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

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“Space–time parallel adaptive simulation of phase-field models on HPC architectures”
Phase-field models

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

Applications

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

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
Previous work: Demixing of alloys

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**

  \[ u_{k+1} - u_{k} = c_{k} = \arg\min_{c} \mathcal{J}^{inc}_{k}(c) \]
Increment minimization problems

- Non-smooth parts, but block-separable

\[ J^{\text{inc}}(c) = J_0(c) + \sum_{i=1}^{m} \phi(c_i) \]

- 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
First results: Nonsmooth multigrid for fracture formation

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

$$\Pi(\dot{u}, \dot{d}) = \int_B \frac{d}{dt} \left[ ((1 - d)^2 + k) \, \psi(u) + gc \gamma(d) \right] + I_{+}(\dot{d}) \, dV$$

with

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

- Time evolution of $u$ and $d$ are determined by minimization principle

$$\{\dot{u}, \dot{d}\} = \arg\{ \inf_{\dot{u} \in \mathcal{W}_\dot{u}} \inf_{d \in \mathcal{W}_d} \Pi(\dot{u}, \dot{d}) \}$$
First results: Nonsmooth multigrid for fracture formation

Benchmark problem: square with a notch

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

STEP (1) Solve $\dot{u} = \arg \min \Pi(\dot{u}, \dot{d})$ with $\dot{d}$ fixed
STEP (2) Solve $\dot{d} = \arg \min \Pi(\dot{u}, \dot{d})$ with $\dot{u}$ fixed
STEP (3) Repeat!
First results: Nonsmooth multigrid for fracture formation

Comparison of TNNMG and Operator split

- 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
Local grid adaptivity

The need for grid adaptivity

- Relevant engineering problems demand a fine grid to properly resolve complex crack patterns.
- Uniform grids too expensive $\rightarrow$ 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
Parallelization in time

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

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

- A great common platform for joint development!
Software infrastructure

Support for grid adaptivity
- Refinement/coarsening
- Different refinement strategies

Support for distributed computing
- Distributed grids
- MPI communication
- Dynamic load balancing

Vectorization
- Work in progress
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