On efficient and robust numerical solution algorithms for nonstationary, nonlinear, coupled problems

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Overview

Multiphysics

Multiphysics:

- Modeling the interaction of various physical phenomena

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For instance:

- Solids (elastic/plastic) u,
- Fluids (Stokes, Navier-Stokes, Darcy) $\{v, p\}$,
- Chemical concentrations c,
- Temperatures T,
- Saturations s.

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Number of couplings:

- Traditionally: 2 PDEs couple
- Nowadays: often more than 2 PDEs couple

Coupling types

- **Volume coupling** (the PDEs live in the same domain) and exchange information via volume terms, right hand sides, coefficients.
- Examples: Biot equations for modeling porous media flow, phase-field fracture, Cahn-Hilliard phase-field models for incompressible flows.
- **Interface coupling** (the PDEs live in different domains) and the information of the PDEs is only exchanged on the interface.
- Example: fluid-structure interaction, sharp interface models.

Details on interface coupling

Two basic methods:

- Interface-Tracking
- Interface-Capturing

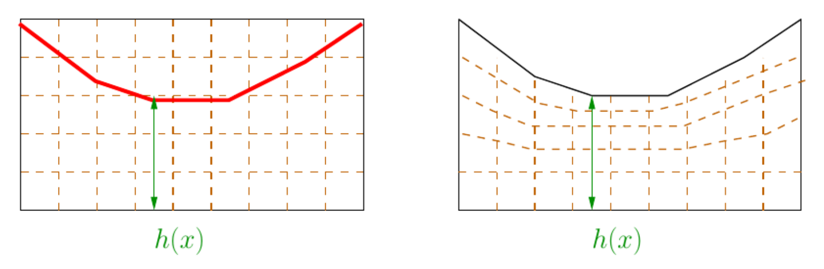

Figure: Left: the mesh is fixed and the interface must be captured. Right: interface-tracking in which the interface is located on mesh edges.

Interface-tracking

- In methods, where the domain is decomposed into elements or cells (finite volumes, finite elements or isogeometric analysis), using interface-tracking aligns mesh edges with the interface.

$\rightarrow$ **fitted methods**.

- For moving interfaces, the mesh elements need to be moved as well;
- However, mesh elements may be deformed too much such that the approach fails if not taken care of (expensive) re-meshing in a proper way.

Interface-capturing

- In interface-capturing methods (unfitted methods), the domain and consequently the single elements stay fixed.
- Here, the interface can move freely through the domain.
- Mesh degeneration is not a problem, but capturing the interface is difficult.
- Topology changes (e.g., contact) are possible

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In this approach a further classification can be made:

- Lower-dimensional approaches
- Diffusive techniques.

Specific realizations:

- The first method comprises extended/generalized finite elements, cut-cell methods, finite cell methods, and locally modified finite elements;
- Diffusive methods are the famous level-set method or phase-field methods.

1 Multiphysics (nonstat., nonlinear, coupled PDEs)

2 Examples of coupled PDEs
- Two prototype examples
- Classifications

3 Numerical algorithms
- Needs
- Two-phase-flow phase-field fracture propagation

4 Towards multiscale phenomena
- Several scales in time: FSI plus chemistry plus solid growth
- A global-local approach in space for phase-field fracture

5 Conclusions

Fluid-structure interaction

Equations for fluid flows (Navier Stokes) - Eulerian

$$\partial_t v + (v \cdot \nabla v) - \nabla \cdot \sigma(v,p) = 0, \quad \nabla \cdot v = 0, \quad \text{in } \Omega_f \times I,$$
$$+\text{bc and initial conditions}$$

with Cauchy stress tensor $\sigma(v,p) = -pI + \rho_f \nu_f (\nabla v + \nabla v^T)$.

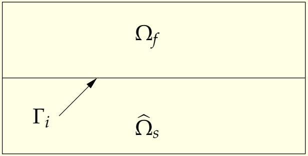
Equations for (nonlinear) elasticity - Lagrangian

$$\partial_t^2 \hat{u} - \hat{\nabla} \cdot (\hat{F}\widehat{\Sigma}(\hat{u})) = 0 \quad \text{in } \widehat{\Omega}_s \times I,$$
$$+\text{bc and initial conditions}$$

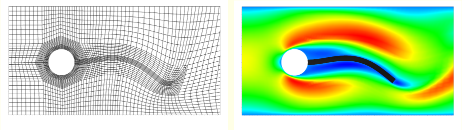
with the stress $\hat{F}\widehat{\Sigma}(\hat{u}) = 2\mu_s \hat{E} + \lambda_s \text{trace}(\hat{E})I$, the strain $\hat{E} = (\widehat{F}\widehat{F}^T - I)$ and $\widehat{F} = I + \widehat{\nabla}\hat{u}$.

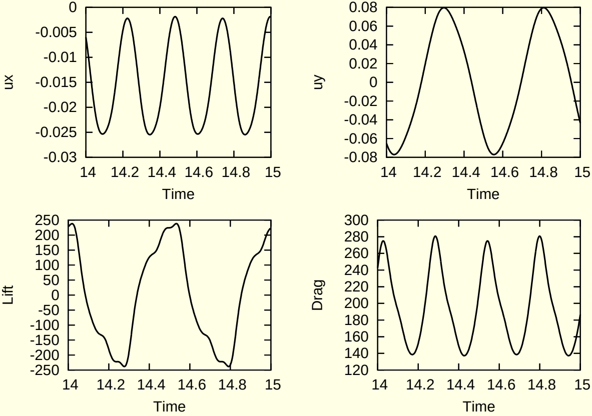
Coupling conditions on $\Gamma_i, \hat{\Gamma}_i$

$$v_f = \hat{v}_s \quad \text{and} \quad \sigma(v,p)n_f = \widehat{F}\widehat{\Sigma}(\hat{u})\hat{n}_s.$$



Example: Hron/Turek benchmark FSI 2 (2006) [1]





