Algebraic MultiGrid Preconditioners for Sparse Linear Solvers at Extreme Scale

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Lawrence Berkeley Laboratory
Sep. 2022

Collaborators, funding and acknowledgments

Pasqua D'Ambra, Consiglio Nazionale delle Ricerche Istituto per le Applicazioni del Calcolo "M. Picone"

Fabio Durastante, Università di Pisa CNR Istituto per le Applicazioni del Calcolo "M. Picone"

Daniele Bertaccini, Università di Roma "Tor Vergata" CNR Istituto per le Applicazioni del Calcolo "M. Picone"

Stefan Kollet, Jülich Forschungszentrum, Institute of Bio- and Geosciences.

Herbert Owen Barcelona Super Computing Center

Project ID: 824158
European Commission
Horizon 2020
European Union funding
for Research & Innovation

What we want to solve

$$\text{Solve}: \; A\mathbf{x} = \mathbf{b},$$

where

- $A \in \mathbb{R}^{n \times n}$ is a very large and sparse matrix $\mathrm{nnz}(A) = O(n)$,
- $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$,

is often the most time consuming computational kernel in many areas of computational science and engineering problems.

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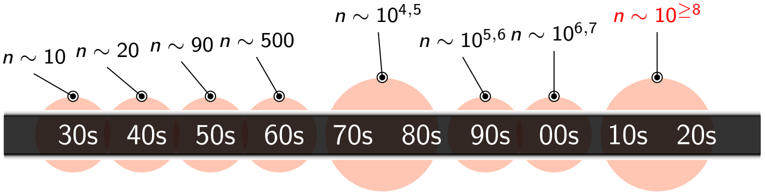


The exascale challenge, using computer that perform 10^{15} Flops, targeting next-gen systems performing 10^{18} Flops to solve problems with tens of billions of unknowns.

Applications

Wind Models

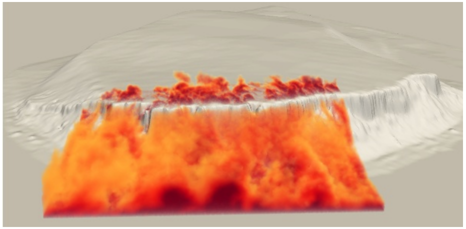
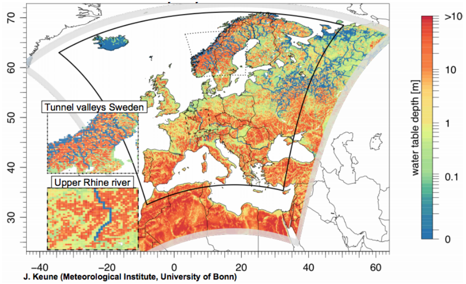


Image credits H. Owen and G. Marin, Barcelona Supercomputing Centre

- Navier-Stokes equations,
- Euler equations,
- Large Eddy Simulations,
- ...

Regional Hydrological Models



- Darcy equation,
- Richards' equation,
- Equations for overland flow
- ...

DoFs: $n \sim 10^{10}$, Processors(cores): $np \sim 10^{6}$

Where we want to solve it

	System	Cores	Rmax (PFlops/s)
1	Frontier	8,730,112	1,102.00
2	Fugaku	7,630,848	442.01
3	Lumi	1,110,144	151.90
4	Summit	2,414,592	148.60
...	...	...	...
21	Marconi-100	347,776	21.64
23	Piz Daint	387,872	21.23
...	...	...	...
82	MareNostrum	153,216	6.47

MareNostrum IV - BSC

Piz Daint - CSCS

- Machines with thousands of MPI cores,
- Hybrid form of parallelism: MPI, OpenMP, CUDA/OpenCL, ...
- but how do we want to solve it?

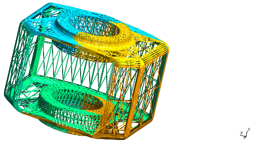
Parallel Sparse Computation Toolkit – psctoolkit.github.io

Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT:

- Existing software standards:
  - MPI, OpenMP, CUDA
  - Serial sparse BLAS,
  - (Par)Metis,
  - AMD
- Attention to performance;
- Research on new preconditioners;
- Data structures are essential, but design for ease of use;
- Tools for large mesh handling: the essential kernel is halo data exchange;
- Krylov subspace solvers;

Parallel Sparse Computation Toolkit – psctoolkit.github.io

Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT: Large mesh handling support



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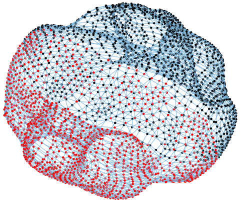


Parallel Sparse Computation Toolkit – `psctoolkit.github.io`

Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT:

- Domain decomposition preconditioners
- Algebraic multigrid with aggregation schemes
  - Parallel coupled Weighted Matching Based Aggregation
  - Smoothed Aggregation (Vaněk, Mandel, Brezina)
- Parallel Smoothers (Block-Jacobi, Hybrid-GS/SGS/FBGS, ℓ_1 variants) that can be coupled with specialized block (approximate) solvers MUMPS, SuperLU, Incomplete Factorizations (AINV, INVK/L, ILU-type)
- V-Cycle, W-Cycle, K-Cycle

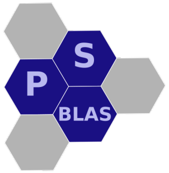
P. D'Ambra, F. Durastante, and S. Filippone. "AMG preconditioners for linear solvers towards extreme scale." SIAM J. Sci. Comp. 43.5 (2021): S679-S703.

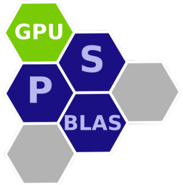
Parallel Sparse Computation Toolkit – psctoolkit.github.io

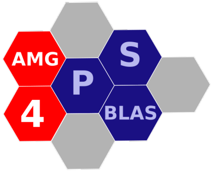
Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT:

- GPU Plugin PSBLAS-EXT
- Support for NVIDIA devices;
- Many data storage formats;
- Fully integrated in PSBLAS, MPI enabled;
- Transparent use from PSBLAS/AMG4PSBLAS

S. Filippone et al., Sparse matrix-vector multiplication on GPGPUs, ACM Trans. Math. Software **43** (2017), no. 4, Art. 30

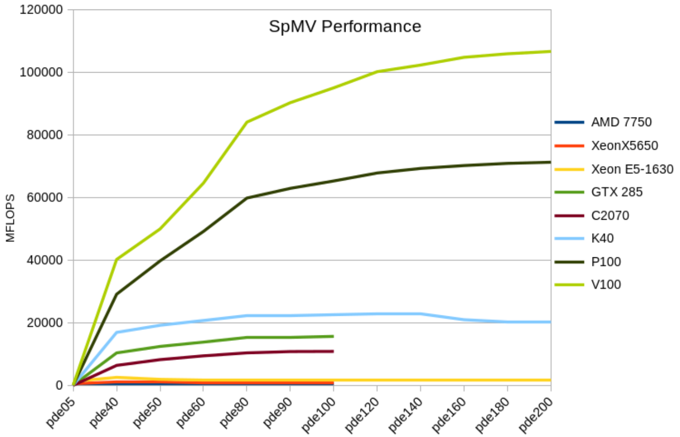






Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT.

