Toward space-time parallel simulations of phase-field models

December 4, 2017 | Robert Speck
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BMBF-Project ParaPhase

High-order space-time parallel phase-field simulations

- interface problems can be modeled with phase-field equations
- wide range of applications, e.g. fracture propagation in ceramics, drying soil etc.
- some key phenomena only emerge when the domain is large and simulation time long enough
- significant computing cost $\Rightarrow$ parallelism in space and time

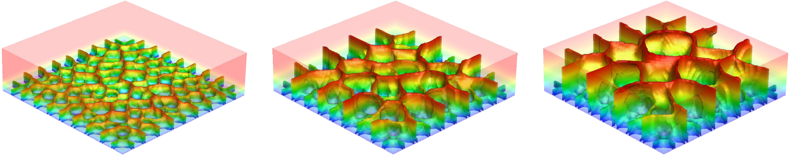

Figure: Modeling of fracture propagation in dry soil

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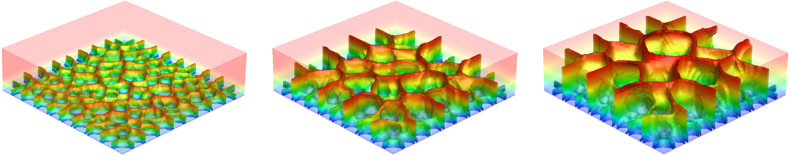

Figure: Modeling of fracture propagation in dry soil

The consortium

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Applications

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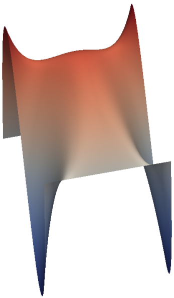
Applications

A very simple toy problem (in space)



Model problem:

$$
\begin{aligned}
-\Delta u &= f \quad \text{on } \Omega := [0,1]^2 \\
u &= g \quad \text{on } \partial\Omega
\end{aligned}
$$

Standard approach: multigrid

- very efficient (mostly)
- supported by a lot of theory
- parallelizable

Parallel multigrid with DUNE

DUNE = Distributed and Unified Numerics Environment

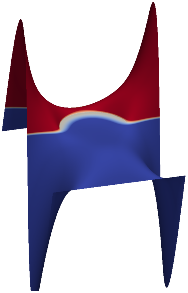
- modular C++ library for the solution of PDEs
- easy implementation of methods like Finite Elements
- slim interfaces, HPC-ready, easy to extend

Parallel multigrid with DUNE

- idea: let core modules handle the parallelization, algorithm should look (more or less) the same
- need: distributed data structures, reduction operations, communication
- allow overlapping and non-overlapping partitioning
- global index for each DoF

A less simple toy problem

Complexity $+=1$



Model problem:

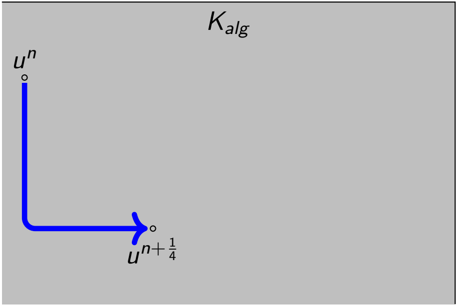
$$\begin{aligned} -\Delta u &= f && \text{on } \Omega := [0,1]^2 \\ u &\leq u_+ && \text{on } \Omega \\ u &= g && \text{on } \partial\Omega \end{aligned}$$

Left: toy problem with

$$u_+(x) = \begin{cases} 0.2 & ||x - x_0|| < r \\ \infty & \text{otherwise} \end{cases}$$

Multigrid for obstacle problems

The TNNMG algorithm



- Pre-smoothing: projected Gauss-Seidel
- Linear multigrid step for reduced problem
- Project on K_{alg}
- Line search to ensure monotonicity

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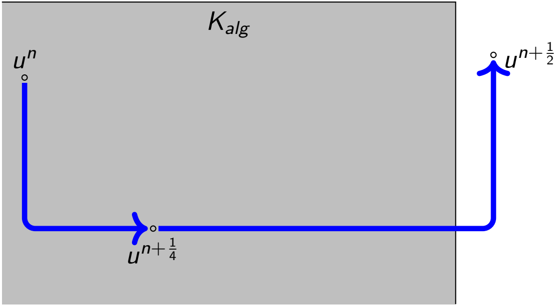