[1] Wick; Comp. Struct, 2011

A parallel block-preconditioned monolithic solver [2]

- At each Newton step, we have:

$$A_h := \begin{bmatrix} \mathcal{M} & \mathcal{C}_{ms} & 0 \\ \mathcal{C}_{sm} & \mathcal{S} & \mathcal{C}_{sf} \\ \mathcal{C}_{fm} & \mathcal{C}_{fs} & \mathcal{F} \end{bmatrix}, \approx \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ \mathcal{C}_{fm}\mathcal{M}^{-1} & \tilde{\mathcal{C}}_{fs}\mathcal{S}^{-1} & 1 \end{bmatrix} \begin{bmatrix} \mathcal{M} & 0 & 0 \\ 0 & \mathcal{S} & 0 \\ 0 & 0 & \mathcal{X} \end{bmatrix} \begin{bmatrix} I & \mathcal{M}^{-1}\mathcal{C}_{ms} & 0 \\ 0 & I & \mathcal{S}^{-1}\mathcal{C}_{sf} \\ 0 & 0 & I \end{bmatrix} \quad (1)$$

with $\mathcal{X} = \mathcal{F} - \tilde{\mathcal{C}}_{fs}\mathcal{S}^{-1}\mathcal{C}_{sf}$.

- Computational performance:

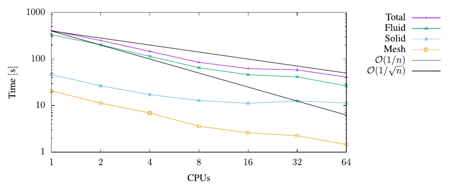


Figure: FSI-2 benchmark: Strong scalability using the preconditioned GMRES scheme for approximately $16 \cdot 10^6$ dofs using $Q(2) - Q(2) - P(1)$ elements and time step size $dt = 0.01s$. Average time given in seconds for the solution of one linear system.

[2] Jodlbauer/Langer/Wick, IJNME, 2019

Phase-field fracture propagation (simplified version)

Formulation (Simplified quasi-static brittle fracture)

For the loading steps $n = 1, 2, 3, \ldots, N$: Find a displacement function $u : B \times I \to R^d$ and a phase-field indicator function $\varphi : B \times I \to [0, 1]$, where $I := (0, T]$ is the 'time'/loading interval, such that

$$-\nabla \cdot (\varphi^2 \nabla u) = f \quad \text{in } B \times I, \quad (u\text{-equation}) \tag{2}$$

$$\varphi |\nabla u|^2 - \epsilon \Delta \varphi - \frac{1}{\epsilon}(1 - \varphi) \leq 0 \quad \text{in } B \times I, \quad (\varphi\text{-equation}) \tag{3}$$

$$\partial_t \varphi \leq 0 \quad \text{in } B \times I, \quad (\text{crack irreversibility}) \tag{4}$$

$$\Big[\varphi |\nabla u|^2 - \epsilon \Delta \varphi - \frac{1}{\epsilon}(1 - \varphi)\Big] \cdot \partial_t \varphi = 0 \quad \text{in } B \times I. \quad (\text{compatibility condition}) \tag{5}$$

To formulate a well-posed problem, boundary and initial conditions are needed:

$$\begin{aligned}
u(x,t) &= u_D(x,t) && \text{on } \partial\Omega_D \times I, \\
u(x,t) &= 0 && \text{on } \partial\Omega_2 \times I, \\
\varphi^2 \nabla u \cdot n &= 0 && \text{on } (\partial\Omega_1 \cup \partial\Omega_0) \times I, \\
\partial_n \varphi &= 0 && \text{on } \partial B \times I, \\
\varphi(x,0) &= \varphi_0 && \text{on } B \times \{0\},
\end{aligned}$$

with an initial fracture φ_0 and with $\epsilon > 0$ as the so-called phase-field regularization parameter.

Single edge notched shear test in mechanics [3]

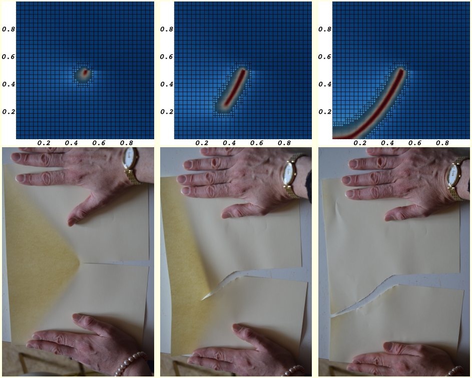


Figure: Comparison of experiment and numerical simulation.

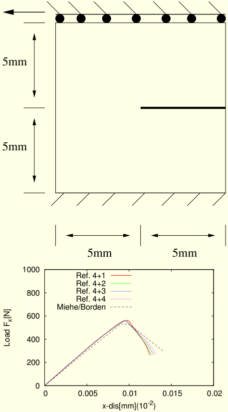


Figure: Setting and functional evaluation in terms of the load-displacement curve

[3] All parameters taken from Miehe/Welschinger/Hofacker (2010) CMAME, (2010) IJNME

Classification of fluid-structure interaction

1. PDE system with $d+d+1$ variables: $(v_x, v_y, v_z, u_x, u_y, u_z, p)$ for $d=3$
2. Nonlinear constitutive models: convection term in the NSE equations, geometric nonlinearities in the elastic strain tensor
3. Interface-coupled PDEs
4. Solid and fluid ask for different conservation properties; solid is wave-like (conservation of energy!)
5. Large solid deformations: different coordinate systems. Eulerian for fluids and Lagrangian for solids

Classification of phase-field fracture

1. PDE system with $d+1$ variables: (u_x, u_y, u_z, φ) (d=3)
2. Nonlinear constitutive models (stress splitting) in the displacement equation
3. Volume-coupled PDEs
4. Variational inequality (crack irreversibility constraint)

$\Rightarrow$ Three types of nonlinearities:

1. nonlinear effects in the model (e.g., stress splitting)
2. nonlinear effects through coupling terms
3. nonlinear effects due to the variational inequality

More information in the GAMM-Leitartikel 02/2018

ZIELORIENTIERTE NUMERIK FÜR MULTIPHYSIKSIMULATIONEN

VON THOMAS WICK

Multiphysik

Multiphysik bezeichnet ein interdisziplinäres Forschungsgebiet, in dem verschiedene physikalische Phänomene miteinander gekoppelt werden. Oft basieren diese Beschreibungen auf kontinuumsmechanischen Modellen, welche auf sogenannte Systeme von Differentialgleichungen (DGL) führen.

