# AMG Preconditioners for Computational and Data Science at Extreme Scale

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Calcolo Scientifico e Modelli Matematici

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# The HPC Team at

Projects Participants :

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- Mauro Carrozzo (IAC-CNR), IT
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- Daniele Bertaccini (Univ. of Rome Tor-Vergata and IAC-CNR), IT

Collaborations :

Mahantesh M. Halappanavar, PNNL (Richland, WA), USA

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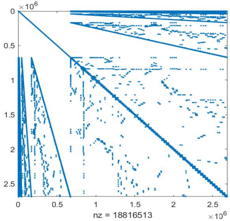
# What we want to solve

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

$n$ **large**

sparsity degree $= 1 - \dfrac{nnz}{n^2} \approx 1$



often the most time consuming computational kernel in many areas of Computational/Data Science

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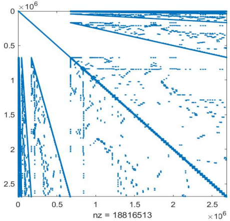

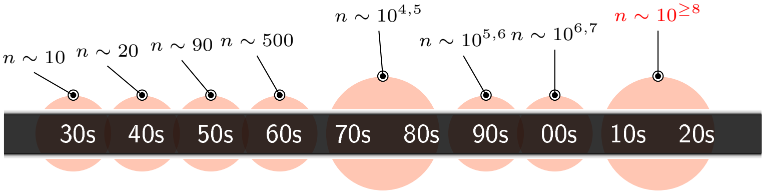

$n \sim 10$

$n \sim 20$

$n \sim 90$

$n \sim 500$

$n \sim 10^{4,5}$

$n \sim 10^{5,6}$

$n \sim 10^{6,7}$

$n \sim 10^{\geq 8}$

30s 40s 50s 60s 70s 80s 90s 00s 10s 20s

The exascale challenge: using computer that do $10^{15}$ Flops, targeting next-gen systems doing $10^{18}$ Flops, to solve problems with tens of billions $(10^{12})$ dofs

# Where we want to solve it[1]

|  | System | Cores | Rmax (TFlops/s) |
|---|---|---|---|
| 1 | Fugaku | 7,630,848 | 442,010.0 |
| 2 | Summit | 2,414,592 | 148,600.0 |
| 3 | Sierra | 1,572,480 | 94,640.0 |
| ⋮ | ⋮ | ⋮ | ⋮ |
| 18 | Marconi-100 | 347,776 | 21,640.0 |
| 20 | Piz Daint | 387,872 | 21,230.0 |
| ⋮ | ⋮ | ⋮ | ⋮ |
| 74 | MareNostrum | 153,216 | 6,470.8 |

- Computers with thousands of CPU cores and GPU accelerators
- Hybrid form of parallelism/programming models: MPI, OpenMP, CUDA/OpenCL/OpenACC, . . .

Marconi 100 - Cineca

Piz Daint - CSCS

[1] TOP500 list, November 2021 – `https://www.top500.org`

# Main issues and challenges

- the cost of data movement dominates the cost of floating-point arithmetic
- accelerators (GPUs, FPGAs, . . .) can run at very high throughput exploiting high levels of data parallelism
- accelerators work very fast on low precision floating-point arithmetic
- minimizing energy consumption is important for sustainability of HPC

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New Mathematics, new algorithms

and new software development tools are needed

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LA FRONTIERA

Il software matematico: le sfide della ricerca sui supercalcolatori

Home > Cultura E Società Digitali

Il software matematico è alla base della simulazione computazionale applicata nei più diversi settori, dalla fluidodinamica all'Intelligenza Artificiale, ed è determinante per lo sviluppo dei supercalcolatori. Cos'è, come funziona, storia, strumenti e metodologie

25 Feb 2022

**Pasqua D'Ambra**
CNR, IAC, CINI HPC-KTT

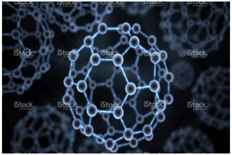
**Salvatore Filippone**
università di Roma "Tor-Vergata" , CINI HPC-KTT