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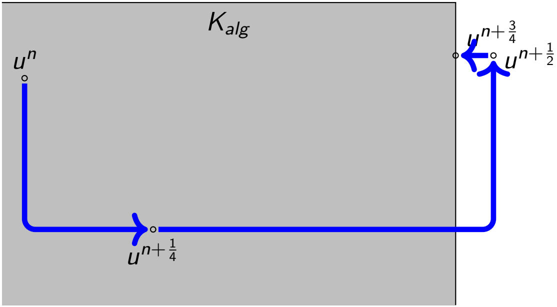

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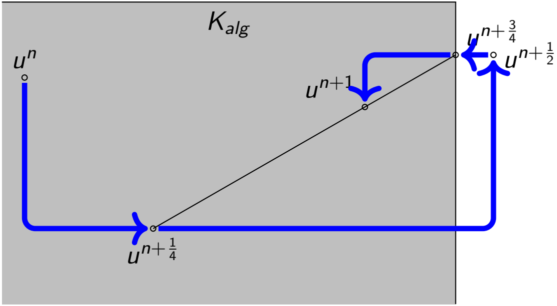

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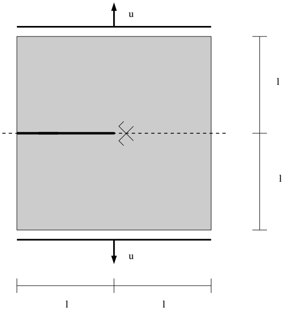
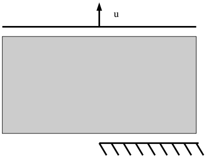
Application: Notched domain under tension

A Boundary Value Problem

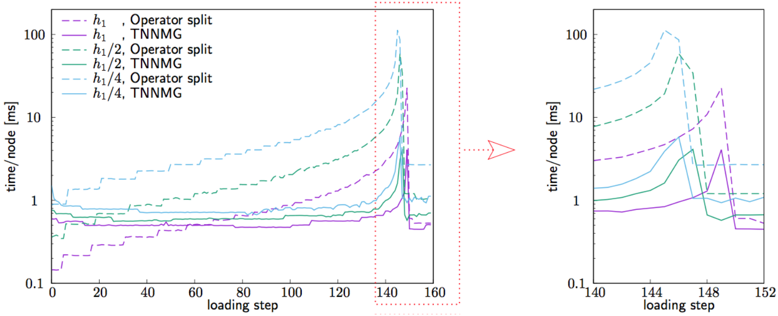




- Single-edge-notched domain under tensile loading
- Only upper half of the specimen is simulated (symmetry)
- Deformation by a linear increasing non-homogeneous Dirichlet boundary condition at the top

Application: Notched domain under tension

TNNMG vs. standard operator splitting



Adding time

Complexity $+= 1$

What if our problems are time-dependent?

- example: Allen-Cahn or Cahn-Hilliard equations: diffuse interface model for phase transition and separation phenomena
- TNNMG allows semi- or fully implicit time-stepping with provable convergence
- parallel TNNMG = parallelization in space for time-dependent phase-field problems

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Are we done, then?

Limits of purely spatial parallelization

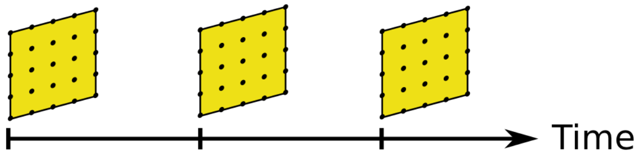

Figure: Time-stepping to solve time-dependent partial differential equations.

- Spatial parallelization reduces runtime **per time-step**
- Strong scaling saturates eventually because of communication
- Costs for **more time-steps** are not mitigated

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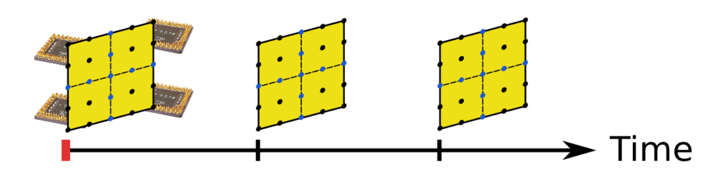

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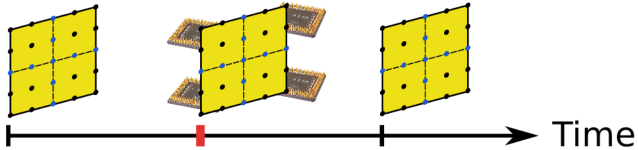

