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), 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)

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 2015

- PhD thesis of J. Steiner on Fluid-Structure Interaction "Coupling Different Discretizations for Fluid Structure Interaction in a Monolithic Approach"
- Development of first prototypes of software libraries (PASSO and moonolith) for the numerical simulation of coupled multiphysixs problems

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Energy Turnaround
National Research Programme NRP 70

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

Cyrill von Planta(ICS-USI), Alessandro Rigazzi(ICS-USI), Thomas Driesner(ETH), Rolf Krause(ICS-USI)

Introduction

Numerical simulations play a key role for a better understanding of the hydraulic stimulation mechanisms. Stimulation leads to a widening of preexisting fractures and as a result to a shearing of the rough rock surfaces against each other in direction of the preexisting strains and stresses. As a mechanical problem 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.

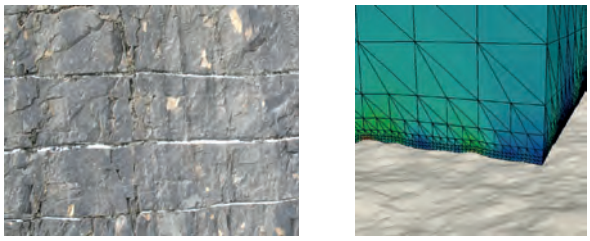


Fig. 1. From rock to model. Fractures in a natural rock formation (right) and contact simulation of two rough surfaces. From [1].

Friction

Using the power spectral density we can construct self-affine rough surfaces. By simulating the force blocking and interlocking in the fine asperities on the microscopic level we can deduce the friction parameter for Coulomb friction on the macroscopic level.

Fig. 2. Left: Generated rough surface. Right: stresses on the rough contact surface of a displaced cube. From [1].

Update of local Constraints

Robust solution methods require that the linearization of the local constraints is updated in every iteration, that is obstacle and domain are not to overlap. Furthermore one needs to take the constraints into consideration in every update of the solution (as in the non-linear Gauss-Seidel step mentioned in fig. 5).

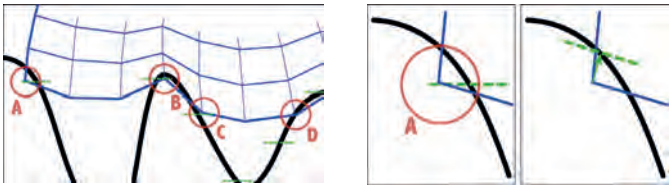


Fig. 3. Iterative update of the local constraints (green) when the body (blue) overlaps with obstacle (black). From [1].

Mortar Methods

Due to deformations of the bodies, the meshes at the contact zone are in general no longer conforming which makes it more difficult to maintain the stability of the discretization. In order to remedy this we will employ the Mortar method.

Computing the needed projections and determining contact zones is computationally expensive. Hence we have developed a library to automatize and parallelize this task [2].

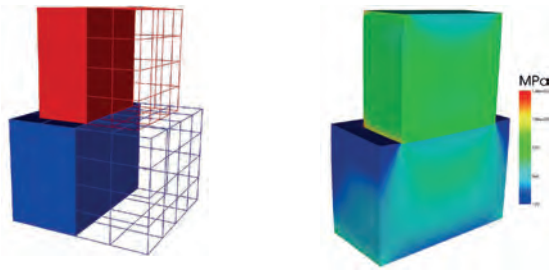
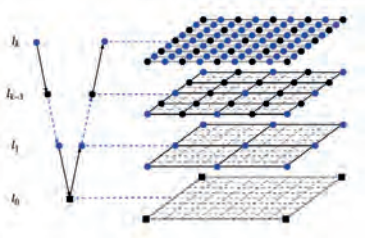


Fig. 4. Left: Nonconforming meshes between 2 cubes. Nodes of the blue and red cubes are not aligned on the boundary. Right: Same cubes showing the Mises Stresses. From [3].

Solver: Parallel non-linear Multigrid Methods

The monotone multigrid method is a recursive iterative method which uses multiple nested meshes. The method approximates the high-frequency parts of the solution on finer meshes and projects the low-frequent remainder of the error on coarser meshes [5].



