

PyAMG: Algebraic Multigrid Solvers in Python

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Statement of need

PyAMG is a Python package of algebraic multigrid (AMG) solvers and supporting tools for approximating the solution to large, sparse linear systems of algebraic equations,

$$Ax = b,$$

where A is an $n \times n$ sparse matrix. Sparse linear systems arise in a range of problems in science, from fluid flows to solid mechanics to data analysis. While the direct solvers available in SciPy's sparse linear algebra package (`scipy.sparse.linalg`) are highly efficient, in many cases *iterative* methods are preferred due to overall complexity. However, the iterative methods in SciPy, such as CG and GMRES, often require an efficient preconditioner in order to achieve a lower complexity. Preconditioning is a powerful tool whereby the conditioning of the linear system and convergence rate of the iterative method are both dramatically improved. PyAMG constructs multigrid solvers for use as a preconditioner in this setting. A summary of multigrid and algebraic multigrid solvers can be found in Olson (2015a), in Olson (2015b), and in Falgout (2006); a detailed description can be found in Briggs et al. (2000) and Trottenberg et al. (2001).

Summary

The overarching goals of PyAMG include both readability and performance. This includes readable implementations of popular variations of AMG (see the Methods section), the ability to reproduce results in the literature, and a user-friendly interface to AMG allowing straightforward access to the variety of AMG parameters in the method(s). Additionally, pure Python implementations are not efficient for many sparse matrix operations not already available in `scipy.sparse` — e.g., the sparse matrix graph coarsening algorithms needed by AMG. For such cases in PyAMG, the compute (or memory) intensive kernels are typically expressed in C++ and wrapped through PyBind11, while the method interface and error handling is implemented directly in Python (more in the next section).

In the end, the goal of PyAMG is to provide quick access, rapid prototyping of new AMG solvers, and performant execution of AMG methods. The extensive PyAMG [Examples](#) page highlights many of the package's advanced AMG capabilities, e.g., for Hermitian, complex, nonsymmetric, and other challenging system types. It is important to note that many other AMG packages exist, mainly with a focus on parallelism and performance, rather than quick access and rapid prototyping. This includes BoomerAMG in `hypre` (Henson & Yang, 2002; `hypre`, 2022), MueLu in Trilinos (The MueLu Project Team, 2020; The Trilinos Project Team, 2020), and GAMG within PETSc (Balay et al., 2021), along with other packages focused on accelerators (Bell et al., 2012), such as AmgX (Naumov et al., 2015), CUSP (Dalton et al., 2014), and AMGCL (Demidov, 2019).

Design

The central data model in PyAMG is that of a `MultiLevel` object, which is constructed in the *setup* phase of AMG. The multigrid hierarchy is expressed in this object (details below) along with information for the *solve* phase, which can be executed on various input data, b , to solve $Ax = b$.

The `MultiLevel` object consists of a list of multigrid `Level` objects and diagnostic information. For example, a `MultiLevel` object named `ml` contains the list `ml.levels`. Then, the data on level i (with the finest level denoted $i=0$) accessible in `ml.levels[i]` includes the following information:

- A : the sparse matrix operator, in CSR or BSR format, on level i ;
- P : a sparse matrix interpolation operator to transfer grid vectors from level $i+1$ to i ;
- R : a sparse matrix restriction operator to transfer grid vectors from level i to $i+1$; and
- `presmoothen`, `postsmoothen`: functions that implement pre/post-relaxation in the solve phase, such as weighted Jacobi or Gauss-Seidel.

Other data may be retained for additional diagnostics, such as grid splitting information, aggregation information, etc., and would be included in each level.

Specific multigrid methods (next section) in PyAMG and their parameters are generally described and constructed in Python, while key performance components of both the setup and solve phase are written in C++. Heavy looping that cannot be accomplished with vectorized or efficient calls to NumPy or sparse matrix operations that are not readily expressed as SciPy sparse (CSR or CSC) operations are contained in short, templated C++ functions. The templates are used to avoid type recasting the variety of input arrays. The direct wrapping to Python is handled through another layer with PyBind11. Roughly 26% of PyAMG is in C++, with the rest in Python.

