Direct solves on a multigrid solver in lattice quantum chromodynamics (QCD)

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Motivation

How we use MUMPS

Advantages

Disadvantages

Outlook

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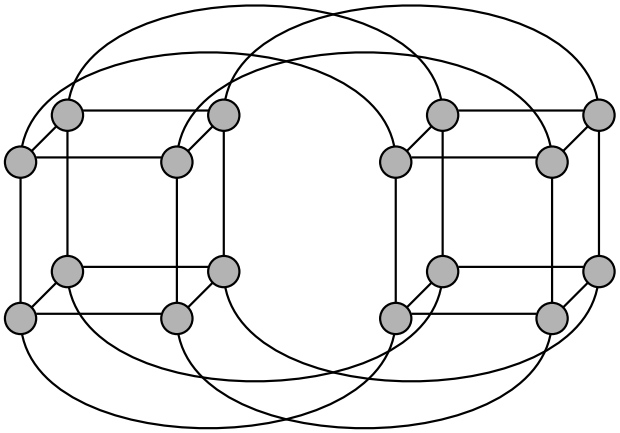
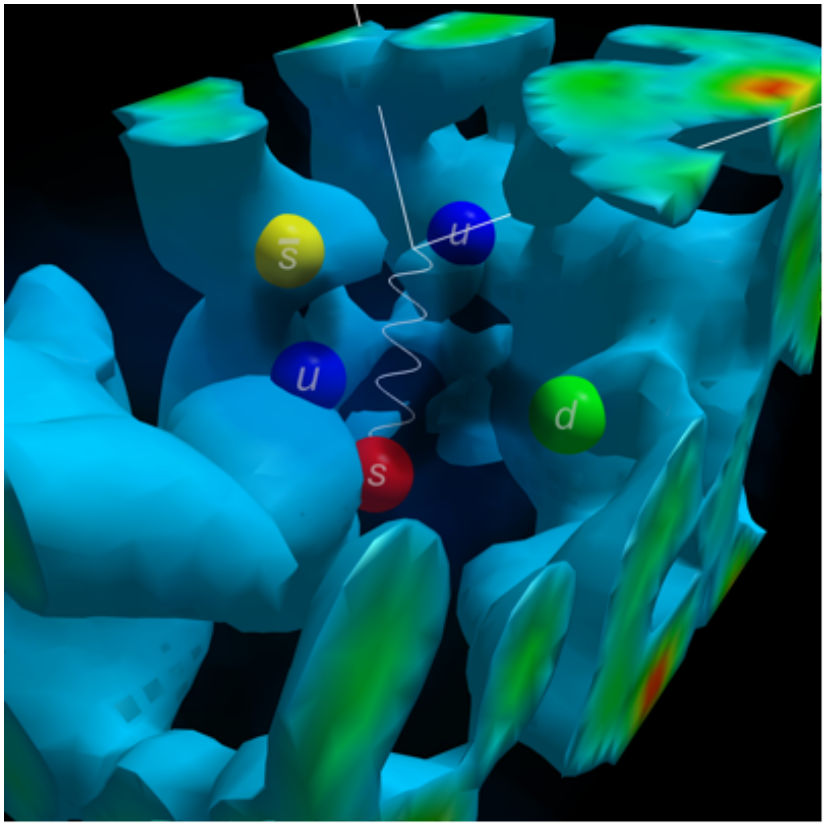
Outline

