PyAMG

Algebraic Multigrid Solvers in Python

Nathan Bell, Nvidia
Luke Olson, University of Illinois
Jacob Schroder, University of Colorado at Boulder

Copper Mountain 2011

Boot disc

- For Mac
  - Press and hold `c` immediately after reboot
- For the usual suspects (Dell, HP, Thinkpad, etc...)
  - Some automatically detect a bootable DVD
  - Pressing `F12`, `F8`, or `F6` at boot window can list boot options
  - Last, an advanced approach changes BIOS boot order
    - Press `F1`, `delete`, or `esc` during initial boot window
    - From the BIOS, change boot order to start with DVD drive first
- After booting, open a terminal (Applications—>Accessories—>Terminal)

Task 0.1: Installing PyAMG

Compile PyAMG (if using boot disc)

```
$ tar -xvf pyamg2.0.tar.gz
$ cd pyamg/
$ sudo python setup.py install
$ cd Examples/WorkshopCopper11
$ ipython
```

Test PyAMG during interactive iPython session, enter:

```python
import pyamg
pyamg.test()
```

What is PyAMG

- Algebraic multigrid (AMG) workbench
  - Readable and reproducible AMG
  - Efficient serial solver
- Python-based
  - Readability and useability
  - C++ backend for speed
- BLAS, LAPACK, optimized routines, etc...

Goal 1: Ease-of-use

- Accessible interface to non-experts
- Extensive documentation and references
- Portability through modular multiplatform Python libraries
- Rapid prototyping of new techniques
    - Organize source code into intuitive reusable components
    - High-level Python allows for rapid swapping of components

Goal 2: Speed

- Solve millions of unknowns on laptop/desktop
- Use hybrid coding strategy (Python as glue)
  - Performance sensitive portions are small fraction of code
  - 80% Python / 20% natively compiled C/C++/Fortran
- Example:
  - High-level multigrid cycling in Python
  - Calls `gauss_seidel(A,x,b,iterations=1)`
  - All computation done in C++ routine

PyAMG features

- Ruge-Stüben AMG
- Smoothed aggregation (standard and adaptive)
- Native complex support
- Nonsymmetric matrices
- Krylov solvers (CG, BiCGStab, GMRES, fGMRES, CGNR)
- Compatible relaxation (experimental)
- Relaxation methods (GS, wJ, SOR, Kacz, Cheby, Schwarz)
- Visualizations (Paraview, Matplotlib)

Dependencies

PyAMG

Multilevel solvers, relaxation methods, Krylov methods

Scipy

LAPACK and sparse matrix operations

Numpy

Array operations (BLAS)

C++/Swig

Easy interface from Python to C++

Nose

Unit tests, i.e., does everything work?

Matplotlib

Visualizations

iPython

Python interpreter, interactive sessions

What PyAMG does not do...

- Solve everything in linear time
- Multicore (coming)
- GPU acceleration (Cusp)
- Large-scale parallel simulations
  - See Hypre (Livermore) and ML (Sandia)

General Structure

- `multilevel.py` (multilevel solver class)
- Main structure for hierarchy (SA or RS)
- Handles cycling and coarse solver
- Contains list of level object instances
- Each level object instance contains:
  - Matrices: `A, P, R`
  - Functions: `presmoother, postsmoother`

Starting from `pyamg/pyamg`

- `multilevel.py` Multilevel solver class
- `strength.py` Strength-of-connection routines
- `classical/` Ruge-Stüben construction routines
- `aggregation/` SA construction routines
- `krylov/` Krylov solvers, e.g., CG, GMRES, fGMRES
- `relaxation/` Relaxation methods, e.g., GS, wJ, Cheby
- `Graph/` Graph algorithms for coarsening, e.g., MIS
- `vis/` Visualizations in Matplotlib and Paraview
- `amg_core/` C++ functions called through Swig
- `gallery/` Construct model problems
- `util/` Utility functions, e.g., spectral radius

Task 1.1: Getting used to Python

- Accessing documentation inside of iPython
  - Use <tab> on object to see its members
  - Use ? on object or function for documentation
  - Use spacebar to page, and q to quit documentation screen
- Inside of iPython ($ ipython), enter:

The most useful things you'll learn today

```
from pyamg import gallery, smoothed_aggregation_solver
A = gallery.poisson( (50,50), format='csr')
ml = smoothed_aggregation_solver(A)
ml.<tab>
    ml.__class__                    ml._multilevel_solver__solve  ml.level
    ml.__doc__                      ml.aspreconditioner           ml.levels
    ml.__init__                     ml.coarse_solver              ml.operator_complexity
    ml.__module__                   ml.cycle_complexity           ml.psolve
    ml.__repr__                     ml.grid_complexity            ml.solve

ml.solve?
gallery.poisson?
```

Task 1.2: Sparse Matrices

- Construct a sparse matrix
- Inside of iPython, enter:

If you ever get lost, exit iPython (`ctrl-d`, `ctrl-d`), re-enter iPython, and type `run taskx.x.py`

```
from scipy.sparse import *
csr_matrix?
from numpy import array
row = array([0,0,1,2,2,2])
col = array([0,2,2,0,1,2])
data = array([1,2,3,4,5,6])
B = csr_matrix( (data,(row,col)), shape=(3,3) )
B.<tab>
print(B.todense())
   [[1 0 2]
    [0 0 3]
    [4 5 6]]
B = B.tocoo()
```

Task 1.3: Using the gallery

- Generate a sparse matrix by running script
- Inside of iPython, enter:

```
run task1.3

print(A[5050,:].data)
    [-0.22 -0.25  0.22 -0.75  2.   -0.75  0.22 -0.25 -0.22]

print(sten)
    [[-0.22 -0.25  0.22]
     [-0.75  2.   -0.75]
     [ 0.22 -0.25 -0.22]]
```

Script: `task1.3.py`

```
from pyamg.gallery.diffusion import diffusion_stencil_2d
from pyamg.gallery import stencil_grid
from numpy import set_printoptions
set_printoptions(precision=2)
sten = diffusion_stencil_2d(type='FD', \
       epsilon=0.001, theta=3.1416/3.0)
A = stencil_grid(sten, (100,100), format='csr')
```

Task 1.4: Building a MG hierarchy

- Inside of iPython, enter:

```
from pyamg import *
ml = smoothed_aggregation_solver(A)
print(ml)
    multilevel_solver
    Number of Levels:     3
    Operator Complexity:  1.126
    Grid Complexity:      1.130
    Coarse Solver:        'pinv2'
      level   unknowns     nonzeros
        0        10000        88804 [88.84%]
        1         1156        10000 [10.00%]
        2          144         1156 [ 1.16%]

print(ml.levels[0].A.shape)
    (10000, 10000)

print(ml.levels[0].P.shape)
    (10000, 1156)

print(ml.levels[0].R.shape)
    (1156, 10000)
```

