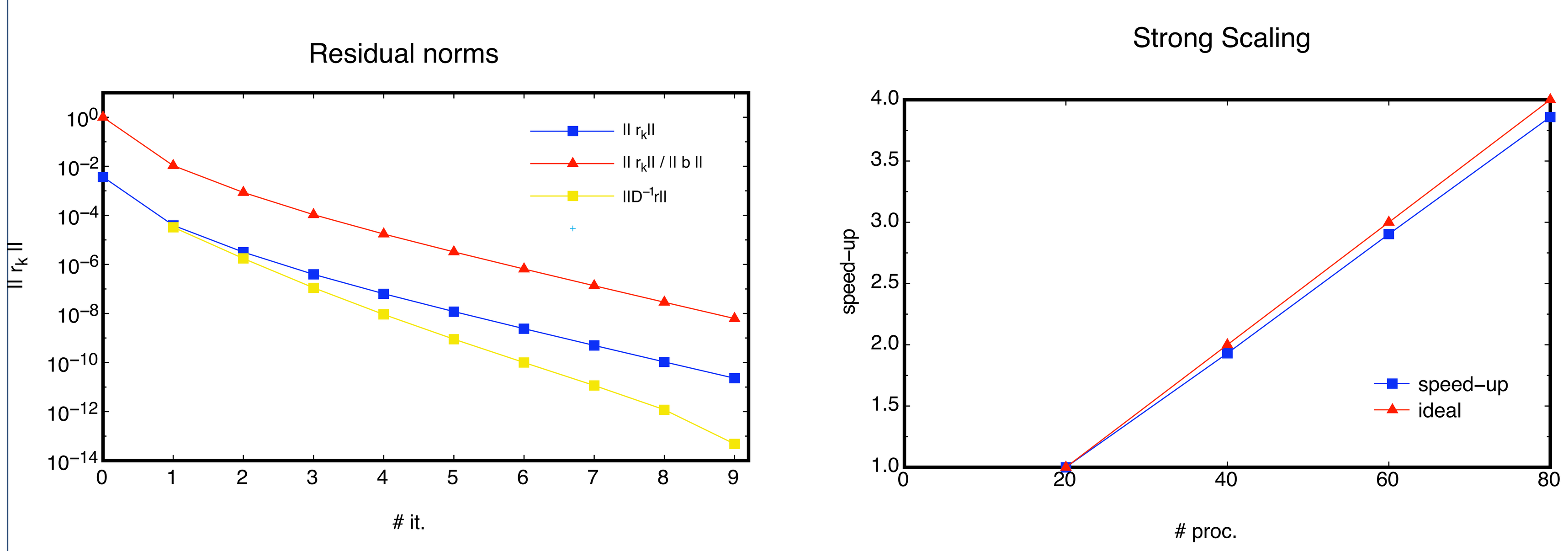
Results

We have conducted scaling experiments for the Newton method which uses a 4 level, V-cycle variant of our Multigrid with 3 pre- and postsmoothing steps for the computation of the step. The testproblem is a phasefield based fracture model included in MOOSE with 1.3 million degrees of freedom.

Figure: Phasefield testproblem with one crack going through the lower right corner.



The results show that the norm of the error r_k decrease by 1-2 orders of magnitude as is expected from Multigrid. Also scaling experiments up to 80 processors show good strong scaling.



Outlook

We will extend the Multigrid-Solver to a true nonlinear solver for contact problems by introducing truncated basis on the coarse grid. The solver will then be extended to solve multibody contact problems using a surface-to-surface variant of our L^2 - Projection.

