ParaPhase: Space–time parallel adaptive simulation of phase-field models on HPC architectures

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ParaPhase

"Space–time parallel adaptive simulation of phase-field models on HPC architectures"

Heike Emmerich
Applications

Carsten Gräser
Numerics

Oliver Sander
Numerics

Robert Speck
HPC

Jiri Kraus
HPC

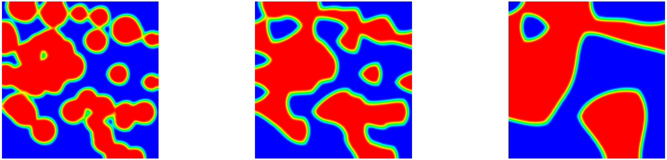
Marc-André Keip
Applications

Phase-field models

- Modelling technique for problem with moving interfaces
- Sharp interfaces are smeared out over a finite width ϵ

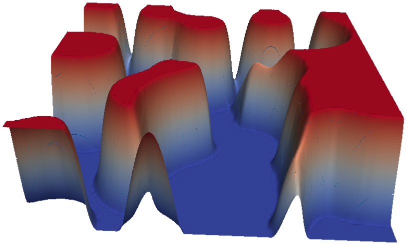
Applications

- Demixing of alloys
- Solidification dynamics
- Viscous fingering
- Fracture formation [Keip, Uni Stuttgart]
- Liquid-phase epitaxy [Emmerich, Uni Bayreuth]



Challenges

- Very localized features
- High grid resolution necessary
- Key phenomena may emerge only for large domains and simulation times



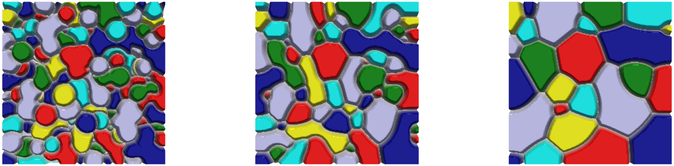
More challenges

- Nonlinear and nonsmooth equations
- Explicit methods: very short time steps
- Implicit methods: Newton-methods work badly, if they work at all

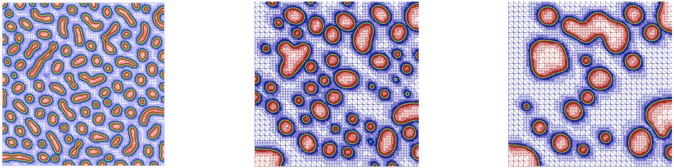
Carsten Gräser, FU Berlin

- Adaptive Finite-Element methods for phase-field demixing problems

Multi-phase Cahn–Hilliard model



Binary Allen–Cahn model



Phase-field models have a common mathematical structure

- Energy functional, e.g.,

$$\mathcal{J}(u) = \int_\Omega \epsilon \|\nabla u\|^2 + \frac{1}{\epsilon}\psi(u)\,dx$$

- Gradient flow

$$\frac{du}{dt} = -\nabla \mathcal{J}(u)$$

- We use implicit time discretization, e.g.,

$$u_{k+1} = u_k - \tau \nabla \mathcal{J}(u_{k+1})$$

- Sequence of non-quadratic minimization problems

$$u_{k+1} - u_k = c_k = \arg\min_c \mathcal{J}_k^{\text{inc}}(c)$$

Nonsmooth multigrid methods [Gräser, Sander]

Increment minimization problems

- Non-smooth parts, but block-separable

$$\mathcal{J}^{\text{inc}}(c) = \mathcal{J}_0(c) + \sum_{i=1}^{m} \phi(c_i)$$

- Frequently convex, or at least close to convex

Nonsmooth multigrid (TNNMG)

- Generalizes standard multigrid to nonsmooth convex minimization problems

Features

- Provable global convergence for strictly convex problems
- No regularization parameters
- Convergence rates independent of the mesh resolution

Project goal

- MPI-parallel implementation

Phase-field models for fracture formation

- Implement TNNMG nonsmooth multigrid for a model of brittle fracture formation
- Model developed and analyzed by Christian Miehe, Stuttgart
- Previously: Operator splitting
- Extend the convergence proof to certain biconvex functionals

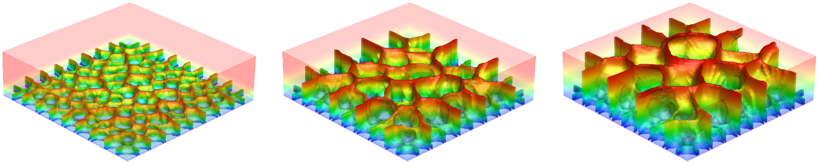


Abb.: Modelling of fracture propagation in dry soil

Phase-field model of brittle fracture

- Unknowns: displacement $\mathbf{u} : \Omega \to \mathbb{R}^d$, fracture phase field $d : \Omega \to [0,1]$
- Elastic bulk energy density $\psi(\mathbf{u}) = \frac{\lambda}{2}(\operatorname{tr} \nabla_{\mathsf{sym}} \mathbf{u})^2 + \mu \operatorname{tr}(\nabla_{\mathsf{sym}} \mathbf{u})^2$
- Regularized crack surface density $\gamma(d) = \frac{1}{2l}(d^2 + l^2 \|\nabla d\|^2)$
- Total energy

$$\Pi(\dot{\mathbf{u}}, \dot{d}) = \int_{\mathcal{B}} \frac{d}{dt}\Big[\big((1-d)^2 + k\big)\ \psi(\mathbf{u}) + g_c \gamma(d)\Big] + I_+(\dot{d})\, dV$$

