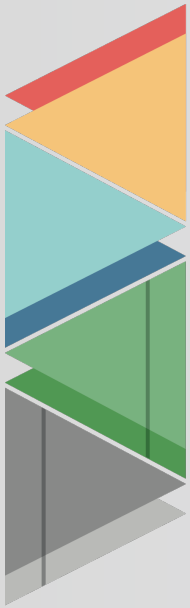

E·C·E²

European Commission | Horizon 2020 European Union funding for Research & Innovation

Demonstration of PSBLAS and AMG4PSBLAS for solving sparse linear systems on parallel hybrid architectures

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Energy Oriented Center of Excellence: toward exascale for energy

The AMG4PSBLAS Team

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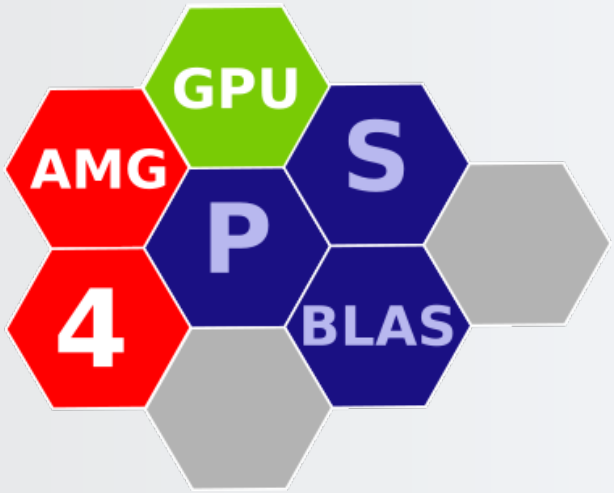
- ~ $ Fabio Durastante

Past Contributors:

- ~ $ Ambra Abdullahi Hassan
- ~ $ Daniela di Serafino
- ~ $ Alfredo Buttari



Freely available from:
psctoolkit.github.io

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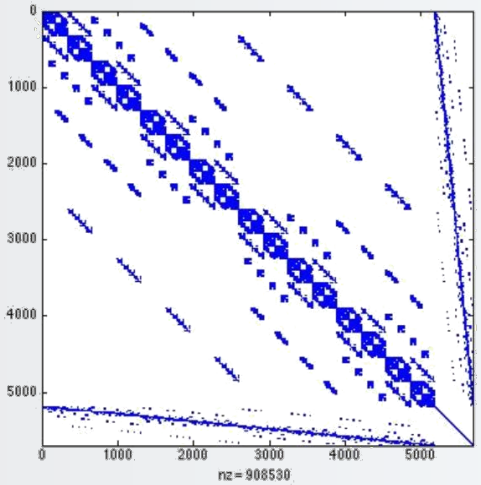
Main Kernel in Computational/Data Science

$A\mathbf{x} = \mathbf{b}, \quad A \in \mathcal{R}^{n \times n}$ (s.p.d.) $\quad \mathbf{x}, \mathbf{b} \in \mathcal{R}^n$

$n >> 10^9$

sparsity degree $\approx 99,9\%$



Applications

numerical simulations: high-resolution models of subsurface flows in water/hydrocarbons/gas resource management require discretization meshes with more than ten billions ($> 10^{10}$) dofs

network analysis: community detection in communication/social networks, e.g., the mobile operator Vodaphone has about 200 million (2×10^8) customers and Google indexes several billion ($> 10^9$) web-pages

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Krylov methods

A matrix is sparse when there are so many zeros (nonzeros are typically $\mathcal{O}(n)$) that it pays off to take advantage of them in the computer representation. James Wilkinson

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Methods of choice: Search for a solution by projection

$$\begin{aligned} \mathbf{x}_m &\in \mathcal{K}_m(A, \mathbf{r}_0) \\ \mathbf{r}_m = \mathbf{b} - A\mathbf{x}_m &\perp \mathcal{K}_m(A, \mathbf{r}_0) \end{aligned}$$

$$\mathcal{K}_m(A, \mathbf{r}_0) = Span\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \ldots, A^{m-1}\mathbf{r}_0\}$$

Krylov subspace (growing with iteration until $\mathbf{x}_m$ is good enough)

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Krylov subspace (growing with iteration until $\mathbf{x}_m$ is good enough)

Conjugate Gradient (CG) for s.p.d. matrices (1952)

CG Convergence

$$\frac{\|\mathbf{e}_k\|_A}{\|\mathbf{e}_0\|_A} \leq 2\left(\frac{a-1}{a+1}\right), \quad a = \sqrt{\mu(A) = \lambda_{max}/\lambda_{min}}$$