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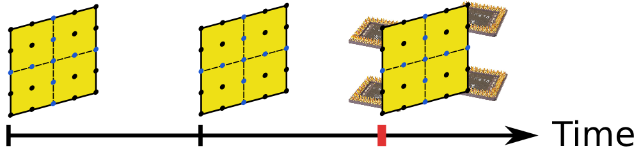

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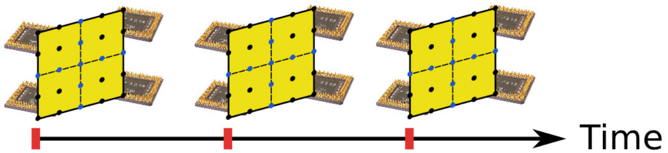

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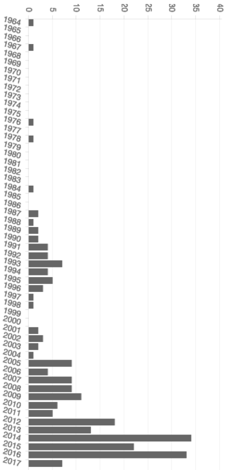
→ Can we compute multiple time-steps simultaneously?

Parallel-in-Time (“PinT”) approaches

“50 years of parallel-in-time integration”, M. Gander (2015)

- Interpolation-based approach (Nievergelt 1964)
- Predictor-corrector approach (Miranker, Liniger 1967)
- Parabolic or time multi-grid (Hackbusch 1984) and (Horton 1992)
- Multiple shooting in time (Kiehl 1994)
- Parallel Runge-Kutta methods (e.g. Butcher 1997) and extrapolation (Richardson 1910)
- Parareal (Lions, Maday, Turinici 2001)
- PITA (Farhat, Chandesris 2003)
- Guided Simulations (Srinavasan, Chandra 2005)
- RIDC (Christlieb, Macdonald, Ong 2010)
- PFASST (Emmett, Minion 2012)
- MGRIT (Falgout et al 2014)



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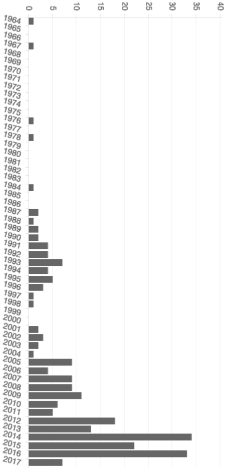

A quick algebraic introduction to PFASST

Basic building block: spectral deferred corrections (SDC)

Consider the Picard form of an initial value problem on $[T_n, T_{n+1}]$

$$u(t) = u_0 + \int_{T_n}^{t} f(u(s))ds,$$

discretized using spectral quadrature rules with nodes t_m:

$$u_m = u_0 + \Delta t QF(u) \approx u_0 + \int_{T_l}^{t_m} f(u(s))ds,$$

then SDC methods can be seen as (approximative) Gauss-Seidel iteration to solve this collocation problem for all u_m.

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$\Rightarrow$ Use this for block smoothing in space-time multigrid = PFASST

A quick algebraic introduction to PFASST

Parallel Full Approximation Scheme in Space and Time

We now glue L time-steps together, using N to transfer information from step l to step $l+1$. We get:

$$\begin{pmatrix} I - \Delta t QF & & & \\ -N & I - \Delta t QF & & \\ & \ddots & \ddots & \\ & & -N & I - \Delta t QF \end{pmatrix} \begin{pmatrix} \vec{u}_1 \\ \vec{u}_2 \\ \vdots \\ \vec{u}_L \end{pmatrix} = \begin{pmatrix} \vec{u}_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

PFASST:

- use (linear/FAS) multigrid to solve this system iteratively
- fine-level smoother: parallel block Jacobi with SDC in the blocks
- coarse-level: serial block Gauß-Seidel with SDC in the blocks

