EoCoE²

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MLD2P4
a Package of Parallel Algebraic MultiGrid Preconditioners for Scalable Linear Solvers

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Energy Oriented Center of Excellence: toward exascale for energy

The MLD2P4 Team

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MLD2P4

Multi-Level Domain Decomposition Parallel Preconditioners Package based on PSBLAS

Main Ref.:
P. D'Ambra, D. di Serafino, S. Filippone, MLD2P4: a package of parallel algebraic multilevel domain decomposition preconditioners in Fortran 95, ACM TOMS, 37, 2010

Freely available from
`https://github.com/sfilippone/mld2p4-2`

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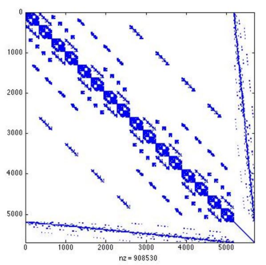
Main Kernel in Computational/Data Science

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

$$n >> 10^9$$

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:

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

Preconditioning

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

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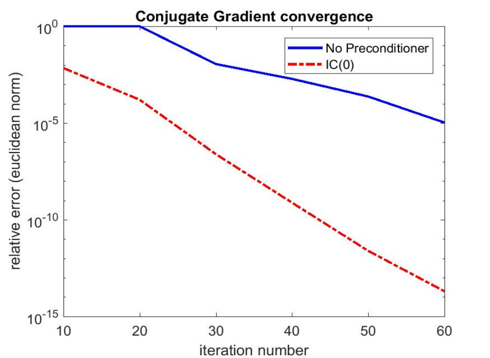
Solving 2D Poisson eq. (2500 dofs, $\mu(A) \approx 1.5 \times 10^3$)



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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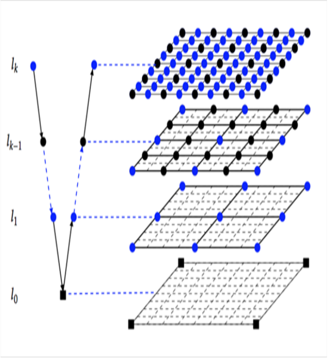
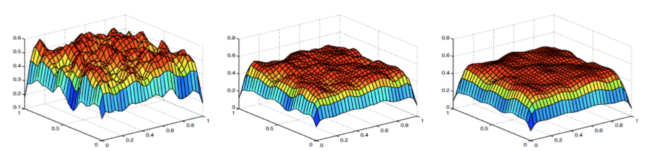
MG Methods

Example: (symmetrized) V-cycle

- Pre-smoothing:
  $x = x + M^{-1}(b - Ax)$
- Residual restriction:
  $r_c = P^T(b - Ax)$
- Solution on coarse grid:
  $A_c e = r_c$, applying recursion
- Error interpolation and
  solution update: $x = x + Pe$
- Post-smoothing:
  $x = x + (M^T)^{-1}(b - Ax)$





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

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

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

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

Algebraic MultiGrid (AMG) Setup

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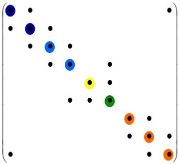
AMG based on Aggregation of dofs

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 aggregationâĂŔ

Given a user-defined threshold ε

Repeat

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

Until all points are marked

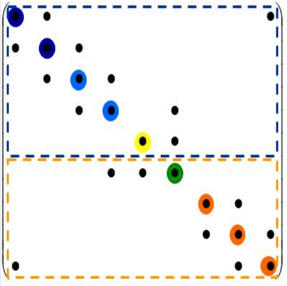
For all leftover points

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

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

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

Endfor



∼ $ embarrassingly parallel but it may produce non-uniform aggregates

∼ $ generally it yields good results in practice on scalar elliptic problems (Tuminaro and Tong, 2000)