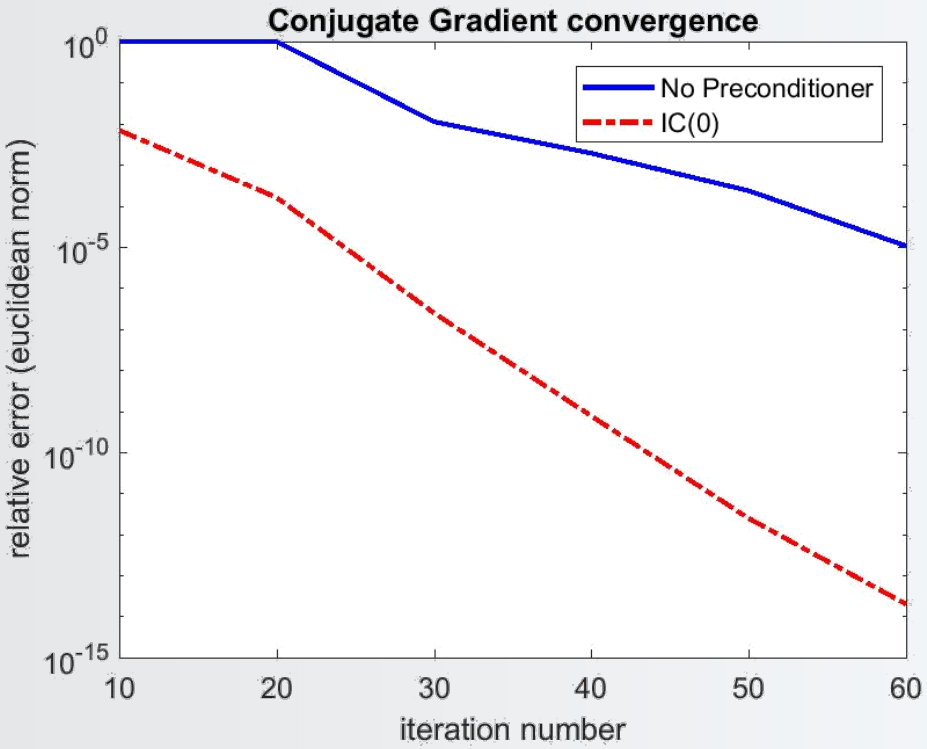
$\mathbf{e}_k = \mathbf{x} - \mathbf{x}_k$ error at iteration k, λ eigenvalue of A

Preconditioning

Solve the system $B^{-1}A\mathbf{x} = B^{-1}\mathbf{b}$, with matrix $B \approx A^{-1}$ (left preconditioner) such that:

$$\mu(B^{-1}A) << \mu(A)$$

Solving 2D Poisson eq.
(2500 dofs, $\mu(A) \approx 1.5 \times 10^3$)



IC(0): $B = LL^T$ with L incompl. Cholesky factor, $\mu(B^{-1}A) \approx 2.2 \times 10^2$

Scalable (optimal) preconditioners

- ~ $ $\mu(B^{-1}A) \approx 1$, being independent of n (algorithmic scalability)
- ~ $ the action of B^{-1} costs as little as possible, the best being $\mathcal{O}(n)$ flops (linear complexity)
- ~ $ in a massively parallel computer, B^{-1} should be composed of local actions, (implementation scalability, i.e., parallel execution time increases linearly with n)

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MultiGrid (MG) Preconditioners

show optimal behaviour for many s.p.d. matrices,
e.g., matrices coming from scalar elliptic PDEs

optimal preconditioner $\neq$ fastest preconditioner

Main Issues for effective parallel MG preconditioners

- ~ $ single-processor performance
- ~ $ memory occupation
- ~ $ balance between computation and communication costs
- ~ $ robustness
- ~ $ flexibility and wide applicability
- ~ $ preconditioner setup time vs. solve time
- ~ $ re-use and efficient updating for varying matrices
- ~ $ ease of use, including interfacing with (legacy) application codes

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Algebraic Multigrid Algorithms

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

Wanted Iterative method B to precondition the CG method:

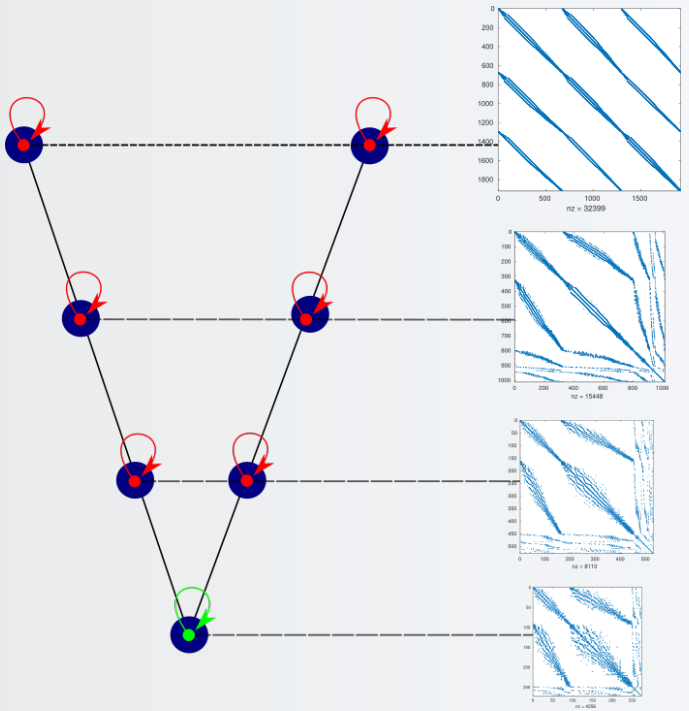
$\sim \$$ Hierarchy of systems

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

$\sim \$$ Transfer operators:

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

Missing Structural/geometric infos



Smoother

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

"High frequencies"

Prolongator

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

"Low frequencies"

Complementarity of Smoother and Prolongator

Algebraic MultiGrid (AMG) Methods

AMG (Brandt, McCormick and Ruge, 1984)

Algebraic MultiGrid methods do not explicitly use the (eventual) problem geometry but rely only on matrix entries to generate coarse-grids by using characterizations of *algebraic smoothness*

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Key issue in effective AMG for general matrices

error not reduced by the (chosen) smoother are called algebraic smoothness:

$$(Aw)_i = r_i \approx 0 \Longrightarrow w_{i+1} \approx w_i$$

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$$(Aw)_i = r_i \approx 0 \Longrightarrow w_{i+1} \approx w_i$$

effective AMG requires that algebraic smoothness is well represented on the coarse grid and well interpolated back $\mathbf{w} = (w_i) \in \mathcal{R}ange(P)$

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Algebraic MultiGrid (AMG) Setup

Recursive application of a two-grid scheme

- $\sim \$$ setup of a convergent iterative solver M (the smoother)
- $\sim \$$ setup of a coarse vector space $\mathcal{R}^{n_c}$ from $\mathcal{R}^n$
- $\sim \$$ build the prolongation P from A
- $\sim \$$ compute coarse grid matrix $A_c = P^T A P$

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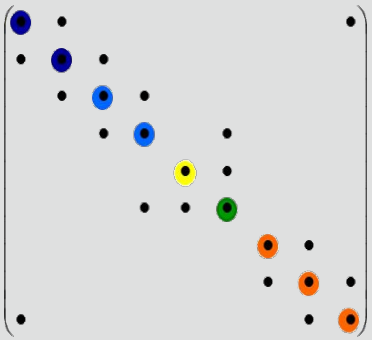
AMG based on Aggregation of dofs

Group the dofs into disjoint sets of aggregates G_j; each aggregate G_j corresponds to 1 coarse dof



Associated prolongation:

$$P := P_{ij} = \begin{cases} w_i & \text{if } i \in G_j \\ 0 & \text{otherwise} \end{cases}$$

$$i = 1, \ldots, n,\ j = 1, \ldots, n_c,$$

or smoothed version of P (Vaněk 1996)

Parallel AMG Setup: decoupled aggregation

Given a user-defined threshold ε

Repeat

- Pick a new root point not adjacent to any existing aggregate
- Add neighbours which are strongly connected $\left(|a^k_{ij}| \geq \varepsilon \sqrt{|a^k_{ii} a^k_{jj}|}\right)$
- Mark all points adjacent to the aggregate

Until all points are marked

For all leftover points

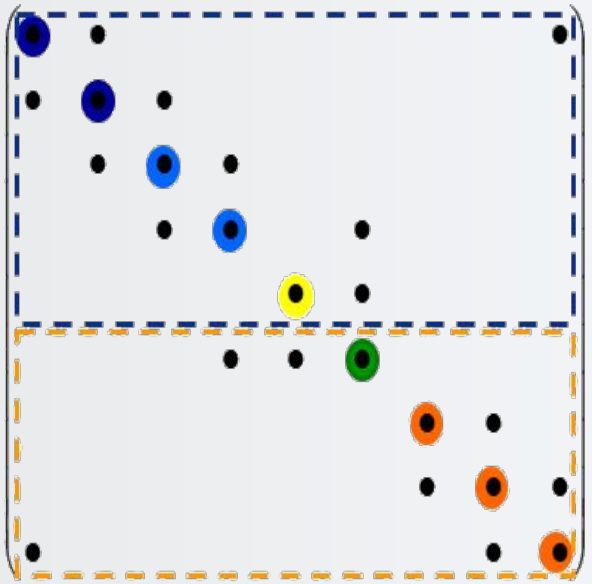
- Add to an aggregated neighbour over threshold; if multiple ones, choose

$$j : |a^k_{ij}| \geq |a^k_{il}| \quad \forall l$$

- If no neighbour is above threshold, start a new aggregate

Endfor

P. Vaněk, J. Mandel and M. Brezina, Algebraic multigrid by smoothed aggregation for second and fourth order elliptic problems, Computing **56** (1996), no. 3, 179–196.



- $\sim$ \$ embarrassingly parallel but it may produce non-uniform aggregates
- $\sim$ \$ generally it yields good results in practice on scalar elliptic problems (Tuminaro and Tong, 2000)

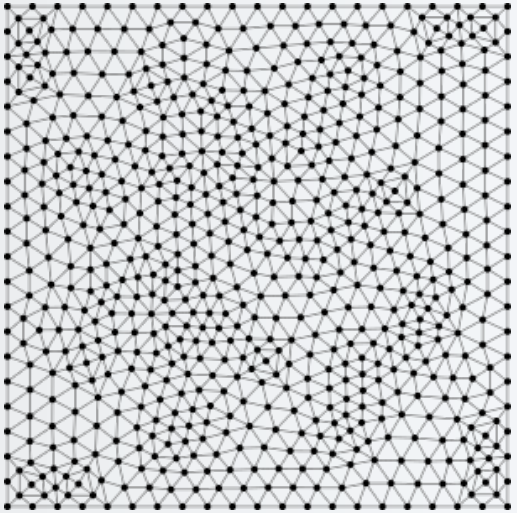
Parallel AMG Setup: Matching based aggregation

AMG based on 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 $\hat{A}$:

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

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



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.

