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SUPPLY of ELECTRICITY

In cooperation with the CTI

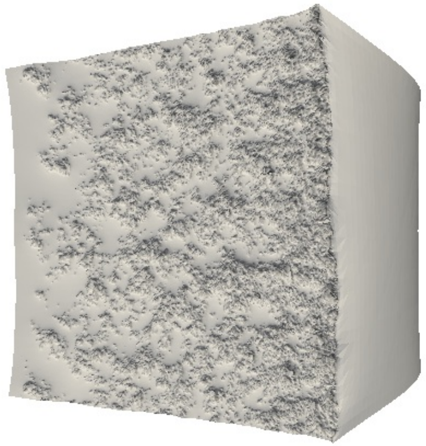
Energy
Swiss Competence Centers for Energy Research

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Commission for Technology and Innovation CTI

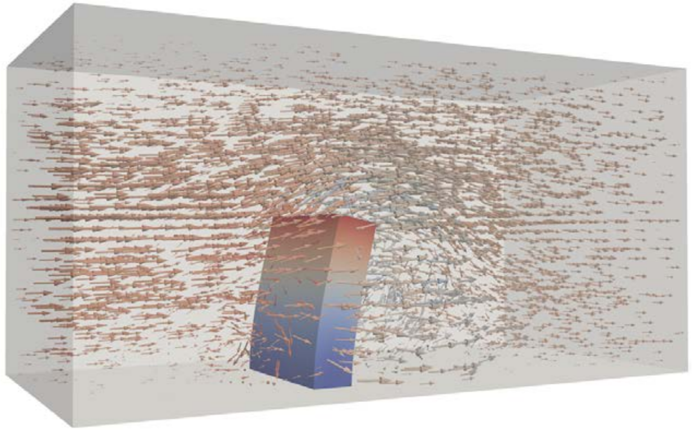
High-end modeling requirements for the energy sector



R. Krause

A, Rigazzi, R. Müller, P. Zulian, T. Dickopf, C. v. Planta. M. Favino, J. Steiner, R. Müller

Institute of Computational Science
USI, Lugano



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4.3 Modeling Facility at USI

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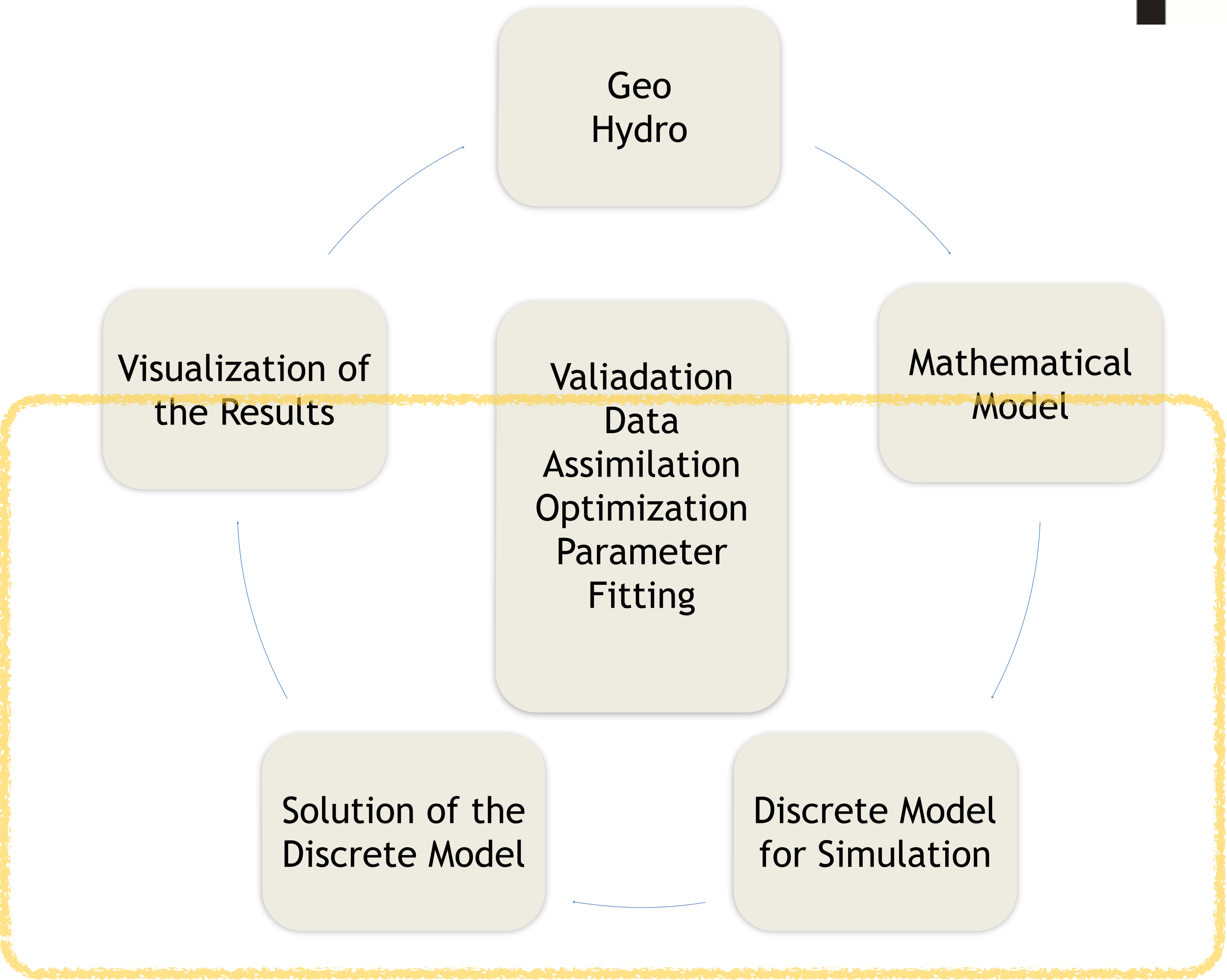
- Alessandro Rigazzi (PostDoc, SCCER-SoE)
- Cyrill von Planta (PhD student, NRP 70)
- Roger Müller (PostDoc, SPP 1748)
- Hardik Kothari (PhD student, SNF/DFG)
- Alessio Quaglino (PostDoc, SERI)

- **NFP 70 "Energiewende"** "Modelling permeability and stimulation for deep heat mining" with T. Driesner (ETH); S. Miller (Neuchâtel)
- **SNF/DFG Schwerpunktprogramm SPP 1748** Project on "Large-scale simulation of pneumatic and hydraulic fracture with a phase-field approach" (Prof.Dr. K. Weinberg (Universität Siegen; Priv.- Doz. Dr. C. Hesch (KIT, Karlsruhe); **SPP 1748 "Reliable simulation techniques in solid mechanics. Development of non-standard discretization methods, mechanical and mathematical analysis"**.
- **SERI (Swiss Space Office)** "Phase unwrapping Parallel Accelerator (PUPAx) " together with P. Pasquali (sarmap, TI)
- **SNF/DFG project** "Parallel multilevel solvers for coupled interface problems" with Prof. Dr. A. Reusken (RWTH Aachen) and Dr. S. Groß (RWTH Aachen).
- **Industry project with Siemens** on Uncertainty Quantification