- GPU Plugin PSBLAS-EXT



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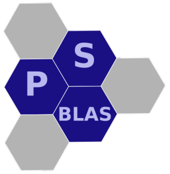
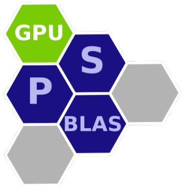
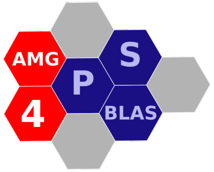


Three central libraries PSBLAS, AMG4PSBLAS and PSBLAS-EXT

- Freely available from: `https://psctoolkit.github.io`,
- Open Source, released under BSD 3 Clause License,
- Interfaced with the Alya multi-physics solver, ParFlow solver, KINSOL non-linear solvers, collaborations with: Barcelona Supercomputing Centre and Jülich Forshungszentrum





Algebraic Multigrid Preconditioners

Given Matrix $A \in \mathbb{R}^{n\times n}$ SPD

Wanted Iterative method B to precondition the CG method:

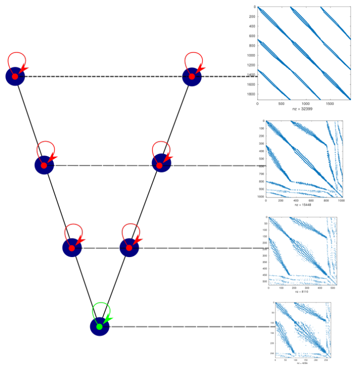
- Hierarchy of systems

$$A_l \mathbf{x}_= \mathbf{b}_l,\ l = 0,\dots,\text{nlev}$$

- Transfer operators:

$$P^l_{l+1} : \mathbb{R}^{n_{l+1}} \to \mathbb{R}^{n_l}$$

Missing Structural/geometric infos



Smoother

$$M_l : \mathbb{R}^{n_l} \to \mathbb{R}^{n_l}$$

"High frequencies"

Prolongator

$$P^l_{l+1} : \mathbb{R}^{n_l} \to \mathbb{R}^{n_{l+1}}$$

"Low frequencies"

Complementarity of Smoother and Prolongator

What are we looking for?

Solve the preconditioned system:

$$B^{-1}Ax = B^{-1}b,$$

with matrix $B^{-1} \approx A^{-1}$ (left preconditioner) such that:

Algorithmic scalability $\max_i \lambda_i(B^{-1}A) \approx 1$ being independent of n,

Linear complexity the action of B^{-1} costs as little as possible, the best being $\mathcal{O}(n)$ flops,

Implementation scalability in a massively parallel computer, B^{-1} should be composed of local actions, performance should depend linearly on the number of processors employed.

What is our *recipe*?

- The smoother M is a standard iterative solver with good parallel properties, e.g., ℓ_1–Jacobi, Hybrid-FBGS, Hybrid-SGS, CG method, etc.
- The prolongator P is built by dofs *aggregation based on matching* in the weighted (adjacency) graph of A.
- The coarse solver can be (again) a preconditioned CG method.

What is our *recipe*?

- The smoother M is an iterative solver with good parallel properties:

GS $A = M - N$, with $M = L + D$ and $N = -L^T$, where $D = \text{diag}(A)$ and $L = \text{tril}(A)$ is intrinsically sequential!

HGS Inexact block-Jacobi version of GS, in the portion of the row-block local to each process the method acts as the GS method.

ℓ_1-HGS On process $p = 1, \ldots, np$ relative to the index set Ω_p we factorize $A_{pp} = L_{pp} + D_{pp} + L_{pp}^T$ for $D_{pp} = \text{diag}(A_{pp})$ and $L_{pp} = \text{tril}(A_{pp})$ then:

$$\begin{aligned} M_{\ell_1-HGS} &= \text{diag}((M_{\ell_1-HGS})_p)_{p=1,\ldots np}, \\ (M_{\ell_1-HGS})_p &= L_{pp} + D_{pp} + D_{\ell_1 p}, \\ (d_{\ell_1})_{i=1}^{nb} &= \sum_{j \in \Omega_p^{nb}} |a_{ij}|. \end{aligned}$$

$$M_{\ell_1-HGS} = \text{diag}((M_{\ell_1-HGS})_p)_{p=1,\ldots np},$$

AINV Block-Jacobi with an approximate inverse factorization on the block $\Rightarrow$ suitable for GPUs

What is our *recipe*?

- The prolongator P is built by dofs *aggregation based on matching* in the weighted (adjacency) graph of A.

Given $\mathbf{w} \in \mathbb{R}^n$, let $P \in \mathbb{R}^{n\times n_c}$ and $P_f \in \mathbb{R}^{n\times n_f}$ be a prolongator and a complementary prolongator, such that:

$$\mathbb{R}^n = \text{Range}(P) \oplus^{\perp} \text{Range}(P_f), \quad n = n_c + n_f$$

$\mathbf{w} \in \text{Range}(P)$: coarse space

$\text{Range}(P_f)$: complementary space

$$[P, P_f]^T A [P, P_f] = \begin{pmatrix} P^T A P & P^T A P_f \\ P_f^T A P & P_f^T A P_f \end{pmatrix} = \begin{pmatrix} A_c & A_{cf} \\ A_{fc} & A_f \end{pmatrix}$$

A_c: coarse matrix

A_f: hierarchical complement

Sufficient condition for efficient coarsening

$A_f = P_f^T A P_f$ as well conditioned as possible, i.e.,
Convergence rate of *compatible relaxation*: $\rho_f = \|I - M_f^{-1} A_f\|_{A_f} \ll 1$

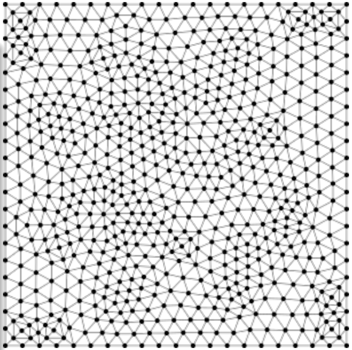
But *how* we achieve it?

