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
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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
Table of Contents

**Motivation**
- Large and sparse linear systems
  - Scalable solvers

**Algebraic MultiGrid Methods**
- Introduction to AMG
- AMG Setup

**MLD2P4**
- MLD2P4’s Features

**User’s Interface**
- Example of use

**Experiments on linear systems from EoCoE**
- Some results
\[ Ax = b, \quad A \in \mathbb{R}^{n \times n} \text{ (s.p.d.)} \quad x, b \in \mathbb{R}^n \]
\[ n \gg 10^9 \]

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 Vodafone has about 200 million (\(2 \times 10^8\)) customers and Google indexes several billion (> \(10^9\)) web-pages
Table of Contents

Motivation
- Large and sparse linear systems

Scalable solvers

Algebraic MultiGrid Methods
- Introduction to AMG
- AMG Setup

MLD2P4
- MLD2P4’s Features

User’s Interface
- Example of use

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Krylov methods

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

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Methods of choice: Search for a solution by projection

$$x_m \in \mathcal{K}_m(A, r_0)$$

$$r_m = b - Ax_m \perp \mathcal{K}_m(A, r_0)$$

$$\mathcal{K}_m(A, r_0) = \text{Span}\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}$$

Krylov subspace (growing with iteration until $x_m$ is good enough)
Krylov methods

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\]

Krylov subspace (growing with iteration until \( x_m \) is good enough)

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

CG Convergence

\[
\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2 \left( \frac{a - 1}{a + 1} \right), \quad a = \sqrt{\mu(A)} = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}
\]

\( e_k = x - x_k \) error at iteration \( k \), \( \lambda \) eigenvalue of \( A \)
Preconditioning

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

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

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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

\[ \mu(B^{-1}A) \approx 1, \text{ being independent of } n \] (algorithmic scalability)

\[ \text{the action of } B^{-1} \text{ costs as little as possible, the best being } O(n) \text{ flops (linear complexity)} \]

\[ \text{in a massively parallel computer, } B^{-1} \text{ should be composed of local actions, (implementation scalability, i.e., parallel execution time increases linearly with } n) \]
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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 ≠ 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
Table of Contents

Motivation
Large and sparse linear systems
Scalable solvers

Algebraic MultiGrid Methods
Introduction to AMG
AMG Setup

MLD2P4
MLD2P4’s Features

User’s Interface
Example of use

Experiments on linear systems from EoCoE
Some results
Example: (symmetrized) V-cycle

1. **Pre-smoothing**: 
   \[ x = x + M^{-1}(b - Ax) \]

2. **Residual restriction**: 
   \[ r_c = P^T (b - Ax) \]

3. **Solution on coarse grid**: 
   \[ A_c e = r_c, \text{ applying recursion} \]

4. **Error interpolation and solution update**: 
   \[ x = x + Pe \]

5. **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 \textit{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*:

\[(Aw)_i = r_i \approx 0 \implies w_{i+1} \approx w_i\]
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Error not reduced by the (chosen) smoother are called algebraic smoothness:

\[(Aw)_i = r_i \approx 0 \implies w_{i+1} \approx w_i\]

effective AMG requires that algebraic smoothness is well represented on the coarse grid and well interpolated back \(w = (w_i) \in \text{Range}(P)\).
Table of Contents

Motivation
   Large and sparse linear systems
   Scalable solvers

Algebraic MultiGrid Methods
   Introduction to AMG

AMG Setup

MLD2P4
   MLD2P4’s Features

User’s Interface
   Example of use

Experiments on linear systems from EoCoE
   Some results
Algebraic MultiGrid (AMG) Setup

Recursive application of a two-grid scheme

\[ M \text{ (the smoother)} \]
\[ \mathcal{R}^n \text{ from } \mathcal{R}^n \]
\[ \text{build the prolongation } P \text{ from } A \]
\[ A_c = P^T A P \]
Algebraic MultiGrid (AMG) Setup

Recursive application of a two-grid scheme

\[ M \] (the smoother)

\[ R^n \] from \( R^n \)

build the prolongation \( P \) from \( A \)

compute coarse grid matrix \( A_c = P^T A P \)

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:

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

or smoothed version of \( P \) (Vaněk 1996)
Parallel AMG Setup: decoupled aggregation