Die Interdisziplinarität erfordert ein Grundverständnis von Theorie, Numerik/Wissenschaftlichem Rechnen und Praxis. Oftmals erfolgt die Spezialisierung auf eines der drei Gebiete, welches nichtsdestotrotz schnell sehr herausfordernd werden kann. Im Folgenden konzentrieren wir uns auf Aspekte des Wissenschaftlichen Rechnens in Multiphysiksimulationen.

Die zugrundeliegenden Differentialgleichungen sind meistens von partieller Natur (PDGL), hängen also von mindestens zwei unabhängigen Variablen ab. Diese PDGL sind im Allgemeinen instationär, nichtlinear, gekoppelt und möglichen Ungleichungsbedingungen unterworfen. Theoretische Ergebnisse sind - wenn überhaupt - lediglich an-

solcher Skalenunterschiede wird in absehbarer Zeit nicht möglich sein, wenngleich Multiskalen-Methoden ein sehr aktives Forschungsfeld darstellen. Auf diesen letzten Punkt wird im weiteren Verlauf des Artikels nicht weiter eingegangen.

Kopplungsbedingungen

Ein entscheidender Aspekt in der Multiphysik betrifft die Analyse, das numerische Design und die Implementierung der Kopplungsbedingungen. Grundsätzlich kann zwischen zwei Klassen unterschieden werden: Volumenkopplungen und Interfacekopplungen. Bei Volumenkopplungen wird über Koeffizienten oder Rechte-Seiten-Terme gekoppelt. Die verschiedenen Gleichungen sind aber im selben Gebiet definiert. Im Gegensatz dazu sind bei Interfacekopplungen die Gleichungen in verschiedenen Gebieten definiert und koppeln an dem inneren Rand, dem sogenannten Interface. Es gibt kein Patentrezept zur allgemeinen Lösung. Im Regelfall sind Interfacekopplungen jedoch viel schwieriger

Efficient and robust numerical solutions

- Respect conservation properties of governing PDEs (e.g., local mass conservation, energy conservation)
- Iterative linear solvers (e.g., CG, GMRES)
- Appropriate nonlinear solvers (fixed-point, Newton, ...)
- Relaxation of possible constraints (e.g., irreversibility condition in phase-field fracture)
- Adaptive methods:
  - Mesh adaptivity in space and/or time
  - Adaptive stopping criteria for linear and nonlinear solvers
  - A posteriori error estimation (possibly goal-oriented)
  - Balancing of errors: e.g., discretization and iteration errors [4]
- Parallelization (MPI, ...) [5]
- Load-balancing when mesh adaptation is combined with parallelization

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[4] Talk by Bernhard Endtmayer

[5] Talk by Daniel Jodlbauer

Practical realization

- The modeling, design and numerical analysis and implementation of multiphysics problems with the previous aims is NOT a one-man-show (resp. one-woman-show) !
- Joint efforts ! (social aspect of research! Try to be open and curious!)
- International interdisciplinarity !

[6] Bangerth et al; since 1998

[7] Heister/Wick; PAMM, 2018

[8] Goll et al; ANS, 2017

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- Governing software must be:
  - sufficiently sophisticated
  - relatively easy to use
  - sustainable
  - flexible
  - must have a good documentation!

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- Governing software must be:
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  - must have a good documentation!
- For me (since the year 2007):
  - Open-source finite element package deal.II[6] `https://www.dealii.org/`
  - Phase-field fracture code[7]
  - Differential and optimization environment library DOpElib[8] `www.dopelib.net`
- But there others as well: dune, fenics, UG4, Gascoigne3D/RoDoBo, NGSolve, FreeFem++, ...

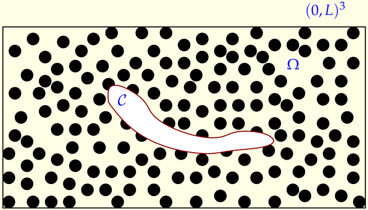
[6] Bangerth et al; since 1998

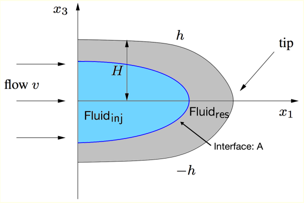
[7] Heister/Wick; PAMM, 2018

[8] Goll et al; ANS, 2017

Example: Two-phase-flow phase-field fracture propagation [9]

- Five PDEs to be coupled: displacements, phase-field, pressure, saturation, fracture-width-calculation
- Illustration: fracture embedded in a porous medium, two-phase Darcy flow inside the fracture





[9]Lee/Mikelic/Wheeler/Wick; SIAM MMS, 2018

Algorithm

Questions:

- Q1: How to discretize the equations?
- Q2: How to couple the equations?
- Q3: how to solve the discretized systems?

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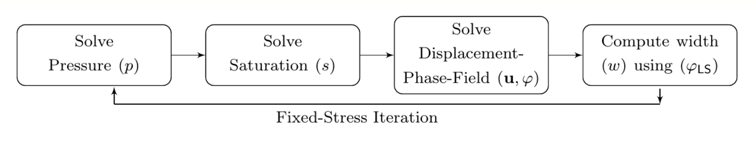
- Q3: how to solve the discretized systems?