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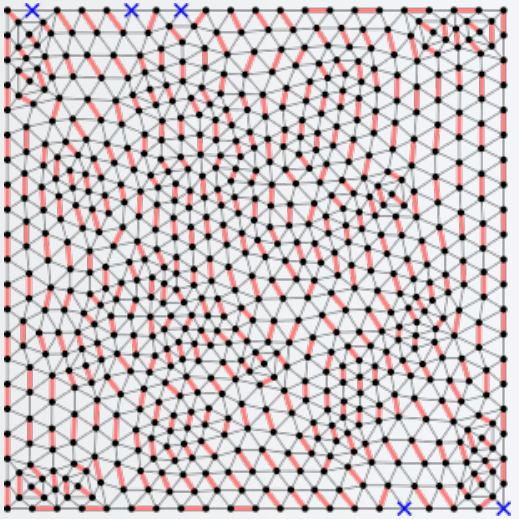

We divide the index set into matched vertexes $\mathcal{I} = \bigcup_{i=1}^{n_p} \mathcal{G}_i$, with $\mathcal{G}_i \cap \mathcal{G}_j = \emptyset$ if $i \neq j$, and unmatched vertexes, i.e., n_s singletons G_i.

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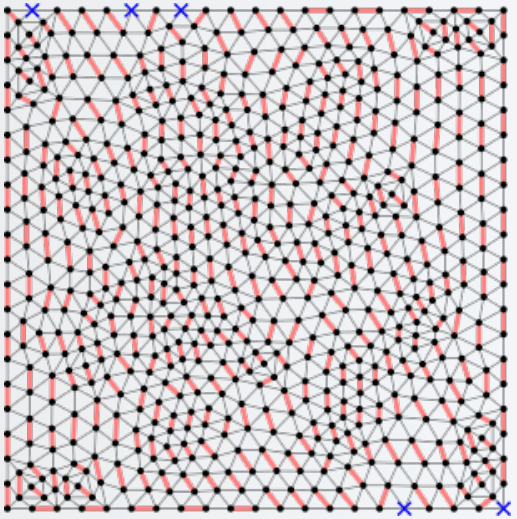

To increase dimension reduction we can perform more than one sweep of matching per step.

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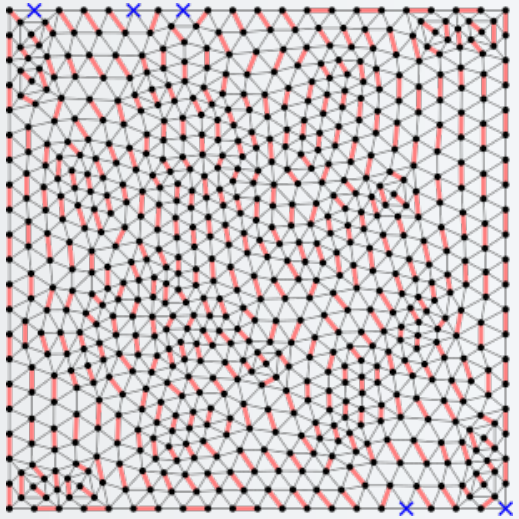

To increase regularity of P_l we can consider a smoothed prolongator by applying a Jacobi step.

Comparison of the Coarsening Strategy

VBM Decoupled aggregation

- ✓ Embarrassingly parallel,
- ✓ Good results with discretized scalar PDEs on a limited number of cores,
- ✗ May produce non-uniform aggregates,
- ✗ Needs user inputted parameters for strength of connection,
- ✗ Issues with anisotropic problems.

Matching-based aggregation

- ✓ Independent of any heuristics or a priori information on the *near kernel* of A,
- ✓ Builds coarse matrices which are well-balanced among parallel processes,
- ✓ No need for special treatment of process-boundary dofs,
- ✓ Works with discretized system of PDEs with arbitrary ordering,
- ✗ May have problems with *highly anisotropic* problems.

