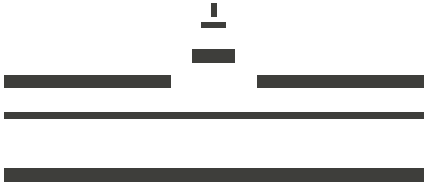

Westfälische
Wilhelms-Universität
Münster

Advances concerning multiscale methods and uncertainty quantification in Exa-Dune

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WWU Münster

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January 25th, 2016

Outline

- Abstraction of Multiscale Methods
- Implementation + Results
- MLMC
- Integration with MLMC Framework

EXA-DUNE:

"Flexible PDE Solvers, Numerical Methods, and Applications"

- 7 groups from 5 german universities
- Aim: develop new numerical, algorithmic and computational techniques to enable exa-scale computing for PDEs on heterogeneous massively parallel architectures
- DUNE and FEAST (TU Dortmund, hardware-oriented numerics)

Problem Statement

Assume we are looking for $u^\epsilon \in U$ solving

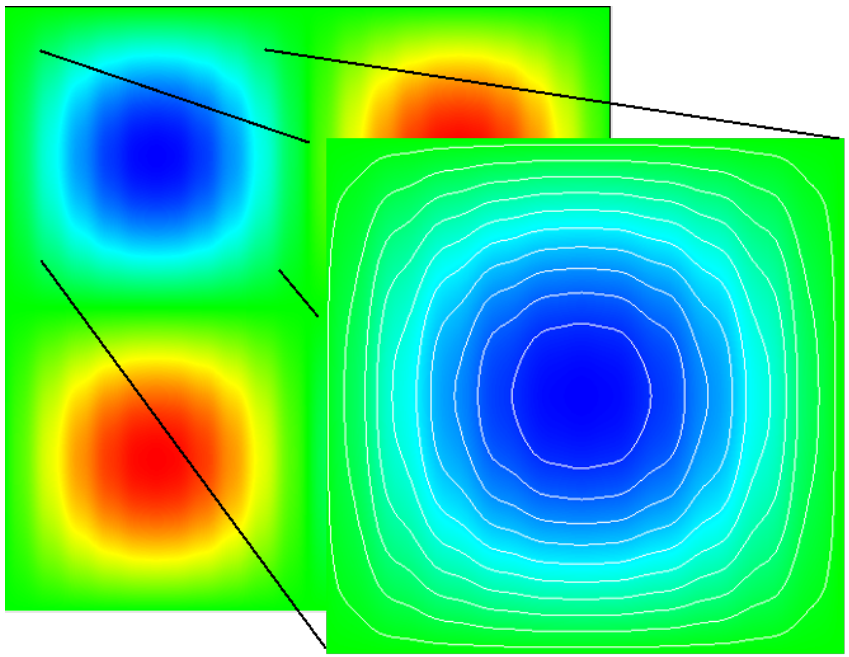
$$R^\epsilon[u^\epsilon](v) = 0 \quad \forall v \in U$$

where $R^\epsilon : U \mapsto U'$
Example:

$$U = H_0^1(\Omega), \qquad R^\epsilon[u] = b^\epsilon[u] - l$$
$$b^\epsilon[u](v) = \int_\Omega A^\epsilon \nabla u \nabla v, \qquad l(v) = \int_\Omega fv$$
$$A^\epsilon(x) = A\left(\frac{x}{\epsilon}\right) : \Omega \mapsto \mathbb{R}^{d\times d}$$

Scales

- Idea: Make use of possible scale-separation
- Macroscopic scale represented by coarse-scale space $U_H \subset U$ on coarse partition $\mathcal{T}_H$ of Ω
- Microscopic scale represented by fine-scale space $U_h \subset U$ on fine partition $\mathcal{T}_h$ of Ω
- Spaces should be nested $U_H \subset U_h \subset U$