Lattice QCD



$$A \cdot x = b$$



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2-level method

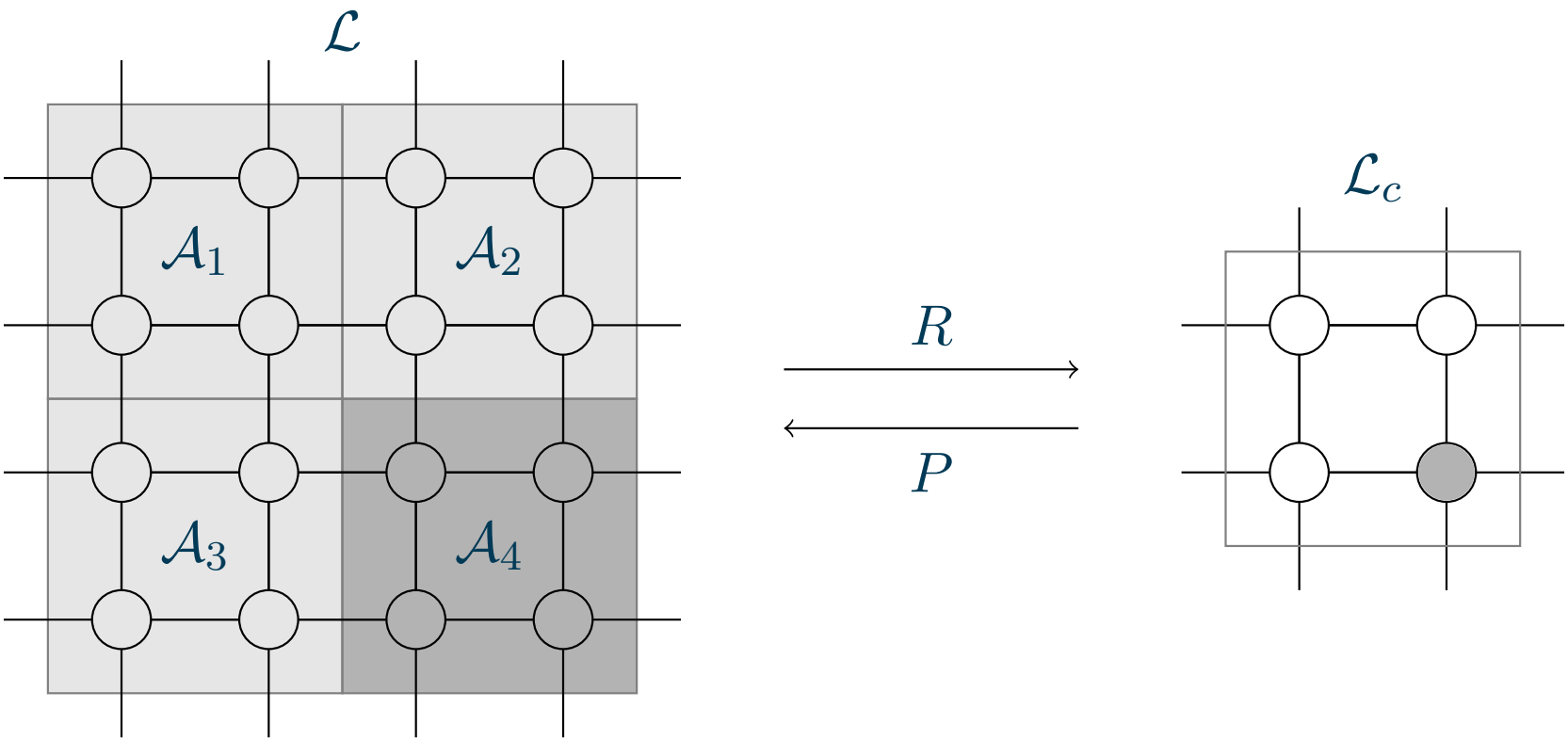

Figure: fine grid left, coarse grid right

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2-level method

$$A_1 = PA_0R = PA_0P^H \tag{1}$$

where $P^H = R \in \mathbb{C}^{n \times s}$ and $P \in \mathbb{C}^{s \times n}$.
With n be the number of lattice sites in $\mathcal{L}$ times $\text{DOF}_{\mathcal{L}}$ and s the number of lattice sites in $\mathcal{L}_c$ times $\text{DOF}_{\mathcal{L}_c}$

From 2-level to multigrid

$$\epsilon = \epsilon_{\text{low}} + \epsilon_{\text{high}} \tag{2}$$

While ϵ_{high} is handled by the smoother on $\mathcal{L}$,
ϵ_{low} must be reduced by a coarse grid correction on $\mathcal{L}_c$.