Answer to Q2:

- iterative coupling (known in subsurface modeling as fixed-stress)
- Flowchart of the algorithm:



Discretization

- (Nonlinear) displacements: standard continuous Galerkin Q_1
- (Nonlinear; variational inequality) phase-field: standard Q_1
- Fracture-width-problem: standard continuous Galerkin Q_1
- (Implicit) Pressure diffraction equation: enriched Galerkin[10] (cont. Galerkin with one extra DoF; DG implementation!)
- (Explicit) Saturation equation: enriched Galerkin

[10] Sun/Liu; 2009

Discretized equations

- Displacements and phase-field are very similar to what we have seen before
- State: width problem, pressure diffraction equation [11] [12] , saturation equation

[11] Ladyzhenskaja/Solonnikov/Uralceva; AMS Vol. 23, 1968

[12] Lions/Magenes, tome 1, chapitre 3, section 4, 1968

Width problem

Formulation

Find $W^l \in C^0([0,T]; V_w(T))$ *such that*

$$A_W(W^l, \psi) = F_W(\psi) \quad \forall \psi \in V_w(T)$$

where

$$A_W(W^l, \psi) = (\nabla W^l, \nabla \psi) + \theta \int_{\Gamma_F^{n,l}} W\psi \, ds,$$

$$F_W(\psi) = \theta \int_{\Gamma_F^{n,l}} W_D^l \cdot \psi \, ds.$$

Pressure diffraction problem

Formulation

At time t^n and the fixed-stress level $l+1$, let U^l, Φ^l, W^l, S^l be given. Furthermore, let the previous time step solutions U^{n-1}, P^{n-1} be given. We iterate for $l = 1, 2, 3, \ldots$ such that: Find $P^{l+1} \in V_{h,k}^{EG}$:

$$S(P^{l+1}, \psi) = F(\psi), \quad \forall \psi \in V_{h,k}^{EG}, \tag{6}$$

where the Incomplete Interior Penalty Galerkin (IIPG) is employed to be compatible with the saturation system. Here the variational form is defined as

$$\begin{aligned} S(P^{l+1}, \psi) := &\sum_{\mathcal{K} \in T_h} \int_{\mathcal{K}} \theta^l \frac{P^{l+1} - P^{n-1}}{\delta t} \psi \, dx + \sum_{\mathcal{K} \in T_h} \int_{\mathcal{K}} K_{\boldsymbol{eff}}^l \nabla P^{l+1} \cdot \nabla \psi \, dx \\ &- \sum_{e \in \mathcal{E}_h^1} \int_e \{\!\{ K_{\boldsymbol{eff}}^l \nabla P^{l+1} \}\!\} [\![\psi]\!] \, d\gamma + \sum_{e \in \mathcal{E}_h^1} \int_e \frac{\alpha_p}{h_e} \{\!\{ K_{\boldsymbol{eff}}^l \}\!\}_{|e} [\![P^{l+1}]\!] [\![\psi]\!] \, d\gamma + \sum_{\mathcal{K} \in T_h} \int_{\mathcal{K}} q^n \psi \, dx, \end{aligned} \tag{7}$$

where $\alpha_p > 0$ is a penalty parameter and the right hand side is defined as

$$F(\psi) := \sum_{\mathcal{K} \in T_h} \int_{\mathcal{K}} f^l \psi \, dx - \sum_{\mathcal{K} \in T_h} \int_{\mathcal{K}} \theta_c^l \nabla P_c(S^l)) \cdot \nabla \psi dx + \sum_{e \in \mathcal{E}_h^1} \int_e \{\!\{ \theta_c^l \nabla P_c(S^l)) \}\!\} [\![\psi]\!] \, d\gamma. \tag{8}$$

Saturation equation

Formulation

Let the previous fixed-stress solutions U^l, Φ^l, W^l, P^l and the previous time step solutions U^{n-1}, P^{n-1}, S^{n-1} be given. At time t^n we iterate for $l = 1, 2, 3, \ldots$: Find $S^{l+1} \in V^{EG}_{h,k_s}$ such that

$$W(S^{l+1}, \psi) = R(\psi), \quad \forall \psi \in V^{EG}_{h,k_s}, \tag{9}$$

where the variational form defined as

$$\begin{aligned} W(S^{l+1}, \psi) := & \sum_{\mathcal{K}\in T_h} \int_{\mathcal{K}} \theta^l_s \frac{S^{l+1} - S^{n-1}}{\delta t} \psi dx + \sum_{\mathcal{K}\in T_h} \int_{\mathcal{K}} \mu^l_{\textbf{stab}} \nabla S^{l+1} \cdot \nabla \psi dx \\ & - \sum_{e\in\mathcal{E}^1_h} \int_e \{\!\{\mu^l_{\textbf{stab}} \nabla S^{l+1}\}\!\} [\![\psi]\!] \, d\gamma + \sum_{e\in\mathcal{E}^1_h} \int_e \frac{\alpha_s}{h_e} \{\!\{\mu^l_{\textbf{stab}}\}\!\}_{|e} [\![S^{l+1}]\!] [\![\psi]\!] \, d\gamma, \end{aligned} \tag{10}$$

where α_s is a penalty parameter and we note that terms with $\mu_{\textbf{stab}}$ are artificial diffusion to stabilize and avoid spurious oscillations for the advection system. Then,

$$R(\psi) := \sum_{\mathcal{K}\in T_h} \int_{\mathcal{K}} V^l \, \nabla \psi dx - \sum_{e\in\mathcal{E}^1_h} \int_e V^l \cdot n \, [\![\psi]\!] \, d\gamma + \sum_{\mathcal{K}\in T_h} \int_{\mathcal{K}} q^l_s \, \psi \, dx. \tag{11}$$

The diffraction coefficients are defined as

$$\theta^l_s := \chi^l_R \cdot 0 + \chi^l_F \, (\varphi^\star_F \rho_{F,\textbf{inj}}), \tag{12}$$

$$\bar{q}^l_s := \chi^l_R \cdot 0 + \chi^l_F \left(\rho_{F,\textbf{inj}} f^n_{F,\textbf{inj}}\right). \tag{13}$$

Numerical solution

- 2D and 3D; code: IPACS (Integrated Phase Field Advanced Crack Simulator) based on deal.II[13]; approx 16 000 lines of code
- Nonlinear quasi-monolithic displacement/phase-field system is solved with Newton's method and line search algorithms. The constraint minimization problem is treated with a semi-smooth Newton method (i.e., a primal-dual active set method).
- Inside Newton: GMRES with block-diagonal preconditioning (AMG from trilinos)
- Width problem: conjugate gradient (CG) solver and symmetric successive over-relaxation (SSOR) preconditioning.
- Pressure and saturation diffraction problems are solved with generalized minimal residual method (GMRES) solvers with diagonal block-preconditioning.