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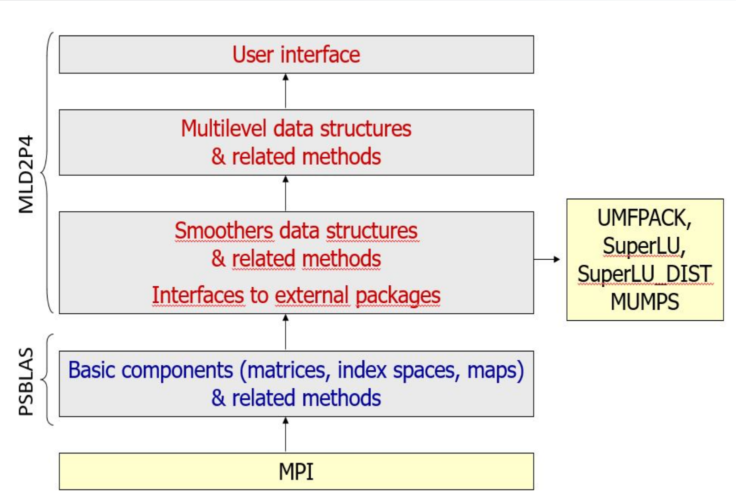
MLD2P4: Parallel Preconditioners based on PSBLAS

- Initially developed as a package of algebraic multigrid Schwarz preconditioners, extended to more general AMG preconditioning within EoCoE
- 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)

MLD2P4 Software Architecture



Current version of MLD2P4 preconditioners

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

- decoupled smoothed 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(icontx,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

- ~ $ `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(mld_dprec_type)  :: P

...
! inizialize parallel environment
  call psb_init(ictxt)
  call psb_info(ictxt,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)
  call P%set(<attribute>, value, info)
...
  call P%set(<attribute>, value, info)
...
! build preconditioner
  call P%hierarchy_build(A,DESCA,info)
! last three optional parameters needed for GPU unning
  call P%smoothers_build(A,DESCA,info,am=ahlg, vm=vgm, im=igm)
! print description of the built preconditioner
  call P%descr(info)