The Simulation Wheel



Computational Science and HPC

Challenges in HPC and Numerical Simulation

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- **Forward Models**
  - Fluid/Solid Mechanics
  - Multi-scale Models
  - Coupled Models (FSI, THM, …)
- **Inverse Models**
  - Parameter/geometry Identification
  - Subsurface flow
- **Large scale: HPC**
  - High resolution
  - Massively parallel
  - Hardware/Software co-design (GPUs, hybrid systems)
  - New methods (time parallel …)
- **Reducing response time**
  - Reduced basis
  - Reduced scale physical model
- **Constrained Optimization**
  - Range of Operation/Efficiency
  - Data assimilation
- **UQ - Uncertainty Quantification**
  - Communication of Results
  - Parameter Sensitivity
- **Free Interfaces and Surface Effects**
  - Contact and Fracture / Erosion
  - Multi-scale approaches
  - Mesh handling
- **Workflow**
  - Simulation - Experiment - Validation - Application
  - Geometry handling, meshing
  - Merging of Data and Simulation: Data driven simulation
- **Software Development and Maintenance**
  - Usability/Maintenance

Challenges in HPC
"Do not save flops, save energy"

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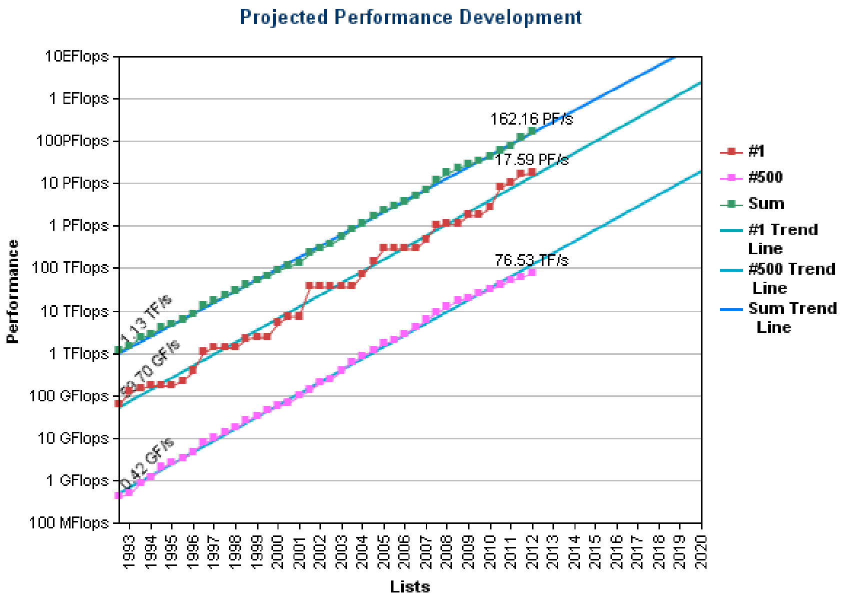
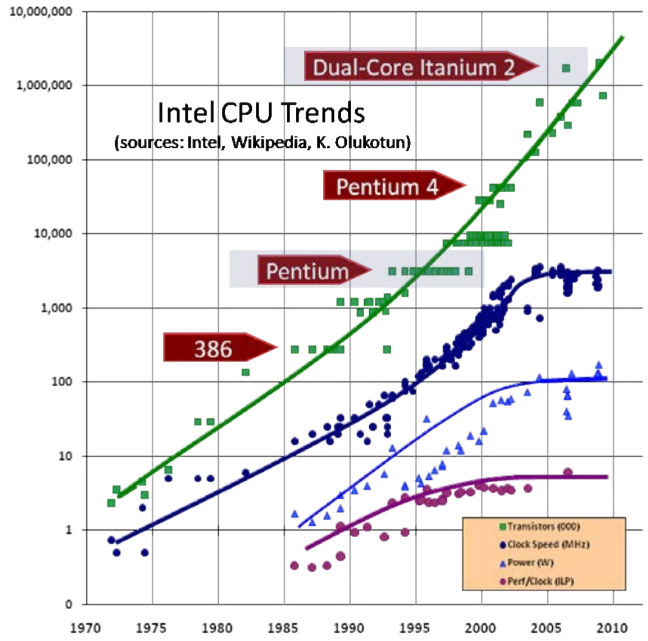


(a) From `http://www.top500.org`



(b) Courtesy of H. Sutter. `http://www.gotw.ca/`

- Accessing data is more energy intensive than computation
- Moving data over large distances takes more time and more energy
- Current hardware is not designed for numerical simulation (many applications run at 2%-5% of peak performance)
- Algorithms have to be adapted:
  - Hardware/software co-design
  - High concurrency (EXASCALE)
  - Increased arithmetic density
  - Asynchronous methods
  - Parallelism in time
  - Adaptivity

How to exploit modern HPC systems?

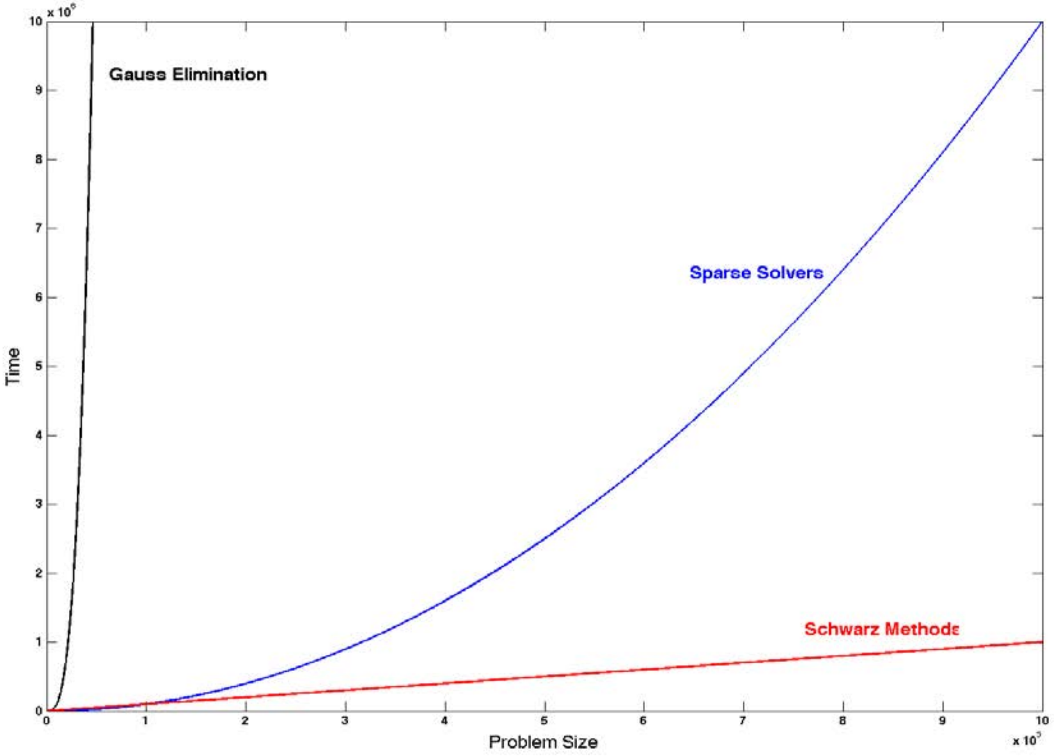
The Supercomputing Paradox Faster hardware can slow you down