Weighted graph matching

Given a graph $G = (\mathcal{V}, \mathcal{E})$ (with adjacency matrix A), and a weight vector $\mathbf{w}$ we consider the weighted version of G obtained by considering the weight matrix $\hat{A}$:

$$(\hat{A})_{i,j} = \hat{a}_{i,j} = 1 - \frac{2a_{i,j}w_iw_j}{a_{i,i}w_i^2 + a_{j,j}w_j^2},$$

- a *matching* $\mathcal{M}$ is a set of pairwise non-adjacent edges, containing no loops;
- a maximum product matching if it maximizes the product of the weights of the edges $e_{i \mapsto j}$ in it.



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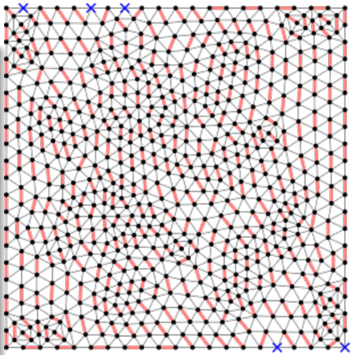
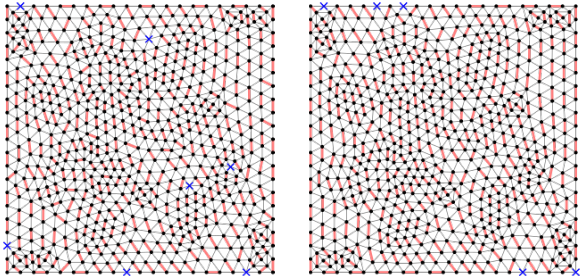


We divide the index set into matched vertices $\mathcal{I} = \bigcup_{i=1}^{n_p} \mathcal{G}_i$, with $\mathcal{G}_i \cap \mathcal{G}_j = \emptyset$ if $i \neq j$, and unmatched vertices, i.e., n_s singletons G_i.

Parallel Matching Algorithms



1. What is the best matching algorithm from a computational point of view?
2. How can we evaluate the quality (in term of the AMG algorithm) of the resulting matching?

With the formalism from (Xu and Zikatanov, 2017) and using a technique from (Napov and Notay, 2011) we associate a quality measure of the aggregates in terms of the convergence properties of the whole AMG method! Better aggregates give better convergence properties.

```
1 Algorithm: Locally Dominant Edge
  Input: Graph $G = (\mathcal{V}, \mathcal{E})$, Weights $\hat{A}$
2 $\mathcal{M} \leftarrow \emptyset$;
3 while $\mathcal{E} \neq \emptyset$ do
4     Take a locally dominant edge $(i, j) \in \mathcal{E}$, i.e., such
       that
              $\arg\max_k \hat{a}_{ik} = \arg\max_k \hat{a}_{jk} = \hat{a}_{ij}$
       Add $(i, j) \in \mathcal{M}$;
5     Remove all edges incident to $i$ and $j$ from $\mathcal{E}$;
6 end
```

Weak Scalability - CPU/GPU Runs - Piz Daint

- Run on the Piz Daint machine up to 28800 cores
- Test: 3D Constant coefficient Poisson Problem with FCG
- DoF: 256k/512k/1M unknowns $\times$ MPI core
- Measure: Solve Time (s).

Scaling

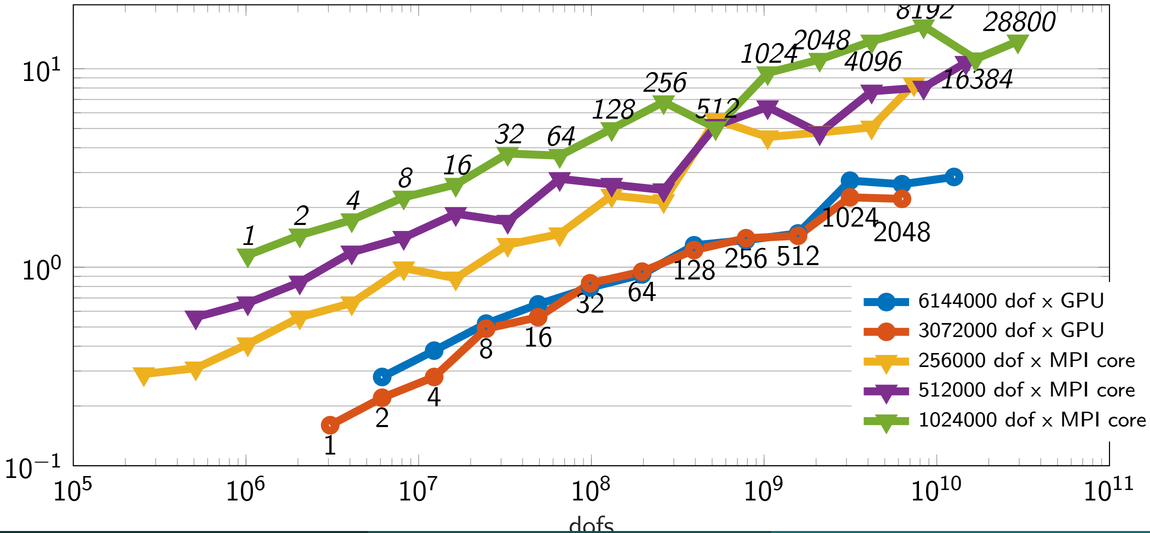
There are two common notions of scalability:

- Strong scaling analysis studies as how the solution time varies with the number of processors for a fixed total problem size.
- Weak scaling analysis studies as how the solution time varies with the number of processors for a fixed problem size per processor.