Multigrid Algorithm

1: Compute $x_{n+1} = x_n + GS(l, b - A * x_n)$
2: Compute $r^{\sim}_{n+1} = I^{l-1}_{l} * (b - A * x_{n+1})$
3: Compute $u = MG(r^{\sim}_{n+1}, l-1, 0)$
4: Compute $r^{\sim}_{n+1} = I^{l}_{l-1} * (b - A * x_{n+1})$
5: Compute $x_{n+2} = x_{n+1} + r^{\sim}_{n+1}$
6: Compute $x_{n+3} = x_{n+2} + GS(l, b - A * x_n)$

Fig. 5. Left: Nested meshes used in the Multigrid algorithm. Right: Monotone multigrid algorithm with one non-linear Gauss-Seidel sweep for pre- and one postsmoothing (step 1 and step 6). The recursion in step 3 leads to the lowest level 0. Picture from [5].

Multigrid in general converges faster than direct solvers. Monotone multigrid makes use of the principle of successive energy-minimization which can be implemented by means of a non-linear Gauss-Seidel algorithm. In particular monotone multigrid has the advantageous properties of scaling well with increasing degrees of freedom and being globally convergent for non-linear problems.

Linear sparse solver pardiso (O.Schenk)

#dof	#nodes	decomp time (s)	peak memory
14.739	4.913	6,58	0,101GB
32.937	10.979	18,7	0,232GB
107.811	35.937	351,62	1,1GB
159.771	53.257	402,89	1,9GB

Linear multigrid for a linear problem
TOL $= 10^{-12}$

#dof	#nodes	solution time
14.739	4.913	3,05
107.811	35.937	29,0
823.875	274.625	238,3

non-linear multigrid for friction
$\mathcal{F} = 0.3$, TOL $= 10^{-12}$

#dof	#nodes	solution time
14.739	4.913	11,59
107.811	35.937	82,81
823.875	27.4625	856,1

Tab 1. Scalability of direct solver (left) vs linear multigrid (middle) vs our non-linear multigrid. Note how the non-linear multigrid scales almost optimal for a non-linear friction problem.

Outlook

We will refactor our existing solvers and methods within our new parallel subspace solver and optimization library “PASSO” and interface it to the complex systems modeling platform CSMP++. PASSO is designed as a parallel library and capable of handling arbitrary n-dimensional problems.`

References

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[5] Krause, SIAM Journal on Scientific Computing, 31(2):1399–1423, 2009
[6] Feng, http://web.utk.edu/~wfeng1/research.html

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Modelling Fatigue in Turbine Blades

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Abstract

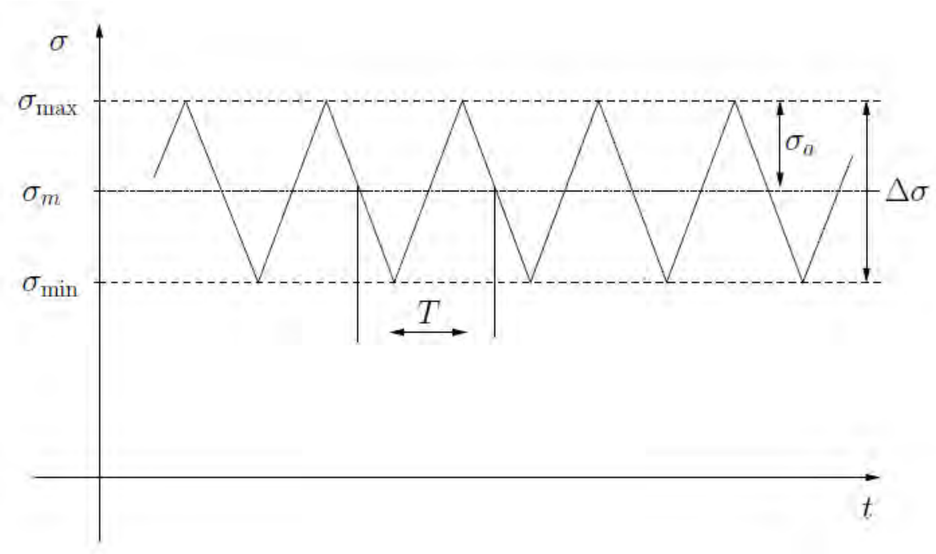
A local and probabilistic model for Low-Cycle Fatigue (LCF) in the context of polycrystalline metal has been studied. It quantifies risks for LCF crack initiation and takes size effects and inhomogeneous strain and temperature fields into account. The model has been calibrated and validated based on fatigue tests with different specimen geometries. Moreover, the probabilistic fatigue life of engineering components, which are already in service, has been analyzed. By varying the geometry of a component to minimize the probability for LCF crack initiation, new designs can be developed according to the local and probabilistic model.