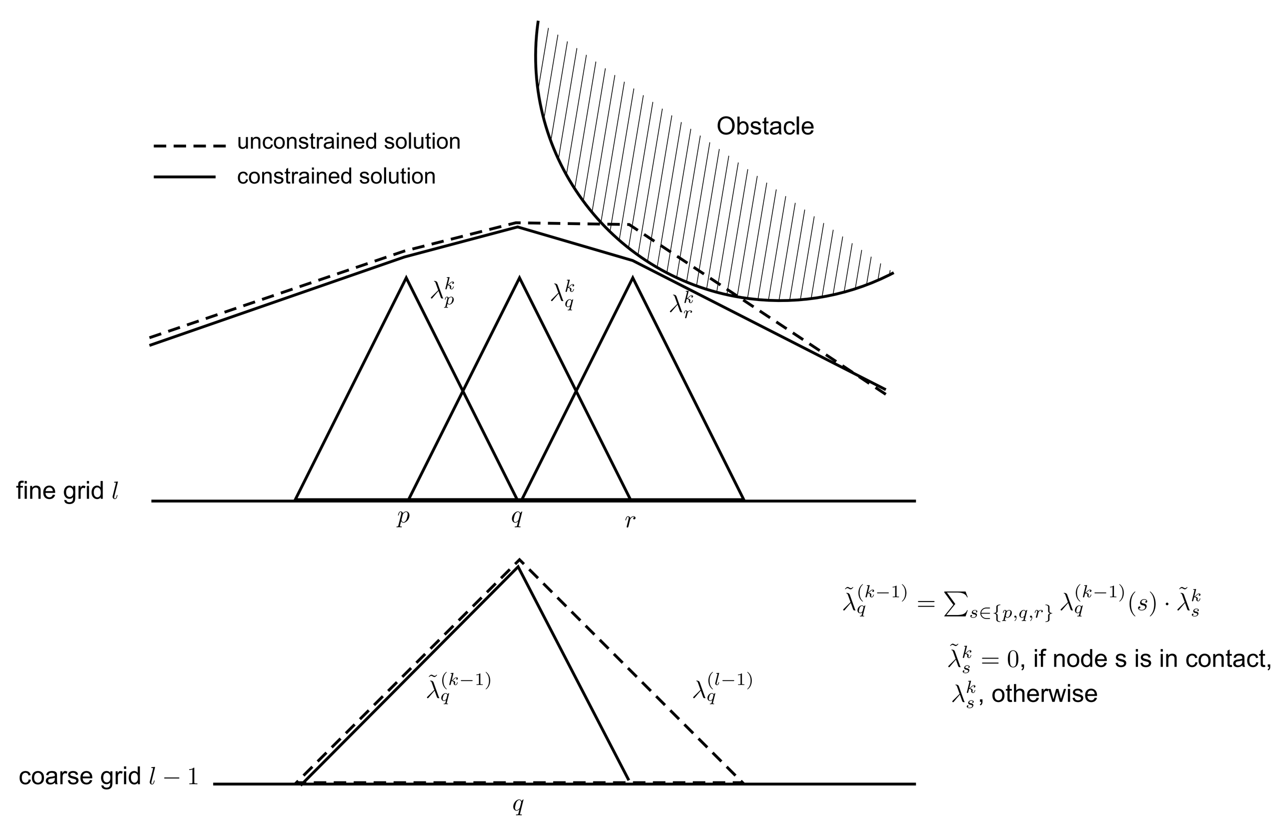


Figure: Example of of truncated basis in 1D for a contact problem. The contribution of the nodes in contact is effectively shut off on the coarse grid.

References
[1] Krause, Zulian SIAM 2016
[2] Dickopf, Krause Int. J. Numer. Meth. Engng 2008; 00:1–2

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A new software for modeling seismic velocity dispersion and attenuation in realistically fractured media

Marco Favino°, Jürg Hunziker, Eva Caspari*, Beatriz Quintal*, Klaus Holliger* and Rolf Krause°*
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Introduction