- Gaußian elimination $O(n^3)$
- Gaußian elimination for sparse Matrices: $O(n^2)$
- Schwarz methods: $O(n)$

n: problem size

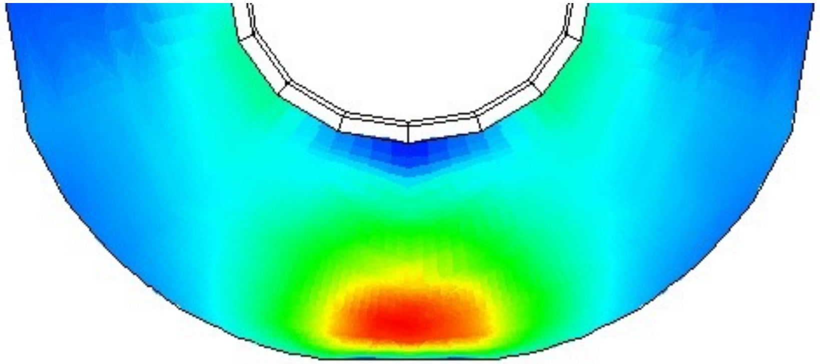
n → 2n

n^3 → $2^3 n^3 = 8n^3$

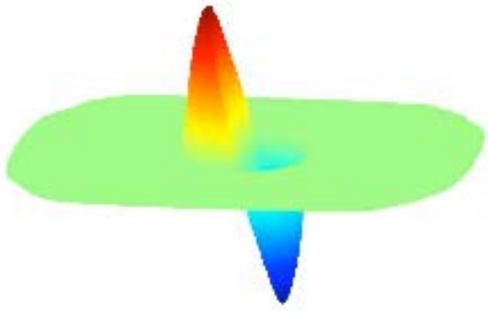


For increasing problem size, methods without optimal complexity will lead to unacceptable computation time.

Efficient Solvers for frictional contact with Finite Elements



von Mises stress



Frictional stresses on the surface

Linear sparse solver pardiso

#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

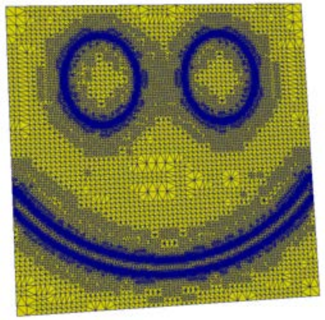
Non-smooth Multigrid for frictional contact [K' 01]

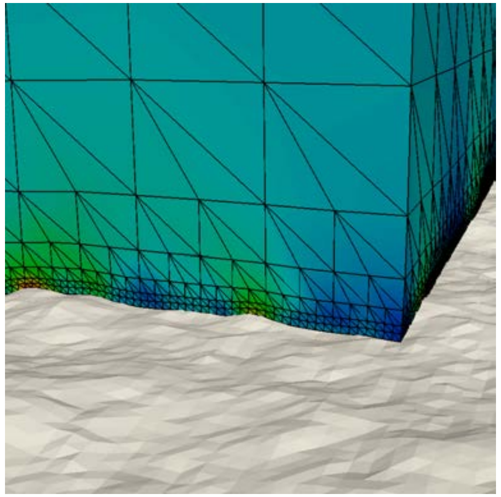
$\mathcal{F} = 0.3$, $\mathrm{TOL} = 10^{-12}$

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

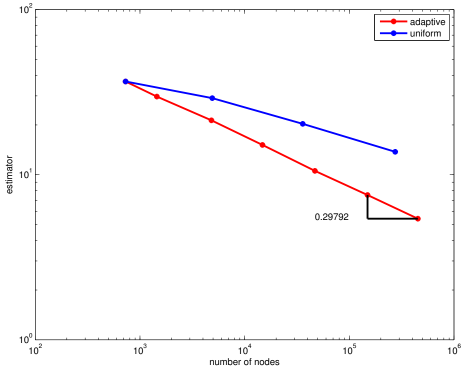
Optimal solvers (right) allow for treating larger problems

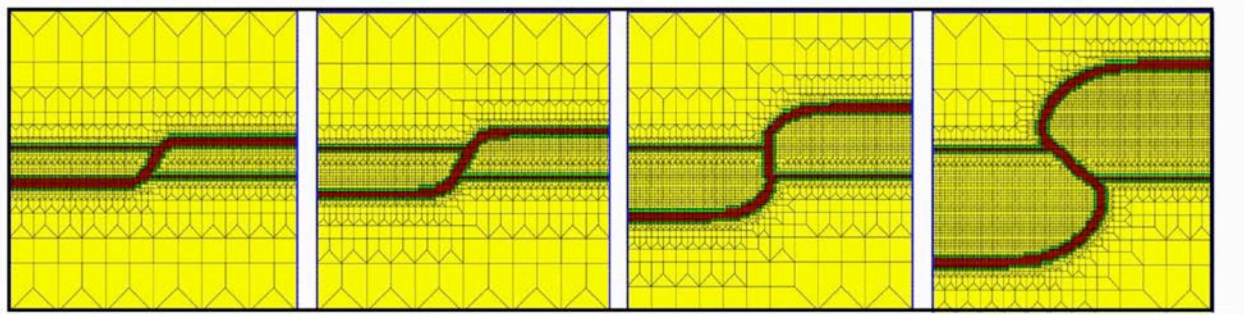
Resolve local effects I- Adaptivity Reliability and Efficiency





Adaptive refinement for contact with a rough surface
[Rigazzi, K' 14]





A posteriori error estimator for contact problems
Adaptive refinement for contact with a "smiley"
error for uniform and adaptive refinement
Sharp upper and lower estimates
[Veeser, Walloth, K' '12]