Given a user-defined threshold $\varepsilon$
Repeat
- Pick a new root point not adjacent to any existing aggregate
- Add neighbours which are strongly connected $\left( \left| a^k_{ij} \right| \geq \varepsilon \sqrt{a^k_{ii}a^k_{jj}} \right)$
- 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 $j: \left| a^k_{ij} \right| \geq \left| a^k_{il} \right| \forall l$
- If no neighbour is above threshold, start a new aggregate
Endfor

$\sim$ 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)
Table of Contents

Motivation
   Large and sparse linear systems
   Scalable solvers

Algebraic MultiGrid Methods
   Introduction to AMG
   AMG Setup

MLD2P4
   MLD2P4’s Features

User’s Interface
   Example of use

Experiments on linear systems from EoCoE
   Some results
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
   $\implies$ modularity and flexibility

~ $ Clear separation between interface and implementation of methods
   $\implies$ 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

- User interface
- Multilevel data structures & related methods
- Smoothers data structures & related methods
- Interfaces to external packages
- Basic components (matrices, index spaces, maps) & related methods
- UMFPACK, SuperLU, SuperLU_DIST, MUMPS
- MPI
Current version of MLD2P4 preconditioners

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

- $\sim$ decoupled smoothed aggregation
- $\sim$ $\sim$ distributed or replicated coarsest matrix

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

- $\sim$ cycles: V, W, K
- $\sim$ $\sim$ smoothers: $l_1$-Jacobi, hybrid (F/B) Gauss-Seidel, block-Jacobi / additive Schwarz with LU, ILU factorizations or sparse approximate inverses for the blocks
- $\sim$ coarest-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
- $\sim$ 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

\[ p\%apply(x,y,\text{desc}_a,\text{info} [,\text{trans},\text{work}]): \text{computes } y = op(B^{-1}) x, \text{where } B \text{ is a previously built preconditioner, stored into } p, \text{and } op \text{ denotes the preconditioner itself or its transpose, according to the value of } \text{trans}. \]

\textit{p\%apply} is called within the PSBLAS method \texttt{psb\_krylov} and hence it is completely transparent to the user.

\[ \sim \$
\]

\[ \sim \$ \text{call } p\%\text{free}(p,\text{info}): \text{deallocates the preconditioner data structure } p \]

\[ \sim \$ \text{call } p\%\text{descr}(\text{info}, [\text{iout}]): \text{prints a description of the preconditioner } p \]
Table of Contents

Motivation
  Large and sparse linear systems
  Scalable solvers

Algebraic MultiGrid Methods
  Introduction to AMG
  AMG Setup

MLD2P4
  MLD2P4’s Features

User’s Interface
  Example of use

Experiments on linear systems from EoCoE
  Some results
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
...
! 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 running
  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)
... 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_SOLVER','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)
...

...!

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)

...
...  
! 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
Table of Contents

Motivation
   Large and sparse linear systems
   Scalable solvers

Algebraic MultiGrid Methods
   Introduction to AMG
   AMG Setup

MLD2P4
   MLD2P4’s Features

User’s Interface
   Example of use

Experiments on linear systems from EoCoE
   Some results
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):

\[
\frac{\partial (\Phi s(p))}{\partial t} + \nabla \cdot \mathbf{u} = f \\
\mathbf{u} = -K \nabla (p - z)
\]

≈ $ 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

\[-\nabla \cdot \mathbf{K} \nabla p = f\]
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 $256 \times 10^3$ rows (dofs) per core up to $4 \times 10^9$ 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:

$\sim \$$ Krylov Solver: Conjugate Gradient, with stopping criterion $\|r_k\| \leq 10^{-6}\|r_0\|$  
\sim \$$ Preconditioner:  
\sim \$$ AMG based on decoupled smoothed aggregation  
\sim \$$ 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.

$\sim \$$ 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

$\sim \$$ 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 $16 \times 10^6$ rows (DOFs) per core up to $8 \times 10^9$ DOFs on 512 GPUs
Work in progress within EoCoE: toward extreme scale

- A 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


~ $ A$. Abdullahi, V. Cardellini, P. D'Ambra, D. di Serafino, S. Filippone, Efficient Algebraic Multigrid Preconditioners on Clusters of GPUs, Parallel Processing Letters, 29, 2019


Thanks for Your Attention