Abstract Method

- Let $\pi_{U_H} : U \mapsto U_H$ denote a projection onto the coarse space with

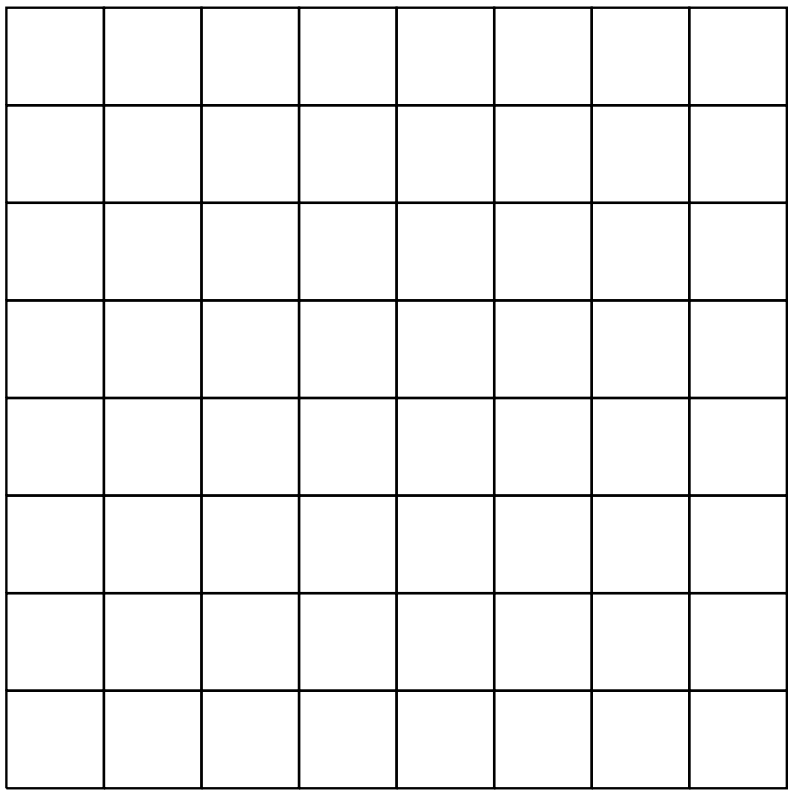
$$U_{f,h} = \{u_h \in U_h : \pi_{U_h}(u_h) = 0\}$$

- Compute and approximate discrete solution

$$\begin{aligned} u^{\epsilon}_{\mu,h} = u_H + u_{f,h} \in & U_H \oplus U_{f,h} \text{ satisfying} \\ R^{\epsilon}_{\mu}[u_H + u_{f,h}](v_H) &= 0 \quad \forall v_H \in U_H \\ R^{\epsilon}_{\mu}[u_H + u_{f,h}](v_{f,h}) &= 0 \quad \forall v_{f,h} \in U_{f,h} \end{aligned}$$

- Concrete choices for U_H, U_h, π_{U_H} and further localization of fine scale equation yield various multiscale methods.

Pure MPI Implementation



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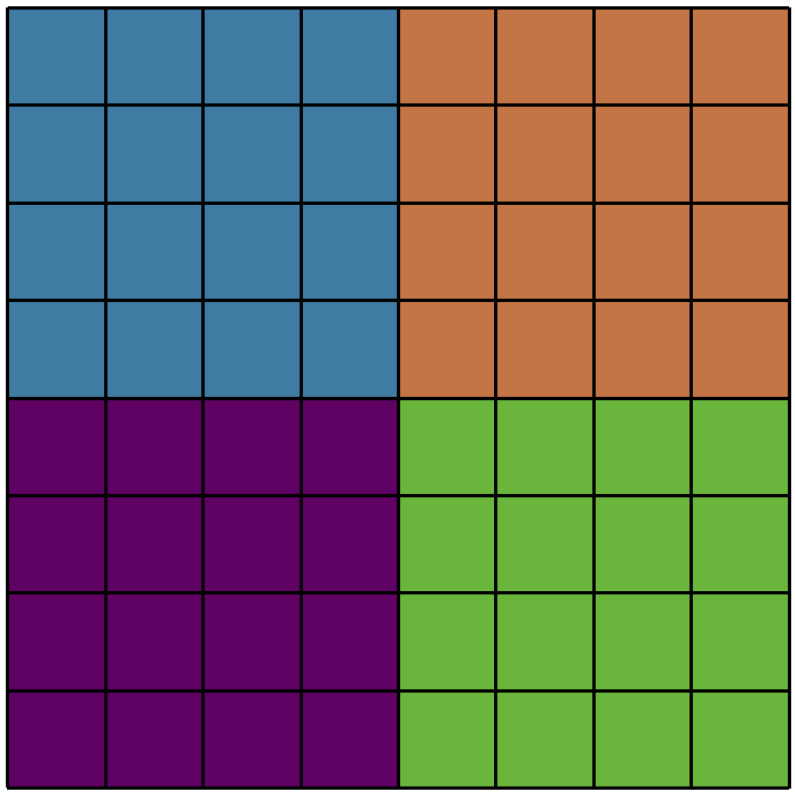