# EoCoE project

## Energy oriented Center of Excellence: toward exascale for energy

applying cutting-edge computational methods to accelerate the transition to the production, storage and management of clean, decarbonized energy

Wind



Materials

Water

Fusion

## Main aim

prepare selected applications to face the exascale challenge

# EoCoE target applications

## Wind Models

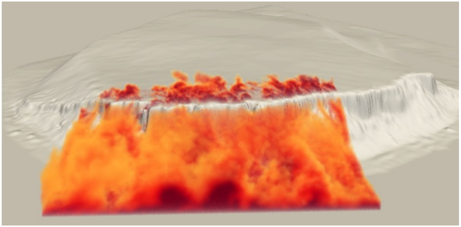
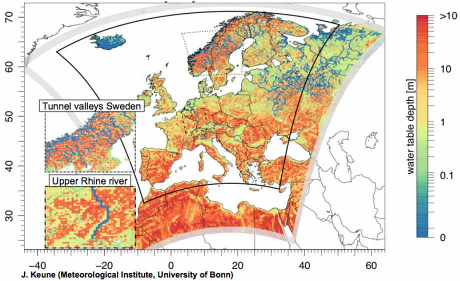


Image credits H. Owen and G. Marin, Barcelona Supercomputing Centre

- Navier-Stokes equations,
- Euler equations,
- Turbulence models,
- ...

## Regional Hydrological Models



J. Keune (Meteorological Institute, University of Bonn)

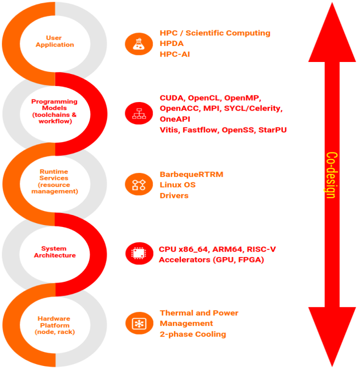
- Darcy equation,
- Richards equation,
- Equations for overland flow
- ...

Target DoFs: $n > 10^{12}$, Computing processes: $np \approx 10^6$

# TEXTAROSSA project

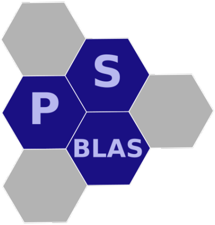
## Towards EXtreme scale Technologies and Accelerators for euROhpc hw/Sw Supercomputing Applications for exascale

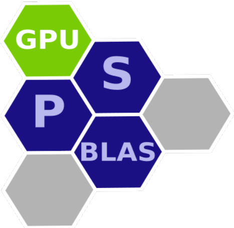
developing new software tools for high-performance and high-energy efficiency on near-future exascale computing systems by multi-directional co-design approach


User Application
HPC / Scientific Computing
HPDA
HPC-AI
Programming Models (toolchains & workflow)
CUDA, OpenCL, OpenMP,
OpenACC, MPI, SYCL/Celerity,
OneAPI
Vitis, Fastflow, OpenSS, StarPU
Runtime Services (resource management)
BarbequeRTRM
Linux OS
Drivers
System Architecture
CPU x86_64, ARM64, RISC-V
Accelerators (GPU, FPGA)
Hardware Platform (node, rack)
Thermal and Power
Management
2-phase Cooling
Co-design