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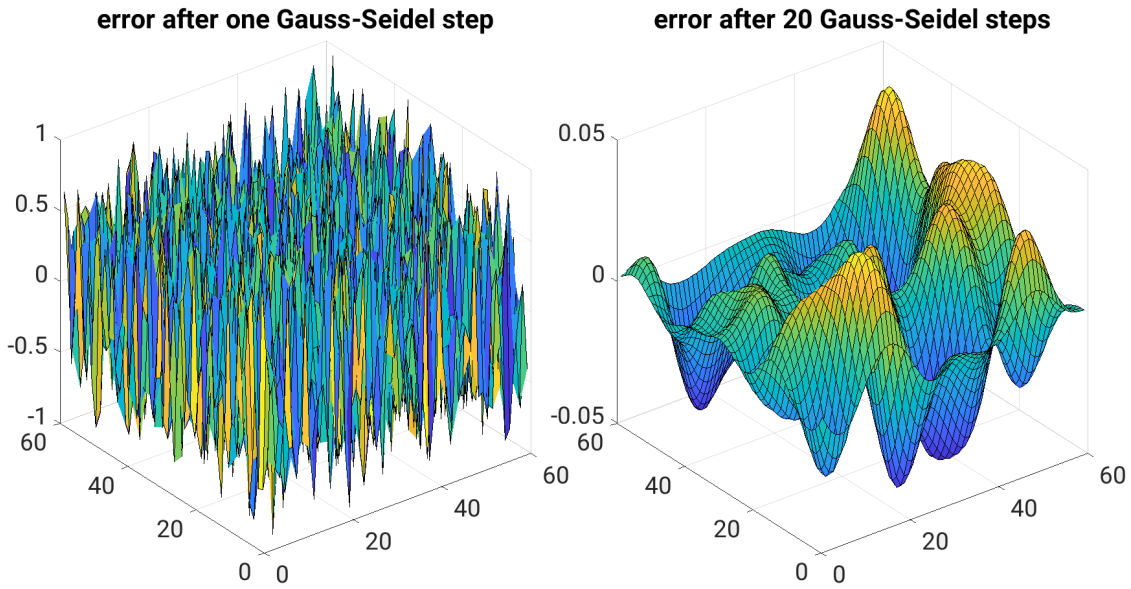

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Coarse Grid Correction

Apply 2-level method again $\rightarrow$ true multilevel method

$\epsilon_{\text{low}} = \epsilon'_{\text{low}} + \epsilon'_{\text{high}}$

- smoother on intermediate level (ϵ'_{high})
- solve coarsest level for CGC (ϵ'_{low})

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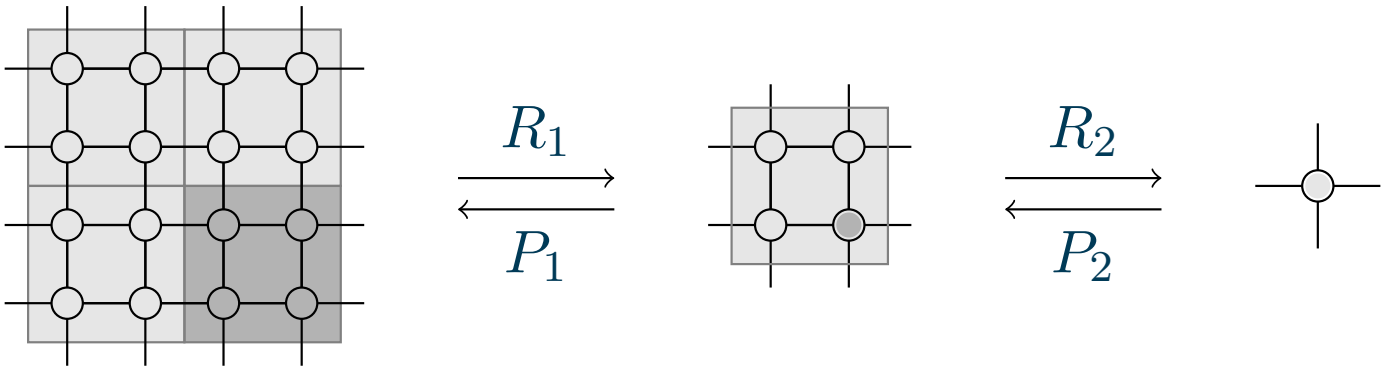
Multigrid method

Keeping geometry intact $\rightarrow$ new lattice with fewer lattice sites while **preserving sparsity and structure of** the corresponding matrix **A**.