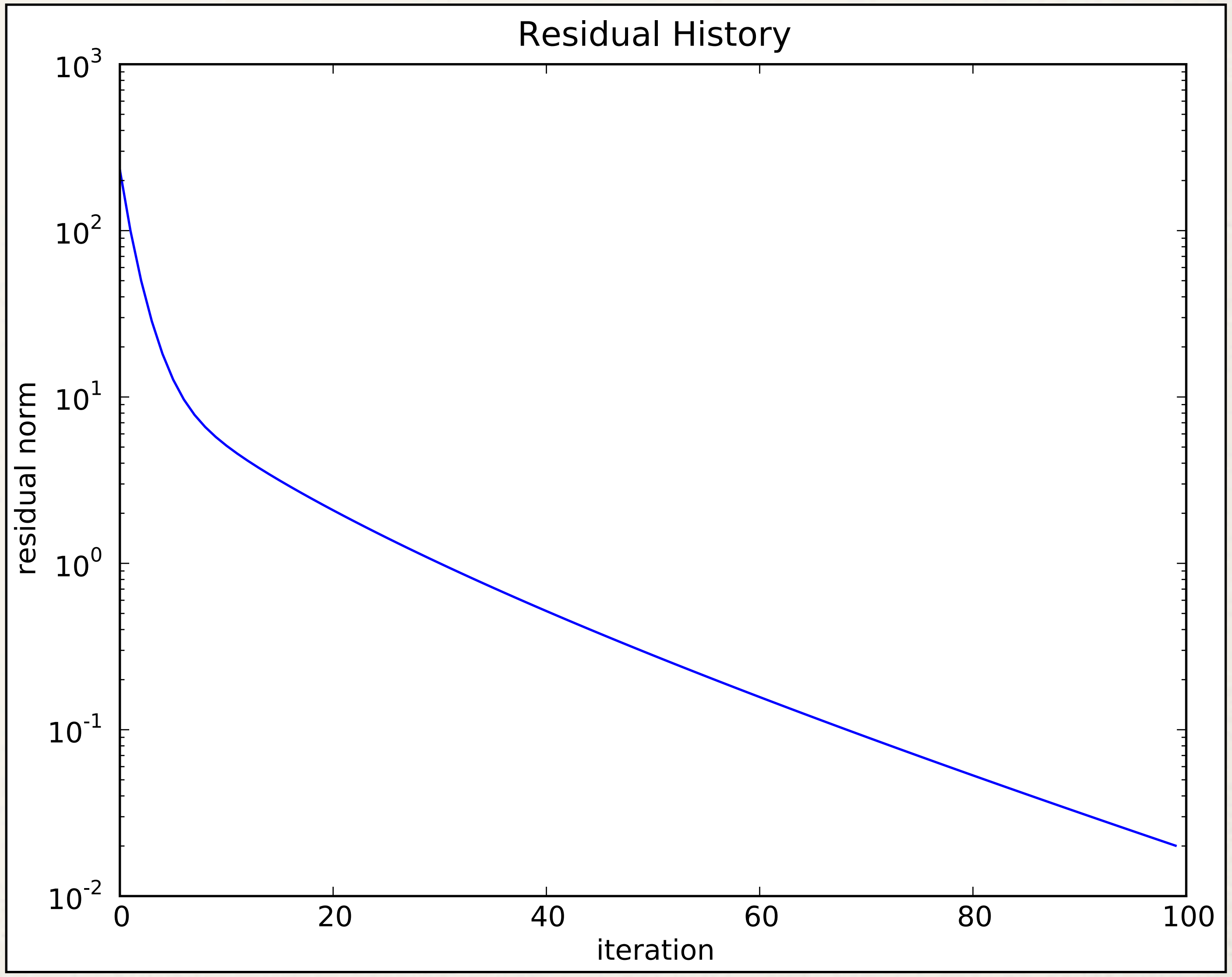
Task 1.5: Solving a problem

- Inside of iPython, enter:

```
run task1.5
```

Script: `task1.5.py`

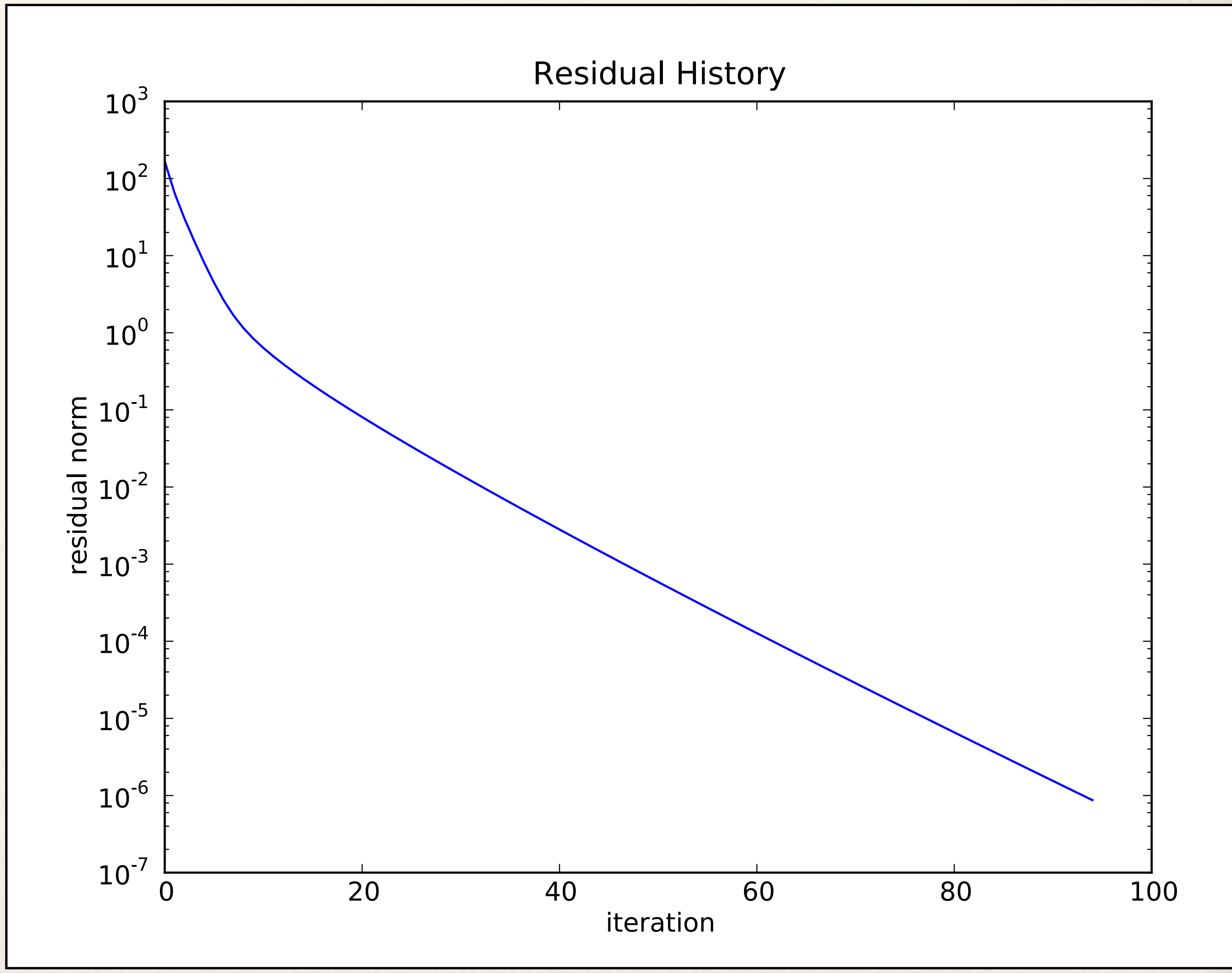
```
from numpy import ones
b = ones((A.shape[0],1))
res = []
x = ml.solve(b, tol=1e-8, \
    residuals=res)

from pylab import *
semilogy(res[1:])
xlabel('iteration')
ylabel('residual norm')
title('Residual History')
show()
```



Task 1.6: Changing MG options

- Use advanced coarsening and prolongation smoothing options
- Inside of iPython, enter:

```
from pyamg import *
from numpy import ones
ml = smoothed_aggregation_solver(A, \
      strength='evolution',         \
      smooth=('energy', {'degree':4}) )
b = ones((A.shape[0],1))
res = []
x = ml.solve(b, tol=1e-8, residuals=res)
from pylab import *
semilogy(res[1:])
xlabel('iteration')
ylabel('residual norm')
title('Residual History')
show()
```



Intermediate Tasks

- Modify existing multilevel hierarchy
- Add new prolongation smoothing function to PyAMG source
- Visualizations with Paraview
- Loading matrix from file
- Blackbox solve