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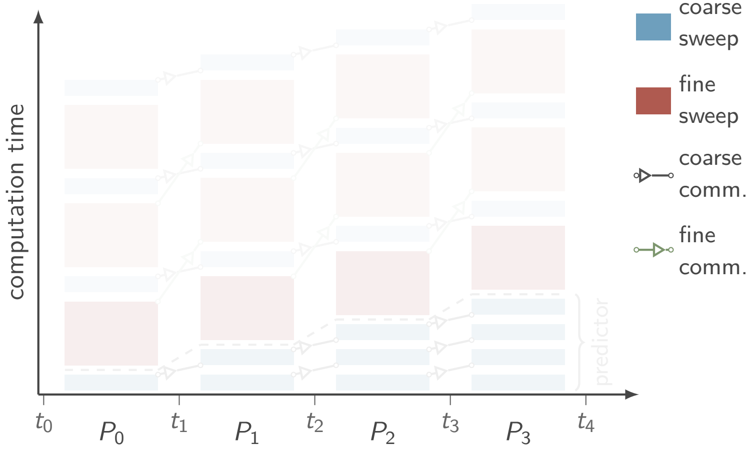
A quick visual introduction to PFASST



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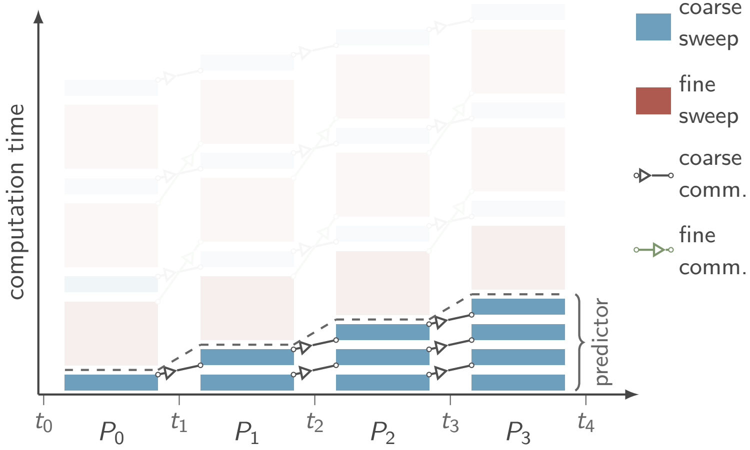

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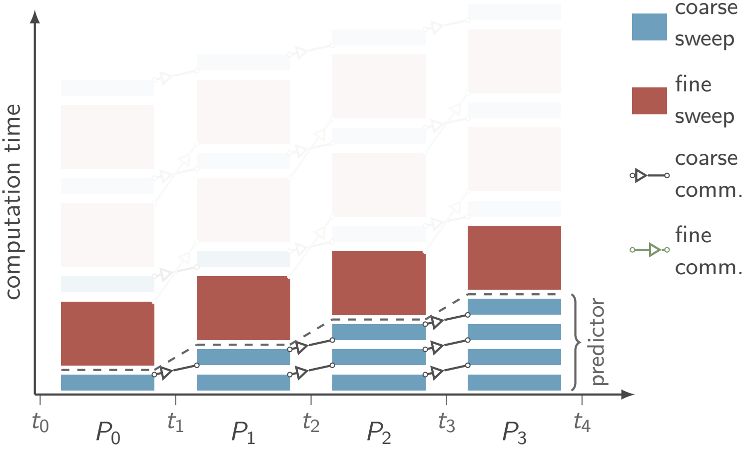

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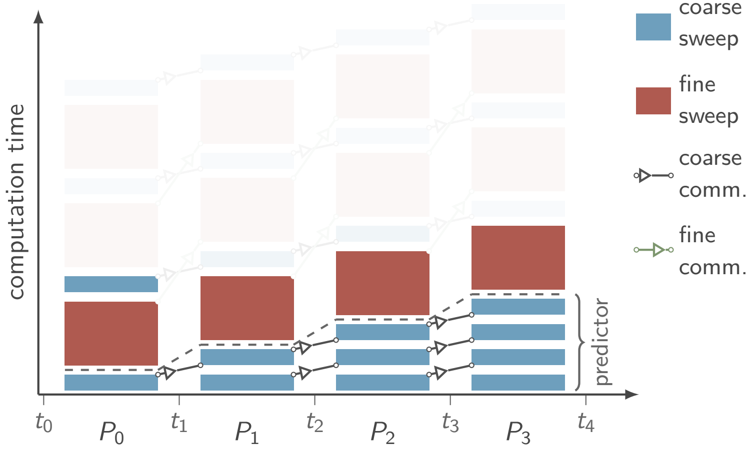