True multigrid:



What did we do so far?

- starting with a large lattice to simulate a large domain
- reduced the size of the corresponding system drastically
- several smoothing steps in between
- kept sparsity intact
- moved computational work to coarsest (smallest) level
- also moved difficulty to coarsest level (?)

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- solve the (very) illconditioned coarsest grid
- with densely packed eigenvalues close to 0

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$\rightarrow$ MUMPS

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Outline

Parameters for MUMPS

DDαAMG as MPI application $\rightarrow$ a lot of processes and OpenMP available

$\rightarrow$ **distributed, assembled format**

A is complex, unsymmetric, well structured and A is implemented stencil-based $\rightarrow$ one must extract I and J coordinates for non-zeros components.

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Multigrid method requires very rough coarsest solves (tol: $\approx 10^{-1}$)

$\rightarrow$ good use of MUMPS' BLR feature.

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MUMPS in DDαAMG

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5. solve with centralized solution in root process
6. scatter solution to all processes

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Outline

Coarse grid properties from finest level large domains

- Eigenvalues are dense and close around zero
- many basis vectors for Krylov subspace required
- to use GMRES, several auxillary parameters have to be introduced, with a lot of hand tuning
- tuning parameters offsets the coarsest level matrix even more from its original form

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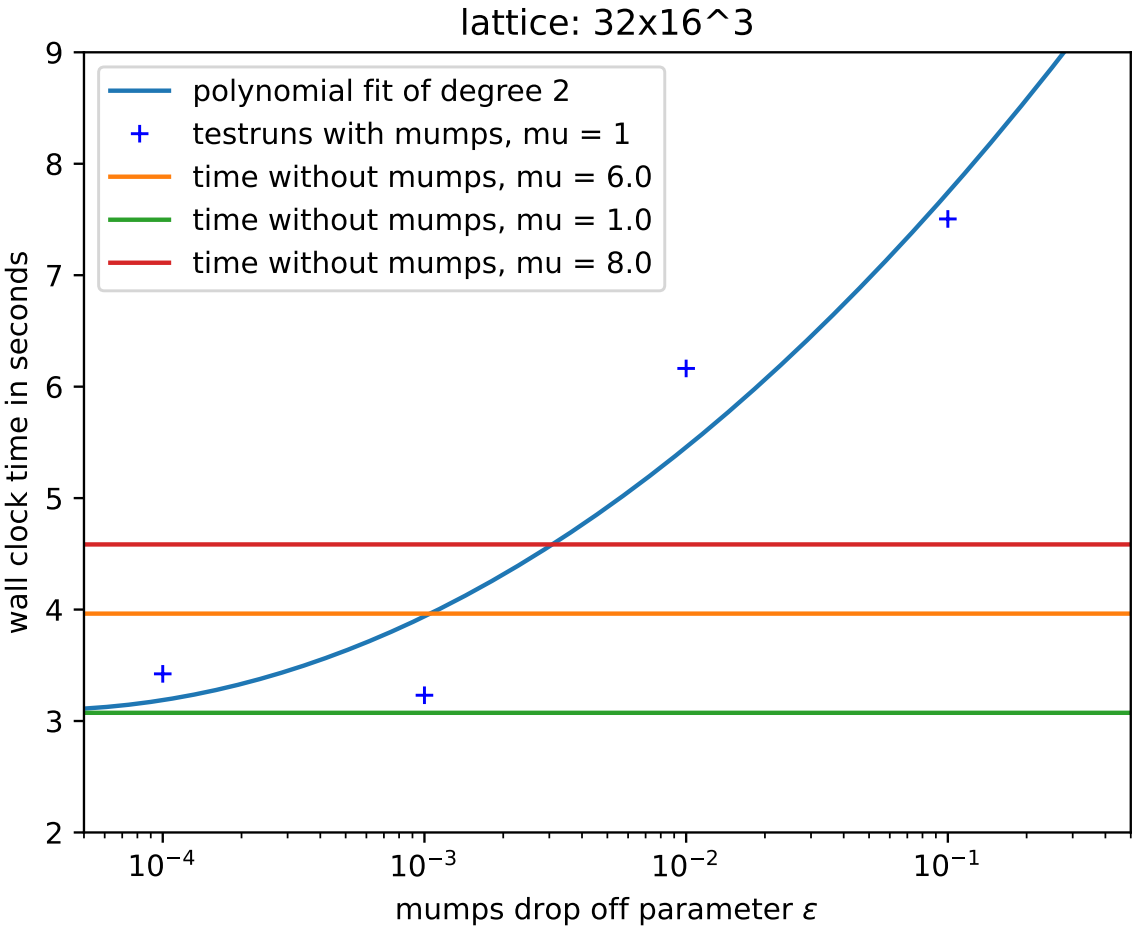
Advantages