Adaptive refinement for a time dependent phase field model
[K', Kornhuber '06]

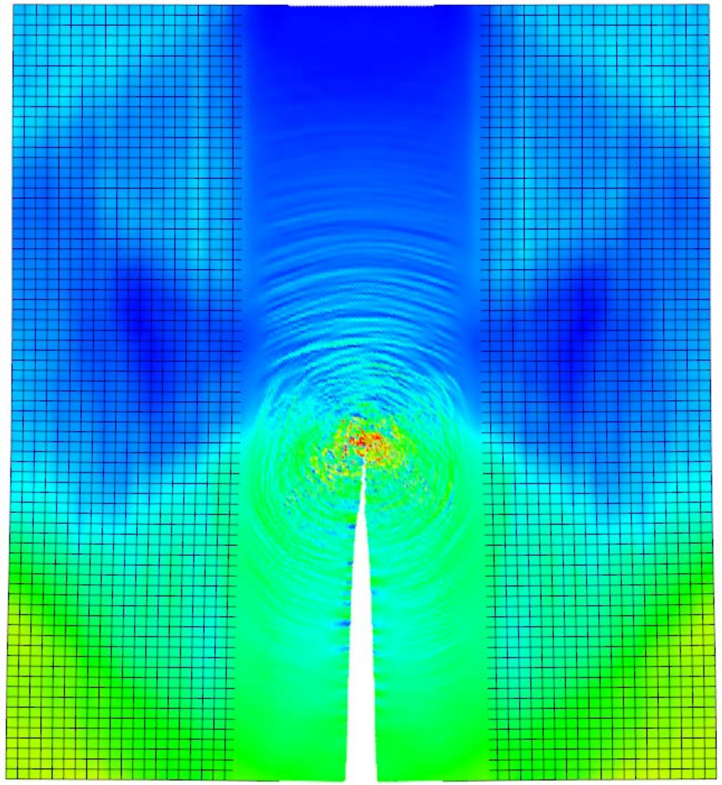
Resolve local effects II
Multiscale Modeling for Fracture

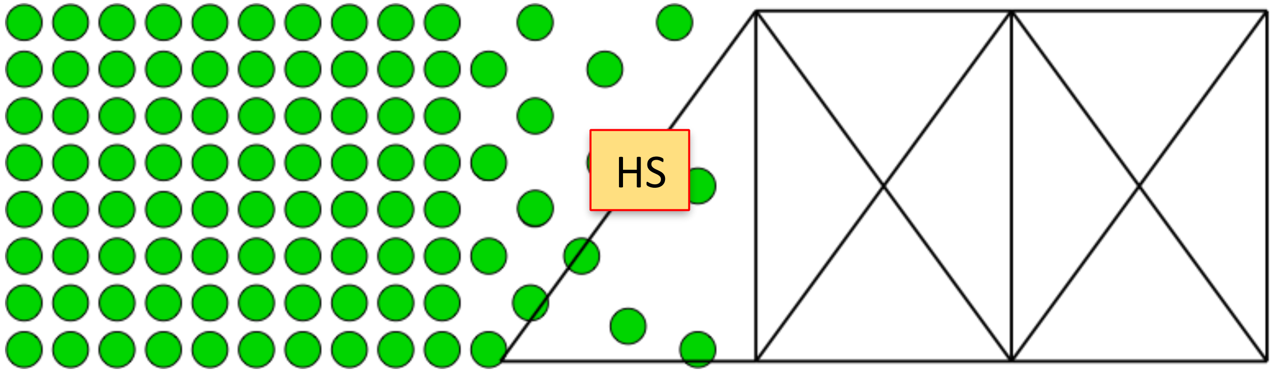
- Finite element method (mostly used)
- Meshless methods (Promising (E.G. Ortiz, Caltech))

Different FE approaches

1. simple models: change of elasticity modules in the body
   - not enough details
   - lost directionality of cracks
   - homogenization techniques remove the discrete nature of cracks
2. Single mesh approach
   - Crack propagates along mesh edges, duplication of nodes
3. adaptive remeshing techniques
   - usually employes different meshes for domain and crack
4. Extended FE methods
   - the discontinuity is not limited to interelement boundaries
   - additional displacement degrees of freedom are introduced but not additional mesh verteces

Multiscale Modeling for Fracture Micro (MD) and Macro (FE)





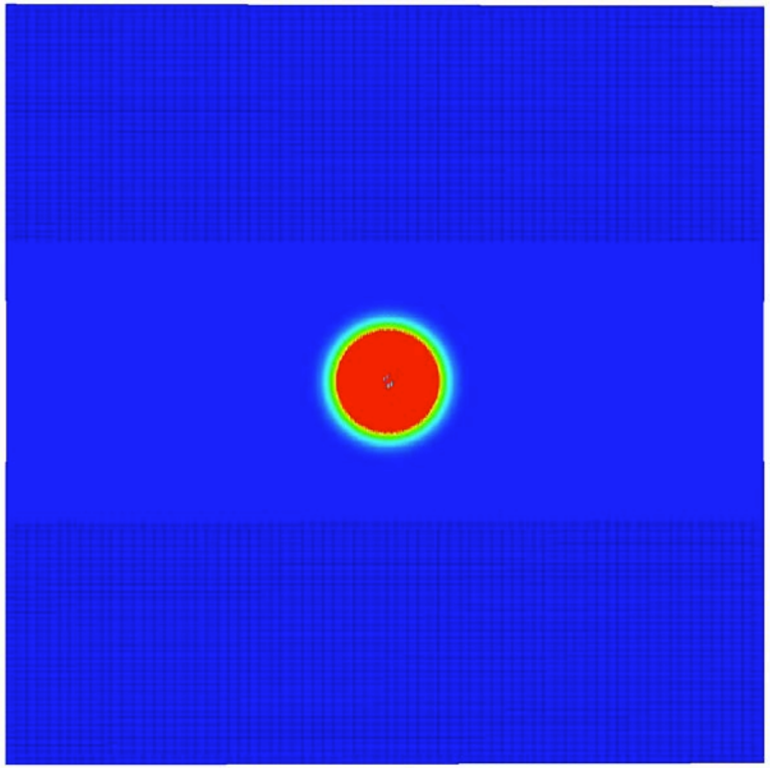
- Hamiltonian $H_{tot} = \alpha h + (1-\alpha)H$ e.g. [Ben Dhia 98, Xiao & Belytschko 04]
- Localized constraints $\boldsymbol{g}(\boldsymbol{u},\boldsymbol{U}) = 0$