Task 2.1: Modifying the hierarchy

- Modify existing multilevel solver object
- Replace existing pre/post-smoothers with new user-provided routine
- Execute commands in shell:

`ctrl-d, ctrl-d` (exit iPython)

```
$ python task2.1.py
```

Set new pre/post-smoother

```
def new_relax(A,x,b):
    x[:] +=  0.125*(b - A*x)

A = gallery.poisson( (100,100), format='csr')
b = ones( (A.shape[0],1))
res = []
ml  = smoothed_aggregation_solver(A)
ml.levels[0].presmoother = new_relax
ml.levels[0].postsmoother = new_relax
x = ml.solve(b, tol=1e-8, residuals=res)

semilogy(res[1:])
show()
```

Task 2.2: Adding a smoother

```
$ gedit ~/pyamg/pyamg/aggregation/aggregation.py
```

At line 409, insert two new lines:

New Lines

```
if fn == 'jacobi':
    P = jacobi_prolongation_smoother(A, T, C, B, **kwargs)
elif fn == 'simple':
    P = T - 0.2*A*T
elif fn == 'richardson':
...
```

```
$ cd ~/pyamg/
$ sudo python setup.py install
$ cd Examples/WorkshopCopper11
$ python task2.2.py
```

```
A = gallery.poisson( (100,100), format='csr')
ml = smoothed_aggregation_solver(A, smooth='simple')
...
```