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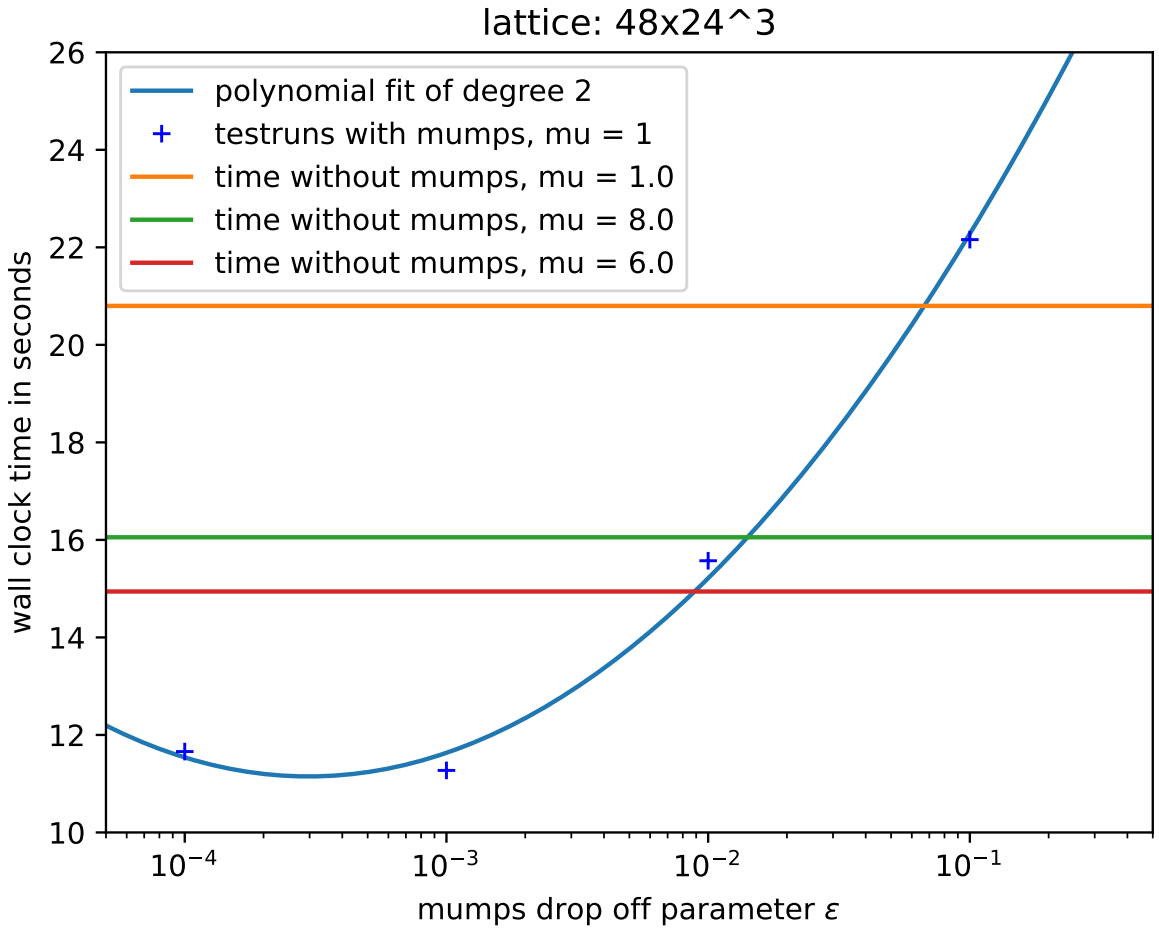

