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Software engineering aspects for a distributed-parallel and h-adaptive high-order space-time wave equation solver based on the deal.II library

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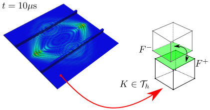
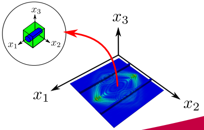
Adaptive algorithms for computational PDEs
Birmingham, January 5-6th, 2016



Numerical Mathematics



Outline

Acoustic Wave Equation

Velocity – Displacement Formulation

$$
\begin{aligned}
\partial_t v - \nabla \cdot a(\boldsymbol{x}) \nabla u &= f && \text{in } \Omega \times I\,, \\
\partial_t u - v &= 0 && \text{in } \Omega \times I\,, \\
\\
u &= 0 && \text{on } \Gamma_D \times I\,, \\
\frac{\partial u}{\partial \boldsymbol{n}} &= 0 && \text{on } \Gamma_N \times I\,, \\
\\
u(\boldsymbol{x}, 0) &= u_0(\boldsymbol{x}) && \text{for } \boldsymbol{x} \in \Omega\,, \\
v(\boldsymbol{x}, 0) &= v_0(\boldsymbol{x}) && \text{for } \boldsymbol{x} \in \Omega\,,
\end{aligned}
$$

where $\Omega \subset \mathbb{R}^d$, and $I = (0, T)$, $0 < T < \infty$.

Solver Suite Overview: `DTM++.Project/xwave`

Variational Space–Time (Time Marching Scheme) Discretisations

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- cG(p)–{dG(0), cG(1)}
- SIPG(p)–{dG(0), cG(1)}
- SIPG(p)–{dG(1), cG(2), cG-C1(3)}

Building Block: Split implementation for space and time

U. Köcher: *Variational Space-Time Methods for the Elastic Wave Equation and the Diffusion Equation*, Ph.D. thesis, HSU Hamburg, 2015, http://nbn-resolving.de/urn:nbn:de:gbv:705-opus-31129

U. Köcher, M. Bause: *Variational space-time discretisations for the wave equation*, J. Sci. Comput. 61(2):424-453, 2014.

Sharply resolved wave fronts
… but expensive since adaptivity is not used

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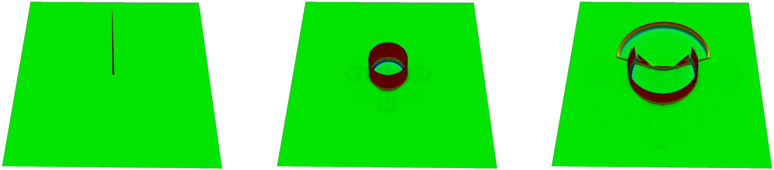

Figure: Heterogeneous media. SIPG(7)–cG(2), 96 Cores, 2013.

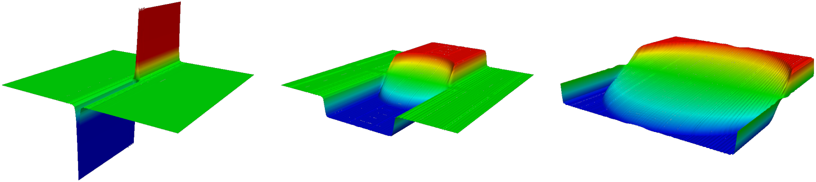

Figure: SIPG(12)–cG-C1(3), 16 Cores, 2015.

Adaptivity: Kelly error estimator

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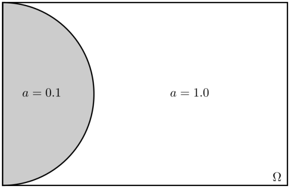
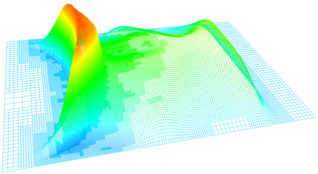
The Kelly error estimator is used for h-adaptivity, which computes space-cell local estimates

$$\eta_K^2 = \sum_{F \in \partial K} c_F \int_F \left[\!\left[a \frac{\partial u_h}{\partial \boldsymbol{n}} \right]\!\right]^2 \mathrm{d}o \,,$$

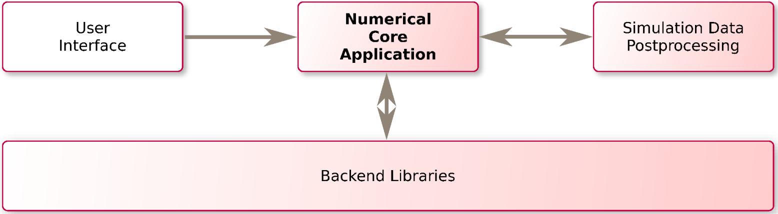
using trace operator $[\![\cdot]\!]$ for the jump in the face F.





