FASP User Guide

FASP Developers

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Chapter 1

Introduction

1.1 General description

The Fast Auxiliary Space Preconditioning (FASP) package provides C source files¹ to build a library of iterative solvers and preconditioners for the solution of large-scale linear systems of equations. The components of the FASP basic library include several ready-to-use, modern, and efficient iterative solvers used in applications ranging from simple examples of discretized scalar partial differential equations (PDEs) to numerical simulations of complex, multicomponent physical systems via the Auxiliary Space Preconditioning framework [19].

The main components of the FASP basic library include:

- Basic linear iterative methods;
- Standard Krylov subspace methods;
- Geometric and Algebraic Multigrid (G/AMG) methods;
- Incomplete factorization methods.

Source files in the package are organized in various abstract levels as follows:

- Level 0 (Aux*.c): Auxiliary functions (timing, memory, threading, ...)
- Level 1 (Bla*.c): Basic linear algebra subroutines (SpMV, RAP, ILU, SWZ, ...)
- Level 2 (Itr*.c): Iterative methods and smoothers (Jacobi, GS, SOR, Poly, ...)
- Level 3 (Kry*.c): Krylov iterative methods (CG, BiCGstab, MinRes, GMRES, ...)
- Level 4 (Pre*.c): Preconditioners (GMG, AMG, FAMG, ...)
- Level 5 (Sol*.c): User interface for FASP solvers (Solvers, wrappers, ...)
- Level x (Xtr*.c): Interface to external packages (Mumps, Umfpack, ...)

¹The code is in the C99 (ISO/IEC 9899:1999) compatible.

The FASP distribution also includes several examples for solving simple benchmark problems. The basic (kernel) FASP distribution is open-source and is licensed under GNU Lesser General Public License or LGPL. Other distributions may have different licensing (contact the developer team for details on this).

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1.2 Roadmap: from basics to complex applications

A distinct feature of the FASP software project is that it is an open ended project. It contains a basic kernel of sources and is maintained by a team of developers with the expertise to build efficient solvers for a wide range of complex numerical models.

As typical for an open-source software, the further development of FASP project will also be based on the involvement of the community. While we have our own plans for expanding FASP's capabilities, we also count on the users' input in providing requests for, as well as, contributions to, the expansion of FASP in different application areas. Our team is ready to provide (or help with) the design and the implementation of efficient solvers based on the FASP kernel to best meet the goals and the requirements of our users.

The FASP software has been successfully used to build efficient solvers for several discretized PDEs and systems of PDEs: general scalar elliptic equations; linear elasticity; Brinkman equation; bi-harmonic equation; Stokes and Navier-Stokes equations; H(curl)/H(div) systems; Maxwell's system. The resulting solvers have been applied in simulations from fluid dynamics, underground water simulation, fluid-structure interactions, Oldryod-B and Johnson-Segalman models, black-oil model, and magnetohydrodynamics (MHD).

Several of these benchmark problems are included as examples in the open-source distribution, others are under development or have more restrictive licensing.

1.3 How to use this guide

This user's guide describes how to use the existing solvers in FASP via a couple of simple tutorial problems. The user's guide is a self-contained document but does *not* provide any details about the algorithms or their implementation. Along with this guide, we provide a reference manual² for

²Available online at http://fasp.sourceforge.net. It is also available in "faspsolver/doc/doc.zip".

technical details on the implementation which includes references. We recommend that the users read these references to better understanding of the code. Furthermore, since FASP is under heavy development, please use this guide with caution because the code might have been changed before this document is updated.

1.4 How to obtain FASP

There are several ways to download the FASP source files. We recommend users download the most updated version from the FASP page on SourceForge.

Downloading from SourceForge

The most updated version of FASP can be downloaded directly from

```
http://fasp.sf.net/download/faspsolver.zip
```

Downloading from BitBucket

FASP is also hosted on $BitBucket.org^3$ using Mercurial (Hg)⁴. A Hg client for GNU Linux, Mac OS X, or Windows can be downloaded from

```
http://mercurial.selenic.com/downloads/
```

There are also many other third-party clients which provides Hg services, for example: EasyMercurial⁵ (cross platform) and SourceTree⁶ (for Mac OS X only).

As a DVCS (Distributed Version Control System) source-control software, Hg is relatively new. But compared with other tools like Git, Hg is considered *friendlier* with a lower learning curve. This is despite the fact that Hg uses two distinct sets of commands and two distinct vocabularies for operations depending upon whether the repository is local or remote. Documentation for Hg is substantially better, including a book⁷. They've also had the advantage of trying the documentation on a fairly savvy group of developers (Mozilla) who gave them lots of feedback that helped polish the rough edges.

Linux or Mac OS X

First, you need to obtain a free copy of FASP kernel functions from our public Hg repository. If you are downloading FASP for the first time, you can clone the repository to your local machine:

```
<sup>3</sup>Official website: https://bitbucket.org/

<sup>4</sup>Official website: http://mercurial.selenic.com/

<sup>5</sup>Official website: http://easyhg.org

<sup>6</sup>Official website: http://www.sourcetreeapp.com

<sup>7</sup>The hgbook, http://hgbook.red-bean.com/
```

```
"Download FASP kernel subroutines via HTTPS"

$ hg clone https://faspusers@bitbucket.org/fasp/faspsolver
```

If you have any problems when clone this repository, please send us an email to faspdev@gmail.com.