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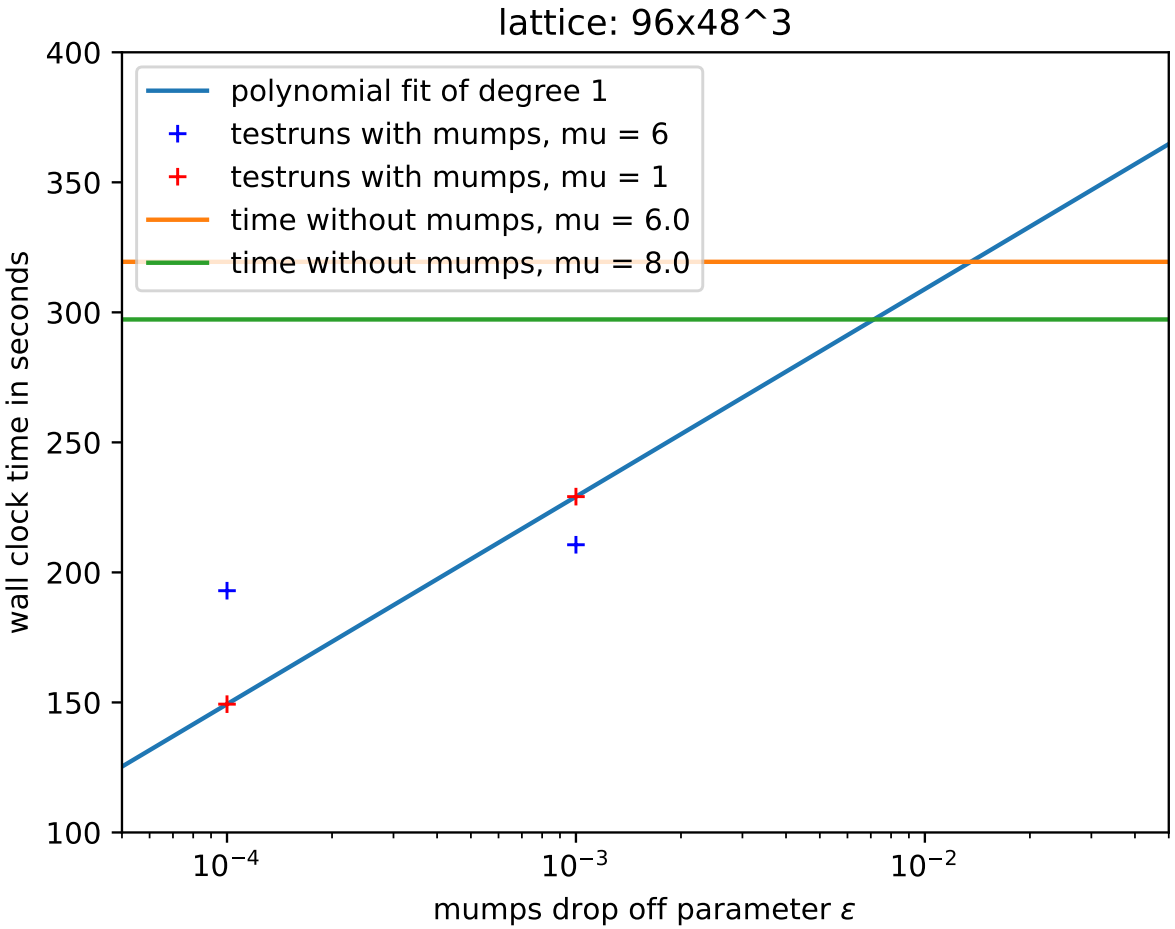

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BLR approximations accuracy: 10^{-4} good choice for all cases

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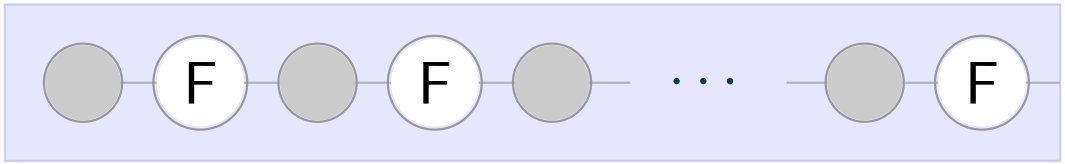
Outline