[13] www.dealii.org

Predictor-corrector mesh adaptivity

- $J(U) = \varphi < c$ with $c = 0.5$ for example.
- The key challenge in phase-field methods is the relation of the model regularization parameter ε and the spatial mesh size h (high mesh resolution required!) since $h < \varepsilon$.
- Wish: Fix a (very) small ε during the entire computation.

$\rightarrow$ Predictor-corrector mesh adaptivity with hanging nodes (the mesh grows with the fracture).

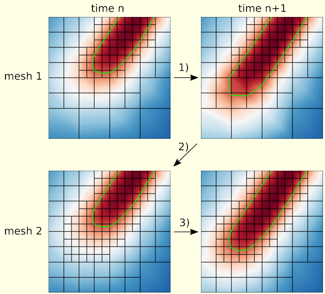


Figure: Predictor-corrector scheme: 1. advance in time, crack leaves fine mesh. 2. refine and go back in time (interpolate old solution). 3. advance in time on new mesh. Repeat until mesh doesn't change anymore. Refinement is triggered for $\varphi < C = 0.2$ (green contour line) here.

Software and parallel solution [14]

- Critical issue: how to solve linear systems efficiently?
- Robustness with respect to ε, κ, h ???

Solution:

- High performance parallel computing with adaptive meshes
- deal.II `www.dealii.org`
- MPI (message parsing interface)
- p4est (parallel dynamic management of a collection of adaptive octrees)
- trilinos (AMG - algebraic multigrid)

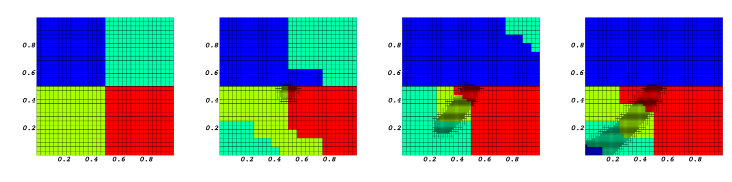


Figure: Exemplified visualization of parallel computing on 4 processors. The different sub-domains are associated with different processors. Depending on mesh refinement, the workload for each processor is adjusted dynamically at each time step.

[14] Heister/Wick; PAMM, 2018

Some brief results [15]

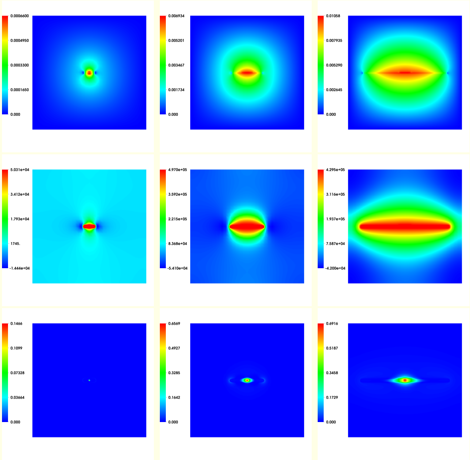


Figure: The width problem, the pressure and saturation distributions at $T = 0.01s, 2s, 10s$.

[15] Lee/Mikelic/Wheeler/Wick; SIAM MMS, 2018

Frei/Richter/Wick (JCP, 2016): Mechano-chemical FSI with solid contact

- Contact of solids (current topic!).
- Different temporal time scales: two-scale approach

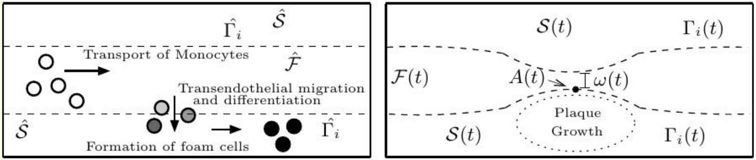


Figure: Configuration of the domain and mechanism of plaque formation. Left: Domain in reference configuration split into fluid part $\hat{\mathcal{F}}$ and solid $\hat{\mathcal{S}}$ divided by the interface $\hat{\Gamma}_i$. Right: Domain in the current (Eulerian) description with plaque formation and narrowing of the vessel.

Multiple scales in time

- Short scale: heart does beat once in about every $[1]s$;
- Long scale: plaque growth takes place in a time span of months, i.e. $[> 1\,000\,000]s$

⇒ a numerical simulation will not be able to resolve each detail while following the long-term process

⇒ consider an averaged flow problem and focus on the long-scale dynamics

⇒ to incorporate effects of the short-scale dynamics, we compute effective wall stresses with the help of isolated small-scale simulations

- Accurate handling of the different time-scales is an open problem.

