A new MATLAB interface to MueLu

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MueMex = MATLAB interface for MueLu
What is MueLu?

MueLu is . . .

. . . the next-generation multigrid framework package in Trilinos.

- provides AMG methods to solve large linear systems of equations
- can be understood as successor but not replacement for ML
- supports both Epetra and Tpetra as linear algebra framework
- is the typical Trilinos package
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MueLu is international: we can give support in

- english (since 2010)
- german (since 2011)
- russian (since 2012)
- french (discontinued in 2012)
Basic concept of Algebraic Multigrid (AMG)

Main idea
Capture errors at multiple resolutions.
Basic concept of Algebraic Multigrid (AMG)

Two main components

- Smoothers
  - Approximate solve on each level
  - "Cheap" reduction of oscillatory error (high energy)
  - $S_L \approx A_L^{-1}$ on the coarsest level $L$

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- **Smoothers**
  - Approximate solve on each level
  - "Cheap" reduction of oscillatory error (high energy)
  - $S_L \approx A_L^{-1}$ on the coarsest level $L$

- **Grid transfers (prolongators and restrictors)**
  - Data movement between levels
  - Definition of coarse level matrices.

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Algorithmic phases
- **Setup phase**
  - Build transfer operators to determine coarse level matrices
  - Initialize level smoothers

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\[ A_i = R_i A_{i-1} P_i \]

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Algorithmic phases

- **Setup phase**
  - Build transfer operators to determine coarse level matrices
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- **Solving phase**
  - Run through multigrid cycle (e.g. V-cycle)
  - Iteratively solve linear system or apply some sweeps with multigrid as preconditioner within an iterative linear solver

Main idea

Capture errors at multiple resolutions.
What is MueMex good for?

What can MueLu provide for MATLAB?

- MueMex runs MueLu as preconditioner in Belos
- Access to all features of Belos (linear solvers, multiple RHS...)
- Access to all preconditioners from Trilinos through MueLu
- Efficient iterative solution of very large linear systems
- Run MueLu multigrid setup once
- Use multigrid hierarchy for solving several (similar) linear systems with varying linear operators and/or right hand sides.

Why is MATLAB useful for MueLu?

- Analyze and tweak multigrid methods using the full functionality of MATLAB.
- Perform basic research on multigrid methods for specific problems.
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1. How to use MueMex
Basic Laplace example — Setup

Define problem:

```matlab
>> [A,coords] = laplacianfun([50,50]);
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Multigrid setup:

Minimal setup: Use default parameters defined by MueLu

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>> [problemID, oc] = muelu('setup', A);
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Multigrid parameters: Provide user parameters (see MueLu user guide)

```matlab
>> [problemID, oc] = muelu('setup', A, 'coarse: max size', 50);
```
Basic Laplace example — Setup

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Multigrid parameters: Provide user parameters (see MueLu user guide)

```matlab
>> [problemID, oc] = muelu('setup', A, 'coarse: max size', 50);
```

XML parameter file: Provide user parameters through xml file

```matlab
```
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...
Basic Laplace example — Solve

Solve problem:

```matlab
>> b = ones(2500,1);
>> [x, numIters] = muelu(problemID, b);
```

MATLAB output:

```matlab
>> [x, numIters] = muelu(problemID, b);
*******************************************************
***** Belos Iterative Solver: Pseudo Block Gmres
***** Maximum Iterations: 1000
***** Block Size: 1
***** Residual Test:
***** Test 1 : Belos::StatusTestImpResNorm<>: (2-Norm Res Vec) / (2-Norm Prec Res0), tol = 1e-08
*******************************************************
Iter  0, [ 1] :  1.000000e+00
Iter  1, [ 1] :  5.608530e-01
Iter  2, [ 1] :  1.953063e-02
Iter  3, [ 1] :  1.303521e-03
Iter  4, [ 1] :  7.361411e-05
Iter  5, [ 1] :  4.277384e-06
Iter  6, [ 1] :  2.581678e-07
Iter  7, [ 1] :  1.169750e-08
Iter  8, [ 1] :  7.920252e-10
Success, Belos converged!
```
Basic Laplace example — Analysis

Visualize solution and error:

```matlab
1  >> plot3(coords(:,1),coords(:,2),x,'.')
2  >> plot3(coords(:,1),coords(:,2),x-A\b,'r. ')
```
Basic Laplace example — Analysis

Visualize solution and error:

1. `>> plot3(coords(:,1), coords(:,2), x, '.' )`
2. `>> plot3(coords(:,1), coords(:,2), x-A\b, 'r.' )`
Complex scalars

MueLu also works with complex scalars:

```matlab
>> A = gallery('tridiag',2500,-1.0,2.0,-1.0) + gallery('tridiag',2500,-100.0,200.0,-100.0) * i;
>> [p,oc] = muelu('setup',A);
```

MATLAB output:

```
--- Multigrid Summary ---
Number of levels    = 2
Operator complexity = 1.33
level   rows   nnz   nnz/row  c   ratio   procs
      0  2500  7498   3.00  1   1
      1   834  2500   3.00  3.00 1
Smoother (level 0) both : "Ifpack2::Relaxation":
   {Initialized: true, Computed: true,
    Type: Symmetric Gauss-Seidel,
    sweeps: 1, damping factor: (1,0),
    Global matrix dimensions: [2500, 2500],
    Global nnz: 7498}
Smoother (level 1) pre : SuperLU solver interface, direct solve
Smoother (level 1) post : no smoother
Set up problem #0
```
Multiple right-hand sides

MueLu can solve multiple right-hand sides:

```matlab
>> b = ones(2500, 2);
>> for j = 1:2500, b(j, 2) = 1/2500*j + 1/(2500*2500)*j.*j*i; end
>> [x, numIters] = muelu(p, b);
```

MATLAB output:

```
*******************************************************
***** Belos Iterative Solver: Pseudo Block Gmres
***** Maximum Iterations: 1000
***** Block Size: 1
***** Residual Test:
      Test 1 : Belos::StatusTestImpResNorm<>: (2-Norm Res Vec) / (2-Norm Prec Res0), tol = 1e-08
*******************************************************
Iter  0, [ 1] :  1.000000e+00  Iter  0, [ 2] :  1.000000e+00
Success, Belos converged!
```

Attention: If the hierarchy is built with a complex operator \( A \), the RHS vector has to contain at least one imaginary value!
Multiple right-hand sides

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```

MATLAB output:

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```

Attention:
If the hierarchy is built with a complex operator \( A \), the RHS vector has to contain at least one imaginary value!
Visualization of results in MATLAB:

```matlab
1 >> plot(real(x(:,1))); hold on; plot(real(x(:,2))); 
2 >> plot(imag(x(:,1))); plot(imag(x(:,2))); hold off;
3 >> plot(imag(A\b-x));
```

Plot of solution vector:  
Plot of imaginary part of error:
2. How to access MueLu data
Study multigrid methods

Example: Study the multigrid effect on a 1d example:

```matlab
>> A = gallery('tridiag',600,-1,2,-1);
>> b=ones(600,1);
>> [problemID,oc] = muelu('setup',A,'coarse: max size',50,'
  multigrid algorithm','unsmoothed');
```

MATLAB output:

```
--- Multigrid Summary
---
Number of levels = 4
Operator complexity = 1.48
level  rows  nnz  nnz/row  c  ratio  procs
  0  600  1798  3.00   1
  1  200  598  2.99  3.00   1
  2  67  199  2.97  2.99   1
  3  23  67  2.91  2.91   1
```

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How to access transfer operators?

Extract (non-smooth) prolongation operators:

1. ```
>> Ptent1 = muelu('get', problemID, 1, 'P');
```  
2. ```
>> Ptent2 = muelu('get', problemID, 2, 'P');
```  
3. ```
>> Ptent3 = muelu('get', problemID, 3, 'P');
```  
4. ```
>> plot(Ptent3(:,15)); hold on; plot(Ptent3(:,15),'o');
```  
Plot of non-smooth basis function #15 of `Ptent3`:
How to access coarse level operators?

Extract coarse level operator on level 3 and solve coarse level problem using MATLAB:

```matlab
>> b1 = P1' * b;
>> b2 = P2' * b1;
>> b3 = P3' * b2;
>> A3 = muelu('get', problemID, 3, 'A');
>> x3 = A3 \ b3;
```

Plot of coarse level solution (level 3):

```matlab
>> plot(x3); hold on;
>> plot(x3, 'o'); hold off;
```

Exact coarse level solution of fine level problem.
Fine level solution and level smoothing

Plot prolonged solution on level 2:

```matlab
>> x2p = Ptent3 * x3;
>> plot(x2p); hold on;
>> plot(x2p,'o'); hold off;
```

Apply one sweep with Jacobi to prolonged solution:

```matlab
>> A2 = muelu('get', problemID, 2, 'A');
>> T = inv(D) * (tril(-A2,-1)+triu(-A2,1));
>> x2s = T * x2p + inv(D) * b2;
>> plot(x2s); hold on; plot(xs2,’o’); hold off;
```
Visualize transfer operator basis functions of 2D Laplace problem:

```matlab
>> [A,coords] = laplacianfun([50 50]);
>> [problemID] = muelu('setup', A);
>> P1 = muelu('get', problemID, 1, 'P');
>> [X,Y]=meshgrid(coords(:,1),coords(:,2));
>> Z = griddata(coords(:,1),coords(:,2),full(P1(:,212)),X, Y);
>> surf(X,Y,Z);
```

Plot of smooth prolongator basis function (associated with aggregate 212):
2D example — non-smooth transfers

Comparison of *smooth* prolongator basis function (associated with aggregate 212) and *non-smooth* basis function (associated with aggregate 234):

```matlab
1 >> [problem2, oc] = muelu('setup', 'A', 'multigrid algorithm', 'unsmoothed');
2 >> Ptent1 = muelu('get', problem2, 1, 'P');
3 >> Z2 = griddata(coords(:,1), coords(:,2), full(Ptent1(:,234)), X, Y);
4 >> surf(X, Y, Z); hold on; surf(X, Y, Z2); hold off;
```
3. Where can I learn more about MueLu?
MueLu resources

- The MueLu user guide
  - can be found here: https://trilinos.org/packages/muelu/muelu-documentation/
  - serves as reference handbook
  - provides an overview of all available user parameters and basic examples

- Examples come with the MueLu sources in the examples folder

- Doxygen
The MueLu tutorial can be found here: www.trilinos.org/packages/muelu/muelu-tutorial

comes with an interactive GUI for individual experiments

no Trilinos installation necessary: we provide a VirtualBox image and a docker container

The MueLu tutorial is divided into

- The beginners tutorial: Chapters 1-5 meant for absolute multigrid beginners. No programming skills necessary. Explains basic usage for standard problems.
- The advanced tutorial: Chapters 6-11 meant for intermediate users of MueLu. Explains design concepts of MueLu and focuses on advanced use concepts.
- Expert topics: Chapters 12-end cover expert topics primarily for developers.
Conclusion

- MueMex: MATLAB interface for MueLu
- allows to use MueLu as solver within MATLAB
- provides easy access to MueLu internals for further analysis
- works also for complex problems and multiple RHS
- ideal tool for research in context of multigrid
  - no C++ knowledge necessary
  - rapid development (no compilation necessary)
  - perfect tool for quick experiments and parameter studies
- MueMex is still under heavy development
One more thing. . .
MueMex — MATLAB extensions for MueLu

- **Advanced software design principles of MueLu**
  - Flexibility through modularity: multigrid framework
  - Strict splitting of algorithms and data
  - Algorithms are implemented in **factories** which use some input data to calculate/generate some other output data

- **MueMex fully integrates in MueLu framework**
  - Use **callback mechanism** to allow to plug in new factories in MueLu written in MATLAB
  - MueMex factories have full access to MueLu framework
  - MueMex factories can use full power of MATLAB
A new MATLAB interface to MueLu

Level: $\ell$

Aggregation
- Phase I
- Phase II
- Phase III

Build level smoother
- Use $A_{\ell+1}$ to build fine level smoother

Generate $\hat{P}_{\ell+1}$
- Build $B_{\ell+1}$ by local QR-decomposition of $B_{\ell}$

Prolongator smoothing
- Generate $P_{\ell+1}$

Galerkin product $R_{\ell+1}A_{\ell}P_{\ell+1}$

Level: $\ell + 1$
Demonstration

Use monochrome picture data to drop entries in input graph of aggregation factory to enforce user-specified aggregates:
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Demonstration

- Write a **factory** in MATLAB which uses
  - the non-filtered matrix $A$ as input
  - drops all off-diagonal entries in $A$ which represent connections between color 1 (e.g. blue) and color 2 (e.g. white).
  - stores the filtered matrix $A$ for being used in aggregation algorithm

- transfer monochrome picture data accordingly to coarse level (this is optional if only two-level method is used)

- **XML file** controls the interconnection and dependencies of factories
  - MATLAB factories fully integrate in existing **MueLu framework** with all factories written in C++/MATLAB
  - optimal **flexibility**
  - **recombination and reuse of factories** without recompilation of source code
  - perfect tool to design new **application-specific preconditioning strategies**
One last thing. . .
Thank you for your attention

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- the MueMex developers, especially
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  - Chris Siefert
- the MueLu developers, especially
  - Jonathan Hu
  - Andrey Prokopenko
  - Jeremie Gaidamour
- the developers of
  - Amesos and Amesos2
  - Ifpack and Ifpack2
  - Zoltan and Zoltan2
  - Epetra and Tpetra
- all Trilinos developers in general