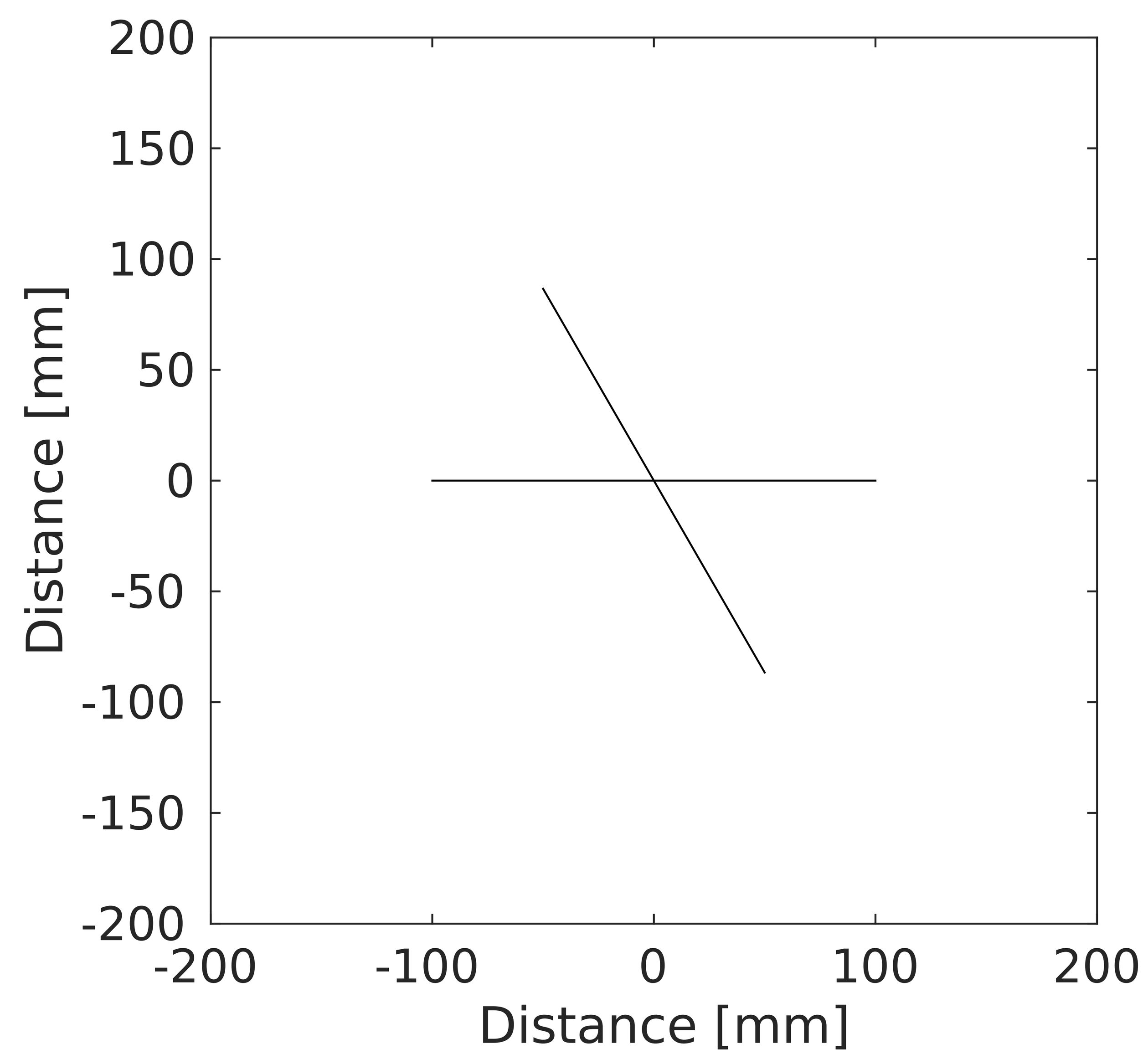
For geothermal and hydrocarbon exploration, nuclear waste disposal and CO_2 storage, knowledge of the fractures in the subsurface is of great relevance. Unfortunately, direct imaging of fractures with seismic methods is not possible, because the seismic wavelength is much larger than the fracture thickness. Indirect imaging is, however, possible, since seismic waves experience velocity dispersion and attenuation in fractured media due to wave-induced fluid flow (WIFF).