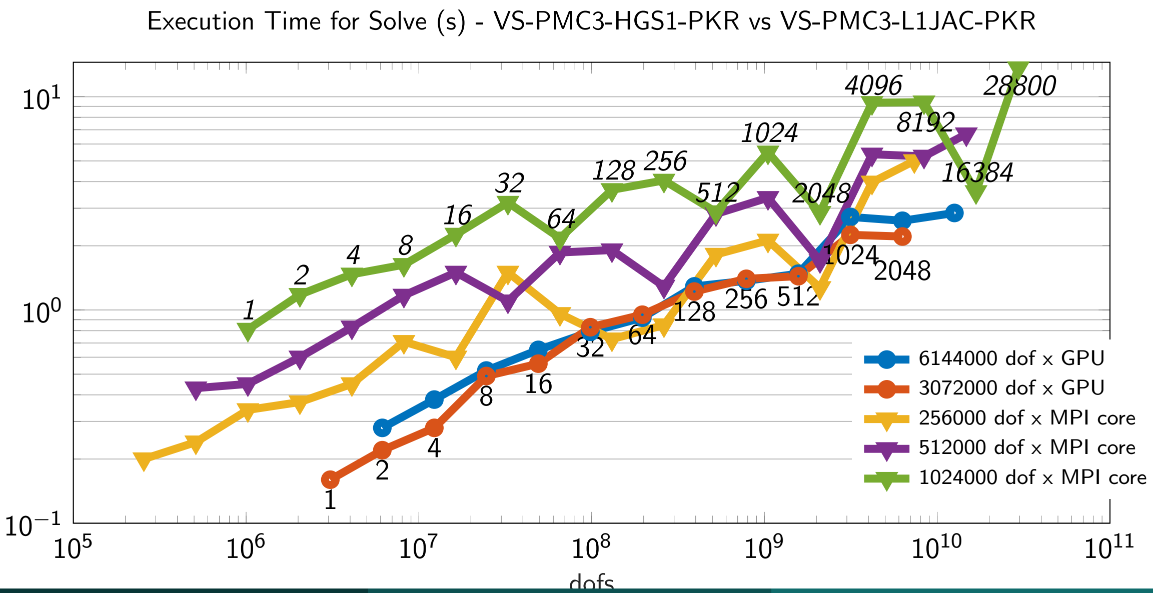
P. D'Ambra, F. Durastante, and S. Filippone. "AMG preconditioners for linear solvers towards extreme scale." SIAM J. Sci. Comp. 43.5 (2021): S679-S703.

Weak Scalability - CPU/GPU Runs - Piz Daint

Execution Time for Solve (s) - K-PMC3-HGS1-PKR vs VS-PMC3-L1JAC-PKR

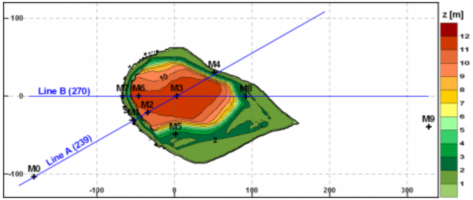


Weak Scalability - CPU/GPU Runs - Piz Daint



A CFD application inside Alya

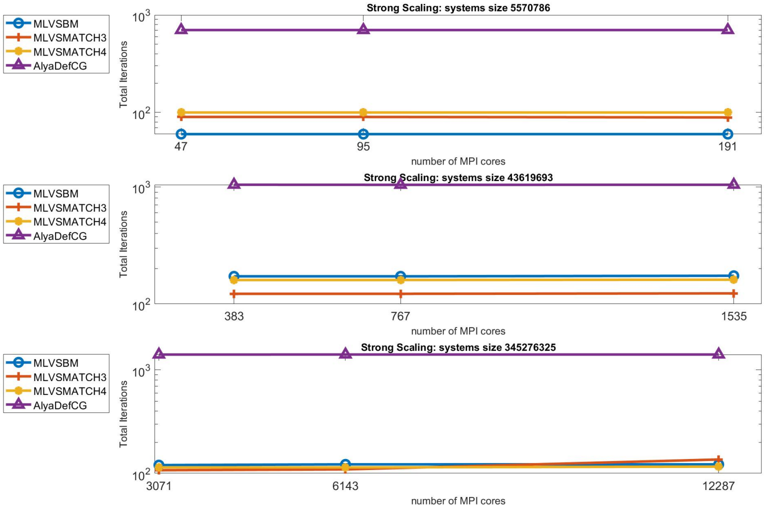
Joint work with
Herbert Owen
Barcelona Super Computing Center



Bolund is an isolated hill situated in Roskilde Fjord, Denmark. An almost vertical escarpment in the prevailing W-SW sector ensures flow separation in the windward edge resulting in a complex flow field.

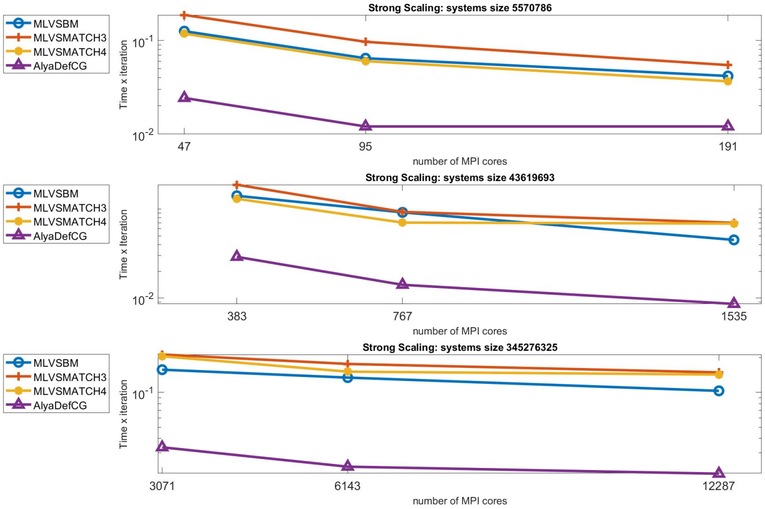
- **Model**: 3D incompressible unsteady Navier-Stokes equations for the Large Eddy Simulations of turbulent flows,
- **Discretization**: low-dissipation mixed FEM (linear FEM both for velocity and pressure),
- **Time-Stepping**: non-incremental fractional-step for pressure, explicit fourth order Runge-Kutta method for velocity.

Bolund Test Case - Strong Scaling - Pressure Equation



- Total number of linear iterations is smaller and stable for increasing number of cores,

Bolund Test Case - Strong Scaling - Pressure Equation



- The time needed per each iteration decreases for increasing number of cores,

The Richards Equation as considered in ParFlow

Collaboration with JÜLICH Forschungszentrum

Richards equation models fluid flow in the *unsaturated* (vadose) zone, it is

- **non-linear** the parameters that control the flow are dependent on the saturation of the media,
- a combination of **Darcy's law** and the principle of **mass conservation**

$$\frac{\partial\left(\rho\,\phi s(p)\right)}{\partial t} + \nabla \cdot q = 0,$$

- $s(p)$ is the saturation at pressure head p of a fluid with density ρ and terrain porosity ϕ,

The Richards Equation: constitutive equations

- q is the volumetric water flux, using Darcy's law it is written as

$$q = -K(p)\left(\nabla p + c\hat{z}\right),$$

  - $K(p)$ the hydraulic conductivity,
  - c the cosine of the angle between the downward z-axis $\hat{z}$ and the direction of the gravity force

To complete the model we need equations for both $s(p)$ and $K(p)$, we use the Van Genuchten formulation [Celia et al. 1990; Van Genuchten, 1980]

$$s(p) = \frac{\alpha(s_s - s_r)}{\alpha + |p|^\beta} + s_r, \text{ and } K(p) = K_s \frac{a}{a + |p|^\gamma},$$

where

- all the parameters $(\alpha, \beta, \gamma, a)$ are fitted on real data and *assumed* to be *constant* in the media;
- K_s is the saturated hydraulic conductivity.