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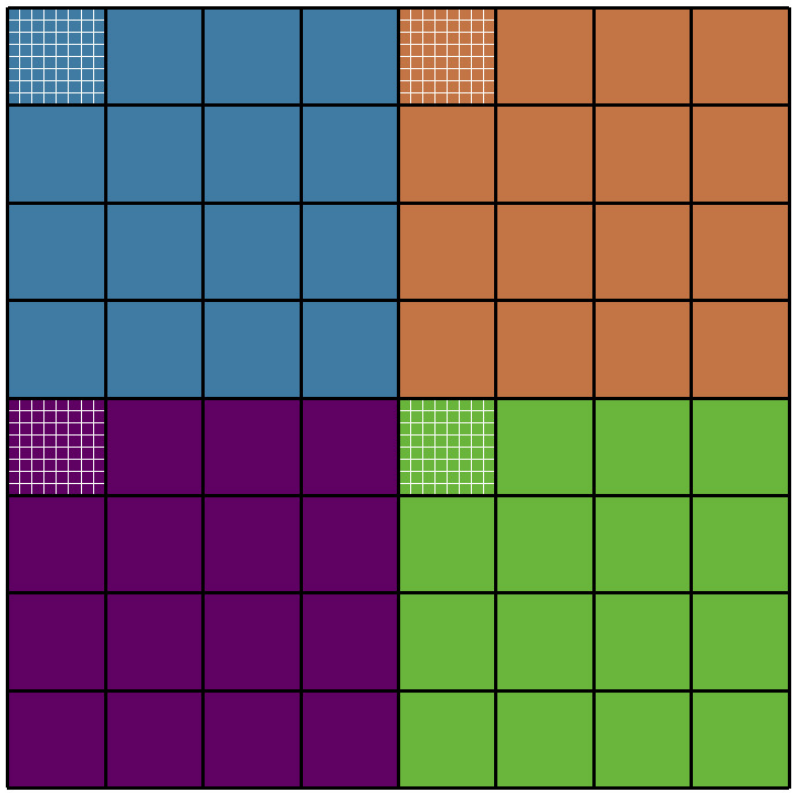


Strong Scaling Setup

- CG-FEM Discretizations via DUNE-gdt with DUNE-pdelab backend
- YASPGRID (cubes) from DUNE-grid on coarse and fine scale
- 64^3 cubes on coarse scale with 8^3 fine cells each, 134.217.728 total
- Hardware: SuperMUC Phase 2, 256 to 8192 MPI ranks
- coarse system: DUNE-istl BiCGStab with ILUT preconditioning
- UMFPACK direct sparse solve for local problems

Testcase Setup

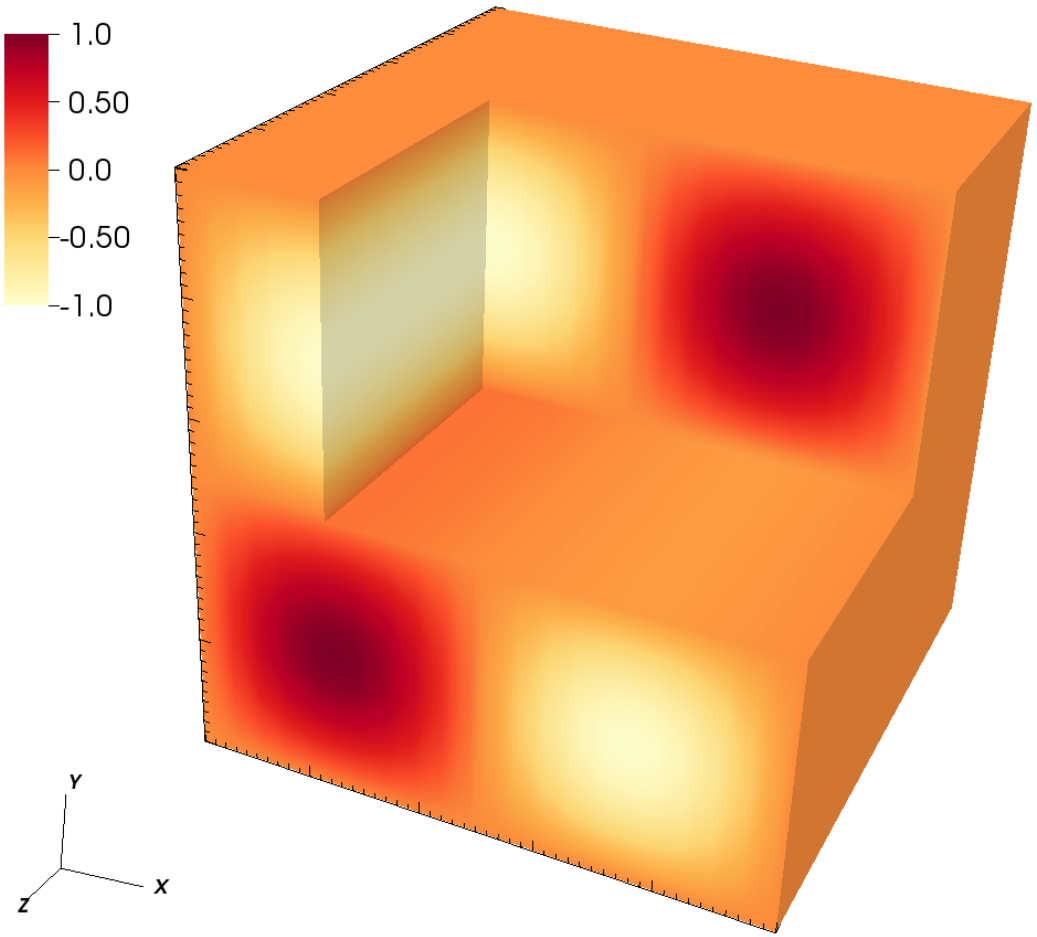
Standard diffusion problem in $\Omega = [0,1]^3$, with boundary conditions $u(x) = 0$ on $\partial\Omega \backslash x_3 \in \{0,1\}$ and Neumann-zero elsewhere. With diffusion A^ϵ and source f^ϵ given as:

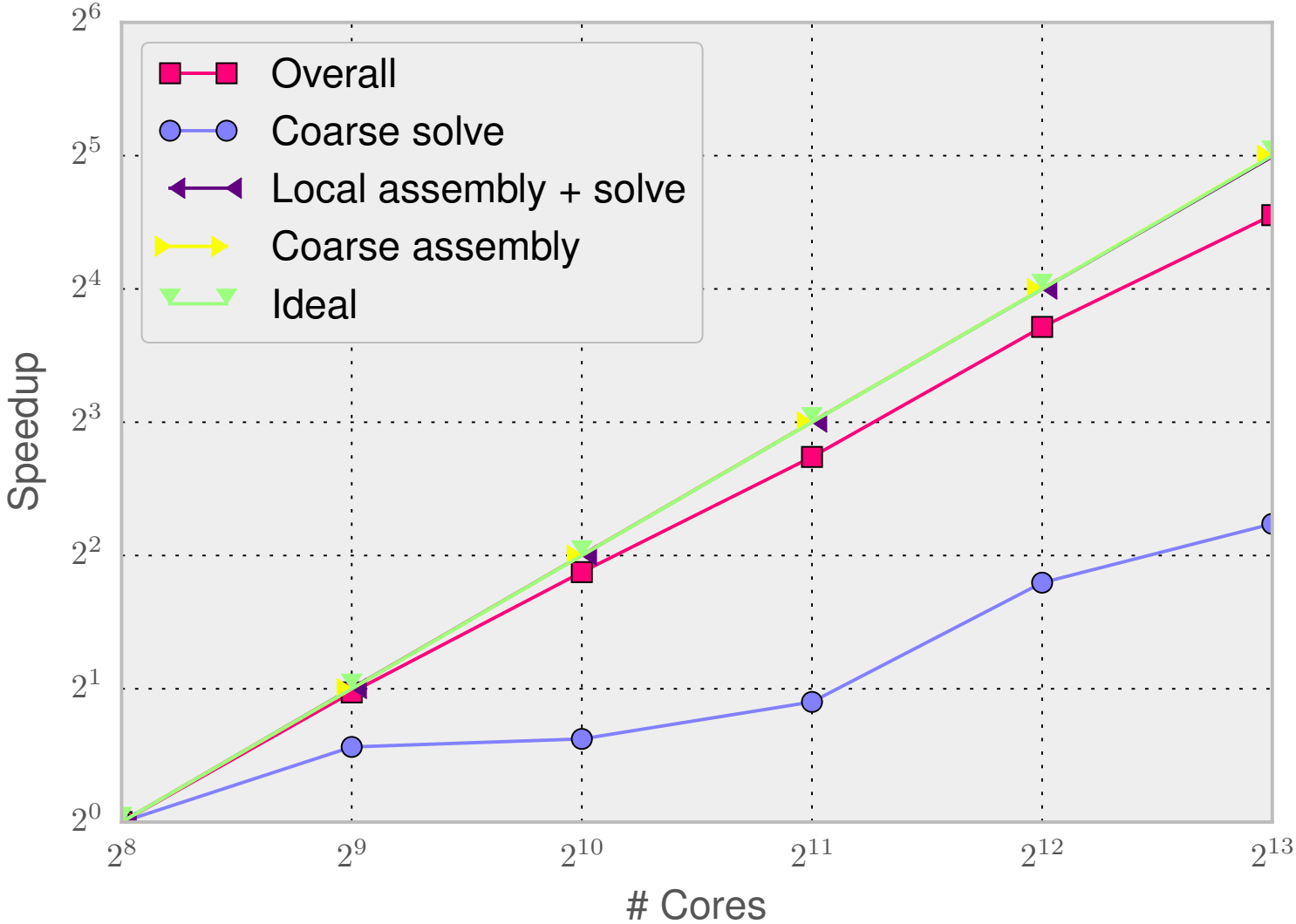
$$A^\epsilon(x_1,x_2,x_3) := \frac{1}{8\pi^2} \begin{pmatrix} 2\left(2+\cos\left(2\pi\frac{x_1}{\epsilon}\right)\right) & 0 & 0 \\ 0 & 1+\frac{1}{2}\cos\left(2\pi\frac{x_1}{\epsilon}\right) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$f^\epsilon(x) := -\nabla\cdot\left(A^\epsilon(x)\nabla v^\epsilon(x)\right)$$