This error estimator is implemented in deal.II.

Numerical Simulation: Software Development



	deal.II	FEnICS	DUNE
FEM:	x	x	x
FV:			x
Mesh:	Quad	Tria, Quad	Tria + Quad
Language:	C++	C++, python	C++

Numerical Simulation: Software Development

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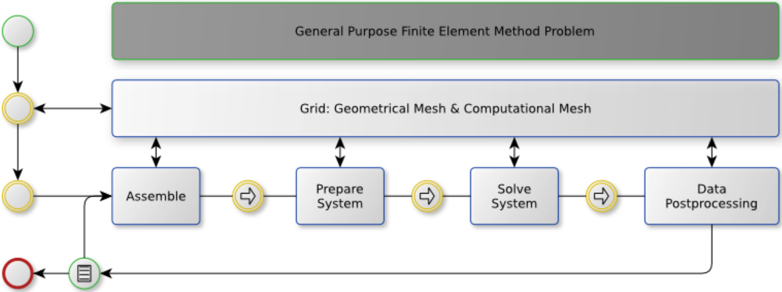
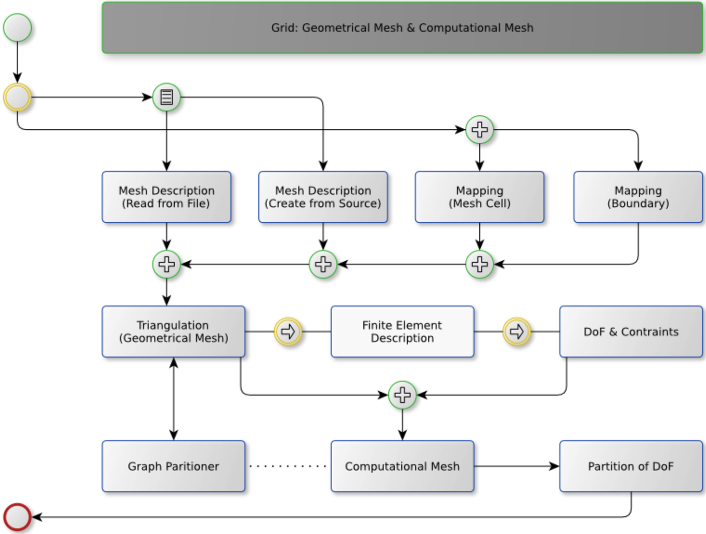


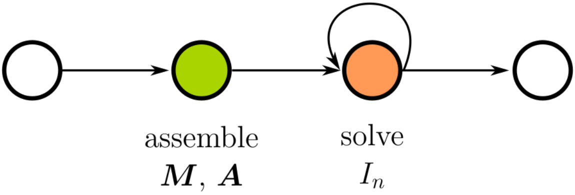
Figure: Numerical Software: Building Blocks

Software Engineering: Grid

Abstraction of the Geometrical and Computational Mesh



Software Engineering: Time Marching Scheme



Software Engineering: Adaptivity

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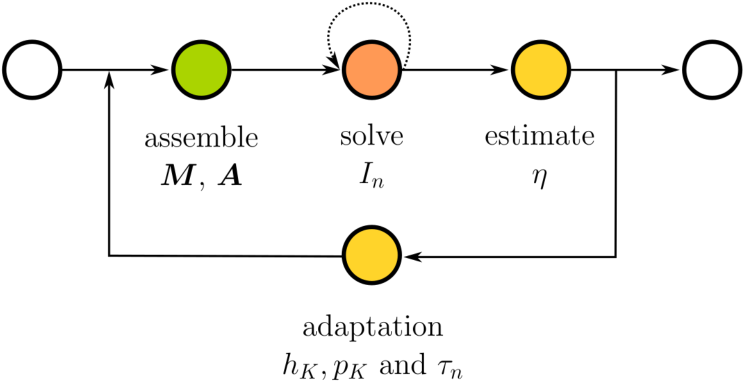