The Richards Equation: constitutive equations

- q is the volumetric water flux, using Darcy's law it is written as

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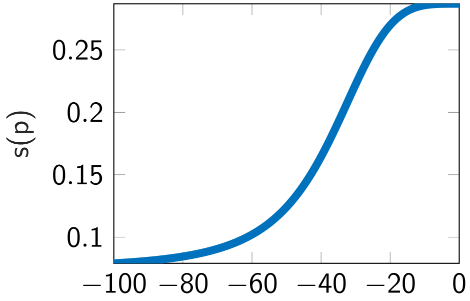
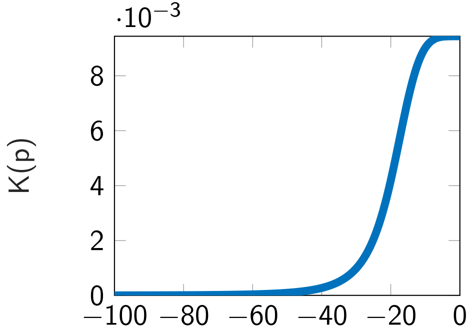




Cell-centered finite difference discretization

We use a cell-centered finite difference **tensor mesh** on

- a parallelepiped discretized with $\mathbf{N} = (N_x, N_y, N_z)$ nodes,
- the cell centers $\{x_{i,j,k} = (ih_x, jh_y, kh_z)\}_{i,j,k=0}^{N-1}$, for $\mathbf{h} = (h_x, h_y, h_z) = (L_x, L_y, L_z)/(\mathbf{N} - 1)$;
- the relative interfaces located at midpoints between adjacent nodes;
- N_t uniform time steps, i.e., the grid $\{t_l = l\Delta\, t\}_{l=0}^{N_t-1}$ for $\Delta\, t = 1/(N_t - 1)$.

This gives the **non-linear equations**:

$$\begin{aligned}\mathbf{\Phi}(p_{i,j,k}^{(l)}) = & \frac{\rho\phi}{\Delta t}\left(s\left(p_{i,j,k}^{(l)}\right) - s\left(p_{i,j,k}^{(l-1)}\right)\right) + q_{i+1/2,j,k}^{(l)} - q_{i-1/2,j,k}^{(l)} + q_{i,j+1/2,k}^{(l)} \\ & - q_{i,j-1/2,k}^{(l)} + q_{i,j,k+1/2}^{(l)} - q_{i,j,k-1/2}^{(l)} + f_{i,j,k} \equiv 0, \\ & \text{for } i,j,k = 1,\ldots,\mathbf{N} - 2,\end{aligned}$$

Cell-centered finite difference discretization

with

$$
\begin{aligned}
q^{(l)}_{i+1/2,j,k} &= -\,{}^{\mathrm{AV}}K^{(l)}_{i+1,i}\left(\frac{p^{(l)}_{i+1,j,k}-p^{(l)}_{i,j,k}}{h_x^2}\right), \qquad q^{(l)}_{i-1/2,j,k} = -\,{}^{\mathrm{AV}}K^{(l)}_{i-1,i}\left(\frac{p^{(l)}_{i,j,k}-p^{(l)}_{i-1,j,k}}{h_x^2}\right),\\
q^{(l)}_{i,j+1/2,k} &= -\,{}^{\mathrm{AV}}K^{(l)}_{j+1,j}\left(\frac{p^{(l)}_{i,j+1,k}-p^{(l)}_{i,j,k}}{h_y^2}\right), \qquad q^{(l)}_{i,j-1/2,k} = -\,{}^{\mathrm{AV}}K^{(l)}_{j-1,j}\left(\frac{p^{(l)}_{i,j,k}-p^{(l)}_{i,j-1,k}}{h_y^2}\right),\\
q^{(l)}_{i,j,k+1/2} &= -\,{}^{\mathrm{AV}}K^{(l)}_{k+1,k}\left(\frac{p^{(l)}_{i,j,k+1}-p^{(l)}_{i,j,k}}{h_z^2}\right)-\frac{K(p_{i,j,k+1})}{2h_z},\\
q^{(l)}_{i,j,k-1/2} &= -\,{}^{\mathrm{AV}}K^{(l)}_{k-1,k}\left(\frac{p^{(l)}_{i,j,k}-p^{(l)}_{i,j,k-1}}{h_z^2}\right)-\frac{K(p_{i,j,k-1})}{2h_z},
\end{aligned}
$$

The Newton method and the sequence of the Jacobians

- Newton step for the solution, at each time step, of the nonlinear systems,
- The Jacobian matrix $J = J_{\mathbf{\Phi}}$ can then be computed in closed form,
- At the core of the (distributed) parallel solution we perform the solution of the (right) preconditioned linear system

$$JM^{-1}(M\mathbf{d}_k) = -\mathbf{\Phi}(\mathbf{p}^{(k,l)}),$$

What did we do in `https://arxiv.org/abs/2112.05051`:

- Describe the asymptotic spectral properties of the sequence $\{J_{\mathbf{N}}\}_{\mathbf{N}}$,
- Analyze the impact of (some) of the different **choices for the interface mean**,
- Use this information to get a matrix sequence $\{M_{\mathbf{N}}\}_{\mathbf{N}}$ for preconditioning $\{J_{\mathbf{N}}\}_{\mathbf{N}}$,
- Approximate such a matrix sequence by a (parallel) AMG method to efficiently solve the systems.

The Newton method and the sequence of the Jacobians

- Newton step for the solution, at each time step, of the nonlinear systems,
- The Jacobian matrix $J = J_{\mathbf{\Phi}}$ can then be computed in closed form,
- At the core of the (distributed) parallel solution we perform the solution of the (right) preconditioned linear system

$$JM^{-1}(M\mathbf{d}_k) = -\mathbf{\Phi}(\mathbf{p}^{(k,l)}),$$

What did we do in `https://arxiv.org/abs/2112.05051`:

- Use this information to get a matrix sequence $\{M_{\mathbf{N}}\}_{\mathbf{N}}$ for preconditioning $\{J_{\mathbf{N}}\}_{\mathbf{N}}$,
- Approximate such a matrix sequence by a (parallel) AMG method to efficiently solve the systems.