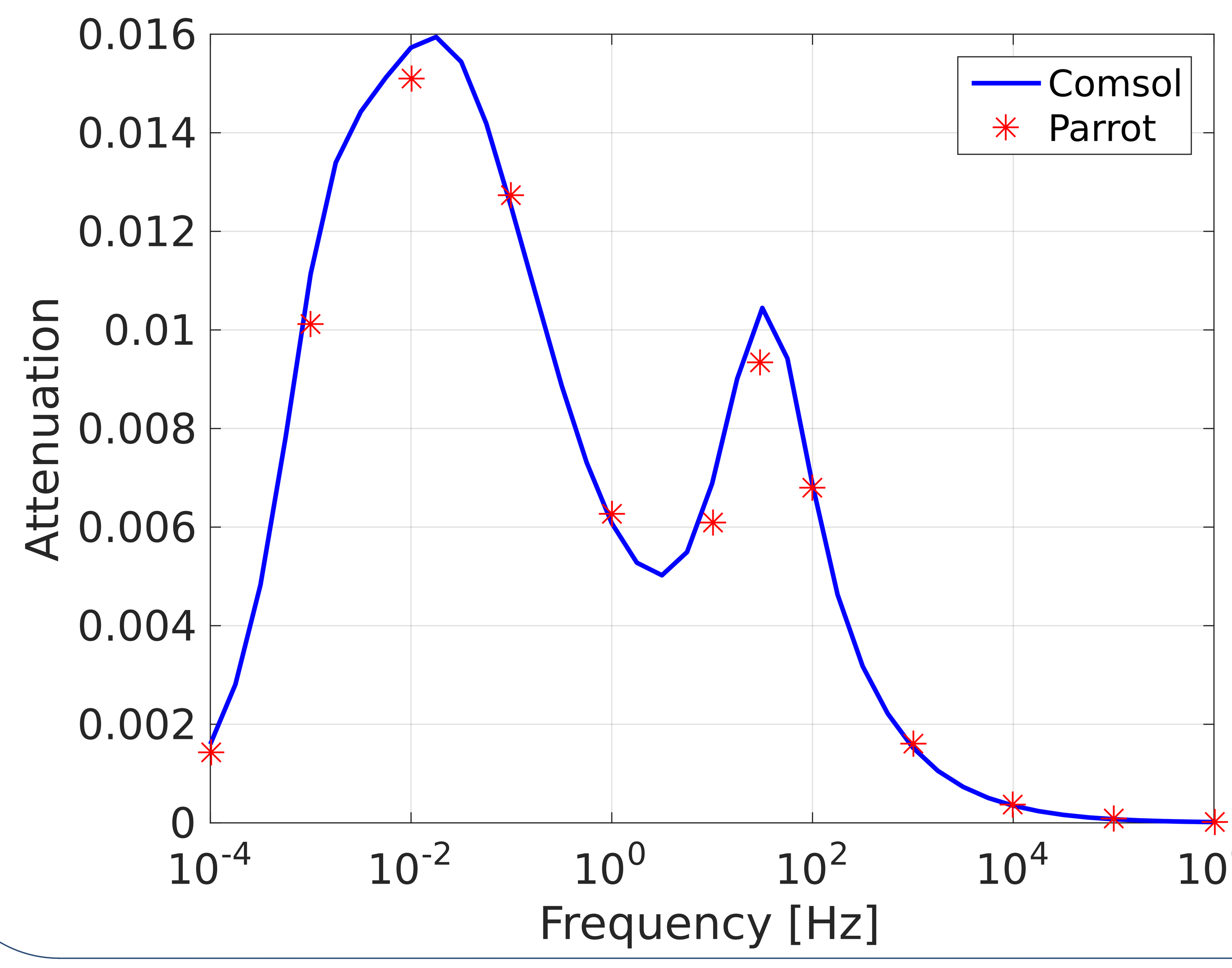
Method

WIFF in fractured media is studied using numerical upscaling experiments as described by the poster by Hunziker et al. (Task 1.2). Because of the fine meshes needed to resolve the fractures, such numerical experiments have been so far limited to rather simple models. To overcome this limitation, we have developed a new code called Parrot inside the finite element framework MOOSE. This software allows us to model realistic two-dimensional fractured rocks employing a fundamentally different approach: fractures are represented as discontinuous changes in the material properties but not explicitly resolved by the mesh. In this way, complex fracture networks can be readily considered without any computationally expensive remeshing. This strategy is coupled with an adaptive mesh refinement technique, which allows to refine the mesh at the fracture locations and hence to capture the complicated physics prevailing at the boundaries between the fractures and their embedding host rock. Starting from a single coarse mesh, this thus allows for a fast and "hands-off" numerical simulation of fracture networks of realistic complexity.

Validation: two fractures

We tested our code on a simple model of two intersecting fractures in order to compare it with the commercial software Comsol Multiphysics.