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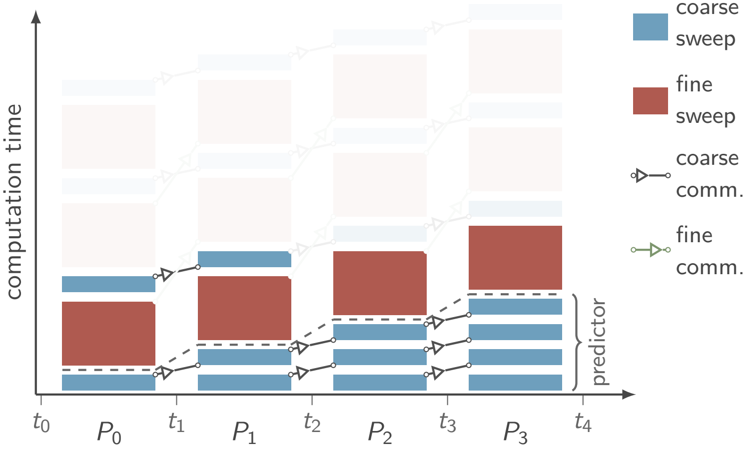

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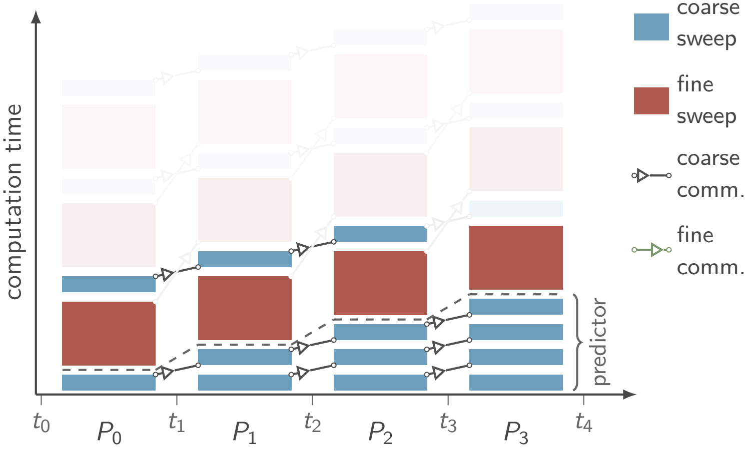

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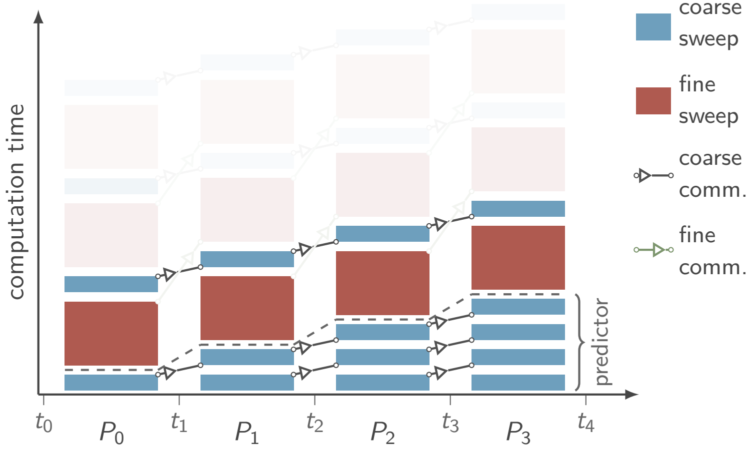

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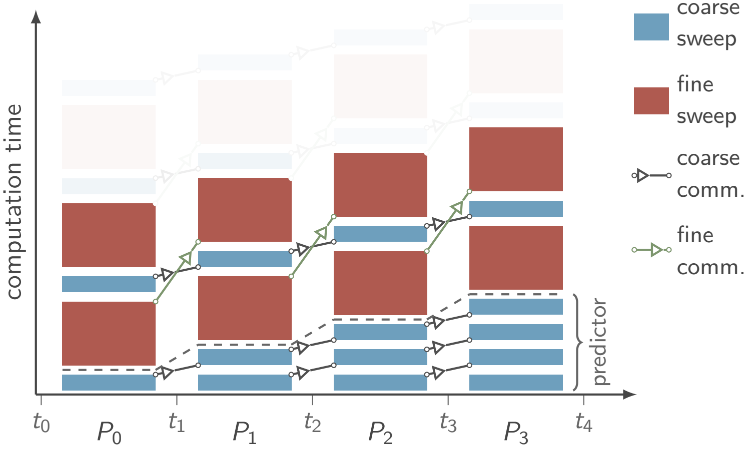