We **focus** here on the **implementation aspects**, for the spectral analysis and the other mathematical information: `https://arxiv.org/abs/2112.05051`

The Theoretical sequence of preconditioners (cont'd)

- The theoretical analysis suggests that we can use the discretization of the diffusion operator to precondition. This is *somewhat natural*, see, e.g., [Jones & Woodward, 2001], **but** now we **have a theoretical underpinning** of why it works,
- The organization of the proof works for **different choices of the fluxes** at the interfaces,
- We use the **G**eneralized **L**ocally **T**oeplitz machinery to achieve the formal result; see the books/papers by [Serra & Garoni 2017], [Barbarino, Serra, Garoni 2020].

But

- We still need to find a way to apply $\{M_{\mathbf{N}}^{-1}\}_{\mathbf{N}}$ sequence. Even if the sequence is simpler.
- Use an Algebraic Multigrid Algorithm to generate a $\{\tilde{M}_{\mathbf{N}}^{-1}\}_{\mathbf{N}}$ sequence.

What do we ask to it?

Solve the preconditioned system:

$$J\tilde{M}^{-1}(\tilde{M}\mathbf{d}_k) = -\mathbf{\Phi}(\mathbf{p}^{(k,l)}),$$

with matrix $\tilde{M}^{-1} \approx J^{-1}$ (right preconditioner) such that:

Algorithmic scalability $\max_i \lambda_i(\tilde{M}^{-1}J) \approx 1$ being independent of $\mathbf{N}$,

Linear complexity the action of $\tilde{M}^{-1}$ costs as little as possible, the best being $\mathcal{O}(\mathbf{N})$ flops,

Implementation scalability in a massively parallel computer, $\tilde{M}^{-1}$ should be composed of local actions, performance should depend linearly on the number of processors employed.

Observe that by the GLT analysis, we know that $\max_i \lambda_i(M^{-1}J) \approx 1$, thus if our multigrid hierarchy is "good enough" we can achieve a "near enough" result with it.

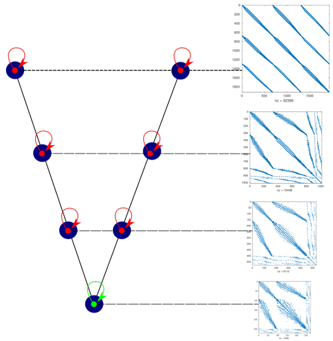
An Algebraic Multigrid Approximation of $\{M_{\mathbf{N}}^{-1}\}_{\mathbf{N}}$

Given Matrix $M_{\mathbf{N}} \in \mathbb{R}^{\mathbf{N}\times\mathbf{N}}$ SPD

Wanted Iterative method $\tilde{M}$ to precondition a Krylov iterative method:

- Hierarchy of systems
$$R_l \mathbf{x}_= \mathbf{b}_l,\ l = 0, \dots, \text{nlev}$$
- Transfer operators:
$$P^l_{l+1} : \mathbb{R}^{n_{l+1}} \to \mathbb{R}^{n_l}$$

Missing Structural/geometric infos



Smoother

$$R_l : \mathbb{R}^{n_l} \to \mathbb{R}^{n_l}$$

“High frequencies”

Prolongator

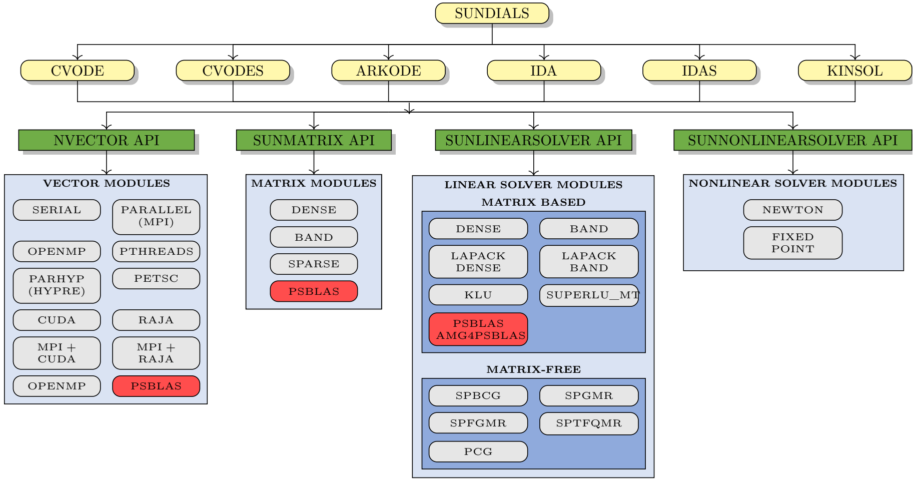
$$P^l_{l+1} : \mathbb{R}^{n_l} \to \mathbb{R}^{n_{l+1}}$$

“Low frequencies”

Complementarity of Smoother and Prolongator

The KINSOL Software Framework

To implement the Newton part of the Newton-Krylov solver we implemented an extension to the SUNDIALS KINSOL package.



From KINSOL to ParFlow

- Wrapping of PSCToolkit *distributed sparse linear algebra* in KINSOL
  - NVECTOR: distributed vectors with all relevant operations (`axpy`, `norms`, `dot`, integrated actions for group of vectors, ...)
  - SUNMatrix: distributed matrix for all the formats in PSBLAS (`CSR`, `CSC`, `COO`, `HYB`, ...) and all the relevant operators (`spmv`, `matrix shift`, ...)
  - SUNLinSol: interface to *all* the Krylov **linear solvers** in PSBLAS (`CG`, `GMRES`, `BiCGStab`, ...) and all the **preconditioner** that can be used (or added in future) to AMG4PSBLAS (Algebraic Multigrid with different aggregation strategies, Domain Decomposition techniques)

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- (PSCToolkit) ⇒ KINSOL ⇒ ParFlow

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- (PSCToolkit) ⇒ KINSOL ⇒ ParFlow
- KINSOL is used in many codes as the supplier of both linear and nonlinear solvers, this first integration is portable for other problems.

Problem and Machine

- Parallelepipedal domain Ω of size $[0, L_x] \times [0, L_y] \times [0, L]$,
- Water at height $z = L$ such that the pressure head becomes zero in a square region at the center of the top layer

$$p(x, y, L, t) = \frac{1}{\alpha} \ln \left[\exp(\alpha h_r) + (1 - \exp(\alpha h_r)) \chi_{[\frac{a}{4}, \frac{3a}{4}] \times [\frac{b}{4}, \frac{3b}{4}]}(x, y, z) \right],$$

- Initial condition is given by $p(x, y, z, 0) = h_r$,
- In all cases we run the simulation for $t \in [0, 2]$ and $N_t = 10$.

Marconi 100

(21th in 06/2022 TOP500)

IBM Power System AC922 nodes
2×16 *IBM POWER93* 3.1 GHz,
256 GB of RAM.