Our contribution: performance/power efficient MathLib

# Parallel Sparse Computation Toolkit



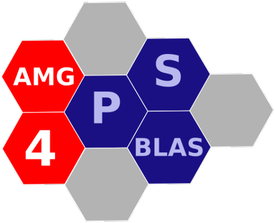


**Parallel Sparse Basic Linear Algebra Subroutines**

Prompted by some works of Iain Duff et al. on standard for Sparse BLAS

+

**its GPU-plugin**



**AMG Preconditioners for PSBLAS**

Available from https://psctoolkit.github.io/

Recently selected as Key Innovation from EU Innovation Radar

# AMG4PSBLAS: AMG Preconditioners for PSBLAS

A software development project started in late 2007

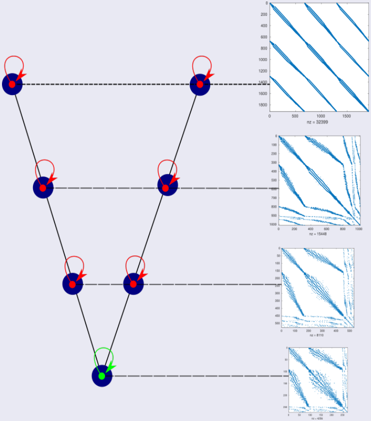
- initially developed as a package of algebraic multigrid Schwarz preconditioners, extended to more general AMG preconditioners
- object-oriented design in Fortran 2003/2008, layered sw architecture on top of PSBLAS
  $\Longrightarrow$ modularity and flexibility
- clear separation between interface and implementation of methods
  $\Longrightarrow$ performance and extensibility (e.g., works transparently on GPUs)
- separated users' interface for setup of the multigrid hierarchy and setup of the smoothers and solvers to have large flexibility at each level

P. D'Ambra et al., MLD2P4: a Package of Parallel Algebraic Multilevel Domain Decomposition Preconditioners in Fortran 95, ACM TOMS, 37, 3, 2010

# AMG Methods

## Example: symmetric V-cycle

```
procedure V-cycle$(k, nlev, A^k, b^k, x^k)$
    if $(k \neq nlev)$ then
        $x^k = x^k + (M^k)^{-1}(b^k - A^k x^k)$
        $b^{k+1} = (P^{k+1})^T\,(b^k - A^k x^k)$
        $x^{k+1} =$ V-cycle$(k+1, A^{k+1}, b^{k+1}, 0)$
        $x^k = x^k + P^{k+1} x^{k+1}$
        $x^k = x^k + (M^k)^{-T}(b^k - A^k x^k)$
    else
        $x^k = \left(A^k\right)^{-1} b^k$
    endif
    return $x^k$
end
```



AMG methods do not explicitly use the problem geometry and rely only on matrix entries to generate coarse grids (setup phase)

# (Two-grid) Convergence

## Theorem

*(Falgout and Vassilevski, 2004) The two-grid preconditioner* $B_{TG}$ *defined from the iteration matrix:*

$$I - B_{TG}^{-1}A = (I - M^{-1}A)(I - P(P^TAP)^{-1}P^TA)(I - M^{-T}A)$$

*is spectrally equivalent to* $A$ *and the following estimate holds:*

$$v^TAv \leq v^TB_{TG}v \leq K_{TG}v^TAv, \text{ with}$$

$$K_{TG} = sup_{v \in \mathcal{R}^n \setminus 0} \frac{v^T\tilde{M}(I - \pi_{\tilde{M}})v}{v^TAv},$$

*where* $\tilde{M} = M(M + M^T - A)^{-1}M^T$ *is the symmetrized smoother and* $\pi_{\tilde{M}} = P(P^T\tilde{M}P)^{-1}P^T\tilde{M}$ *is the* $\tilde{M}-$*based projection.*

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## Ideal prolongator

Assume that $R$ and $S$ form an orthogonal decomposition of $\mathcal{R}^n$, i.e., $RS = 0$, and $P$ is such that $PR$ is a projection onto $\mathcal{R}ange(P)$, the best constant is $K^* = (\lambda_{\text{min}}((S^T\tilde{M}S)^{-1}S^TAS))^{-1}$ and the corresponding minimizer is $P^* = (I - S(S^TAS)^{-1}S^TA)R^T$

# Scalable preconditioners

Solve the system:

$$BAx = Bb,$$

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

- $\max_i \lambda_i(B^{-1}A) \approx 1$ being independent of $n$ (algorithmic scalability)
- the action of $B$ costs as little as possible, the best being $\mathcal{O}(n)$ flops (linear complexity)
- in a massively parallel computer, $B$ should be composed of local actions, **(implementation scalability, i.e., performance linearly proportional to the number of processors employed)**

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## MultiGrid performance parameters