$$v^\epsilon(x_1,x_2,x_3) := \sin(2\pi x_1)\sin(2\pi x_2) + \frac{\epsilon}{2}\cos(2\pi x_1)\cos(2\pi x_2)\sin\left(2\pi\frac{x_1}{\epsilon}\right)$$

Analytical Solution





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- Very few degrees of freedom per MPI-rank. Strong Scaling ends with only 32 cells per rank.

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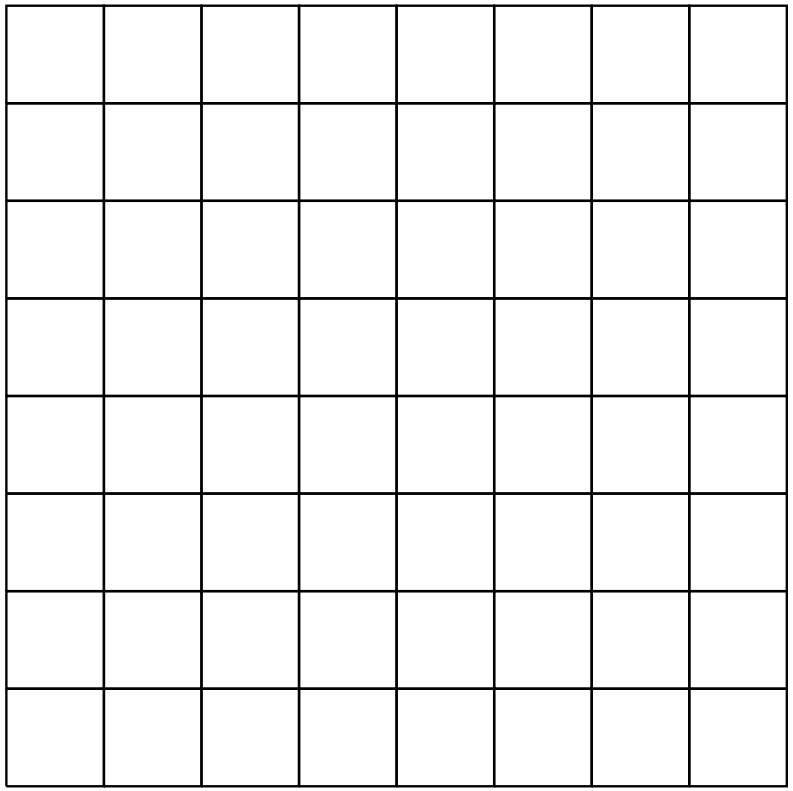
- Decrease number of ranks while increasing amount of work per rank!
- Simple for local problems: they're already embarrassingly parallel