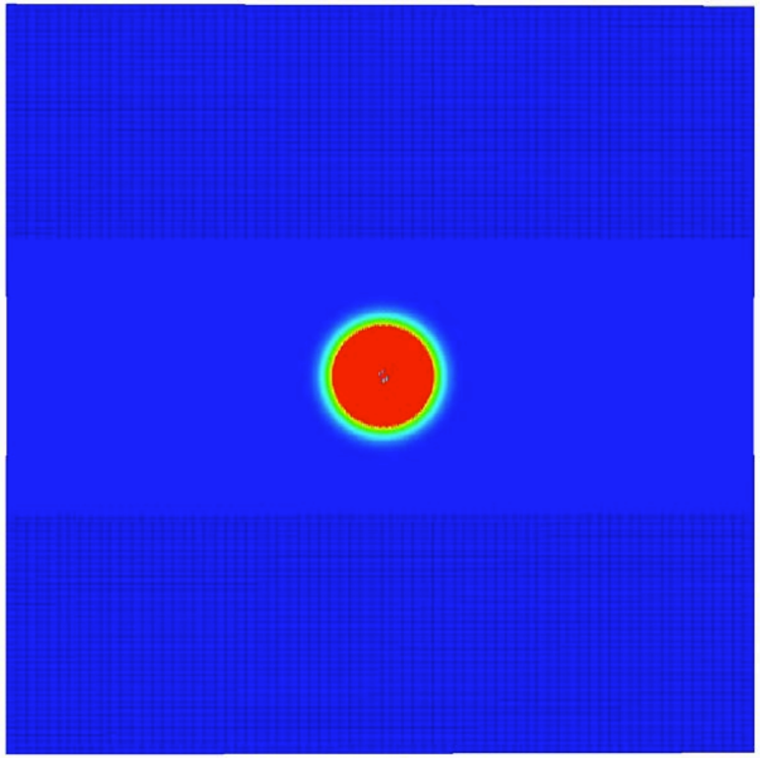
MD displ $\in \mathbf{R}^{3N}$ FE displ $\in H^1$

- Introduce Lagrange multiplier $\lambda \in M$: $H_{tot} = \alpha h + (1-\alpha)H + \lambda \cdot \boldsymbol{g}$
  Differential Algebraic Equations

Multiscale Coupling
Molecular Dynamics - Finite Elements

- Scale transfer can lead to pollution effects at the interface
- Our approach: variational transfer (discrete L^2 projection) and PML at the interfaces





- RATTLE with $\tau = 0.005$
- Damping at interface
- Lennard-Jones Potential with $\varepsilon = 1, \sigma = 1$ and linear elasticity

[K. Fackeldey, D. Krause, R. Krause 2008]

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Crack - Multiscale Simulation
MD - FEM

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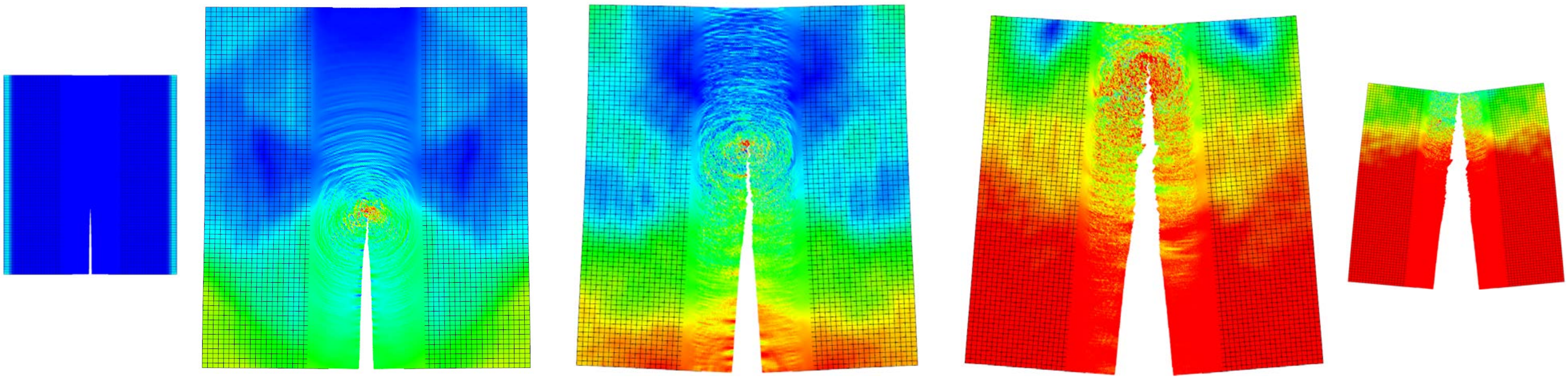


- Resolve crack-tip region with molecular dynamics (MD) simulation
- MD region must follow crack (adaptively) or must be chosen sufficiently large (a-priori)
- But: branching/bifurcation, emission of line dislocations, … destroy locality
- Huge computational demand
- Complex coding, load balancing difficult

[D. Krause, R. Krause 2009]

Phase Field Approach for Fracture

Introduce free energy for damage parameter d

1-d crack formation

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

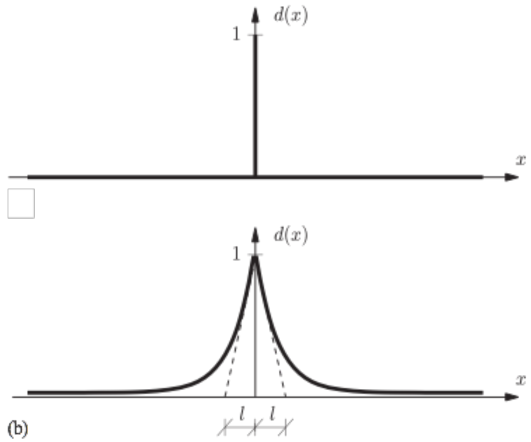
This solves the diff. equation:

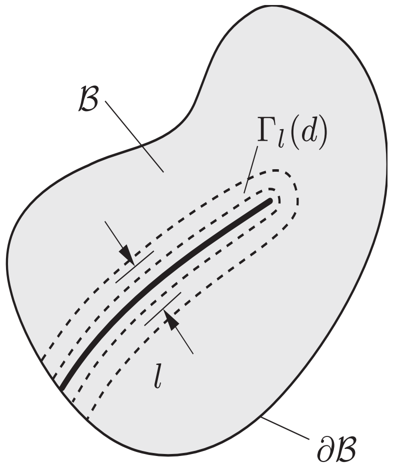
$$d(x) - l^2 d''(x) = 0$$

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

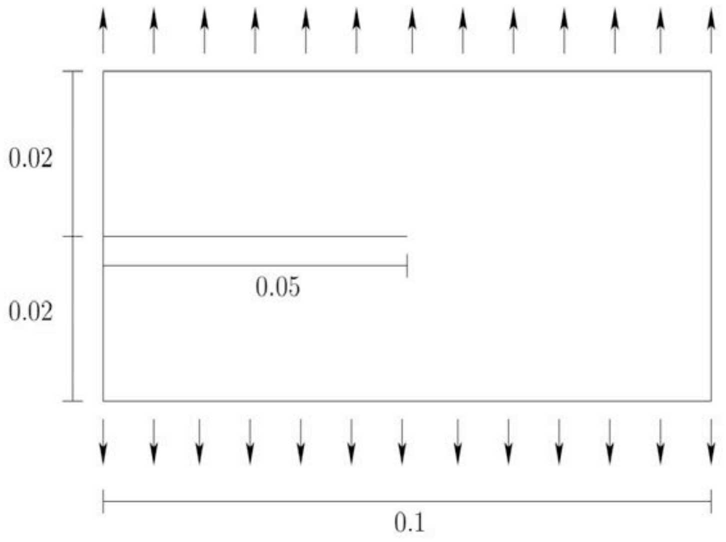
$$I(d) = \frac{1}{2}\int_B \{d^2 + l^2 d'^2\} dV$$

in 3D $\Gamma_l(\mathbf{d}) := \int_B \frac{1}{2l}\mathbf{d}^2 + \frac{l}{2}\nabla(\mathbf{d}) \cdot \nabla(\mathbf{d}) dV$

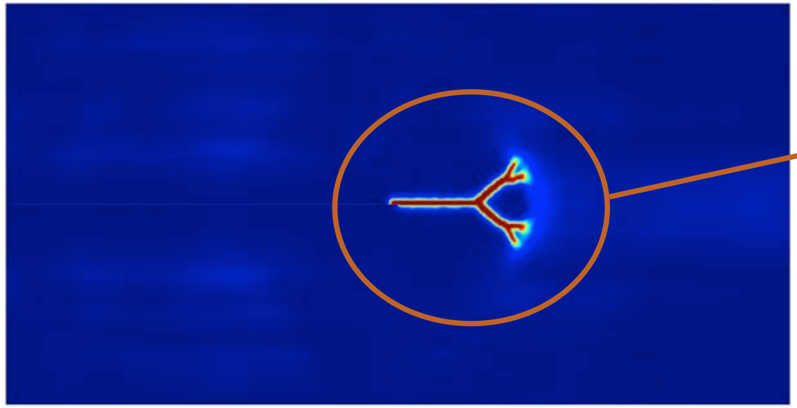


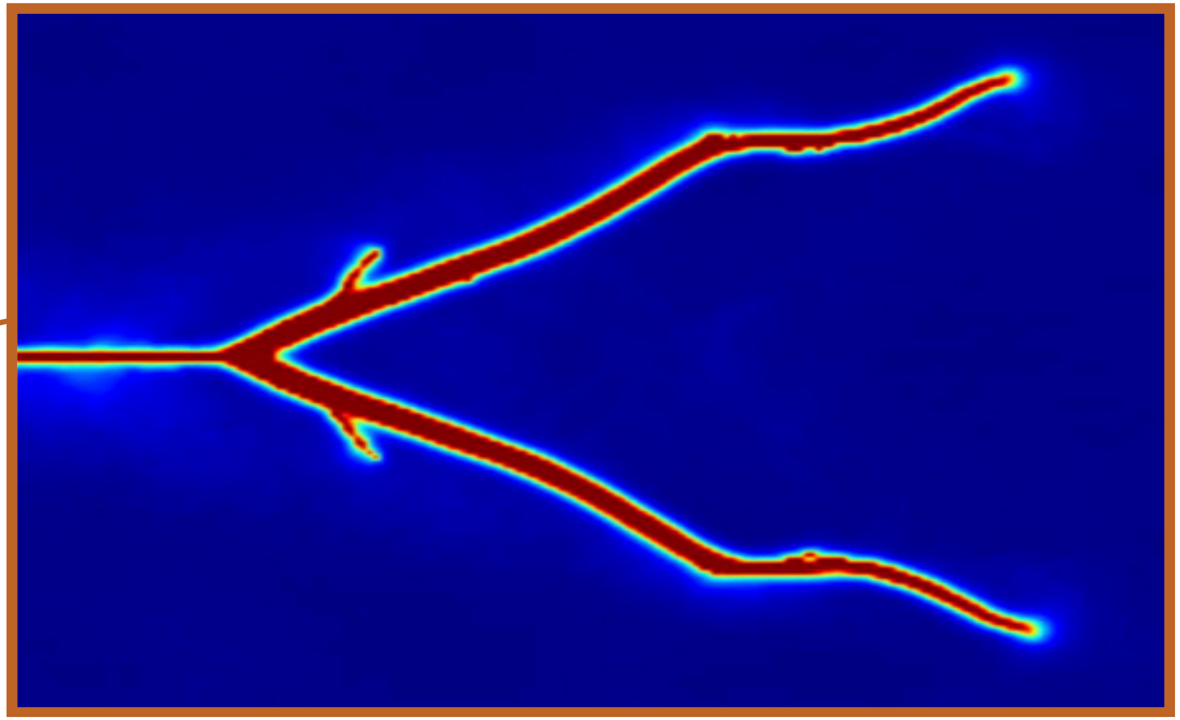


Phase Field Models for Fracture



- Coupling of phase field model (damage field) and elastic material
- Fine but structured mesh for the damage parameter
- Unstructured mesh for the displacements/stresses
- snf/DFG project [Weinberg, Hesch, Krause] within “DFG-Schwerpunktprogramm SPP 1748”

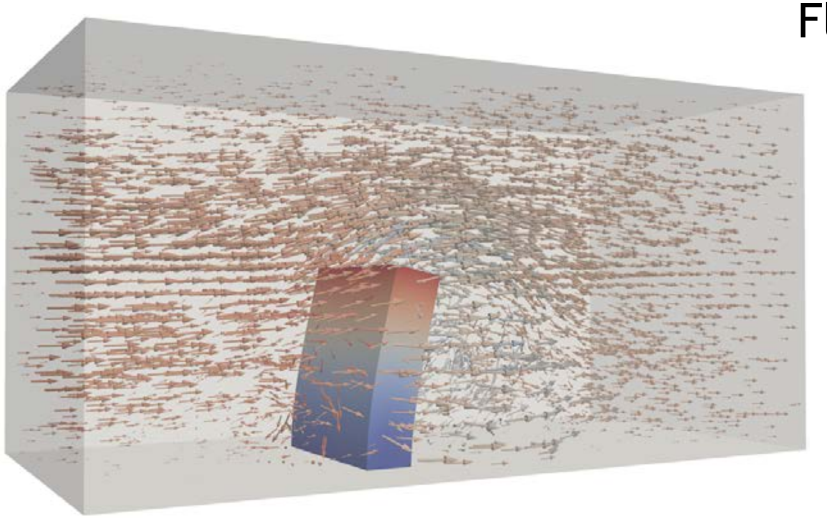




Pictures from: C. Hesch, K. Weinberg; *Int. J. Numer. Meth. Engng*. **99**(1097), 2002