- convergence rate $\rho < 1$: affects number of solver iterations
- operator complexity $opc = \frac{\sum_{k=0}^{nlev-1} nnz(A^k)}{nnz(A^0)}$: affects memory requirements and cycle time
- average stencil size $s(A^k) = nnz\_row(A^k)$: affects computation and communication both in setup and in cycle time

# Our recipies: CMATCH parallel coarsening

Let $\mathbf{w} \in \mathcal{R}^n$ smooth vector, let $P_c \in \mathcal{R}^{n \times n_c}$ and $P_f \in \mathcal{R}^{n \times n_f}$ be a prolongator and a complementary prolongator, such that:

$$\mathcal{R}^n = \mathcal{R}ange(P_c) \oplus^{\perp} \mathcal{R}ange(P_f), \quad n = n_c + n_f$$

$\mathbf{w} \in \mathcal{R}ange(P_c)$ : coarse space $\qquad$ $\mathcal{R}ange(P_f)$ : complementary space

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

$A_c$ : coarse matrix $\qquad$ $A_f$ : hierarchical complement

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## Efficient coarsening (Falgout and Vassilevski, 2004)

Good convergence rate of compatible relaxation:
$\rho_f = \|I - M_f^{-1} A_f\|_{A_f} << 1$ with $M_f = P_f^T M P_f$

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## Our idea (D'Ambra et al., 2013, 2016, 2018)

build $P_c$ (and $P_f$) by dofs **aggregation based on matching in the weighted (adjacency) graph of** $A$, to make $A_f$ **as diagonally-dominant as possible**

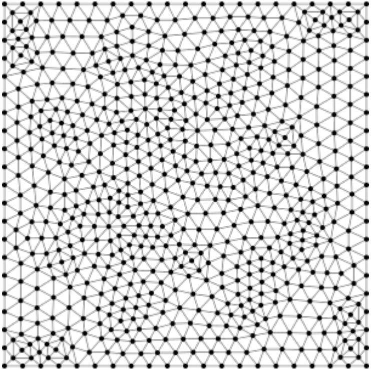
# CMATCH (cont'd)

## Weighted graph matching

Given an (undirected) graph $G = (\mathcal{V}, \mathcal{E})$ (with adjacency matrix $A$), and a weight (smooth) vector $\mathbf{w}$ we consider the weighted version of $G$ with 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
- a maximum weight matching maximizes the sum of the weights of its edges $e_{i \mapsto j}$



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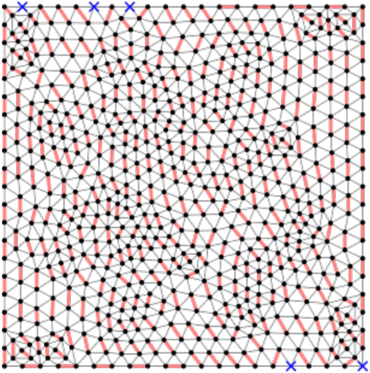

We divide the index set into matched vertices $\mathcal{I} = \bigcup_{i=1}^{n_p} \mathcal{G}_i$, with $\mathcal{G}_i \cap \mathcal{G}_j = \emptyset$ if $i \neq j$, and (possible) unmatched vertices, i.e., $n_s$ singletons $G_i$

# From the matching to the prolongator

We can formally define a *prolongator*:

$$P_c = \underbrace{\left[\begin{array}{cc} \underbrace{\left[\begin{array}{ccc} \mathbf{w}_{e_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \mathbf{w}_{e_{n_p}} \end{array}\right]}_{n_p} 2n_p & \mathbf{0} \\ \mathbf{0} & \underbrace{\left[\begin{array}{ccc} w_1/|w_1| & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & w_{n_s}/|w_{n_s}| \end{array}\right]}_{n_s} n_s \end{array}\right]}_{n_c = n_p + n_s = J} \; n = 2n_p + n_s$$

$$= \begin{bmatrix} \tilde{P} & O \\ O & W \end{bmatrix} = [\mathbf{p}_1, \ldots, \mathbf{p}_J], \qquad \mathbf{w}_e = \frac{1}{\sqrt{w_i^2 + w_j^2}} \begin{bmatrix} w_i \\ w_j \end{bmatrix}$$