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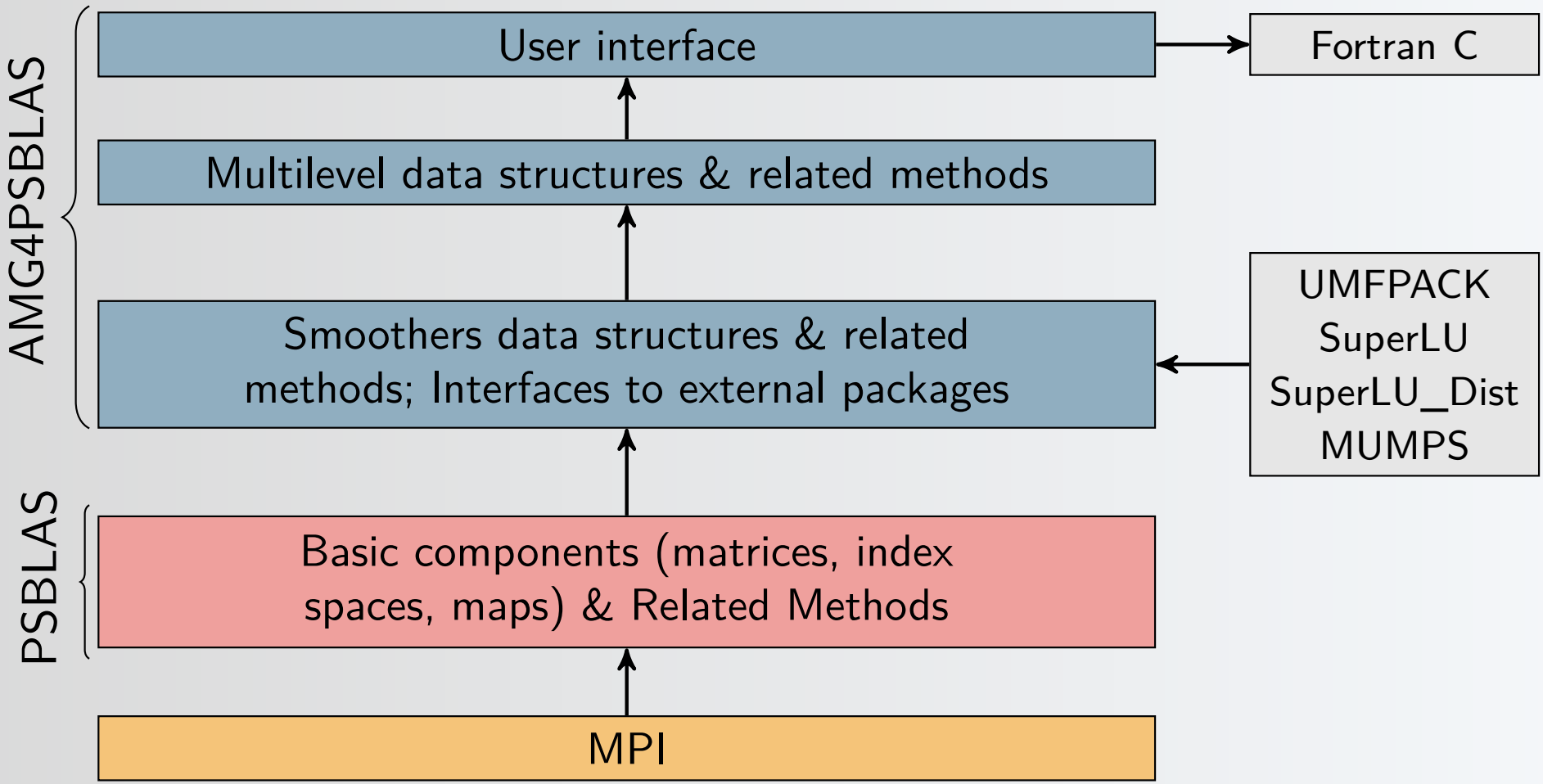
AMG4PSBLAS: Parallel Preconditioners based on PSBLAS

- Improves on the previous versions of the package, initially developed for algebraic multigrid Schwarz preconditioners, upon the extension to more general AMG preconditioning done within EoCoE-I
- Object-oriented design in Fortran 2003, layered sw architecture on top of PSBLAS
  $\Longrightarrow$ modularity and flexibility
- Clear separation between interface and implementation of methods
  $\Longrightarrow$ performance and extensibility
- Separated users' interface for setup of the multigrid hierarchy and setup of the smoothers and solvers to have large flexibility at each level
- Plugin for GPU exploitation (work in progress)
- C and Octave interfaces (work in progress)

AMG4PSBLAS Software Architecture



Current version of AMG4PSBLAS preconditioners

setup phase: **GPU implementation is work in progress**

- ∼ $ decoupled smoothed aggregation
- ∼ $ parallel coupled matching-based aggregation
- ∼ $ distributed or replicated coarsest matrix

solve phase: **already available on GPU** for some methods

- ∼ $ cycles: V, W, K
- ∼ $ smoothers: l_1-Jacobi, hybrid (F/B) Gauss-Seidel, block-Jacobi / additive Schwarz with LU, ILU factorizations or sparse approximate inverses for the blocks
- ∼ $ coarsest-matrix solvers: sparse LU, l_1-Jacobi, hybrid (F/B) Gauss-Seidel, block-Jacobi with LU, ILU factorizations or sparse approximate inverses of the blocks, iterative PCG
- ∼ $ LU factorizations for smoothers & coarsest-level solvers: UMFPACK, MUMPS, SuperLU, SuperLU_Dist