Methods

PyAMG implements several base AMG methods, each with a range of options. The base forms for a solver include

- `ruge_stuben_solver()`: the classical form of C/F-type AMG (Ruge & Stüben, 1987);
- `smoothed_aggregation_solver()`: smoothed aggregation based AMG as introduced in (Vaněk et al., 1996);
- `adaptive_sa_solver()`: a so-called adaptive form of smoothed aggregation from (Brezina et al., 2005); and
- `rootnode_solver()`: the root-node AMG method from (Manteuffel et al., 2017), applicable also to some nonsymmetric systems.

In each of these, the *base* algorithm is available but defaults may be modified for robustness. Options such as the default pre/postsmoother or smoothing the input candidate vectors (in the case of smoothed aggregation AMG), can be modified to tune the solver. In addition, several cycles are available, including the standard V and W cycles, for the solve phase. The resulting method can also be used as a preconditioner within the Krylov methods available in PyAMG or with SciPy's Krylov methods. The methods in PyAMG (generally) support complex data types and nonsymmetric matrices.

Example

As an example, consider a five-point finite difference approximation to a Poisson problem, $-\Delta u = f$, given in matrix form as $Ax = b$. The AMG setup phase is called with

```

1 import pyamg
2 A = pyamg.gallery.poisson((10000,10000), format='csr')
3 ml = pyamg.smoothed_aggregation_solver(A, max_coarse=10)

```

For this case, with 100M unknowns, the following multilevel hierarchy is generated for smoothed aggregation (using `print(ml)`):

```

MultilevelSolver
Number of Levels:      9
Operator Complexity:  1.338
Grid Complexity:      1.188
Coarse Solver:        'pinv'
  level  unknowns  nonzeros
    0    100000000  499960000 [74.76%]
    1    16670000  149993328 [22.43%]
    2     1852454   16670676 [2.49%]
    3     205859   1852805 [0.28%]
    4      22924   208516 [0.03%]
    5       2539   23563 [0.00%]
    6        289   2789 [0.00%]
    7         34    332 [0.00%]
    8          4     16 [0.00%]

```

In this case, the hierarchy consists of nine levels, with SciPy's pseudoinverse (`pinv`) being used on the coarsest level. Also displayed is the ratio of unknowns (nonzeros) on all levels compared to the fine level, also known as the grid (operator) complexity.

The solve phase, using standard V-cycles, is executed with the object's `solve`:

```

1 import numpy as np
2 x0 = np.random.rand(A.shape[0])
3 b = np.zeros(A.shape[0])
4 res = []
5 x = ml.solve(b, x0, tol=1e-8, residuals=res)

```

This leads to the residual history shown in [Figure 1](#).

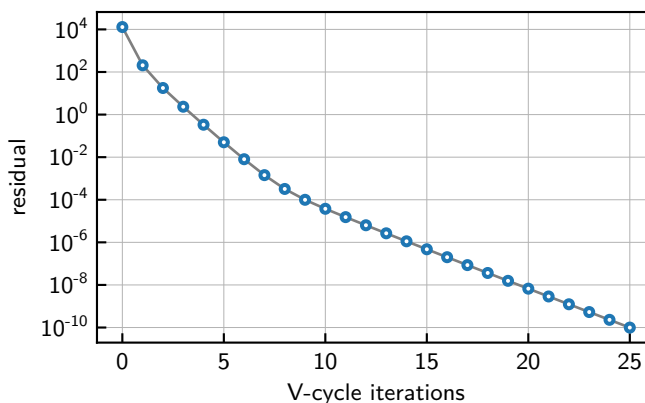


Figure 1: Algebraic multigrid convergence (relative residual).

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