Exploiting Parallelism: Solution Methods

Coupled Problems

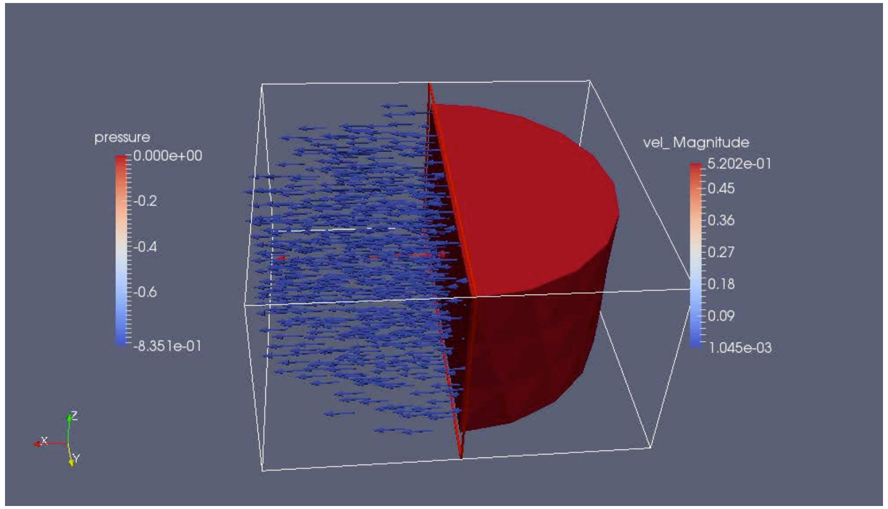


Fluid Structure Interaction
[Steiner, K, '14]

Optimal parallel solution methods

- Domain Decomposition (Schwarz methods)
- Multigrid methods

But: Scalability requires global communication



Poroelasticity:
Compression of a cylindrical specimen
[Favino, K', '13, '15]

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Fluid Structure Interaction

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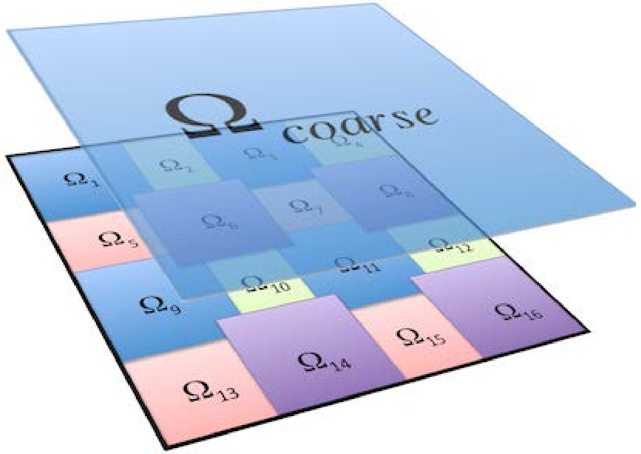


Bi-Conjugate-Gradient Stabilized (BiCGStab) with different preconditioner

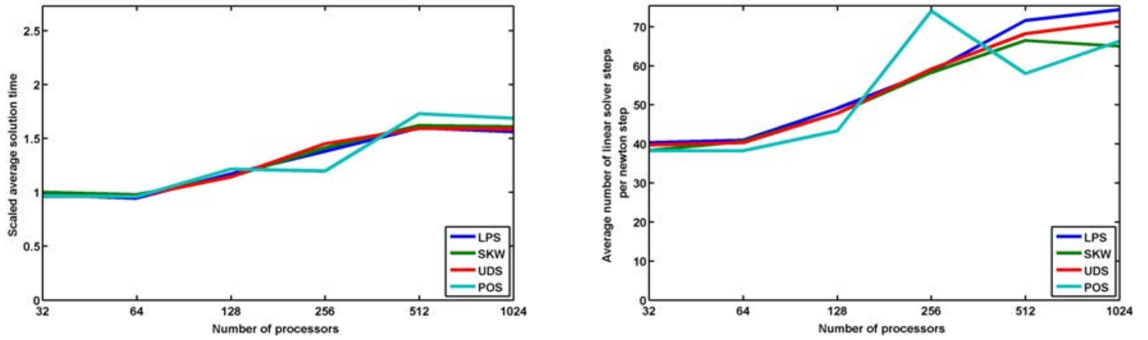
- Restricted additive Schwarz method

$$U^{k+1} = U^k + (\sum_{i=1}^{M} Q_i)(f - AU^k)$$

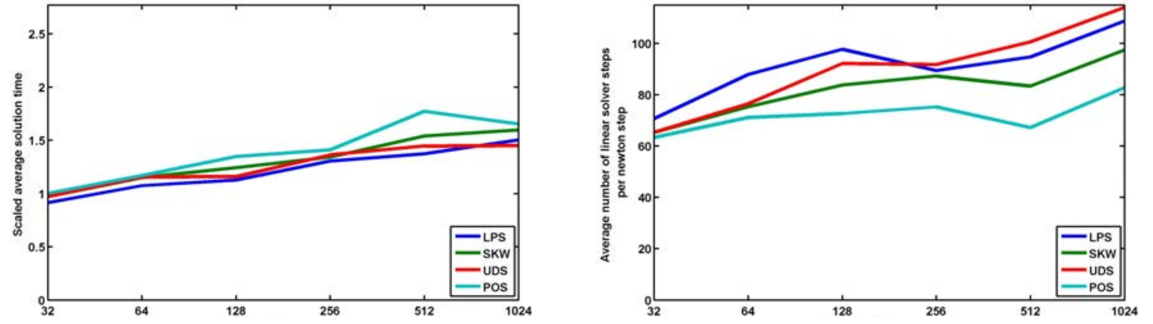
with a preconditioner

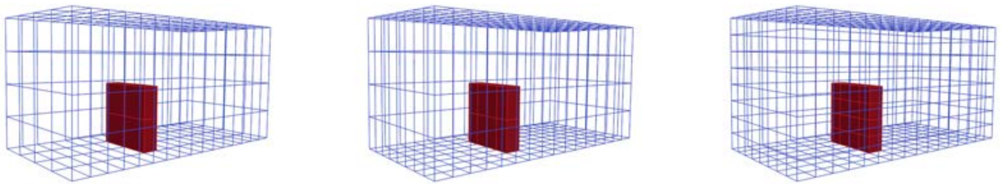
$$\sum_{i=1}^{M} Q_i = (R_0)^T A_0^{-1} R_0 + \sum_{j=1}^{N} (R_j^0)^T A$$