User's interface for preconditioner setup

- ~ $ `p%init(contx,ptype,info)`: allocates and initializes the preconditioner `p`, according to the preconditioner type chosen by the user
- ~ $ `p%set(what,val,info [,ilev, ilmax, pos, idx])`: sets the parameters defining the preconditioner `p`, i.e., the value contained in `val` is assigned to the parameter identified by `what`
- ~ $ `p%hierarchy_build(a,desc_a,info)`: builds the hierarchy of matrices and restriction/prolongation operators for the multilevel preconditioner `p`
- ~ $ `p%smoothers_build(a,desc_a,p,info[,am,vm,im])`: builds the smoothers and the coarsest-level solvers for the multilevel preconditioner `p`
- ~ $ `p%build(a,desc_a,info[,am,vm,im])`: builds the preconditioner `p` (it is internally implemented by invoking the two previous methods)

User's interface for preconditioner apply

- `call p%apply(x,y,desc_a,info [,trans,work])`: computes $y = op(B^{-1})\,x$, where B is a previously built preconditioner, stored into `p`, and op denotes the preconditioner itself or its transpose, according to the value of `trans`.
  `p%apply` is called within the PSBLAS method `psb_krylov` and hence it is completely transparent to the user.

- `call p%free(p,info)`: deallocates the preconditioner data structure `p`
- `call p%descr(info, [iout])`: prints a description of the preconditioner `p`

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Example of use for CPU/GPU

```
! sparse matrix
type(psb_dspmat_type) :: A
! variable declaration needed for GPU running
type(psb_d_hlg_sparse_mat), target   :: ahlg
type(psb_d_vect_gpu)  :: vgm
type(psb_i_vect_gpu)  :: igm
! sparse matrix descriptor
type(psb_desc_type)   :: DESC_A
! preconditioner data
type(amg_dprec_type)  :: P
...
! inizialize parallel environment
call psb_init(ctxt)
call psb_info(ctxt,iam,np)
! read and assemble matrix A and rhs b using
! PSBLAS facilities
```

Example of Use for CPU/GPU (cont'd)

```
! setup AMG preconditioner
call P%init('ML', info)
! Setting up the options (more of this later...)
call P%set(<attribute>, <value>, info)
! build preconditioner
call P%hierarchy_build(A,DESCA,info)
! last three optional parameters for GPU running
call P%smoothers_build(A,DESCA,info,am=ahlg, &
^^I& vm=vgm, im=igm)
! print description of the built preconditioner
call P%descr(info)
! conversions & vector assembly for GPU running
call DESCA%cnv(mold=igm)
call A%cscnv(info,mold=ahlg)
call psb_geasb(x,DESC_A,info,mold=vgm)
call psb_geasb(b,DESC_A,info,mold=vgm)
```

Example of Use for CPU/GPU (cont'd)

```
! set solver parameters and initial guess
...
! solve Ax=b with precond CG
call psb_krylov('CG',A,P,b,x,tol,DESC_A,info,&
^^I& <further options>)
...
! cleanup storage
call P%free(info)
...
!
! leave PSBLAS
call psb_exit(ctxt)
```

And that's all there is to it!

Parameter Setting for Preconditioner Setup

```
...
! build a V-cycle preconditioner with 1
! block-Jacobi sweep (with ILU(0) on the
! blocks) as pre- and post-smoother, and
! 8 block-Jacobi sweeps (with ILU(0)
! on the blocks) as coarsest solver
call P%init('ML',info)
call P%set('SMOOTHER_TYPE','BJAC',info)
call P%set('COARSE_SOLVE','BJAC',info)
call P%set('COARSE_SWEEPS',8,info)
call P%hierarchy_build(A,desc_A,info)
call P%smoothers_build(A,desc_A,info)
...
```

Parameter Setting for Preconditioner Setup (cont'd)

```
...
! build a W-cycle preconditioner with 2
! hybrid Gauss-Seidel sweeps as pre- and
! post-smoother, a distributed coarsest
! matrix, and MUMPS as coarsest-level solver
call P%init('ML',info)
call P%set('ML_CYCLE','WCYCLE',info)
call P%set('SMOOTHER_TYPE','FBGS',info)
call P%set('SMOOTHER_SWEEPS',2,info)
call P%set('COARSE_SOLVE','MUMPS',info)
call P%set('COARSE_MAT','DIST',info)
call P%hierarchy_build(A,desc_A,info)
call P%smoothers_build(A,desc_A,info)
...
```

Parameter Setting for Preconditioner Setup (cont'd)

```
...
! set 1-lev Restricted Additive Schwarz
! with overlap 2 and ILU(0) on the local
! blocks
call P%init('AS',info)
call P%set('SUB_OVR',2,info)
call P%build(A,desc_A,info)
...
```

Example tests directories are available in the library both for reading data from file and for solving a classic scalar elliptic PDE