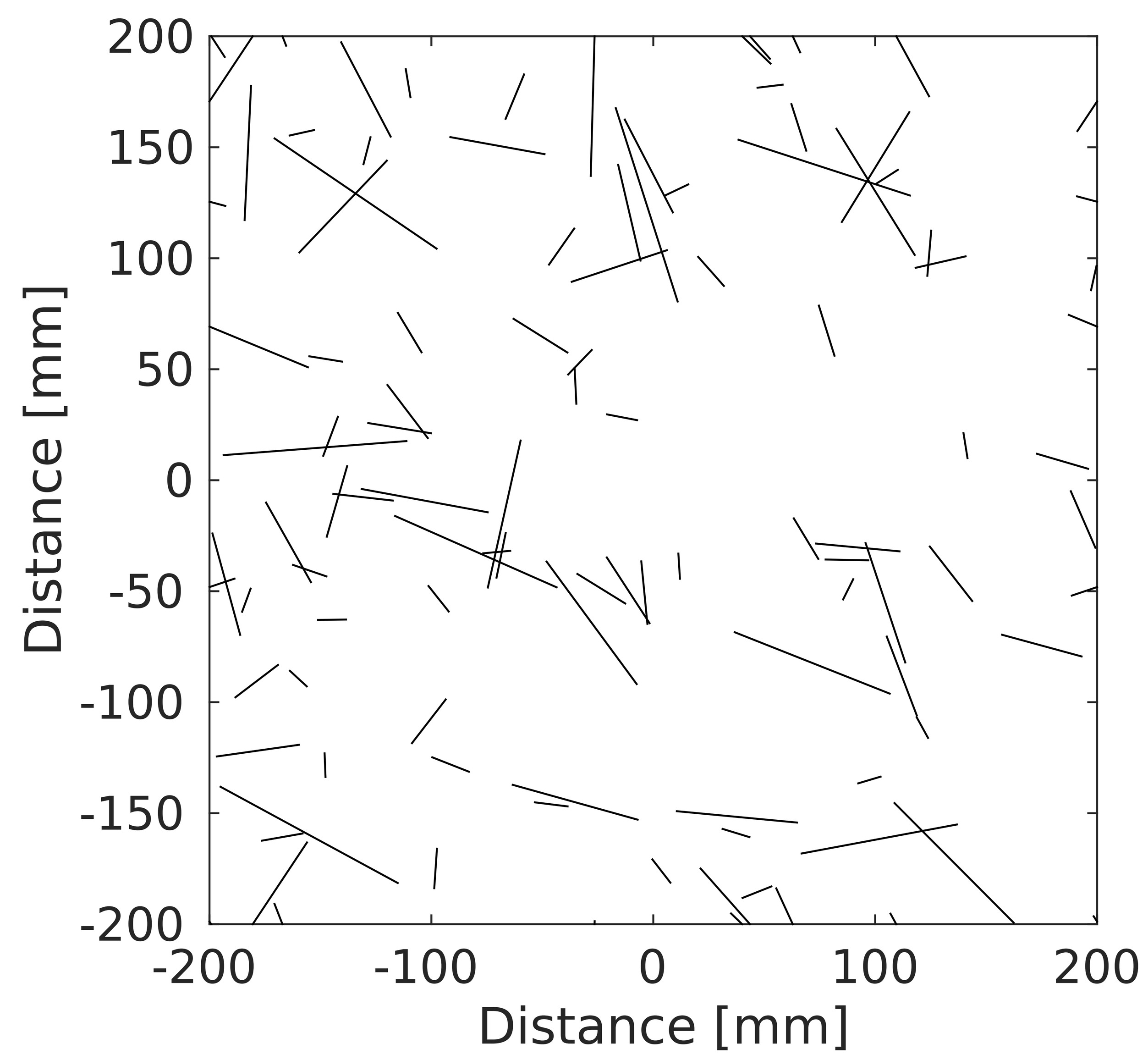


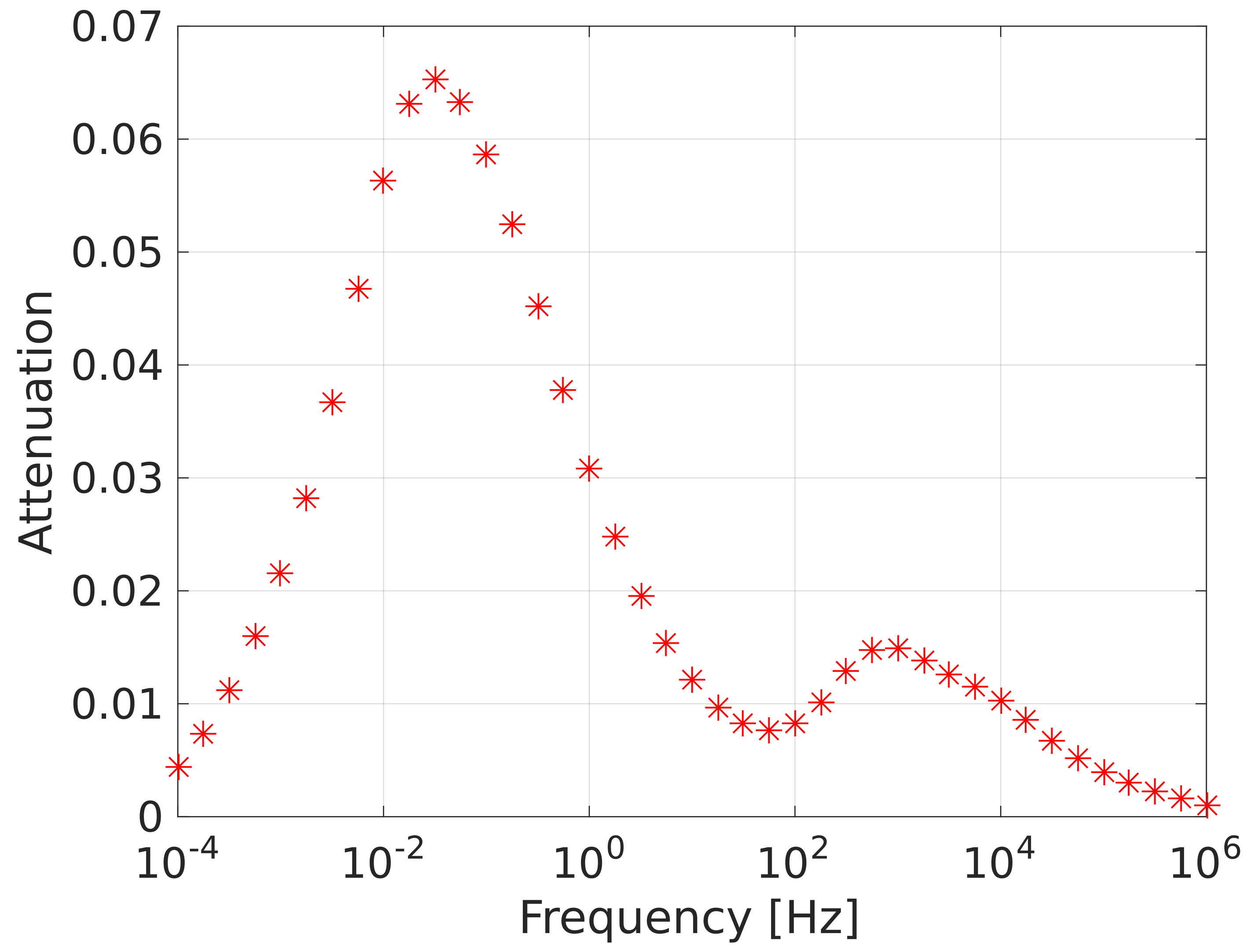


We observe a good agreement with regard to the attenuation computed by the two softwares. The small differences are mainly due to different meshes: unstructured triangular mesh following the geometry in Comsol and refined structured rectangular mesh independent of the geometry in Parrot.

Results: realistic fracture network

We employed software Parrot to determine the attenuation of seismic waves on a sample that features a realistic fracture network.





As in the case with only two fractures, the frequency dependent attenuation for the realistic fracture network contains two peaks. The low-frequency peak is due to WIFF between the fractures and the background, while the high-frequency peak is caused by WIFF between connected fractures. Relative to the amount of fractures, there are less connections between fractures in the second example. Therefore, the high-frequency attenuation peak is much lower in amplitude than the low-frequency attenuation peak.

Conclusions

Our software is able to perform simulations of seismic attenuation and velocity dispersion in realistic fracture networks. Thanks to an adaptive mesh refinement technique, no human interaction is needed to describe the fracture network.

Outlook

In the future, we shall use this new code to investigate WIFF in relation to connectivity and effective storativity of realistic fracture network, and we plan to extend it for three-dimensional simulations.