Task 2.3: Plotting aggregates

- Visualization with Paraview

```
$ python task2.3.py
$ paraview&
```

load data

create hierarchy

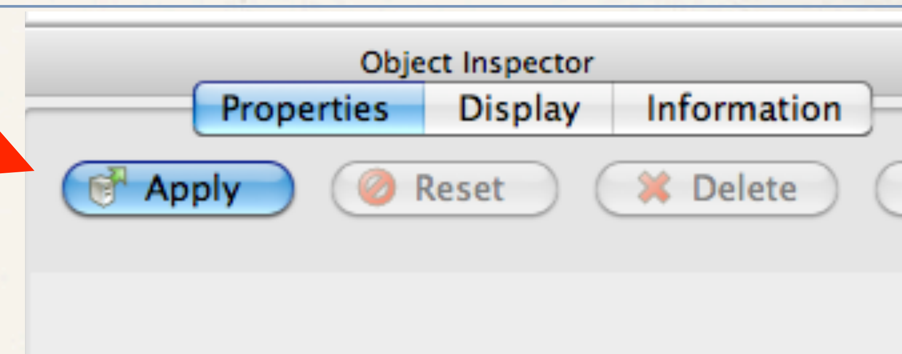
save aggregates

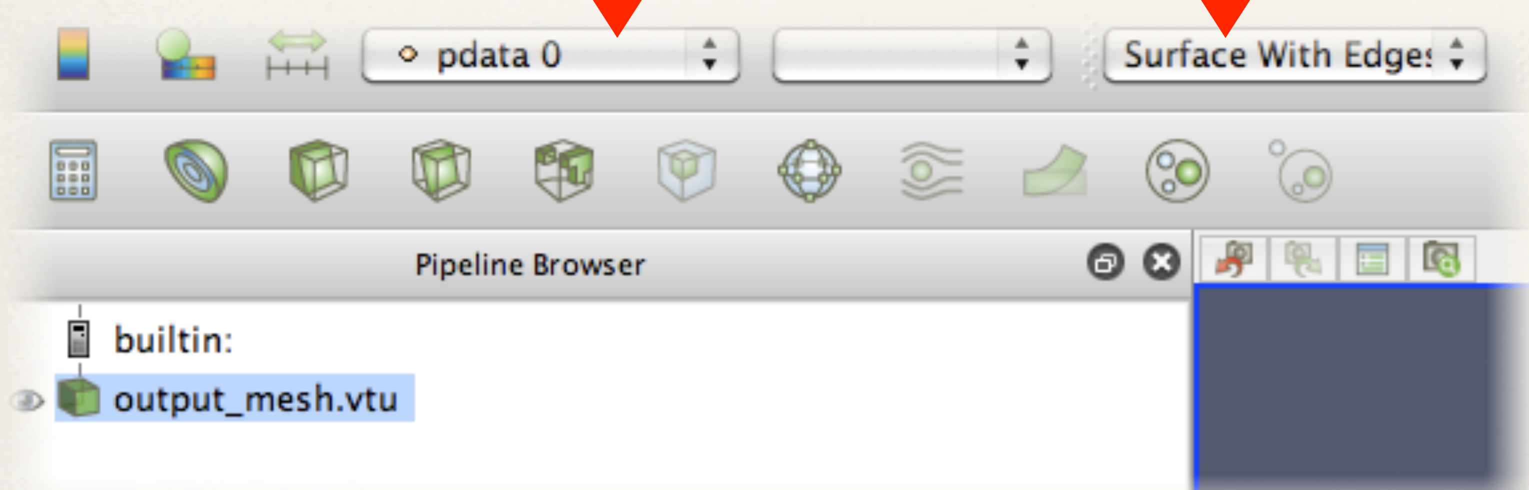
save mesh

```
data = load_example('unit_square')
A = data['A'].tocsr()
V = data['vertices']
E2V = data['elements']

ml = smoothed_aggregation_solver(A,keep=True,max_coarse=10)
b = sin(pi*V[:,0])*sin(pi*V[:,1])
x = ml.solve(b)

vis_coarse.vis_aggregate_groups(Verts=V, E2V=E2V,
        Agg=ml.levels[0].AggOp, mesh_type='tri',
        output='vtk', fname='output_aggs.vtu')

vtk_writer.write_basic_mesh(Verts=V, E2V=E2V,
                            pdata = x,
                            mesh_type='tri',
                            fname='output_mesh.vtu')
```