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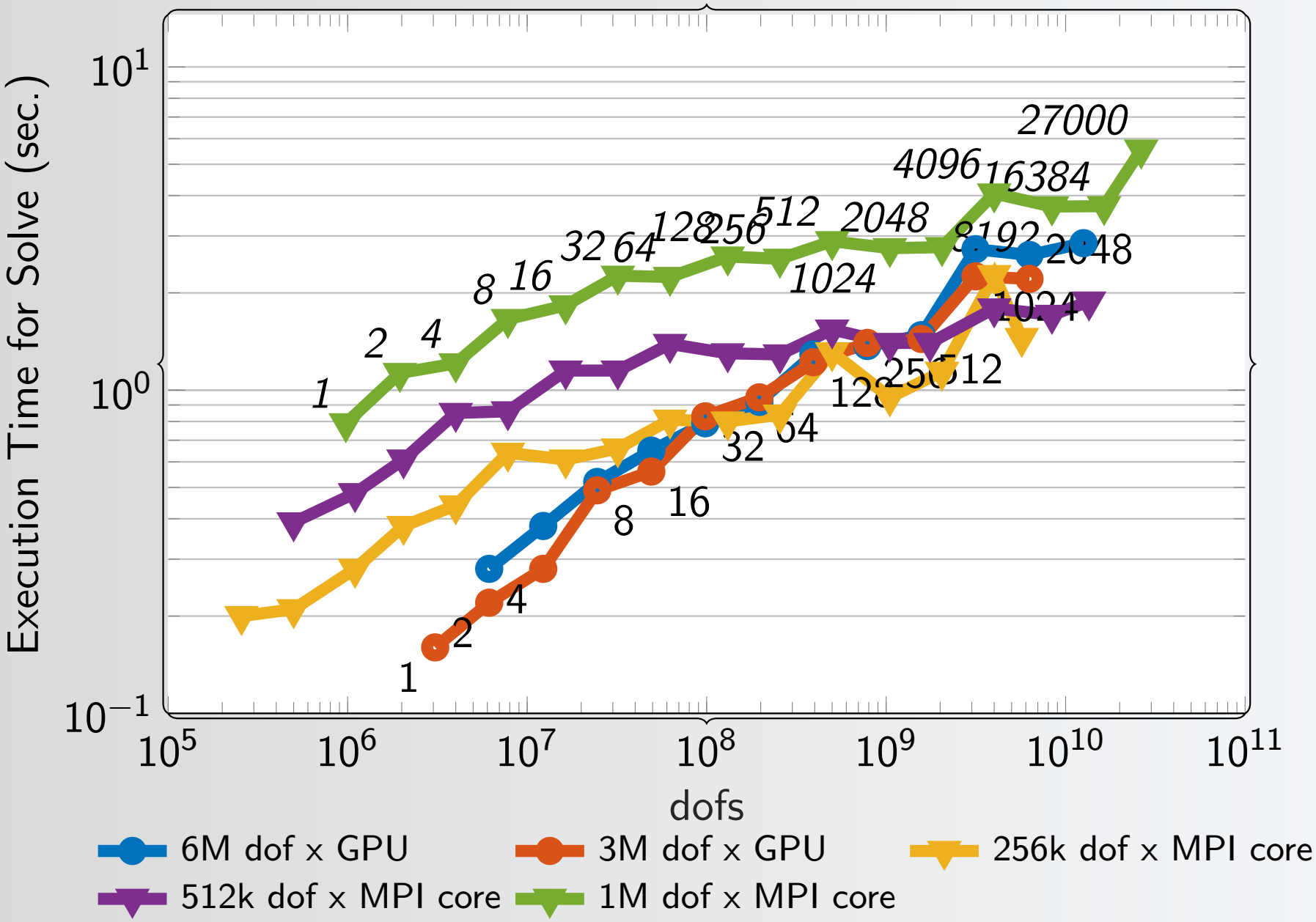
Weak scalability on Piz Daint operated by CSCS

- Poisson problem on the unit cube with 7-point stencil,
- Krylov Solver: Conjugate Gradient, with stopping criterion $\|r_k\| \leq 10^{-6}\|r_0\|$
- Preconditioner:
  - AMG based on coupled smoothed aggregation based on graph-matching
  - V-cycle with 4 point-wise Jacobi sweeps as pre/post-smoother (on the GPU), and 1 sweep of forward/backward Hybrid Gauss-Seidel sweep as pre/post-smoother (on the CPU). Parallel CG preconditioned with Block-Jacobi and ILU(0) at the coarsest level.

Machine Configuration (hybrid Cray XC40/XC50 system): at 21.2 petaflops, rank 6 in Top 500.

- 5704 compute nodes with Intel Xeon E5-2690 v3 CPUs per node and NVIDIA Tesla P100 16GB, 1813 compute nodes equipped with 2 Intel Xeon E5-2695 v4
- Aries routing and communications ASIC with Dragonfly network topology

Weak scalability on Piz Daint operated by CSCS



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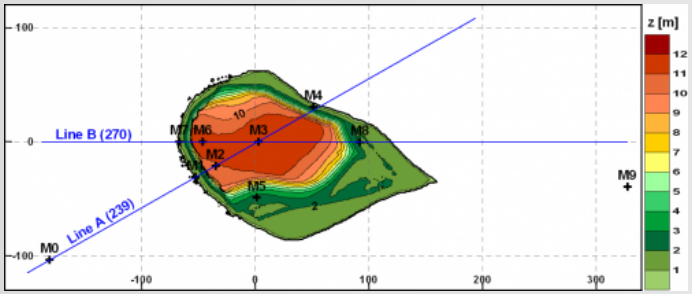
Preliminary results on a CFD application inside Alya

From a 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.