Dual-rail *Mellanox EDR*

Infiniband network by *IBM* 220/300

GB/s.

Preconditioners

	Multigrid		One-Level	
Cycle	1 sweep of V-cyle		Additive Schwarz	Type
Aggregation	Parallel **Decoupled** smoothed aggregation [Vaněk. Mandel, Brezina, 1996]	Parallel **Coupled** smoothed aggregation based on graph matching aggregate size: 8 [D'Ambra, Filippone, Vassilevski, 2018]	1 layer of mesh points in each grid direction	Overlap
Pre/post-smoother	1 iteration of hybrid backward/forward Gauss-Seidel		ILU(0)	Local solver
Coarsest solver	preconditioned `CG` method with ILU(1)-block-Jacobi preconditioner			
Label	VDSVMB	VSMATCH	AS	Label

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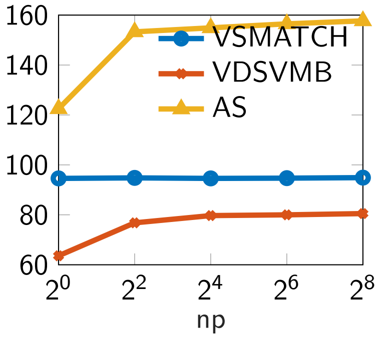
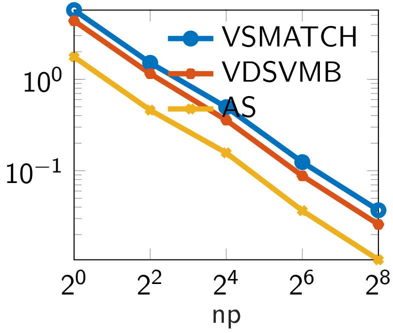
Strong Scalability Analysis

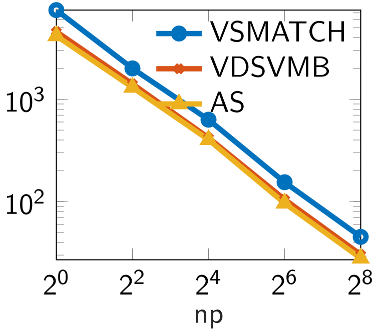
- Parallelepiped $[0,64] \times [0,64] \times [0,1]$, discretized with $N_x = N_y = 800$, and $N_z = 40 \Rightarrow$ 20 millions of dofs,
- Computational cores from 1 to 256, i.e., $np = 4^p$, $p = 0, \dots, 4$,



Average number of linear iterations



Average time per linear iteration T (s)



Total solution time T (s)

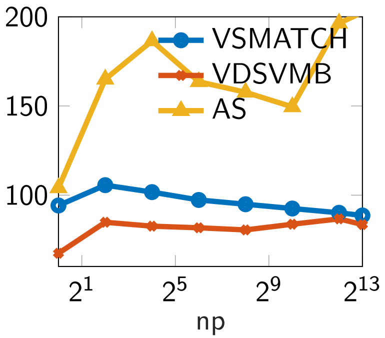
Strong Scalability Analysis

	VDSVBM		VSMATCH		AS	
np	N Jac.s	NLin It.s	N Jac.s	NLin It.s	N Jac.s	NLin It.s
1	3	36	3	38	3	43
4	3	37	3	38	4	39
16	3	37	3	38	4	39
64	3	37	3	38	4	39
256	3	37	3	38	4	39

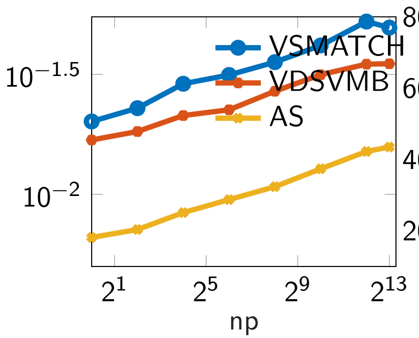
Number of **nonlinear iterations** (NLin It.s), and number of **computed Jacobians** (N Jac.s) for the three preconditioners.

Weak scalability analysis

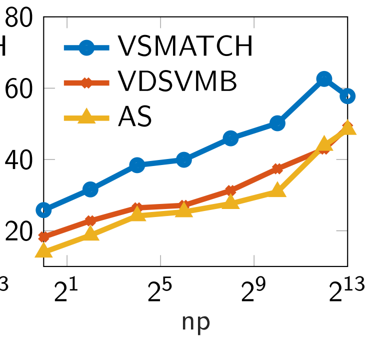
- $N_x = N_y = 50$, and $N_z = 40$, $\Omega(np) = [0, 2^p \times 4.0] \times [0, 2^q \times 4.0] \times [0, 1.0]$
- $np = p \times q$ processes, $p = 0, \dots, 7$, $q = 0, \dots, 6$, and a corresponding mesh $N(p \times q) = (2^p N_x, 2^q N_y, N_z) \Rightarrow$ 820 millions of dofs.



Average number of linear iterations



Average time per linear iteration T (s)



Total solution time T (s)

Weak scalability analysis

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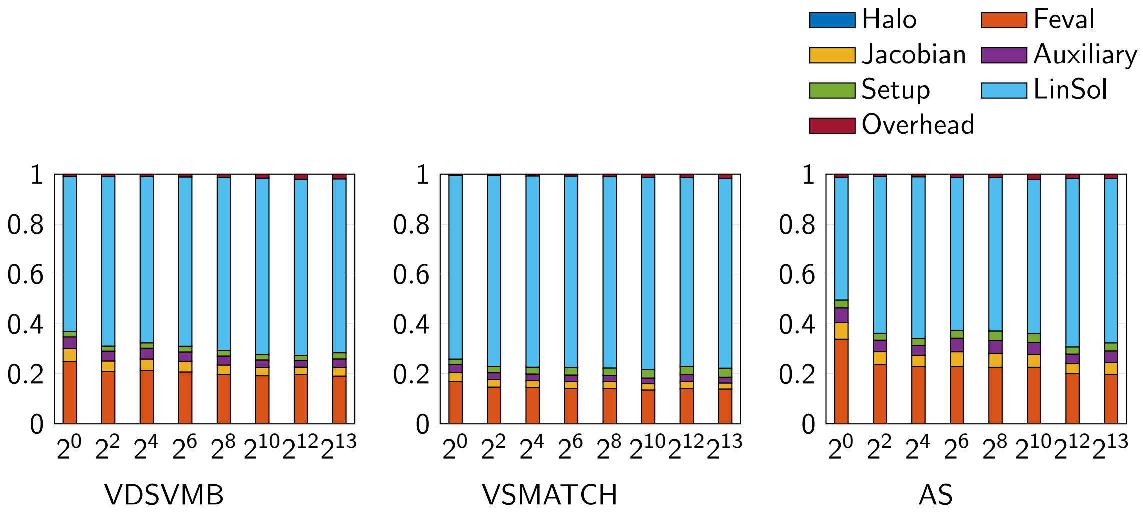
np	N Jac.s	NLin It.s	N Jac.s	NLin It.s	N Jac.s	NLin It.s
1	3	37	3	36	3	40
4	3	38	3	38	3	36
16	3	38	3	38	3	40
64	3	37	3	38	4	37
256	3	37	3	38	4	39
1024	3	39	3	38	4	41
4096	3	41	3	38	4	47
8192	3	40	3	38	4	48

Number of **nonlinear iterations** (NLin It.s), and number of **computed Jacobians** (N Jac.s) for the three preconditioners.