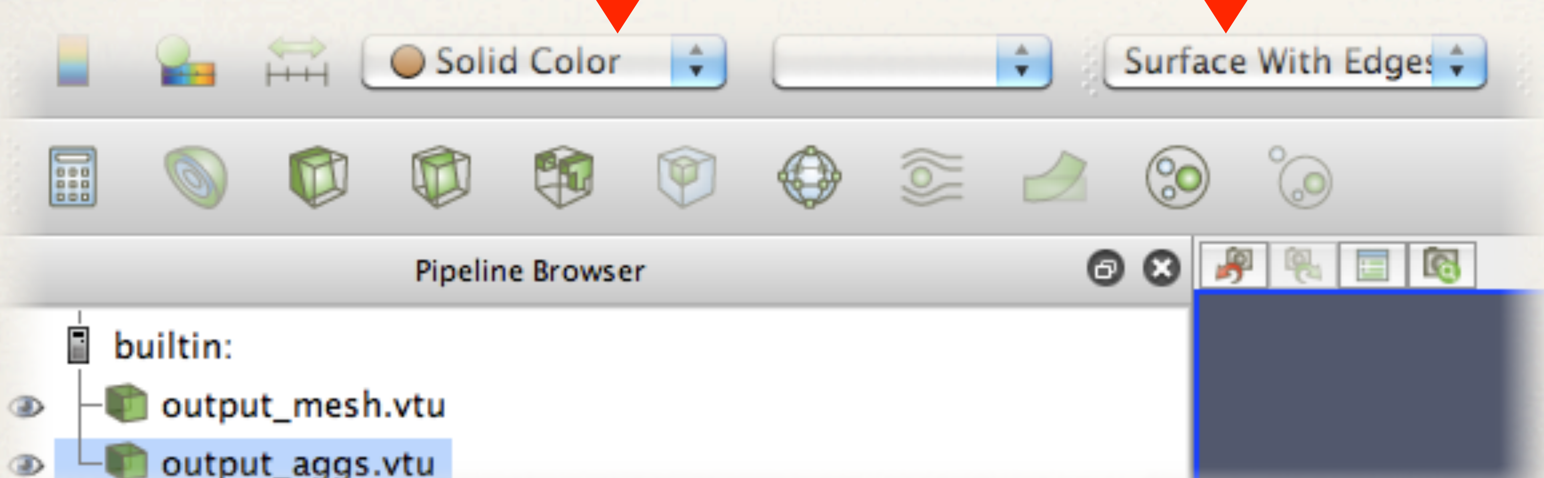
Task 2.3: Plot mesh and aggregates