Hybrid MPI/Shared Memory Implementation



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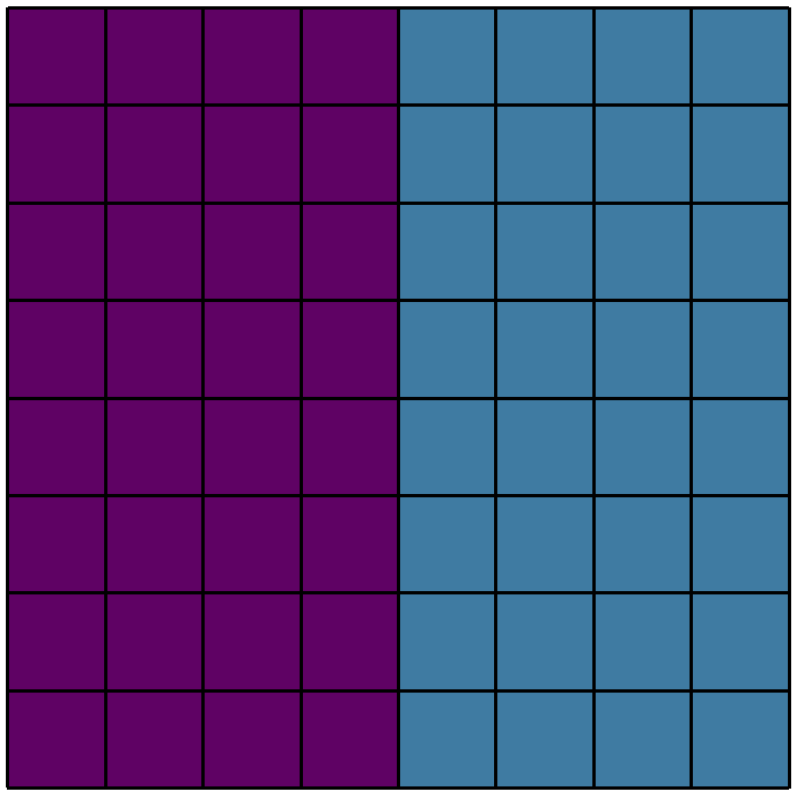