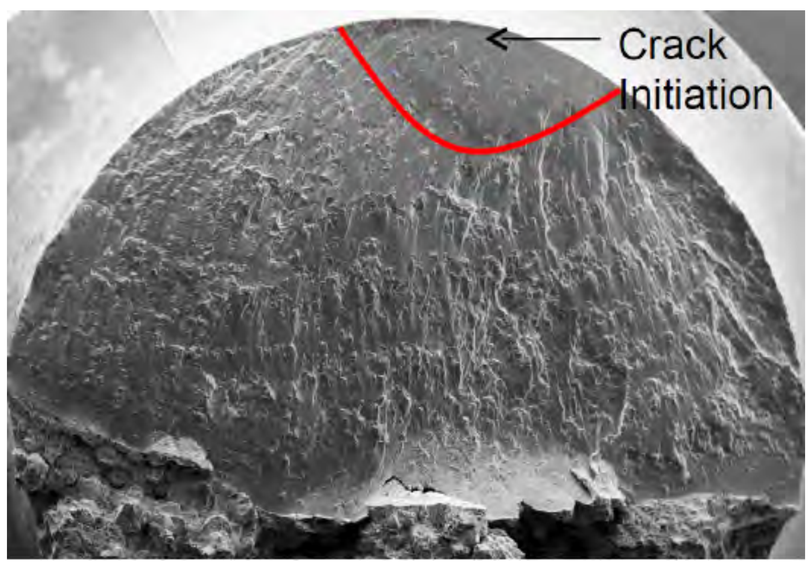
Introduction

Fatigue describes crack formation in material under cyclic loading which can often result in failure of engineering components. Activation and deactivation operations of technical units are common examples in engineering, where fatigue and, in particular, low-cycle fatigue play an important role. For many materials, fatigue life is marked by significant scatter. Furthermore, size effects influence the fatigue life of components. The deterministic safe-life approach in fatigue design employs results of standardized specimen tests to estimate the design life of a component. Thereby, safety factors are applied to consider the inherent scatter in fatigue life, size effects, and uncertainties such as those in the loading and temperature conditions.

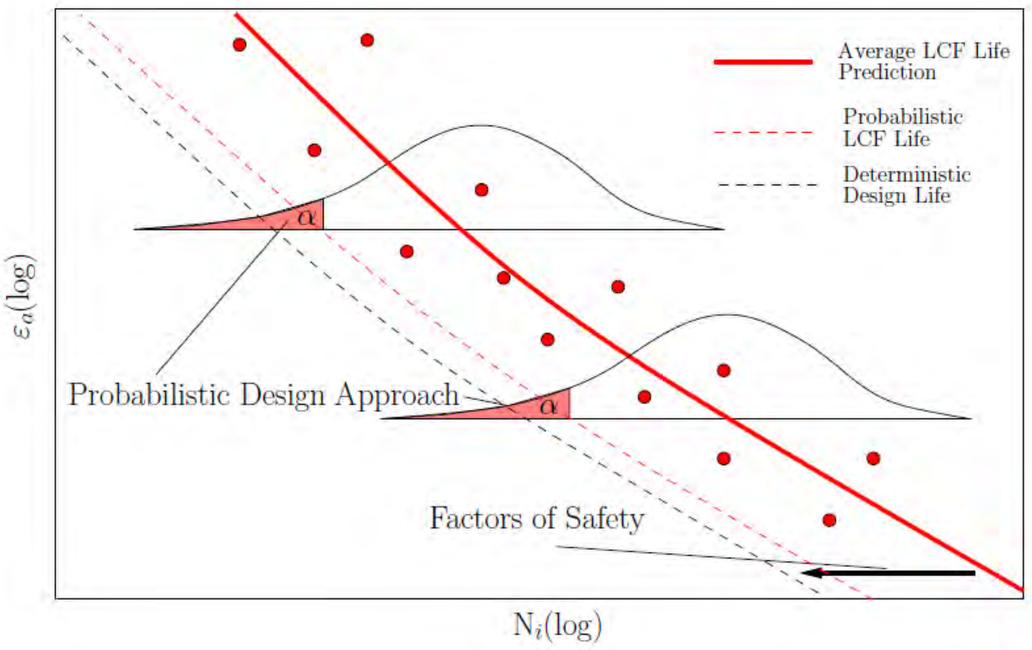
Failure mechanism [Radaj et al. 2007]