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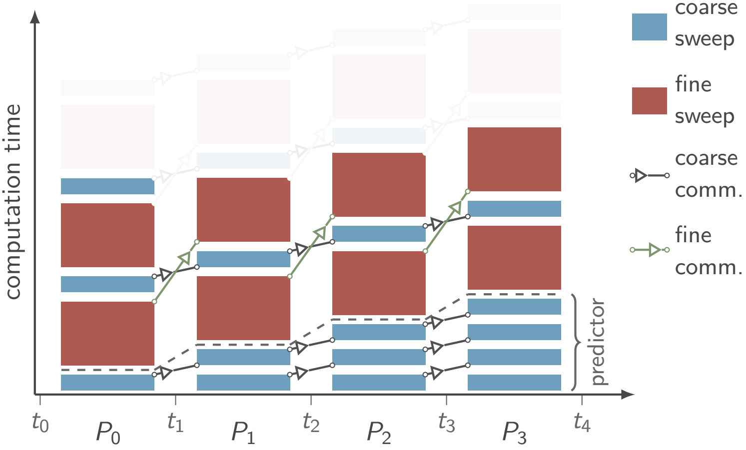

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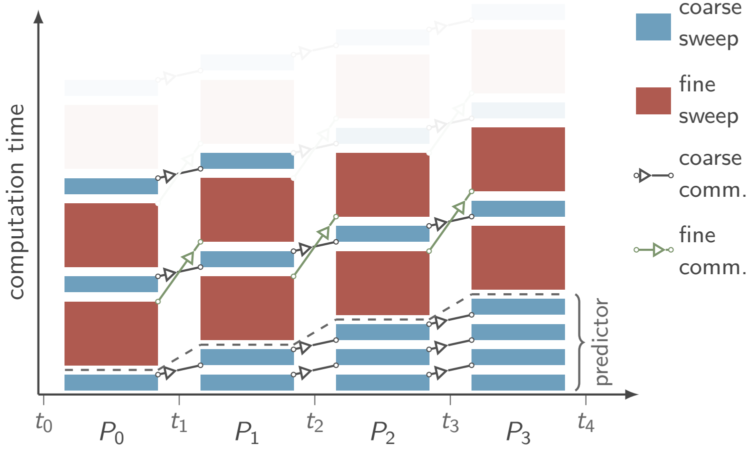

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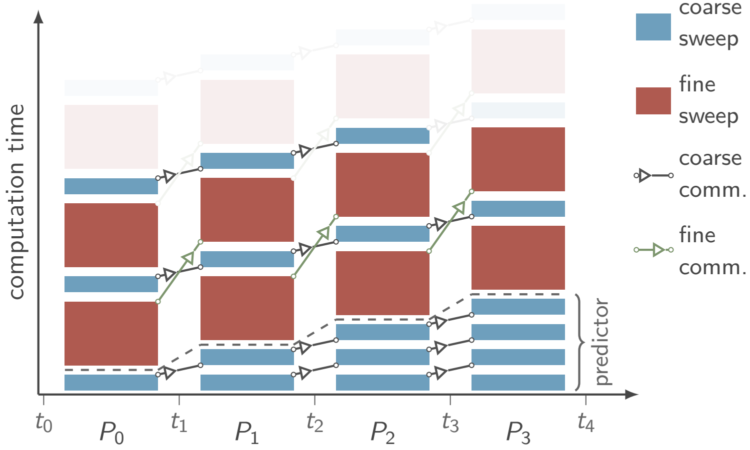

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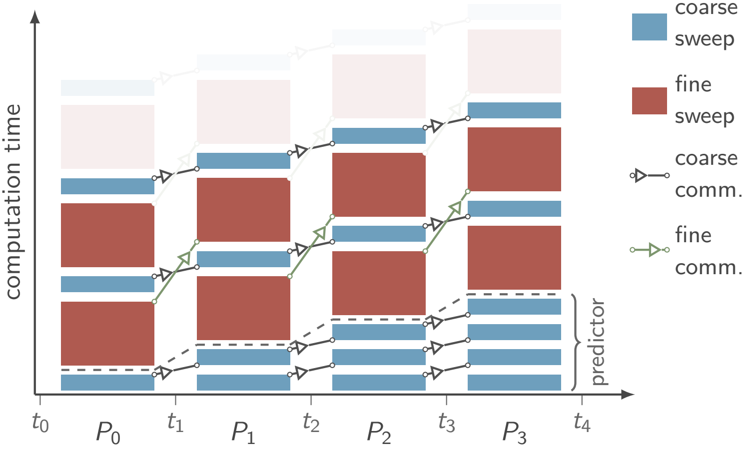