Solution algorithms: Long-scale/short-scale

Initialize $v^0 = 0$, $u^0 = 0$, $g^0 = 0$ and the vessel-width $\omega^0 = 2$. Set time-step $k_l = [1]day = [86\,400]s$. Iterate for $n = 1, 2, \ldots$:

1.a) Solve quasi-stationary long-scale problem:

$$\{c_s^{n-1}, \omega^{n-1}\} \mapsto \{v^n, u^n, p^n\}$$

1.b) Compute the vessel width in the point $A(\tau_n)$

$$\omega^n = 2 - 2u_{s,2}^n(A(\tau_n), \tau_n)$$

2.a) Set $v^{s,0} = v^n$, $u^{s,0} = u^n$ and solve the short-scale problem in $I_n = [[\tau_n]days, [\tau_n]days + [1]s)$

$$\{v^{s,0}, u^{s,0}, c_s^{n-1}, \omega^n\} \mapsto \{v^{s,m}, u^{s,m}, p^{s,m}\},\ m = 1, \ldots, N_s$$

2.b) Compute average wall stress in main stream direction

$$\sigma_{WS}^n = \frac{1}{N_s} \sum_{m=1}^{N_s} \int_{\Gamma_i} |\sigma_f(v^{s,m}, p^{s,m})\vec{n} \cdot \vec{e}_1| \, do$$

2.c) Update the foam cell concentration

$$c_s^n = c_s^{n-1} + k_l \gamma_0 \left(1 + \sigma_{WS}^n / \overline{\sigma}\right)^{-1}$$

Long-scale problem: clogging

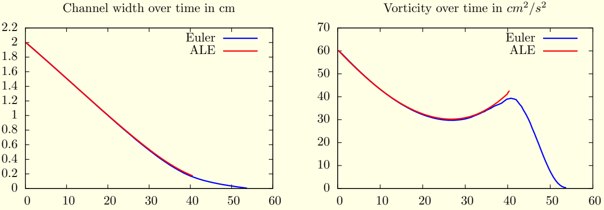


Figure: Channel width and vorticity for a long-scale simulation with reduced inflow velocity. The inflow velocity goes to zero when the channel closes. This makes the complete closure of the channel possible.

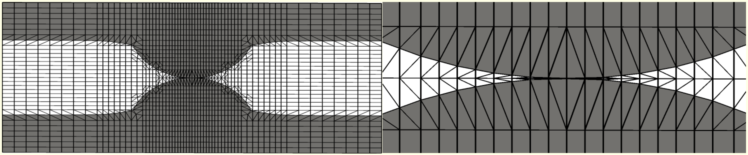


Figure: Fully Eulerian deformation when the channel is completely closed at $\tau = [55.8] days$. The standard classical ALE technique cannot close the channel!

Multiscale in space: Motivation [16]

- Fracture process is a local event but is embedded in a big reservoir. How to choose ε? What is the meaning of ε? How to embed local fine-scale features into a macroscale framework with less detailed information?

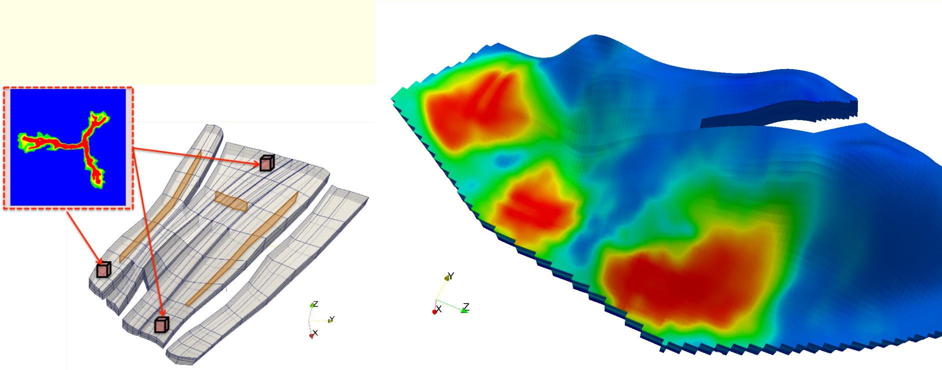


Figure: Phase-field as fractured well model in a 3d large-field porous medium.

[16] Wick/Singh/Wheeler; 2015, SPE Journal

A predictor-corrector global-local approach [17]

- The previous situation is too difficult. Simplify the situation in the following.

→ Global-local approach

- Global (macroscale) problem: linearized elasticity without phase-field
- Local (microscale) problem: elasticity with stress-splitting, nonlinear constitutive laws, and phase-field
- Coupling of both problems via Lagrange multipliers

[17] Noii/Aldakheel/Wick/Wriggers; 2019, arXiv:1905.07519v1

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- Local (microscale) problem: elasticity with stress-splitting, nonlinear constitutive laws, and phase-field
- Coupling of both problems via Lagrange multipliers
- Challenge: crack path a priori unknown

→ local domain a priori unknown!

- Local domain is adapted during the simulation

→ predictor-corrector adaptive global-local approach

[17] Noii/Aldakheel/Wick/Wriggers; 2019, arXiv:1905.07519v1

The global-local algorithm

Algorithm 1 *Global-Local iterative scheme combined with Robin-type boundary conditions.*

Input: loading data $(\bar{\boldsymbol{u}}_n, \bar{\boldsymbol{\tau}}_n)$ on $\partial_D\mathcal{B}$ and Γ_N, respectively;
solution $(\boldsymbol{u}_{G,n-1}, \boldsymbol{u}_{L,n-1}, d_{L,n-1}, \boldsymbol{u}_{\Gamma,n-1}, \boldsymbol{\lambda}_{C,n-1}, \boldsymbol{\lambda}_{L,n-1})$ and $\mathcal{H}_{L,n-1}$ from step $n-1$.