Parallel Simulation: Distributed Mesh and DoF

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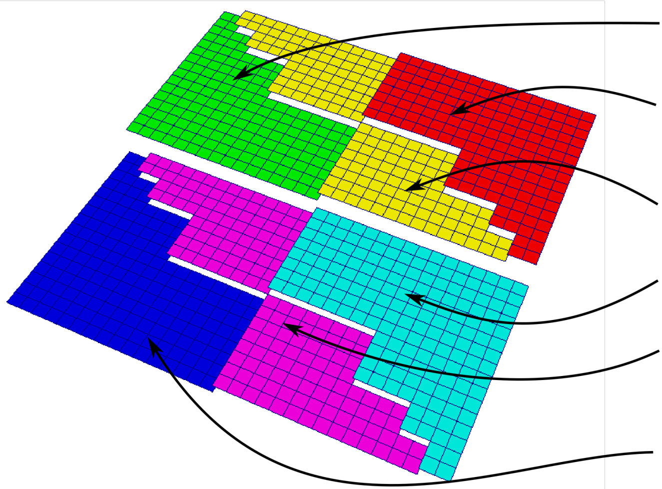

$$\begin{bmatrix} u_1^1 \\ \cdots \\ u_{n_1}^1 \\ u_1^2 \\ \cdots \\ u_{n_2}^2 \\ u_1^3 \\ \cdots \\ u_{n_3}^3 \\ u_1^4 \\ \cdots \\ u_{n_4}^4 \\ u_1^5 \\ \cdots \\ u_{n_5}^5 \\ u_1^6 \\ \cdots \\ u_{n_6}^6 \end{bmatrix}$$

Experimental Strong Parallel Scaling

Time-Domain Elastic Wave Equation, SIPG(3)–cG-C1(3)

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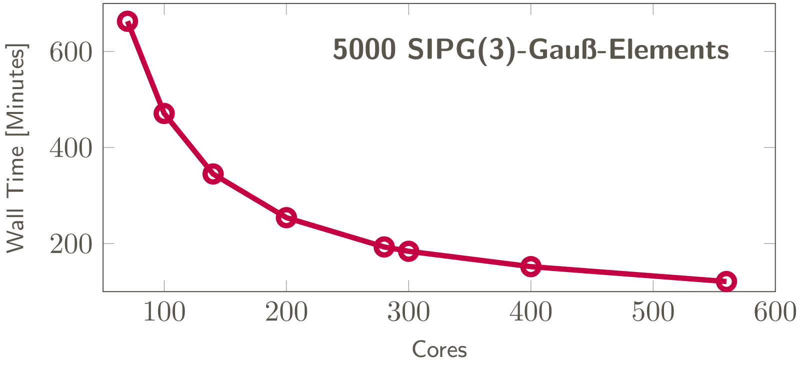

- Building Block: Parallel Grid
- Building Block: Parallel Linear Algebra
- Building Block: Parallel Assembly

DTM++.Project/Biot, 2015

Poroelasticity Solver

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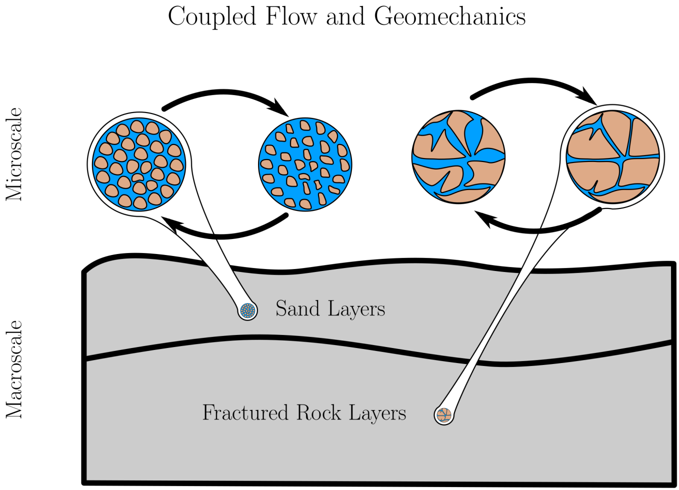

DTM++.Project/Biot, 2015

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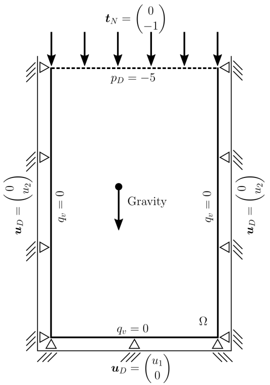

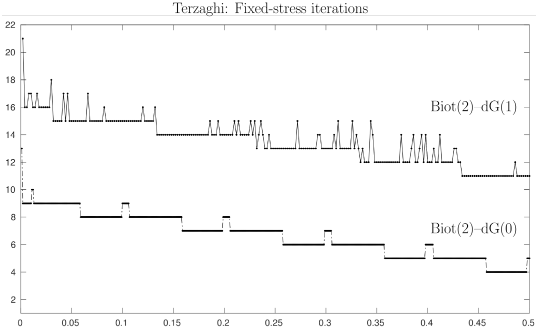

- Building Block: FE-System: cG(p+1)-RT(p)-dG(p)
- Building Block: Time Discretisations: dG(0), dG(1), cG(1)*
- Building Block: Fixed point iteration