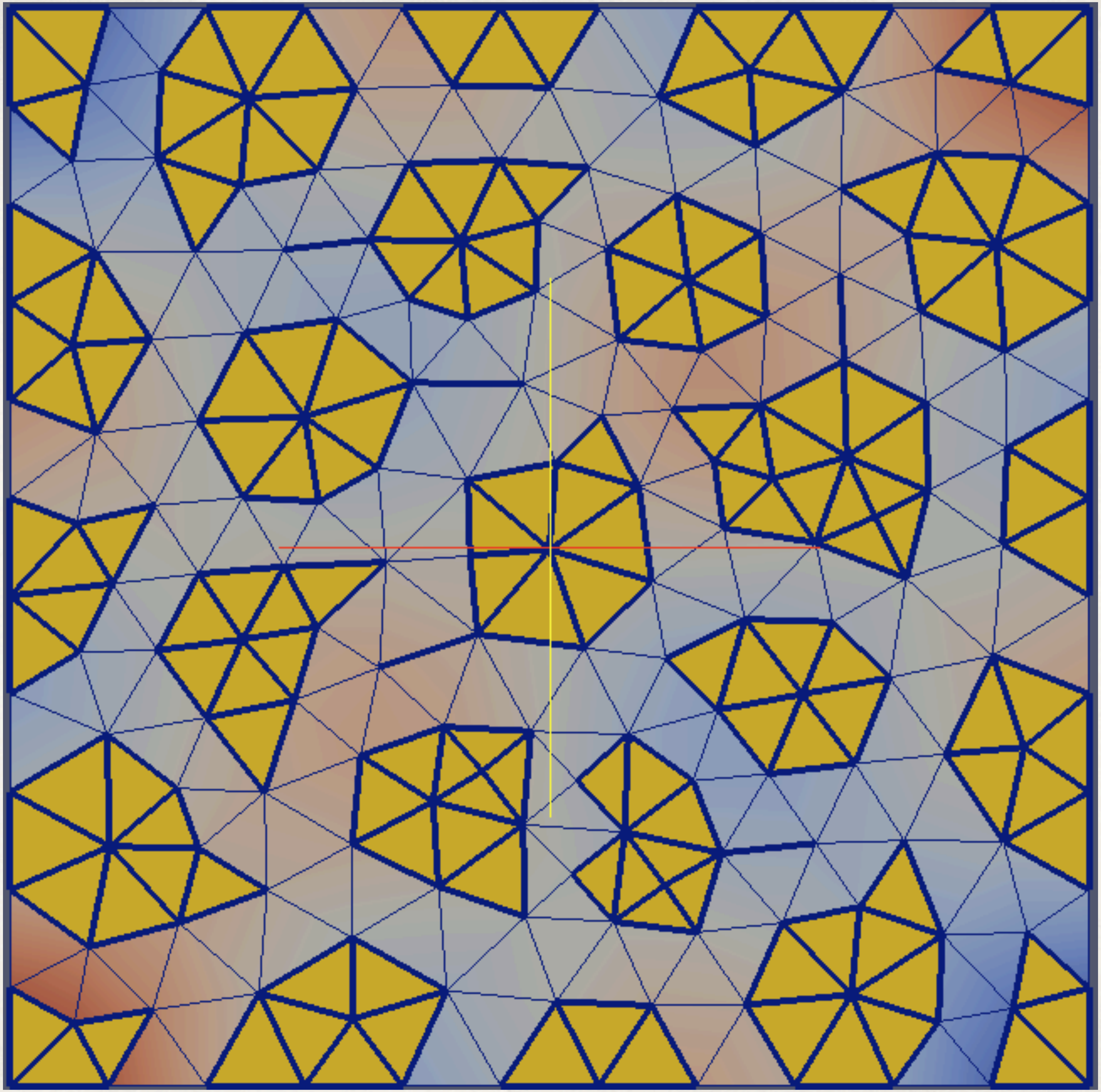
- Open `output_mesh.vtu`, then click apply
- Select options