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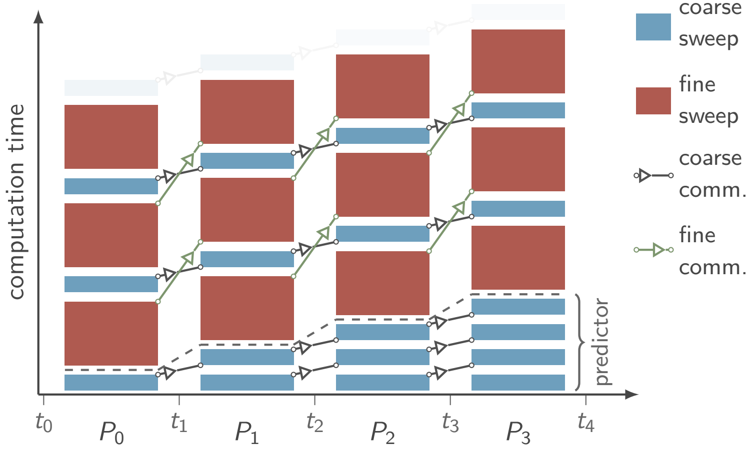

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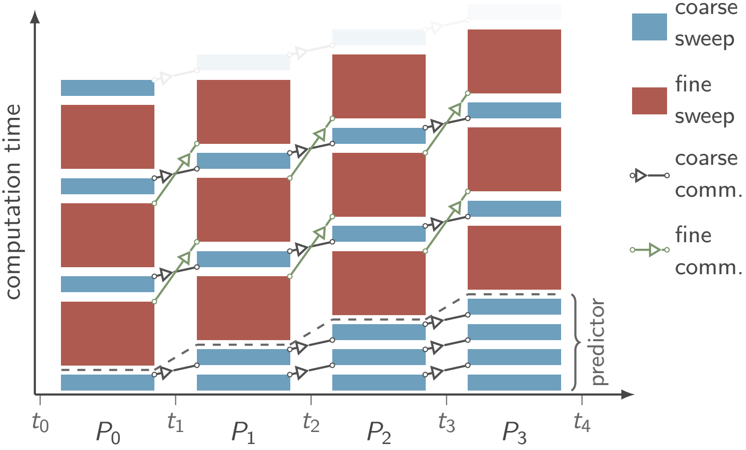

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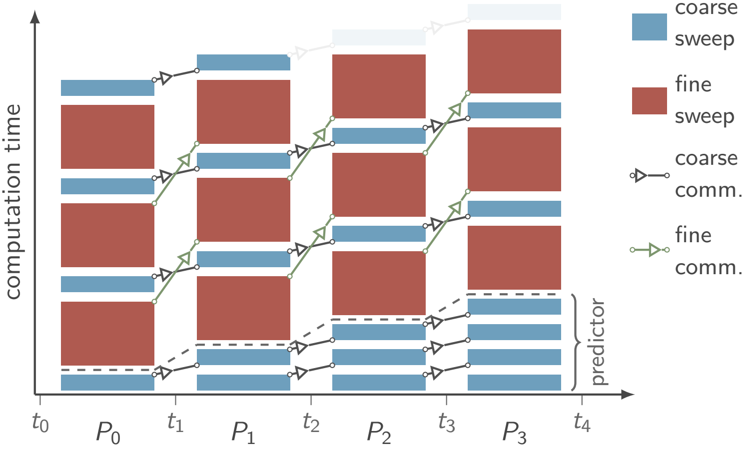