Global-Local iteration $k \geq 1$:

Local boundary value problem:

- given $\mathbb{A}_L, \boldsymbol{\Lambda}_L^{k-1}, \mathcal{H}_{L,n-1}$; solve
  phase-field part:
  $$(1-\kappa)\int_{\mathcal{B}_L} d_{L+}\mathcal{H}(\boldsymbol{\varepsilon}(\boldsymbol{u}_L)).\delta d_L \mathrm{d}\boldsymbol{x} + G_c\int_{\mathcal{B}_L}\frac{1}{l}(d_L-1).\delta d_L \mathrm{d}\boldsymbol{x}$$
  $$+G_c\int_{\mathcal{B}_L} l\nabla d_L.\nabla(\delta d_L)\mathrm{d}\boldsymbol{x} + G_c\int_{\mathcal{B}_L}\alpha l\nabla d_L.\boldsymbol{M}.\nabla(\delta d_L)\mathrm{d}\boldsymbol{x} = 0,$$
  mechanical part:
  $$\begin{cases} \int_{\Omega_L}\boldsymbol{\sigma}(\boldsymbol{u}_L, d_L) : \boldsymbol{\varepsilon}(\delta\boldsymbol{u}_L)\,\mathrm{d}\boldsymbol{x} - \int_\Gamma \boldsymbol{\lambda}_L\cdot\delta\boldsymbol{u}_L\,\mathrm{d}s = 0, \\ \int_\Gamma \boldsymbol{\lambda}_L\cdot\delta\boldsymbol{u}_\Gamma\,\mathrm{d}s + \mathbb{A}_L\int_\Gamma \boldsymbol{u}_\Gamma\cdot\delta\boldsymbol{\lambda}_C\,\mathrm{d}s = \boldsymbol{\Lambda}_L^{k-1}, \\ \int_\Gamma (\boldsymbol{u}_\Gamma - \boldsymbol{u}_L)\cdot\delta\boldsymbol{\lambda}_L\,\mathrm{d}s = 0, \end{cases}$$
  set $(\boldsymbol{u}_L, d_L, \boldsymbol{u}_\Gamma, \boldsymbol{\lambda}_L) =: (\boldsymbol{u}_L^k, d_L^k, \boldsymbol{u}_\Gamma^{k,\frac{1}{2}}, \boldsymbol{\lambda}_L^k)$,
- given $(\boldsymbol{u}_L^k, \boldsymbol{\lambda}_L^k; \mathbb{A}_G)$, set
  $$\boldsymbol{\Lambda}_G^k = \mathbb{A}_G\int_\Gamma \boldsymbol{u}_L^k\cdot\delta\boldsymbol{\lambda}_C\,\mathrm{d}s - \int_\Gamma \boldsymbol{\lambda}_L^k\cdot\delta\boldsymbol{u}_\Gamma\,\mathrm{d}s.$$

Global boundary value problem:

- given $\mathbb{A}_G, \boldsymbol{\Lambda}_G^k, \boldsymbol{u}_\Gamma^{k,\frac{1}{2}}$, solve
  $$\begin{cases} \int_{\Omega_G}\boldsymbol{\sigma}(\boldsymbol{u}_G) : \boldsymbol{\varepsilon}(\delta\boldsymbol{u}_G)\,\mathrm{d}\boldsymbol{x} - \int_\Gamma \boldsymbol{\lambda}_F\cdot\delta\boldsymbol{u}_G\,\mathrm{d}s - \int_\Gamma \boldsymbol{\lambda}_C\cdot\delta\boldsymbol{u}_G\,\mathrm{d}s - \int_{\Gamma_N}\bar{\boldsymbol{\tau}}\cdot\delta\boldsymbol{u}_G\,\mathrm{d}s = 0, \\ \int_\Gamma \boldsymbol{\lambda}_C\cdot\delta\boldsymbol{u}_\Gamma\,\mathrm{d}s + \mathbb{A}_G\int_\Gamma \boldsymbol{u}_\Gamma\cdot\delta\boldsymbol{\lambda}_C\,\mathrm{d}s = \boldsymbol{\Lambda}_G^k, \\ \int_\Gamma (\boldsymbol{u}_\Gamma^{k,\frac{1}{2}} - \boldsymbol{u}_G)\cdot\delta\boldsymbol{\lambda}_C\,\mathrm{d}s = 0, \end{cases}$$
  set $(\boldsymbol{u}_G, \boldsymbol{u}_\Gamma, \boldsymbol{\lambda}_C) =: (\boldsymbol{u}_G^k, \boldsymbol{u}_\Gamma^k, \boldsymbol{\lambda}_C^k)$,
- given $(\boldsymbol{u}_G^k, \boldsymbol{\lambda}_C^k; \mathbb{A}_L)$, set
  $$\boldsymbol{\Lambda}_L^k = \mathbb{A}_L\int_\Gamma \boldsymbol{u}_G^k\cdot\delta\boldsymbol{\lambda}_C\,\mathrm{d}s - \int_\Gamma \boldsymbol{\lambda}_C^k\cdot\delta\boldsymbol{u}_\Gamma\,\mathrm{d}s.$$
- if fulfilled, set $(\boldsymbol{u}_G^k, \boldsymbol{u}_L^k, d_L^k, \boldsymbol{u}_\Gamma^k, \boldsymbol{\lambda}_C^k, \boldsymbol{\lambda}_L^k) =: (\boldsymbol{u}_{G,n}, \boldsymbol{u}_{L,n}, d_{L,n}, \boldsymbol{u}_{\Gamma,n}, \boldsymbol{\lambda}_{C,n}, \boldsymbol{\lambda}_{L,n})$ and stop;
  else $k+1 \to k$.

Output: solution $(\boldsymbol{u}_{G,n}, \boldsymbol{u}_{L,n}, d_{L,n}, \boldsymbol{u}_{\Gamma,n}, \boldsymbol{\lambda}_{C,n}, \boldsymbol{\lambda}_{L,n})$ and $\mathcal{H}_{L,n}$.