Construction of multigrid



set up

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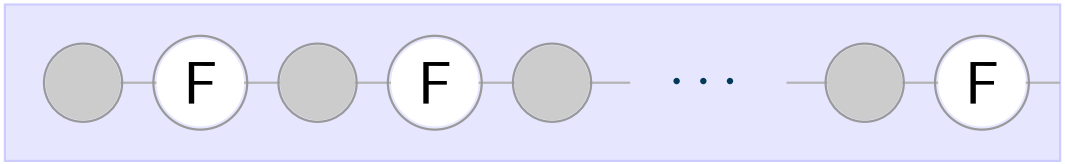
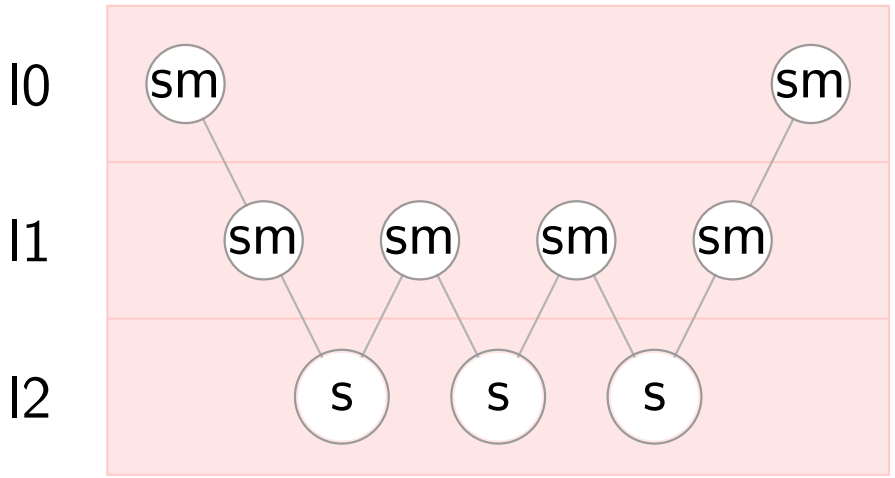


set up

- requires several coarsest level updates
- using more levels reduces factorize time

Disadvantages



solve

- solve phase does not make good use of multithreading
- solution is gathered to root process
- MPI_Scatter done by user
- strong scaling hard to keep up with more levels

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Future possibilities:

future systems will be more ill-conditioned due to

- more realistic physical values
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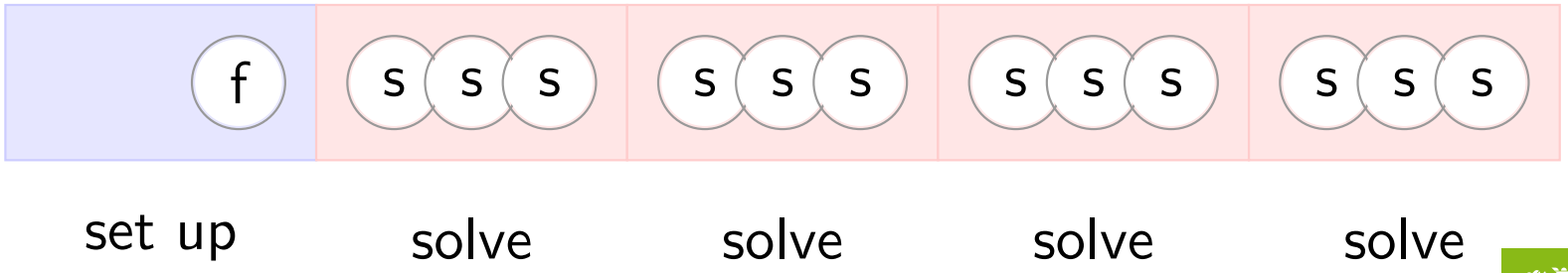
Our research group interests:

- stochastic methods with a lot of sequential solves for one factorization



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Thank you for your attention!

Questions are welcome ....

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