- and a geometric multigrid method



Additive Schwarz (geometric explicit):





[J. Steiner, R. Krause 2014]

Parallelize in space saturates

- Traditionally, decomposition is done only in space
- Time is discretized sequentially

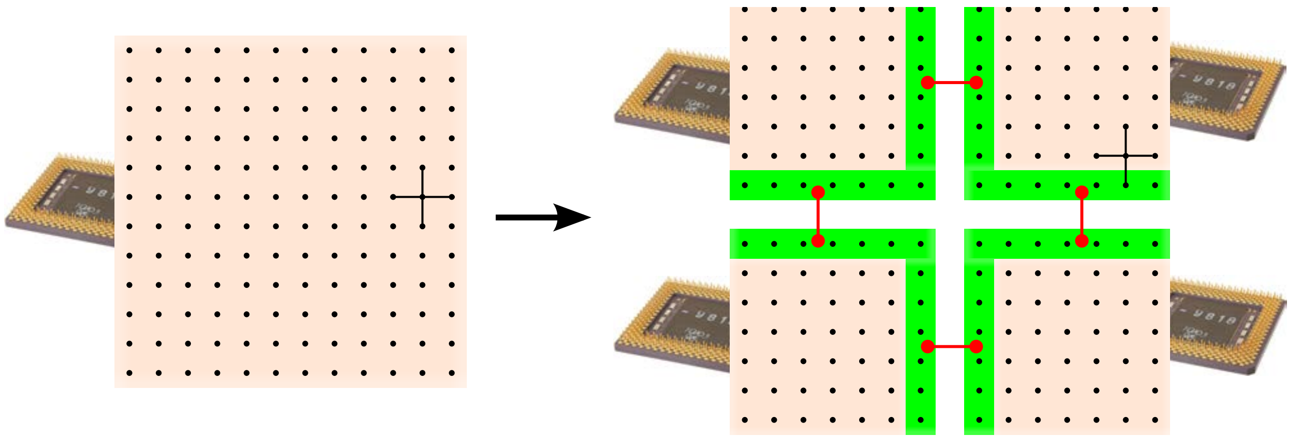


Figure : CPU photo courtesy of Eric Gaba.

Use time as an additional direction for parallelization
(PARAREAL, PFASST, MGRIT, ...)

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Parallelize in time and space

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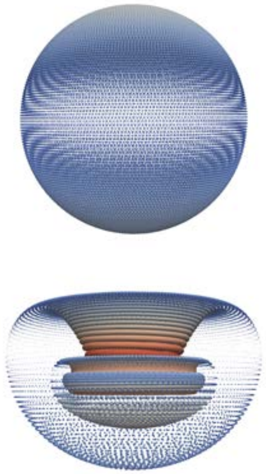
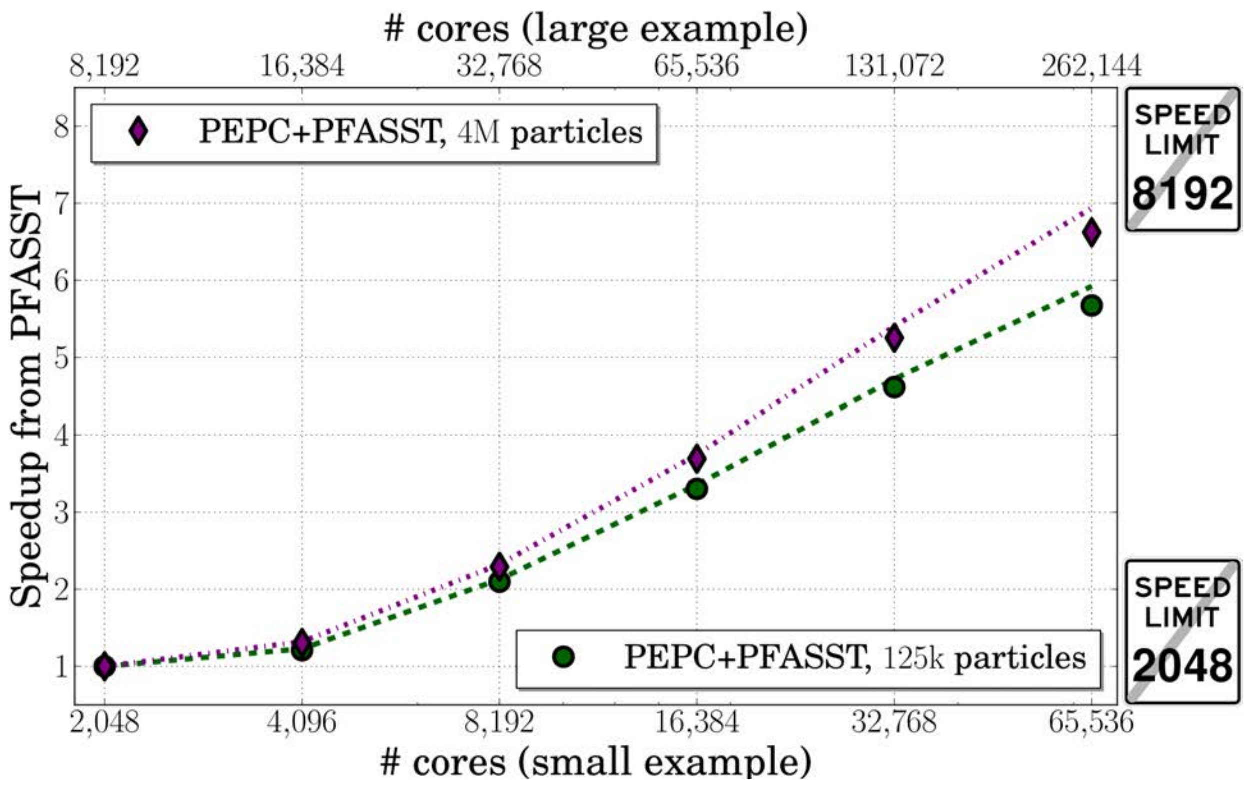
- multiphysics, hybrid implementation of the 'Hashed Oct-Tree' scheme
- here: vortex particle method
- 4th order time integration with $dt = 0.5$ and $[0, T] = [0, 16]$
- small setup with 125k and large setup with 4M particles
- strong scaling saturates at approx. $2,048$ and $8,192$ cores on IBM BG/P





Speedup through parallelization in time for fluid flow (Navier Stokes)

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- …
- Fluid Structure Interaction
- PDE constrained Optimization (Turbine Design)
- Coupled Structures in Fractured Reservoirs
- Data Assimilation

Fundamental Research

Modeling Facility
Numerical Methods
Mathematical Models
Numerical Analysis
Simulation Software
Education and Exchange

↔

High Performance Computing CSCS