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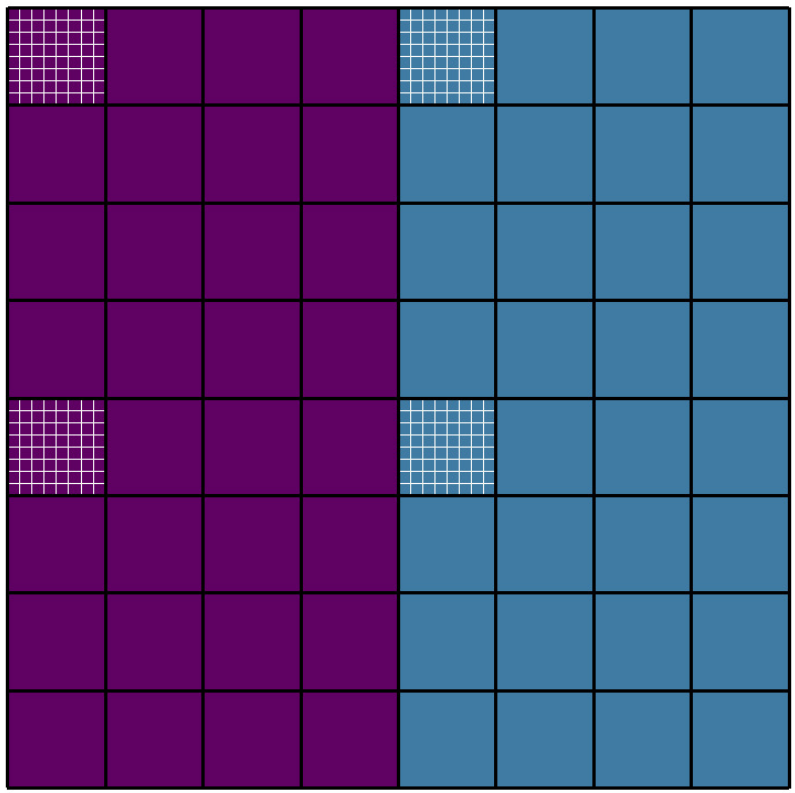
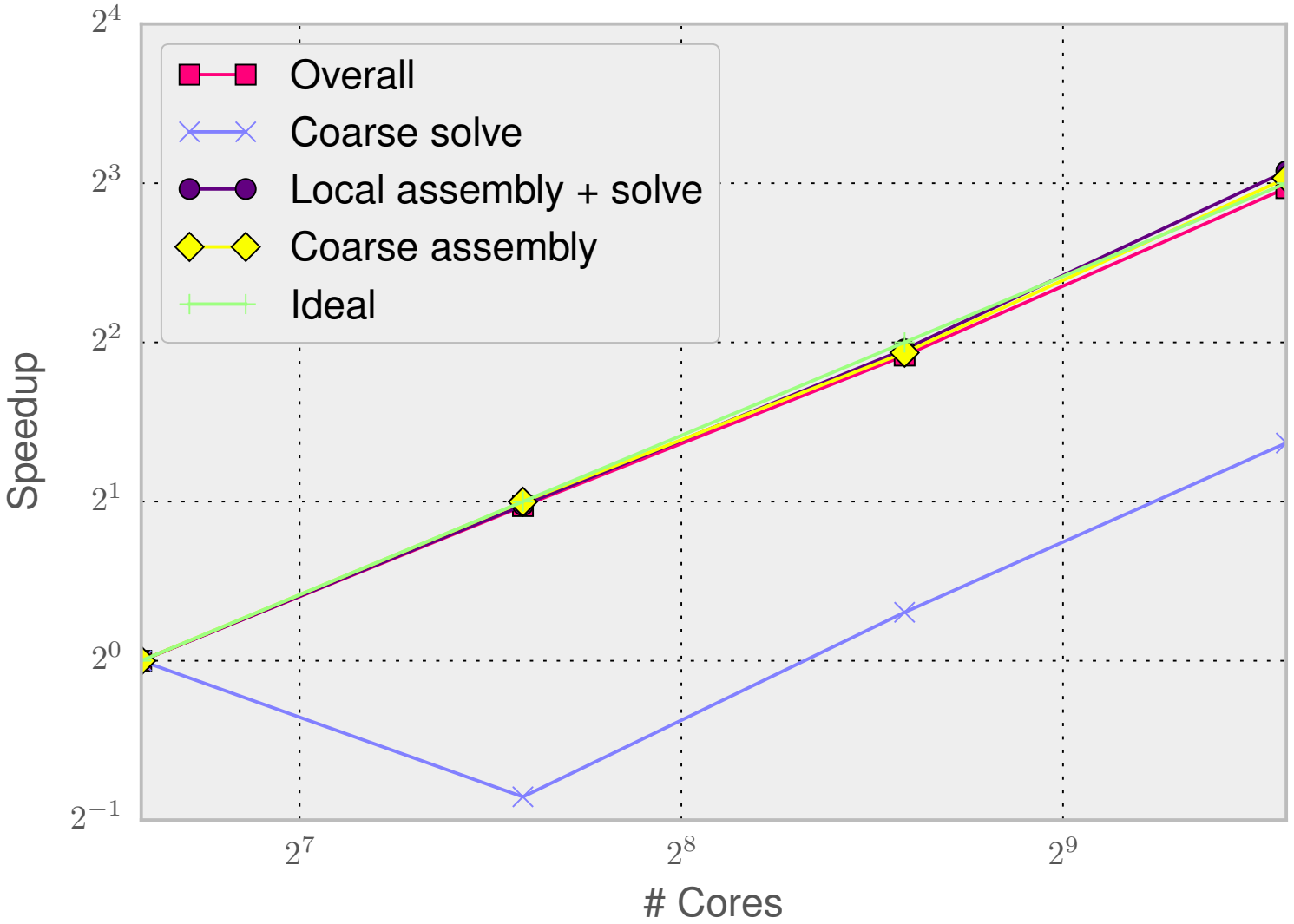


Hybrid Strong Scaling Setup

- 8^3 cubes on coarse scale with 32^3 fine cells each, 16.777.216 total
- Hardware: CHEOPS (RRZK Cologne)
- 16 to 128 MPI-ranks, one hexacore CPU per rank: 96 to 768 cores used



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- Conventionally this uncertainty is quantified by means of Monte Carlo methods
- But: Notoriously bad convergence

MLMC Ideas

The main idea behind Multi Level Monte Carlo Method is to split

$$Q(\omega) = Q_0(\omega) + Q_1(\omega) - Q_0(\omega) + \cdots + Q_L(\omega) - Q_{L-1}(\omega) + Q(\omega) - Q_L(\omega)$$

with $L + 1$ increasingly accurate (+ time intensive) solvers. We reduce its variance accordingly, with many quick evaluations for the coarse solution and few slower solves for the differences. These solves are independent of one another $\rightarrow$ trivial parallelization. MLMC can greatly improve order of convergence compared with MC.