- Open `output_aggs.vtu`, then click apply
- Select options



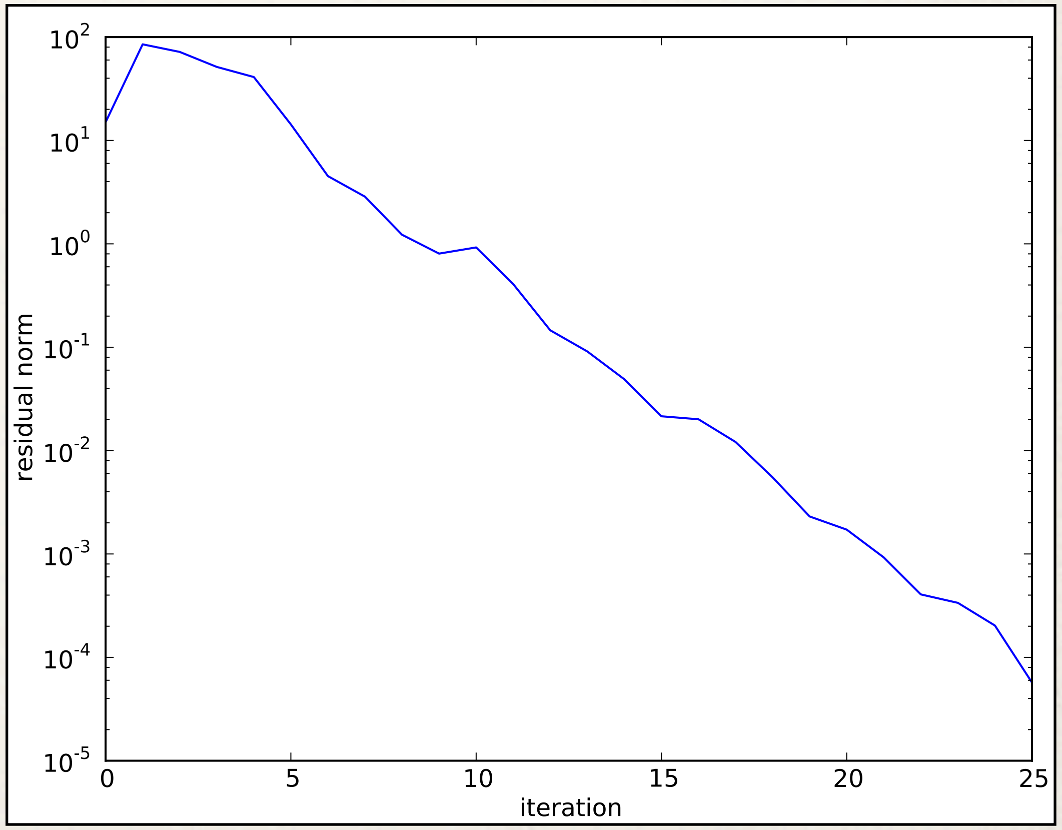


Task 2.4: Loading a matrix

nonsymmetric

$ python task2.4.py

```
data = loadmat('../../pyamg/gallery/example_data/recirc_flow.mat')
A = data['A']

from pyamg import *
ml = smoothed_aggregation_solver(A, symmetry='nonsymmetric',max_coarse=5)
```



Try it with...

```
ml = smoothed_aggregation_solver(A, symmetry='symmetric',max_coarse=5)
```

Task 2.5: Running blackbox solve

Inside of iPython, enter:

- "blackbox" solve attempts to pick the most robust options
- solve once
- solve again (same hierarchy)

```
from scipy import rand
from numpy import arange, array
from pyamg import solve
from pyamg.gallery import poisson
from pyamg.util.linalg import norm

# Run solve(...) with the verbose option
n = 100
A = poisson((n,n),format='csr')
b = array(arange(A.shape[0]))
x = solve(A,b,verb=True)

# Return the solver for re-use
(x,ml) = solve(A, b, verb=True,
               return_solver=True, tol=1e-8)

# Run for a new right-hand-side
b2 = rand(b.shape[0],)
x2 = solve(A, b2, verb=True,
           existing_solver=ml, tol=1e-8)
```

Advanced Tasks

- SWIG
  - SWIG interfaces between C++ and Python
  - Replace slow Python segments with C++
  - This task compares pure Python and hybrid Python/C++ versions of forward and backward substitution

- Important files for example
  - `numpy.i` interface between NumPy and C++ (esp. arrays)
  - `complex_ops.h` interface for complex data types
  - `splinalg.i` IN, INPLACE and OUT types, templating
  - `splinalg.h` headers, function definitions (plan vanilla C++)

```
$ cd ~/pyamg/Examples/SWIG
```

Task 3.1: Calling C++

splinalg.h defines the C++:

```
template<class I, class T>
void forwardsolve(const I Ap[], const I Aj[], const T Ax[],
                        T  x[], const T  b[], const I n)
{...
}
```

splinalg.i defines the C++ interface for SWIG:

```
 /* INPLACE types */
%define T_INPLACE_ARRAY1( ctype )
%apply ctype * INPLACE_ARRAY {
  ctype    x [ ]
};
```

SWIG compiles and creates the python interface:

```
$ swig -c++ -python splinalg.i
```

```
splinalg.forwardsolve(L.indptr,L.indices,L.data,x,b,n)
```

Task 3.1: Calling C++

To compile example:

`ctrl-d, ctrl-d` (exit iPython)

```
$ cd ~/pyamg/Examples/SWIG
$ sudo python setup.py install
```

Run example calling C++ routines with SWIG:

```
$ python testbasic.py
```

Task 3.1: Calling C++

- C++ call:

```
time for one LU solve  = 0.1998 ms
```

- `$ gedit precondition.py`
  - change line 74 to

```
def preconditioner_matvec(L,U):
    def matvec(x):
        return lusolve_reference(L,U,x)
```

- `$ python testbasic.py`

```
time for one LU solve  = 34.15 ms
```

1 or 2 magnitude difference

PyAMG

Algebraic Multigrid Solvers in Python

http://www.pyamg.org

Nathan Bell, Nvidia
Luke Olson, University of Illinois
Jacob Schroder, University of Colorado at Boulder

Thanks To NSF