- Surface driven
- Surface roughens itself due to dislocations
- Plastic deformations accumulate → LCF crack Initiation

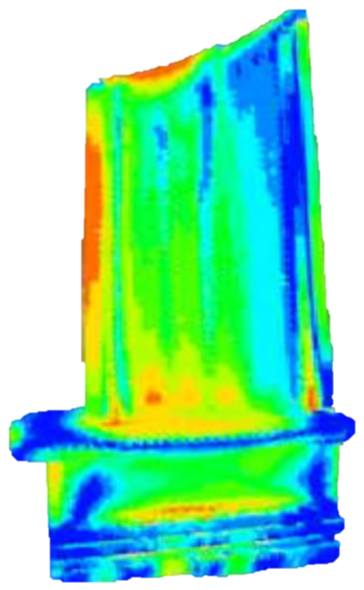




Probabilistic fatigue analysis [Schmitz et al. 2013]:



We applied the probabilistic model to a gas-turbine blade which is subjected to thermo-mechanical loading during the operating state. Having computed the total Probability of Failure we also consider and visualize the hazard density on the blade's surface, shown in red in the image on the right. This approach is general and can be applied to other classes of problems where a probabilistic model can be derived.



Project details

This is a closed joint project between Siemens AG and the Institute of Computational Science, which is part of USI (Università della Svizzera Italiana).

General FEA and Contact Problems

- Thermoelastic Analysis is a crucial input for deterministic and probabilistic life of a turbine blade
- In particular, contact areas are effected by crack initiations
- How sensitive is the deterministic and probabilsitic life regarding contact problems and its modelling?
- Conduct shape optimization w.r.t. the probabilistic cost functional via the adjoint method
- Further validation of the probabilistic model [Schmitz et al. 2013]

References

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- S. Schmitz, G. Rollmann, H. Gottschalk, and R. Krause, 2013, *Risk Estimation for LCF Crack Initiation Life of aTurbine Blade under Thermomechanical Loading*, Proceedings of the Seventh International Conference on Low Cycle Fatigue, Aachen, Germany
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Large-scale simulation of pneumatic and hydraulic fracture with a phase-field approach

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Abstract

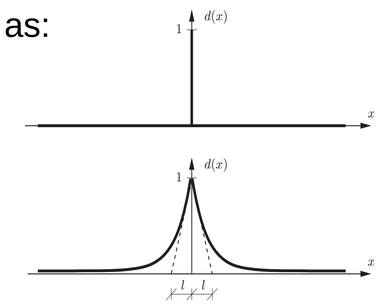
The phase-field method is an non-local approach which allows the computation of the dynamical evolution of an interface. The basic idea is to differentiate multiple phases by means of an order parameter. The variation of the systems free energy with respect to this order parameter then reveals the time evolution of the interface. Phase-field models of fracture are conceptually similar to models of continuum damage mechanics, whereby the order parameter weights the damage (or integrity) of the structure. Generally, a phase-field model may be considered as a gradient-type material model with a free energy function that is composed of classical bulk energy and a gradient-type regularized surface energy. Phase-field approaches to fracture offer important new perspectives towards the computational modeling of complex crack topologies.

Phase-field

Simulating the evolution of a crack-interface by describing the free energy of the system in terms of an order-parameter allows us to model its kinetics by minimizing the free energy with respect to this order parameter.