⇒ The $\mathcal{M}$ on (a log transformation of) $\hat{A}$ produces $A_f$ with dominant diagonal entries, for $P_f$ such that $P_c^T D P_f = 0$, with $D = \mathrm{diag}(A)$ (Olschowka et al. 1996, Duff et al., 2001)

# CMATCH (cont'd)

```
Input: $A$ matrix, $\mathbf{w}$ (smooth) vector,
maxsize maximum coarsest size
Output: hierarchy of coarse matrices $A^k$
1  $A^1 = A$, $k = 1$, $\mathbf{w^1} = \mathbf{w}$
2  while size($A^k$) $>$ maxsize
    2.1  apply parallel matching-based pairwise aggregation to the graph of $A^k$ with
         weigths depending on $\mathbf{w}^k$
    2.2  build $P_c^k$, $R_c^k = (P_c^k)^T$ and $A_c^k = R_c^k A^k P_c^k$
    2.3  $A^{k+1} = A_c^k$, $\mathbf{w}_c = R_c^k \mathbf{w}^k$
    2.4  $k = k + 1$
   endwhile
```

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  endwhile
```

## Increasing Coarsening Ratio for Reducing Complexity

Consecutive levels based on pairwise aggregation can be combined, e.g., double pairwise can be obtained by:

$$\overline{P_c}^k = P_c^{2k-1} P_c^{2k}, \quad \overline{R_c}^k = (\overline{P_c}^k)^T, \quad \overline{A_c}^k = A_c^{2k}, \quad k = 1, \dots \lceil nl/2 \rceil$$

# CMATCH (cont'd)

## Approximation matching algorithms & parallel software

efficient (sub-optimal) algorithms (Catalyürek et al. 2012, Manne et al. 2014)

- quality guarantee of the computed matching, generally $1/2-$approximation to a maximum weight matching
- linear-time $\mathcal{O}(nnz)$ complexity
- available software in source form (MatchBox-P by Halappanavar et al.)

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- a completely automatic procedure applicable to general s.p.d. systems, independent of any heuristics or a priori information on the near kernel of A

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- well-balanced coarse matrices among parallel processes, no need for special treatment of process-boundary dofs accounting for inter-processes coupling
- significant flexibility in the choice of the size of aggregates, almost arbitrarily aggressive coarsening

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- linear-time $\mathcal{O}(nnz)$ complexity
- available software in source form (MatchBox-P by Halappanavar et al.)

## Main advantages of CMATCH

- a completely automatic procedure applicable to general s.p.d. systems, independent of any heuristics or a priori information on the near kernel of A