Adaptive Stabilized Convection-Diffusion-Reaction

K. Schwegler, M. Bause

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Model problem

$$\partial_t u + \boldsymbol{b} \cdot \nabla u - \nabla \cdot \epsilon \nabla u + r\, u = f\,, \quad 0 < \epsilon \ll 1\,.$$

- Theorem to discretise: *"First Dualise Then Stabilise"* (FDTS)
- Space-time (time marching scheme) discretisation:
  - primal: cG(p)–dG(0)
  - dual: cG(p+1)–cG(1)
- Streamline Upwind Petrov-Galerkin stabilisation (SUPG)

Implemented in python with dolfin (FEnICS) by K. Schwegler.

Adaptive Stabilized Convection-Diffusion-Reaction

Numerical Test: Moving Hump Problem (John et. at. '08)

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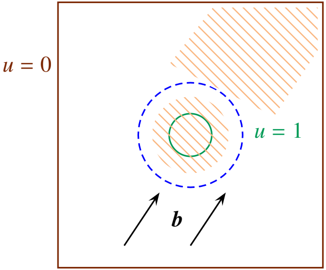

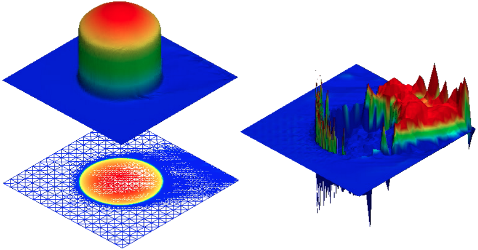

Analytic solution:

$$u(\boldsymbol{x},t) = 16\sin(\pi t)\, x_1(1-x_1)x_2(1-x_2)\left[\frac{1}{2} + \frac{1}{\pi}\arctan(2\epsilon^{-0.5}(0.25^2 - (x_1-0.5)^2 - (x_2-0.5)^2))\right]$$

Goal quantity:

$$\mathcal{J}(u) = \|u(T)\|^{-1}_{L^2(\Omega)}\,(e(T),u(T))_{L^2(\Omega)}\,, \quad |\mathcal{J}(u) - \mathcal{J}(u_{\tau,h})| \overset{!}{\leqslant} \text{tol}$$

Adaptive Stabilized Convection-Diffusion-Reaction

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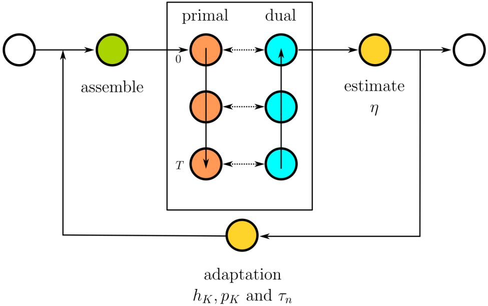
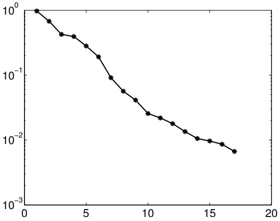


it	$n_{\max}$	DoF	$\mathcal{I}_{\text{eff}}$	it	$n_{\max}$	DoF	$\mathcal{I}_{\text{eff}}$
1	25	735	0.55	9	95	6184	1.03
2	29	1002	0.63	10	113	7785	1.11
3	34	1255	0.78	11	135	9051	1.04
4	40	1786	1.07	12	161	12557	1.03
5	47	2300	1.11	13	193	16484	1.00
6	56	3067	1.13	14	231	20192	1.02
7	67	3857	1.26	15	277	25415	1.01
8	80	4611	1.23	16	332	36091	1.01

$$\mathcal{I}_{\text{eff}} = \left| \frac{\eta}{\mathcal{J}(u) - \mathcal{J}(u_{\tau,h})} \right|$$



Error over DWR iterations

Recent Publications

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- **U. Köcher**: *Variational Space-Time Methods for the Elastic Wave Equation and the Diffusion Equation*, Ph.D. thesis, HSU Hamburg, 2015, http://nbn-resolving.de/urn:nbn:de:gbv:705-opus-31129
- **M. Bause, F. Radu and U. Köcher**: *Error analysis for discretizations of parabolic problems using continuous finite elements in time and mixed finite elements in space*, submitted, arXiv:1504.04491, 2015.
- **K. Schwegler**: *Adaptive goal-oriented error control for stabilized approximations of convection-dominated problems*, Ph.D. thesis, HSU Hamburg, 2014.