In one dimension we can model a crack interface as:

$$d(x) = e^{|x|/l}$$

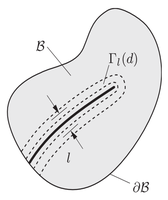


This is the solution of the differential equation

$$d(x) - l2d''(x) = 0$$

which is the Lagrange equation that results from the variation of the functional:

$$I(d) = \frac{1}{2}\int_B \{d^2 + l^2 d'^2\} dV$$ this Integral we can identify with the crack surface density Γ_l



$I(e^{-|x|/l}) = l\Gamma$ and in 3 dimensions this becomes:

$$\Gamma_l(\mathbf{d}) := \int_B \frac{1}{2l}\mathbf{d}^2 + \frac{l}{2}\nabla(\mathbf{d})\cdot\nabla(\mathbf{d}) dV$$

Finite deformation field

Material governed by Helmholtz free energy Ψ

$$\Psi := \Psi(C), \quad C = F^T F, \text{ def. gradient: } F = D\varphi$$

Fracture is due to tension, this leads to fracture insensitive part of F

$$\tilde{F} = \sum_a (\lambda_a^+)^{(1-\mathbf{d})}(\lambda_a^-)\mathbf{n}_a \otimes \mathbf{N}_a, \qquad \lambda^{\pm}\text{…tensile /compressive princ. stretches}$$

This leads to:

$\mathbf{P} = \partial_F \Psi(\tilde{F}(F,\mathbf{d}))$ First Piola stress

$H = \partial_{\mathbf{d}} \Psi(\tilde{F}(F,\mathbf{d}))$ Driving force of phase field

Local balance of linear momentum

Lagrangian form:

$$\rho_0 \dot{\mathbf{v}} = DIV(\mathbf{P}) + \bar{\mathbf{B}}$$
$$0 = H = \frac{g_c}{2l}\mathbf{d} - g_c l \Delta(\mathbf{d})$$

Boundary conditions:

$$\varphi = \bar{\varphi}, \quad \partial B^{\varphi} \times [0,T]$$
$$\mathbf{PN} = \bar{\mathbf{T}}, \quad \partial B^{\sigma} \times [0,T]$$
$$\mathbf{d} = \bar{\mathbf{d}}, \quad \partial B^{\mathbf{d}_D} \times [0,T]$$
$$\nabla\mathbf{d}\cdot\mathbf{N} = 0, \quad \partial B^{\mathbf{d}_N} \times [0,T]$$

Weak formulation

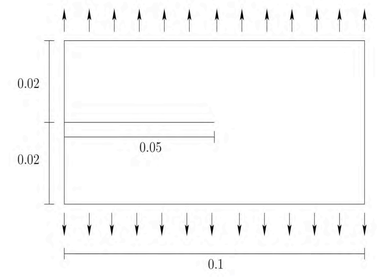
$$G_\varphi := \int_B \rho_0 \delta\varphi\cdot\ddot{\varphi} + \mathbf{B} : \nabla_x(\delta\varphi) - \delta\varphi\cdot\bar{\mathbf{B}} dV - \int_{\partial B^\sigma} \delta\varphi\cdot\bar{\mathbf{T}} dA = 0$$

$$G_{\mathbf{d}} := \int_B \delta\mathbf{d}\left(H + \frac{g_c}{2l}\right) + g_c l \nabla(\delta\mathbf{d})\cdot\nabla(\mathbf{d}) = 0$$

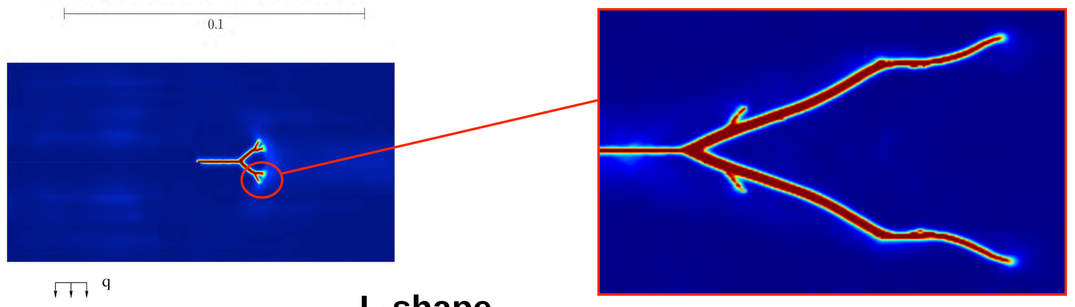
Dynamic crack branching

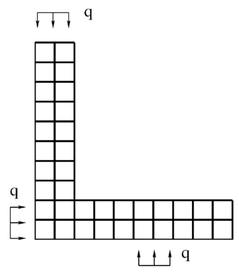
Plate loaded on the upper and lower side, using pure Neumann boundaries with a uniform dead load in both directions.
We consider a **hyperelastic Neo-Hookean** material with free energy:

$$\Psi(C^e) = \frac{\mu}{2}\left(\sum_{a=1}^{n}(\lambda_a^e)^2 - n\right) + \frac{\lambda}{2}(\ln(J))^2 - \mu\ln(J)$$



After 300 time steps with $\Delta t=10^{-7}$, the time-step size has been reduced to $\Delta t=2\text{x}10^{-8}$ to account for further branching after the main branch.

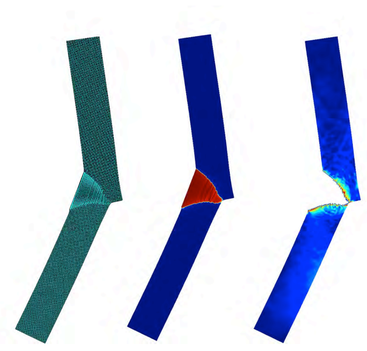




L-shape

Here the motion of a L-block is considered. The mesh consists of 9867 elements and 30600 unknowns.

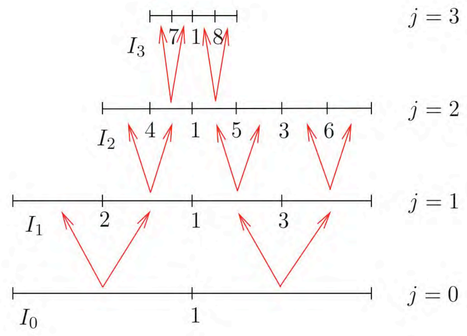
Phase-field and stress distribution at t=0.8, the L-shape has just ripped apart.



Examples taken from [1]

Multigrid method for Allen-Cahn equation

When using **implicit time discretization** methods, multigrid methods are among the fastest solvers for large systems.



Major property of the multigrid method: **convergence** does **not depend** on the **element size** (level independence). It also presents a method of **optimal complexity** for a broad class of large and sparse linear systems, arising when discretizing elliptic boundary problems. Adaptive methods provide a sequence of discretization of partial differential equations with optimal approximation quality. Further we can tag elements for refinement on basis of their **local error**.

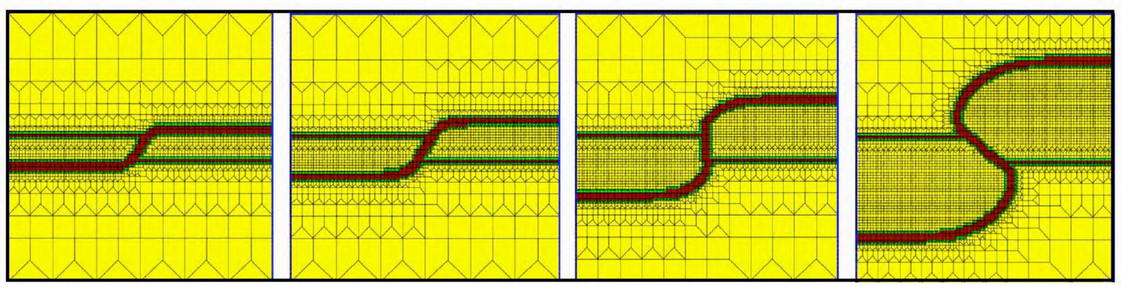


Image out of [2]

Conclusion

A novel approach for crack propagation for large deformation problems and finite strains along with a consistent numerical framework for the spatial as well as the temporal discretization is proposed. this project will provide a number of new and non-standard computational tools for the simulation of pneumatic and hydraulic fracturing and a most general framework for the simulation of fracture for nonlinear materials. This will allow us large-scale simulations of variationally and thermodynamically consistent multi-physics phase-field fracture models undergoing finite deformations throughout the time domain of interest.

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