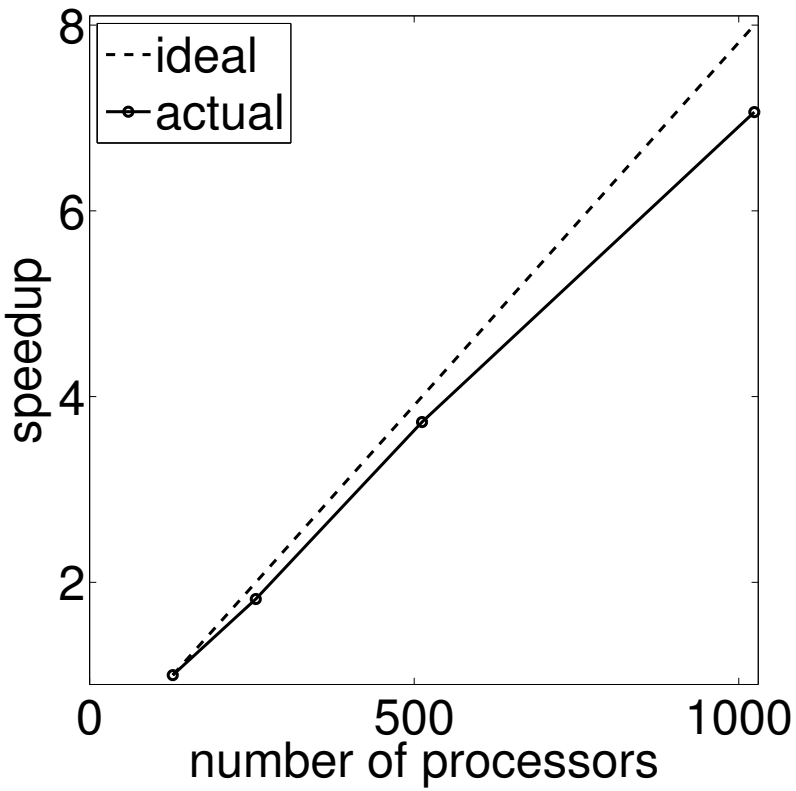
MLMC Implementation

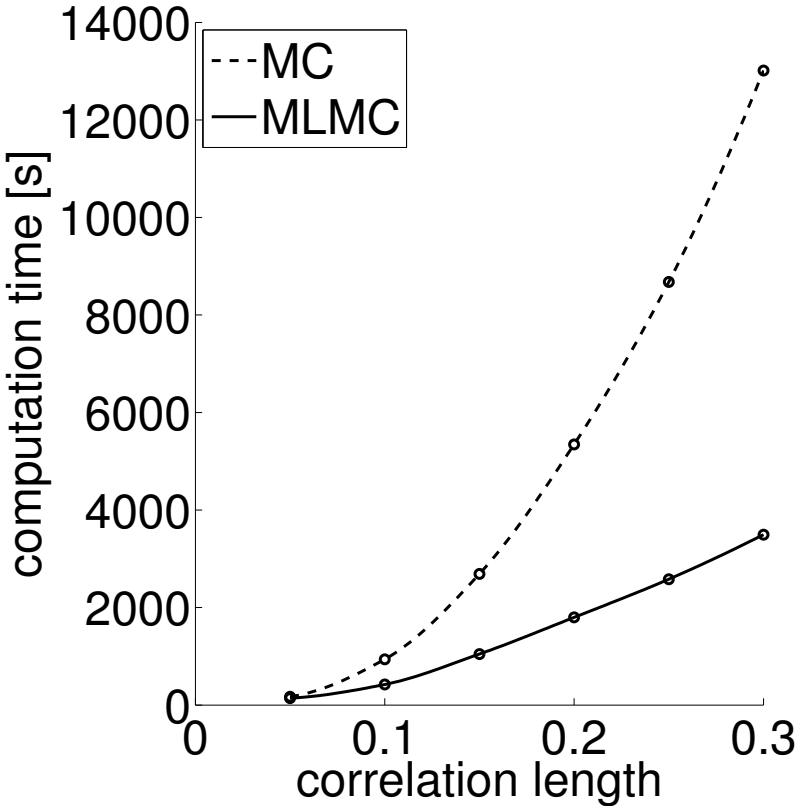
- DUNE module with very little requirements on pluggable solvers
- Optimizes selection of slow/fast solves to minimize time to solution
- Distributes work across groups of MPI-Ranks
- Tries to mimimize the communication overhead for estimating mean times and variances

MLMC Testcase setup

- stationary single phase flow through a unit cube
- random permeability field
- Boundary condition: constant pressure difference between left and right end faces
- Aggregate quantity $Q(\omega)$ sought is the total flow through the cube
- up to 1024 CPUs of the ITWM Cluster in Kaiserslautern

Scaling of a 2-level MsFEM/FEM and comparison with Standard MC





Thank you for your attention.

Get the code:

`https://github.com/wwu-numerik/dune-multiscale`

`https://github.com/wwu-numerik/dune-mlmc`