Mode of operation of the predictor-corrector scheme

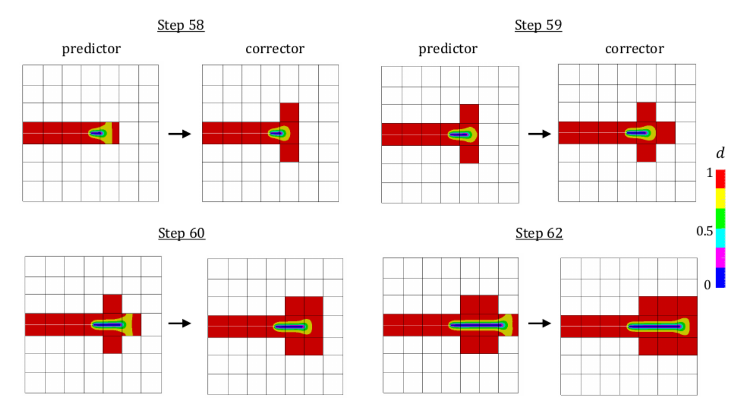

Figure: Mode of operation: predictor-corrector adaptive global-local approach

Heterogeneous L-shaped panel test: configuration

- Original L-shaped panel test based on Dissertation of B.J. Winkler (2001)
- We now add imperfections in parts of the domain

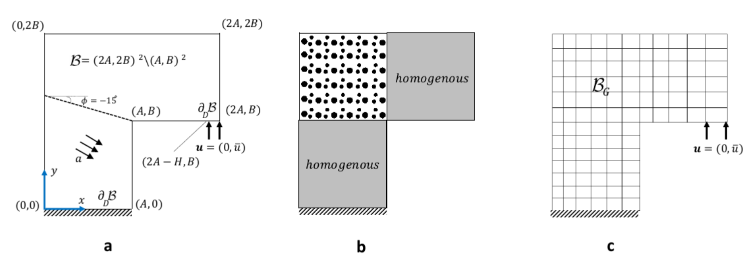

Figure: Heterogeneous L-shaped panel test. (a) Geometry and loading setup with a structural director a inclined under an angle $\varphi = -15$ (b) partitioning of domain into the heterogeneity and homogeneity counterparts and (c) global finite element mesh without potential fictitious zones.

Heterogeneous L-shaped panel test: stress evaluations

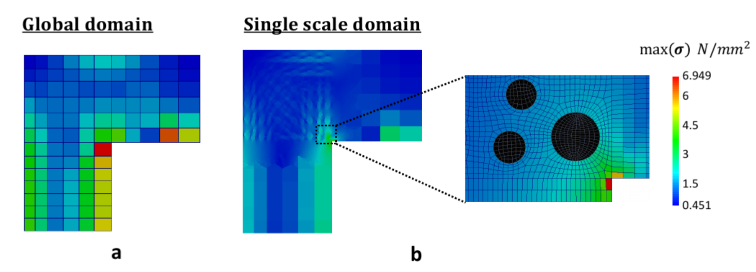

Figure: Maximum stress state in the heterogeneous L-shaped panel test. (a) Global stress state and (b) single scale stress state.

Heterogeneous L-shaped panel test: fracture path

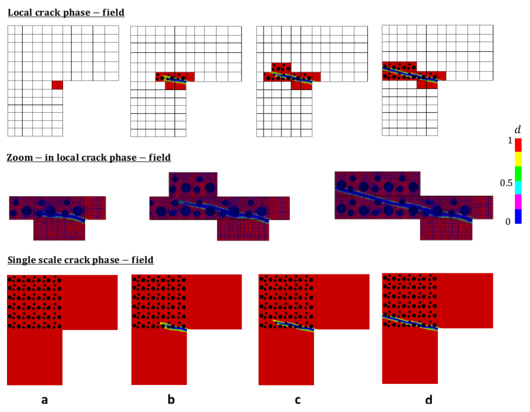

Figure: Crack phase-field pattern for the transversely isotropic heterogeneous L-shaped panel test with fiber direction angle of $\varphi = -15^\circ$. First row: local crack phase-field based on the adaptive scheme; Second row: mesh evolution for local domain by considering the influence of inclusions; Third row: resulting single scale phase-field solution at (a) $\bar{u} = 0.15\ mm$, (b) $\bar{u} = 0.324\ mm$, (c) $\bar{u} = 0.333\ mm$ and (d) $\bar{u} = 0.58\ mm$.

Heterogeneous L-shaped panel test: comparison to a single-scale solution and computational cost

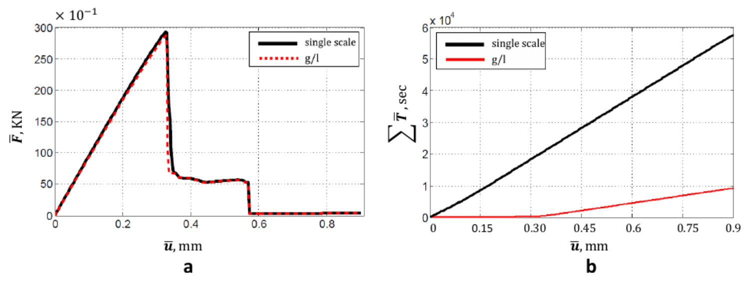

Figure: Heterogeneous L-shaped panel test. (a) Comparison of the load-displacement curves and (b) accumulated time-displacement curves.

Almost done ...

Conclusions

- ✓Examples of nonlinear, coupled PDEs (multiphysics)
- ✓Details on possible interactions and interfaces
- ✓Numerical techniques, coupling algorithms, and simulations; in particular for more than only 2 coupled PDEs
- ✓Towards multiscale phenomena in time and space

Some open questions

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→ Model order reduction (simplifying the equations!)

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5. More validation comparisons between experiments and simulations

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1. **DFG SPP 1962: Optimizing Fracture Propagation Using a Phase-Field Approach**

   `https://spp1962.wias-berlin.de/project.php?projectID=17`

2. **DFG SPP 1748: Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis**

   `https://www.uni-due.de/spp1748/`

3. **FWF project P-29181: Goal-oriented error control for phase-field fracture coupled to multiphysics problems**

   `http://www.numa.uni-linz.ac.at/Research/Projects/P29181/index.shtml`

4. **PhoenixD (funded by the DFG) under Germany's Excellence Strategy within the Cluster of Excellence (EXC 2122)**

   `https://www.phoenixd.uni-hannover.de/`

The End

Thank you so much for your valuable time today!

Thanks a lot to the organizers for this kind invitation
to deliver this lecture here in Strobl!

Questions?

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