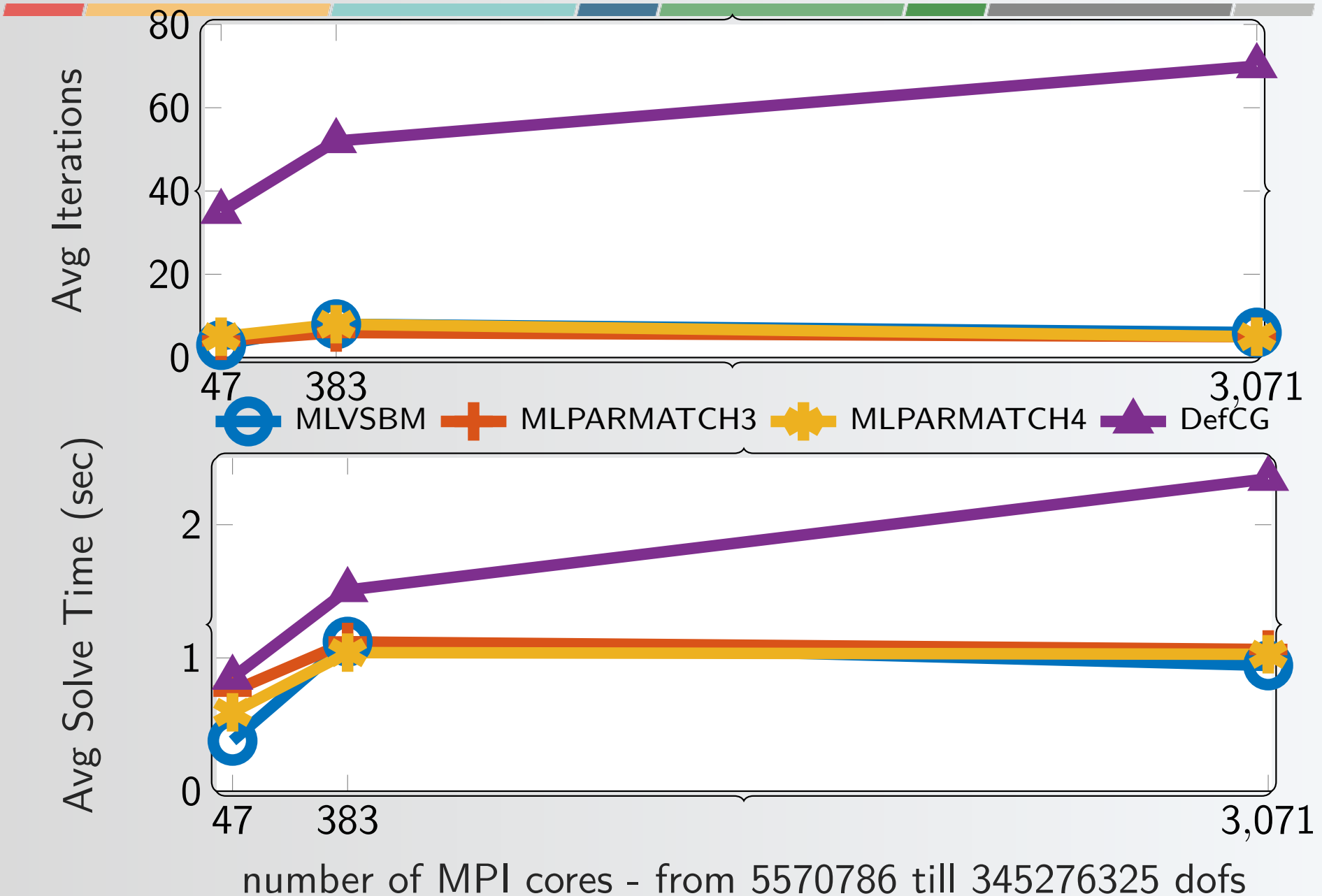
Weak scalability on Marenostrum 4 - operated by BSC

- Solution of the pressure equation for 20 subsequent time-steps with fixed preconditioner,
- Krylov Solver: Conjugate Gradient, with stopping criterion $\|r_k\| \leq 10^{-6}\|r_0\|$
- Preconditioner:
  - AMG based on decoupled smoothed aggregation
  - AMG based on coupled matching
  - V-cycle with 1 sweep of forward/backward Hybrid Gauss-Seidel sweep as pre/post-smoother and parallel CG preconditioned with Block-Jacobi and ILU(0) at the coarsest level

Machine Configuration: at 11,14 Petaflops, rank 29 in Top 500

- Intel Xeon Platinum 8160 CPU at 2.10GHz (Skylake); 3456 nodes, 48 cores per node
- Intel Omni-Path high-performance interconnection network

Weak scalability on Marenostrum 4 - operated by BSC



Work in progress within EoCoE: toward extreme scale

- ~ $ New matching with multi-objective functions trading off between maximum cardinality and maximum weight to treat *highly anisotropic* problems,
- ~ $ new smoothers for efficient hybrid CPU/GPU versions,
- ~ $ efficient implementation of hybrid CPU/GPU version of preconditioners setup phase,
- ~ $ integration within KINSOL by LLNL for non-linear solvers,
- ~ $ testing within Alya from BSC and Parflow from JSC

Main References

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Thanks for Your Attention