- well-balanced coarse matrices among parallel processes, no need for special treatment of process-boundary dofs accounting for inter-processes coupling
- possible improving in V-cycle convergence, by smoothing of matching-based prolongators as in classic smoothed aggregation

$$P_s^k = (I - \omega (D^k)^{-1} A^k) P_c^k, \text{ for } D^k = \mathrm{diag}(A^k)$$

# Quality and Convergence: *a posteriori* analysis

## Theorem

*(D'Ambra, Durastante, Filippone, Zikatanov, 2022) Our TG-AMG $B_{TG}$ with convergent smoother $M$ and BCMATCH exact algorithm has the following property:*

$$\|I - B_{TG}^{-1} A\|_A \leq 1 - \frac{\mu_c}{c^D}$$

$$\text{with} \quad \mu_c = \min_{1 \leq j \leq J} \mu_j(V_j^c) = \min_{1 \leq j \leq J} \left[ \max_{\mathbf{v}_j \in V_j} \min_{\mathbf{v}_j^c \in V_j^c} \frac{\|\mathbf{v}_j - \mathbf{v}_j^c\|_{D_j}^2}{\|\mathbf{v}_j\|_{A_j}^2} \right]$$

*and $c^D$ the continuity constant of the smoother.*

- The constants $c^D$ depends on the symmetrized $\tilde{M}$ convergent smoother

$$c_D \|\mathbf{v}\|_D^2 \leq \|\mathbf{v}\|_{\tilde{M}^{-1}}^2 \leq c^D \|\mathbf{v}\|_D^2$$

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

# Our recipies: highly parallel smoothers

Gauss-Seidel (GS): $A = M - N$, with $M = L + D$ and $N = -L^T$, where $D = \mathrm{diag}(A)$ and $L = \mathrm{tril}(A)$

It is intrinsically sequential!

# Our recipies: highly parallel smoothers

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

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$\ell_1$-HGS On process $p = 1, \ldots, np$ relative to the (row) index set $\Omega_p^{nb}$: $A_{pp} = L_{pp} + D_{pp} + L_{pp}^T$ where $D_{pp} = \mathrm{diag}(A_{pp})$ and $L_{pp} = \mathrm{tril}(A_{pp})$

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$$D_{\ell_1 p} = diag((d_{\ell_1})_i)_{i=1,\ldots,nb}, \; d_{\ell_1} = \sum_{j \in \Omega_p^{nb}} |a_{ij}|$$

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HINVK $M_{HINVK} = \mathrm{diag}((M_{HINVK})_p)_{p=1,\dots np}$

with $(M_{HINVK})_p = A_{pp}^{-1} \approx ZD^{-1}Z^T$ suitable for GPUs

# The weak approximation constant

Let be $P_c$ the CMATCH prolongator and $P_f$ its D-orthogonal complement, with $D = \mathrm{diag}(A)$. Our weak approximation constant is:

$$K = (\lambda_{\mathsf{min}}((P_f^T \tilde{M} P_f)^{-1}(P_f^T A P_f)))^{-1}$$

Unsmoothed prolongator with 3 sweeps of pairwise aggregation

| m | np | HGS | $\ell_1$−HGS | HINVK | $\ell_1$−INVK |
|---|---|---|---|---|---|
| 4096 | 1 | 1.3766 | 1.3766 | 1.5562 | 1.5562 |
| 2048 | 2 | 1.4194 | 1.5270 | 1.5273 | 1.7196 |
| 1024 | 4 | 1.4587 | 1.6621 | 1.6093 | 2.2149 |
| 512 | 8 | 1.4744 | 1.7803 | 1.8284 | 2.6713 |
| 256 | 16 | 1.4945 | 1.8230 | 1.8608 | 2.7307 |
| 128 | 32 | 1.5149 | 1.8682 | 1.8977 | 2.7972 |
| 64 | 64 | 1.5335 | 1.9162 | 1.9390 | 2.8715 |
| 32 | 128 | 1.5880 | 2.0343 | 2.0272 | 3.0707 |
| 16 | 256 | 1.6406 | 2.1594 | 2.1440 | 3.3688 |
| 8 | 512 | 1.6665 | 2.3088 | 2.3137 | 3.7280 |
| $l_1$-Jacobi | | | | 5.6220 | |

homogeneous 3D Laplacian problem with mesh size $m = 16^3$ over $np$ processes.

# Test Case: Poisson Equation

$$-\Delta u = 1 \text{ on unit cube, with DBC}$$

- 7-point finite-difference discretization
- cartesian grid with uniform refinement along the coordinates for increasing mesh size

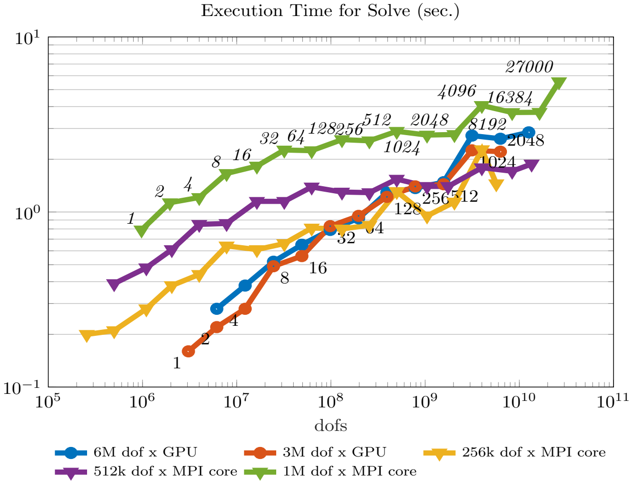
## Solver/preconditioner settings

- AMG as preconditioner of CG, stopped when $\|\mathbf{r}^k\|_2/\|\mathbf{b}\|_2 \leq 10^{-6}$, or $itmax = 500$

  VSCMATCH V-cycle, CMATCH building aggregates of max size $8$, smoothed prolongators
- coarsest matrix size $n_c \leq 200np$, with $np$ number of cores
- 1 sweep of forward/backward Hybrid Gauss-Seidel smoother (4 sweeps of $l_1-$Jacobi on GPU), parallel PCG coupled with Block-Jacobi+ILU(0) at the coarsest level

Platform: Piz Daint, Cray Model XC40/Cray XC50 with 5704 hybrid compute nodes (Intel Xeon E5-2690 v3 with Nvidia Tesla P100)

# Results at extreme scale: MPI vs hybrid MPI-CUDA



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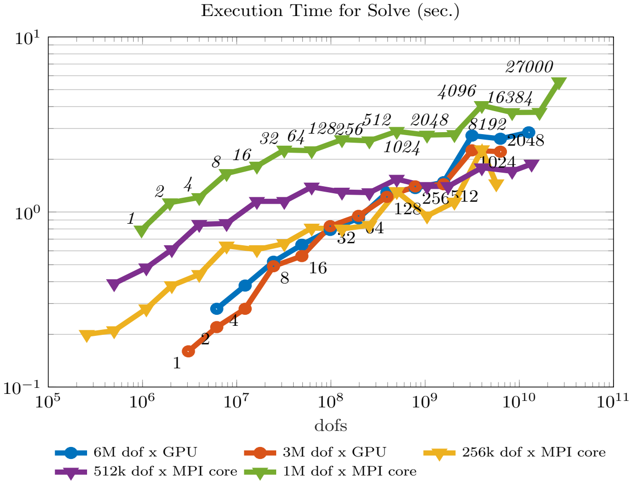
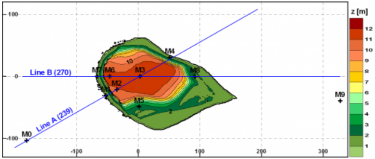


## Performance/Power efficiency

the hybrid approach permits savings in solve time and energy consumption

# A CFD application inside Alya

Joint work with
Herbert Owen
Barcelona Super Computing Center

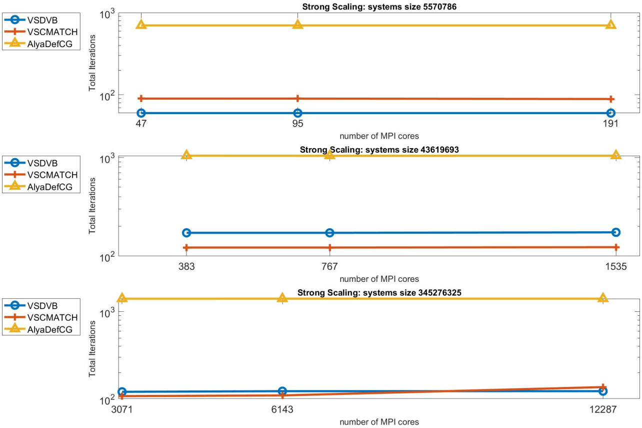


Bolund is an isolated hill situated in Roskilde Fjord, Denmark. An almost vertical escarpment in the prevailing W-SW sector ensures flow separation in the windward edge resulting in a complex flow field.