Weak scalability analysis - Time Fractions



Conclusions and future perspectives

We focused on **two main objectives**

- ✓ prove some asymptotic spectral properties of the sequence of Jacobian matrices generated discretizing the Richards equation;
- ✓ prove the efficiency, flexibility and robustness of a software framework for parallel sparse matrix computations.

Our plans for the future

- extension of the PSCToolkit interface to KINSOL, in order to use the ability of the PSCToolkit linear solvers in exploiting GPU architectures;
- integration of the software stack into the ParFlow code for realistic simulations in hydrological applications.

Conclusions and Future Directions

We have proved

- ✓ Aggregation procedure with certified quality,
- ✓ Scalability results on tens of thousands of cores,
- ✓ Comparable results with state of the art libraries,
- ✓ Interfacing with large scale scientific applications,
- ✓ Multi-GPU support.

Algorithmic and software extensions to AMG4PSBLAS (future work)

- Multi-objective matching to increase coarsening ratio,
  - Collaboration with Pacific Northwest National Laboratory (Richland, WA), and Purdue University (IN)
- Process remapping for coarse grid solutions,
  - Collaboration with Centre national de la recherche scientifique (Toulouse)
- GPU data and preconditioner setup improvements,
- Communication avoiding Krylov methods,
- Mixed-precision arithmetic.

Essential bibliography

- Multigrid based on matching

- P. D'Ambra and P. S. Vassilevski, Adaptive AMG with coarsening based on compatible weighted matching, Comput. Vis. Sci. **16** (2013), no. 2, 59–76.
- P. D'Ambra, S. Filippone and P. S. Vassilevski, BootCMatch: a software package for bootstrap AMG based on graph weighted matching, ACM Trans. Math. Software **44** (2018), no. 4, Art. 39, 25 pp.
- M. Bernaschi, P. D'Ambra and D. Pasquini, AMG based on compatible weighted matching for GPUs, Parallel Comput. **92** (2020), 102599, 13 pp.
- P. D'Ambra, F. Durastante, S. Filippone and L. Zikatanov, Automatic coarsening in Algebraic Multigrid utilizing quality measures for matching-based aggregations. arXiv preprint (2022), `arXiv:2001.09969`.

- Scalability results

- P. D'Ambra, F. Durastante, and S. Filippone. "AMG preconditioners for linear solvers towards extreme scale." SIAM J. Sci. Comp. 43.5 (2021): S679-S703.

- PSBLAS

- S. Filippone and A. Buttari, Object-oriented techniques for sparse matrix computations in Fortran 2003. ACM Trans. Math. Software **38** (2012), no. 4, 1–20 pp.
- S. Filippone et al., Sparse matrix-vector multiplication on GPGPUs, ACM Trans. Math. Software **43** (2017), no. 4, Art. 30, 49 pp.

Thank You!

Quality and Convergence: *a posteriori* analysis

Convergence Theorem (D'Ambra, Durastante, Filippone, Zikatanov)

The exact TL–AMG with convergent smoother M, and prolongator P based on the maximum weight matching applied on a SPD matrix A has a convergence rate of

$$\|I - B^{-1}A\|_A \leq 1 - \frac{\mu_c}{c^D}, \text{ for } \mu_c = \min_{1 \leq j \leq J} \mu_j(V_j^c) = \min_{1 \leq j \leq J} \left[\max_{\mathbf{v}_j \in V_j} \min_{\mathbf{v}_j^c \in V_j^c} \frac{\|\mathbf{v}_j - \mathbf{v}_j^c\|_{D_j}^2}{\|\mathbf{v}_j\|_{A_j}^2} \right].$$

and c^D the continuity constant of the smoother. Moreover, the $\mu_j^{-1}(V_j^c)$ are such that

$$\lambda_2^{-1}(D_j^{-1}A_j) \leq \mu_j^{-1}(V_j^c) \leq \lambda_1^{-1}(D_j^{-1}A_j).$$

Furthermore, if either $(\mathbf{w}_{e_{i \to j}}, \lambda_1(D_j^{-1}A_j))$, or $(\mathbf{w}_{e_{i \to j}}^{\perp}, \lambda_2(D_j^{-1}A_j))$ are eigencouples of $D_j^{-1}A_j$, then

$$\mu_j^{-1}(V_j^c) = \lambda_2^{-1}(D_j^{-1}A_j)$$

- The local constants $\mu_j^{-1}(V_j^c)$ are then a quality measure for the single aggregates

Fixing the parameters

We can fix the weight vector **w**, and evaluate the performance of the matching algorithms.

Theorem (Optimal prolongator)

Let $\{\lambda_j, \mathbf{\Phi}_j)_{j=1}^n$ be the eigenpairs of $\overline{T} = \overline{M}A$ for the symmetrized smoother $\overline{M}$. Let us also assume that $\mathbf{\Phi}_j$ are orthogonal w.r.t. $(\cdot,\cdot)_{\overline{M}^{-1}}$. The convergence rate $\|E(P)\|_A$ is minimal for P such that

$$\text{Range}(P) = \text{Range}(P^{opt}),$$

where $P^{opt} = \{\mathbf{\Phi}_1, \dots, \mathbf{\Phi}_{n_c}\}$. In this case,

$$\|E\|_A^2 = 1 - \lambda_{n_c+1}$$

⚠A good candidate can be obtained by exploiting the symmetrized smoother $\overline{M}$ to select as a weight vector an ε–smooth algebraic vector, i.e., for a given $\epsilon \in (0,1)$, **v** an algebraically ϵ-smooth with respect to A if

$$\|\mathbf{v}\|_A^2 \leq \epsilon \|\mathbf{v}\|_{\overline{M}^{-1}}^2.$$

For our choice of P we know that:

- There exists $\mathbf{h} \in \mathbb{R}^{n_c}$ such that $P\mathbf{h} = \mathbf{w}$