! conversions and vector assembly needed 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,...)
  ...
! cleanup storage
  call P%free(info)
  ...
!
! leave PSBLAS
  call psb_exit(ictxt)
```

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%bld(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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Parflow Model

Simulations of subsurface flow for regional hydrology studies

Richard's equation

Filtration through variably saturated porous media for incompressible flows (3D model based on Darcy's law):

$$
\begin{aligned}
\frac{\partial(\Phi s(p))}{\partial t} + \nabla \cdot \mathbf{u} &= f \\
\mathbf{u} &= -\mathbf{K}\nabla(p - z)
\end{aligned}
$$

- implicit time integration method
- finite difference discretization of spatial operator on a structured Cartesian mesh
- Newton-Krylov solver for non-linear algebraic equation coupled with a linear geometric preconditioner
- MPI-based parallel code written in C

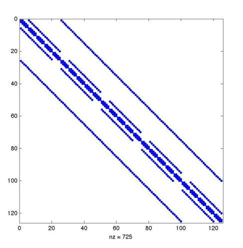
Test cases for PSBLAS and MLD2P4

Simplified steady-state model

$$-\nabla \cdot \mathsf{K} \nabla p = f$$

on unit cube, with no-flow boundary conditions

- discretization obtained by a PSBLAS code reproducing a Matlab mini-app provided by JSC
- isotropic conductivity tensor
- cartesian grid with uniform refinement along the coordinates for increasing mesh size
- hepta-diagonal spd matrices



Weak scalability on Marenostrum 4 - operated by BSC

Selected PSBLAS/MLD2P4 preconditioned iterative solvers:

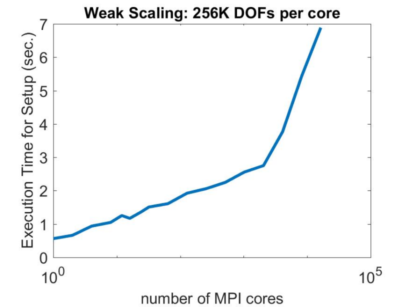
- Krylov Solver: Conjugate Gradient, with stopping criterion $\|r_k\| \leq 10^{-6}\|r_0\|$
- Preconditioner:
  - AMG based on decoupled smoothed aggregation
  - V-cycle with 1 sweep of forward/backward Hybrid Gauss-Seidel sweep as pre/post-smoother and parallel CG preconditioned with Block-Jacobi and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

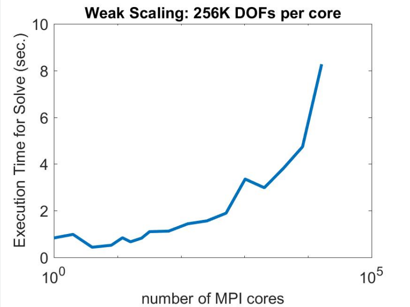
Machine Configuration: at 11,14 Petaflops, rank 29 in Top 500

- 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

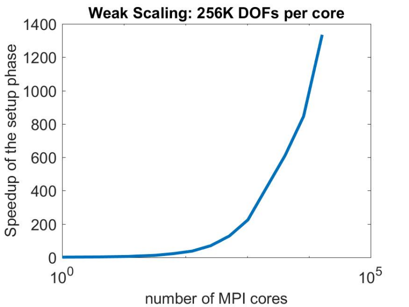
Row-block distribution of the matrix obtained
by a 3d decomposition of the grid

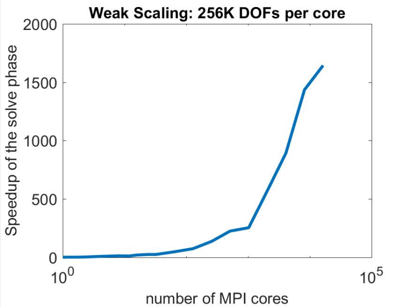


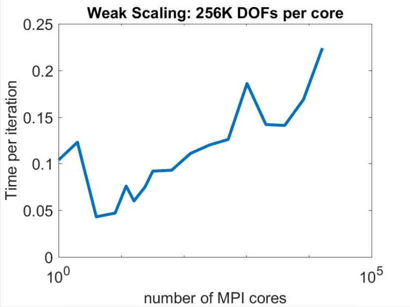


matrix with 256×10^3 rows (dofs) per core
up to 4×10^9 dofs on 16384 cores

Weak scalability on Marenostrum 4 - operated by BSC







Weak scalability on Piz Daint operated by CSCS

Selected PSBLAS/MLD2P4 preconditioned iterative solvers:

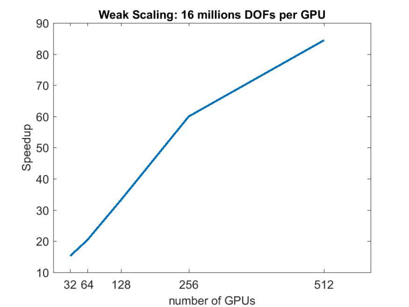
- Krylov Solver: Conjugate Gradient, with stopping criterion $\|r_k\| \leq 10^{-6}\|r_0\|$
- Preconditioner:
  - AMG based on decoupled smoothed aggregation
  - V-cycle with 2 point-wise Jacobi sweeps as pre/post-smoother and 10 sweeps of parallel Block-Jacobi, with approximate inverse applied to the blocks at the coarsest level

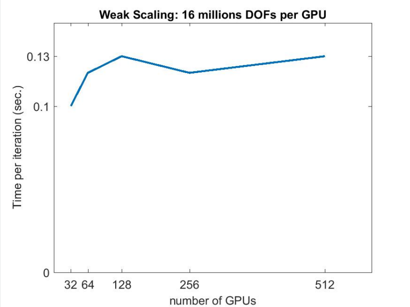
Machine Configuration (hybrid Cray XC40/XC50 system): at 21.2 petaflops, rank 6 in Top 500.

- 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

Row-block distribution of the matrix obtained
by a 3d decomposition of the grid





matrix with 16×10^6 rows (DOFs) per core
up to 8×10^9 DOFs on 512 GPUs

Work in progress within EoCoE: toward extreme scale

- ∼ $ new coupled aggregation scheme based on maximum weight matching in graphs
- ∼ $ 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