- **Model**: 3D incompressible unsteady Navier-Stokes equations for Large Eddy Simulations of turbulent flows $Re_\tau = 10^7$
- **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

Three fixed size problems ($\approx 6 \times 10^6,\ 4.4 \times 10^7,\ 0.35 \times 10^9$), for increasing number of cores, 20 time steps in the fully development flow phase



- AMG preconditioners largely reduce the total number of iterations

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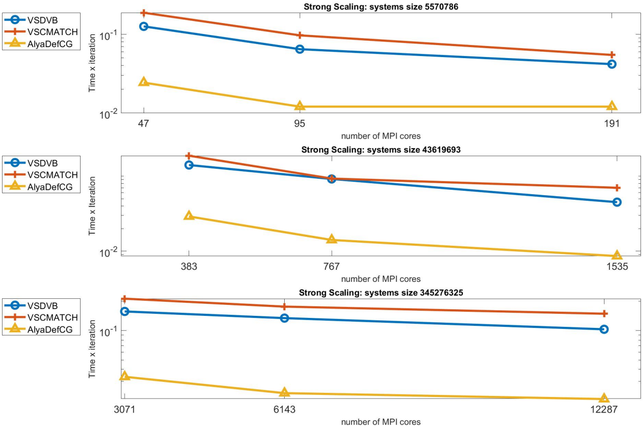

- solve time needed per each iteration decreases for increasing number of cores

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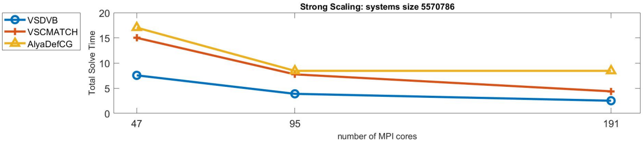

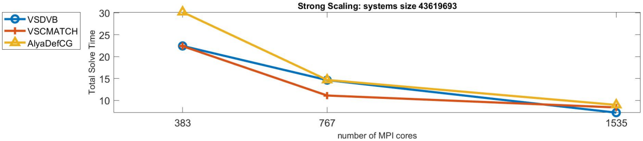

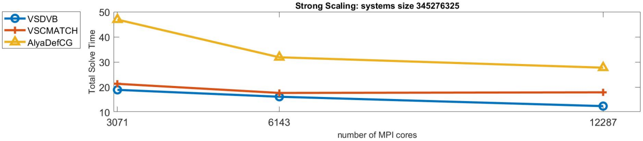

- the trade-off between cost-per-iteration and number of iterations advantages the AMG preconditioners

# Concluding Remarks and Work in Progress

- PSCToolkit is a software project addressing scalability, flexibility and robusteness for high-performance scientific computing at extreme scale
- our new parallel coarsening algorithm based on compatible weighted matching, used in conjunction with smoothed prolongators and highly parallel smoothers, shows algorithmic and implementation scalability
- we solve systems with size larger than $10^{10}$ on current pre-exascale computers, embedding hybrid CPU-GPU nodes, saving time and energy
- scalability results and comparison with available software demonstrates the validity of our approaches both in terms of algorithms and in terms of software development
- integration and testing within very large scale wind simulations and hydrology applications, in collaborations with BSC and JSC, gave very promising results
- we want to explore extreme scalability beyond $10^5/10^6$ computing cores and trillions $(10^{18})$ of dofs

# Main recent references

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## Thanks for Your Attention

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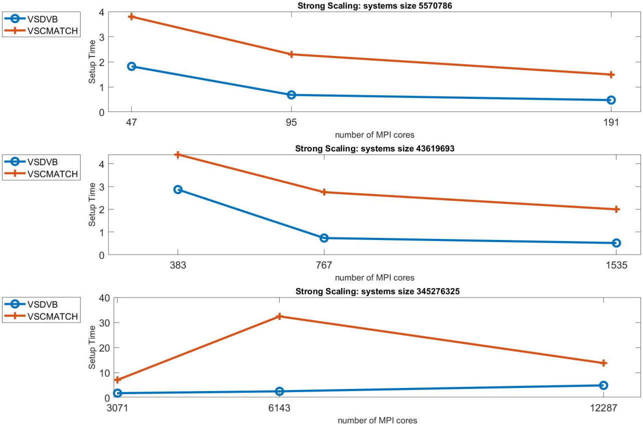
# Preconditioners Setup Time in Alya


Strong Scaling: systems size 5570786
VSDVB
VSCMATCH
Setup Time
number of MPI cores
Strong Scaling: systems size 43619693
VSDVB
VSCMATCH
Setup Time
number of MPI cores
Strong Scaling: systems size 345276325
VSDVB
VSCMATCH
Setup Time
number of MPI cores