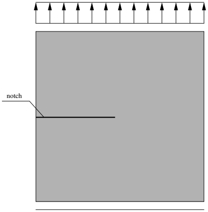
with

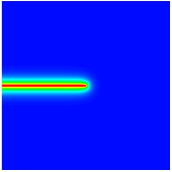
$$I_+(\dot{d}) = \begin{cases} 0 & \text{for } \dot{d} \geq 0 \\ \infty & \text{otherwise} \end{cases}$$

- Time evolution of $\mathbf{u}$ and d are determined by minimization principle

$$\{\dot{\mathbf{u}}, \dot{d}\} = \arg\{\inf_{\dot{\mathbf{u}} \in \mathcal{W}_{\dot{\mathbf{u}}}} \inf_{\dot{d} \in \mathcal{W}_{\dot{d}}} \Pi(\dot{\mathbf{u}}, \dot{d})\}$$

Benchmark problem: square with a notch





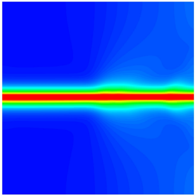
- State-of-the-art solution scheme (Operator split):

STEP (1) Solve $\dot{\mathbf{u}} = \arg\min \Pi(\dot{\mathbf{u}}, \dot{d})$ with $\dot{d}$ fixed

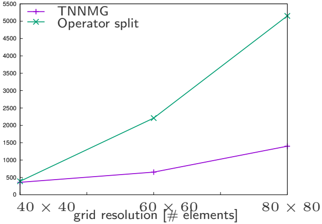
STEP (2) Solve $\dot{d} = \arg\min \Pi(\dot{\mathbf{u}}, \dot{d})$ with $\dot{\mathbf{u}}$ fixed

STEP (3) Repeat!

Comparison of TNNMG and Operator split



Operator split

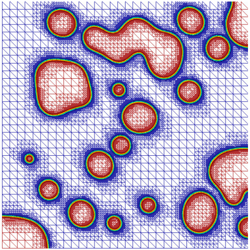


TNNMG

- TNNMG and operator split perform at the same speed for small problems
- With increasing grid resolution, the operator split method needs more and more iterations
- Iteration numbers for the nonsmooth multigrid method remain bounded

The need for grid adaptivity

- Relevant engineering problems demand a fine grid to properly resolve complex crack patterns.
- Uniform grids too expensive $\longrightarrow$ adaptive methods are needed
- Previous work: adaptive phase field simulations for demixing [Gräser]



Project goals

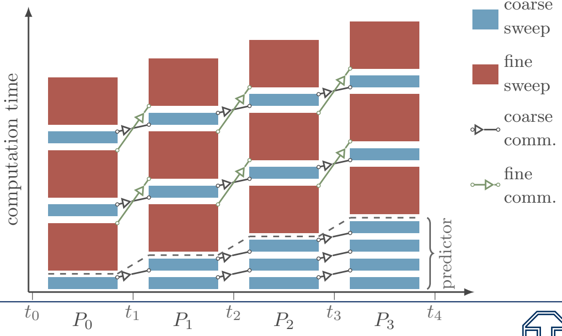
- Nonsmooth multigrid in an MPI-parallel situation for nonlinear/nonsmooth equations
- Dynamic load balancing

Scaling problems

- Dynamic load-balancing will not scale to large processor numbers
- Therefore: parallelize in time!

PFASST: Parallel Full Approximation Scheme in Space and Time [Speck, Jülich]

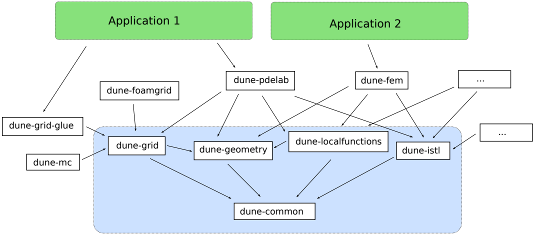
- Parallel-in-time method
- Compute fine and coarse defect problems in parallel
- Related to space–time multigrid
- Expected to integrate nicely with nonsmooth multigrid method TNNMG



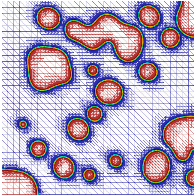
Open-source C++ toolbox for solving partial differential equations

Distributed and Unified Numerics Environment

- Separate libraries for
  - Grids
  - Shape functions
  - Linear algebra
  - etc.

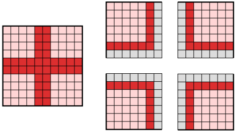


- A great common platform for joint development!



Support for grid adaptivity

- Refinement/coarsening
- Different refinement strategies



Support for distributed computing

- Distributed grids
- MPI communication
- Dynamic load balancing

Vectorization

- Work in progress

SPPEXA

Open-source PFASST implementation [Speck, FZ Jülich]

- C++ implementation of the parallel full approximation scheme in space and time algorithm
- Time parallel algorithm for solving ODEs and PDEs
- Contains basic implementations of the spectral deferred correction (SDC) and multi-level spectral deferred correction (MLSDC) algorithms
- Transparent development through Github: `https://github.com/Parallel-in-Time/PFASST`

(Further) goals

Parallel nonlinear multigrid

- MPI-parallel version of TNNMG
- Dynamic load-balancing

Advanced discretization methods for phase-fields

- Discontinuous-Galerkin discretizations
- Increase arithmetic density
- Towards GPU programming

Parallel-in-time

- Combine PFASST and FE and multigrid
- Apply to simple phase-field equations

Application

- Test the TNNMG method for the brittle-fracture model
- Combine with grid adaptivity
- Extend to ductile materials