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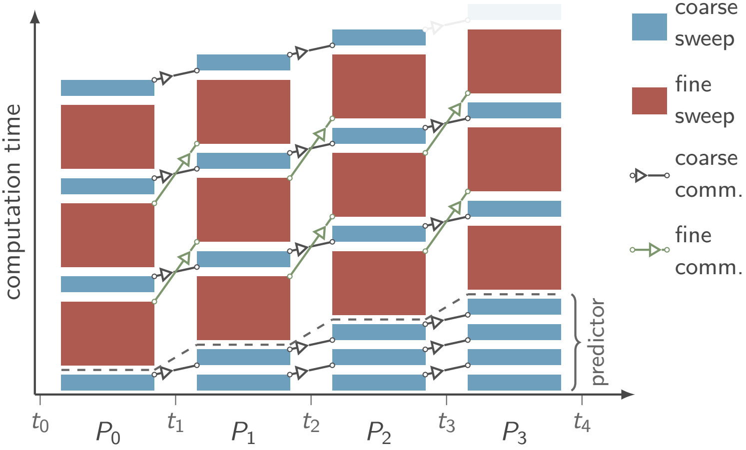

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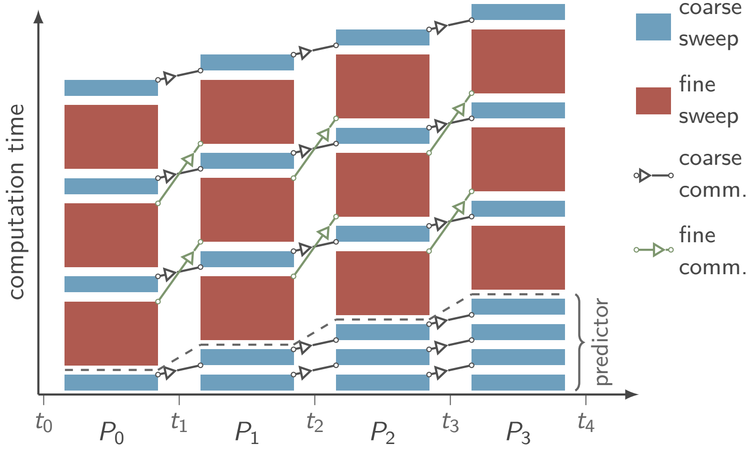
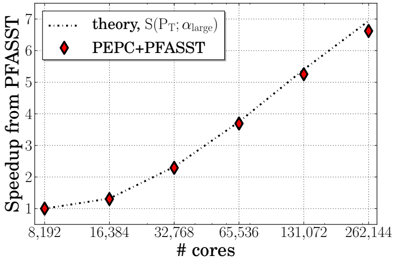
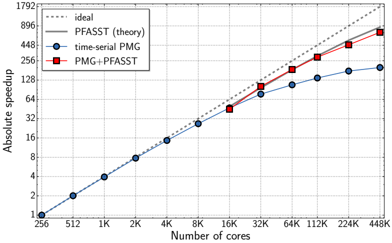


Examples: vortex particles and space-time multigrid



- vortex particles with Barnes-Hut tree code in space
- reduced force calculation on coarse level

→ 7x additional speedup



- 3D heat equation with multigrid solver in space
- coarsening via reduction of grid points and discretization order

→ 4x improved speedup

And phase-field problems?

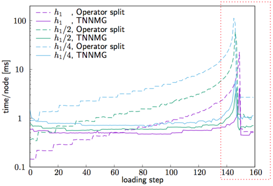
Done

- PFASST in time and finite elements in space ☑
- dune-PFASST: a DUNE module for parallel-in-time integration ☑
- PFASST for reaction diffusion problems, e.g. Allen-Cahn ☑
- coupling of PFASST in time with (serial) TNNMG in space ☑

To-do

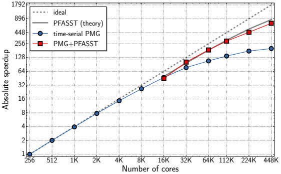
- coupling of PFASST with space-parallel solver ☐
- non-smooth problems ☐
- adaptivity in space and time ☐

Three takeaways



Parallel TNNMG method provides reliable and efficient solver for phase-field problems

Parallel-in-Time integration (PinT) can help to extend prevailing scaling limits



images/lego-pile.jpg

Space-time parallelization within **DUNE** leaves us with a ton of things to play with

The PinT Community

To learn more about PinT check out the website

`www.parallelintime.org`

and/or join one of the PinT Workshops, e.g.

7th Workshop on Parallel-in-Time Integration

- May 2-4, 2018
- Roscoff, France
- by Yvon Maday et al.

Also, there is a mailing list, join by writing to

`parallelintime+subscribe@googlegroups.com`

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