After a long pause⁸, you should have obtained "faspsolver" in your current directory successfully. If you have already cloned the repository before, you can just pull a new version and update your local version with it: Go to your local "faspsolver" directory and then

```
"Pull a new version from BitBucket"

$ hg pull

"Update you local version to the new version"

$ hg update
```

Windows OS

If you are using Windows, you may want to install TortoiseHg⁹. After installing it, the TortoiseHg menu has been merged into the right-click menu of Windows Explore. You could download FASP copy from BitBucket.org. Choose "TortoiseHg" --> "Clone" in the pop-up menu, the source address is

```
https://faspusers@bitbucket.org/fasp/faspsovler
```

Then press "Clone" and you will obtain "faspsolver" in the directory you set.

1.5 Building and installing the FASP library and examples

FASP has been tested using the compilers and built-in libraries of several Linux distributions (Cent OS, Debian, Fedora, RedHat, Ubuntu) Mac OS X 10.6 and later (Leopard, Snow Leopard, Lion, Mavericks, Yosemite, El Capitan), and Windows (XP, Win 7) with several compliers, including gcc, g++, clang, icc, VC++. FASP also easily links to applications written in Fortran and this has been tested with gfortran, g95, ifort Fortran compilers.

⁸In fact, a very long pause. This is because the initial clone with copy all the history data which is about 400MB in total. Depending on the speed of your network, it could take 15 minutes to one hour.

⁹Official website: http://tortoisehg.bitbucket.org/

FASP on Linux or Mac OS X

To build the FASP library for these operating systems. Open a terminal window, where you can issue commands from the command line and do the following: (1) go to the main FASP directory (we will refer to it as \$(faspsolver) from now on); (2) modify the "FASP.mk.example" file to math your system and save it as "FASP.mk"; (3) then execute:

```
$ make config
$ make install
```

These two commands build the FASP library/header files. It installs the library in \$(faspsolver)/lib and the header files in \$(faspsolver)/include. It also creates a file \$(faspsolver)/Config.mk which contains few of the configuration variables and can be loaded by external project Makefiles (see §1.6 for details on \$(faspsolver)Config.mk).

If you do not have "FASP.mk" present in the current directory, default settings will be used for building and installation FASP.

Next, if you would like to try some of the examples that come with FASP, you can build the "test" and "tutorial" targets as follows:

```
$ make test
$ make tutorial
```

Equivalently, you may also build the test suite and the tutorial examples by using the "local" Makefile(s) in \$(faspsolver)/test and \$(faspsolver)/tutorial.

```
$ make -C test
$ make -C tutorial
```

Note: While these two approaches to build the FASP test suite and the FASP examples produce equivalent result in most cases, we note an important difference. The former approach uses a CMake installation process. The latter works without invoking Cmake and represents an example of how one may link an external project with the FASP library. We refer to §1.6 below for more details.

If everything went all right, you can go to the "faspsolver/test" directory and try to run a test problem:

```
$ ./test.ex
```

If you need help with the available options, type

```
$ make help
```

and you will get the following screen

```
Fast Auxiliary Space Preconditioners (FASP)
                                                 | | |
Quick start:
To build FASP, copy "FASP.mk.example" to "FASP.mk" and put user-defined setting
there and then type "make config; make install".
More options:
                       # Configure the building environment
$ make config
$ make config debug=yes  # Configure with compiler debug options ON
$ make config debug=all  # Configure with FASP internal debug options ON
$ make config openmp=yes # Configure with OpenMP support
$ make config prefix=/dir # Configure installation of FASP library and header
                          files in "/dir/lib" and "/dir/include"
$ make
                        # Compile the library (after "make config")
$ make install
                      # Install FASP library and header files
$ make test | tutorial  # Install FASP test or tutorial examples
                      # Remove the files installed by "make install"
$ make uninstall
$ make headers
                        # Generate function declarations automatically
$ make docs
                        # Generate the FASP documentation with Doxygen
$ make clean
                        # Remove obj files but retain configuration options
                      # Remove build directory and cleans test & tutorial
$ make distclean
$ make version
                       # Show version information
                        # Show this screen
$ make help
```

Many options can be changed in "FASP.mk", as well as from the command line. For example,

```
$ make config CC=gcc49 prefix=/usr/local
$ sudo make install
```

will install in the FASP library in /usr/local/lib and the include files in /usr/local/include so that they may be accessed by multiple users.

The example given above in most cases will require administrative privileges from the user, i.e. using sudo or other equivalent mechanism, to install in a system directory (such as /usr/local in our example). We do not recommend such way of installing FASP, although it will work in most cases if the user has administrative privileges. We recommend installation of FASP library/headers locally and then, if needed, copying them to a different location.

To uninstall FASP and clean up the working directory, you can run

```
$ make uninstall
$ make distclean
```

Windows 7

We provide a Visual Studio 2010 (VS10) distribution and a VS10 distribution of FASP for Windows users. For example, you can just open "faspsolver/vs10/faspsolver-vs10.sln" if you are using VS08 as your default developing environment. Then a single-click at the "Build Solution" on the menu or "F7" key will give you all the FASP libraries and the test programs in "faspsolver/test/". The way for building in VS10 is similar.

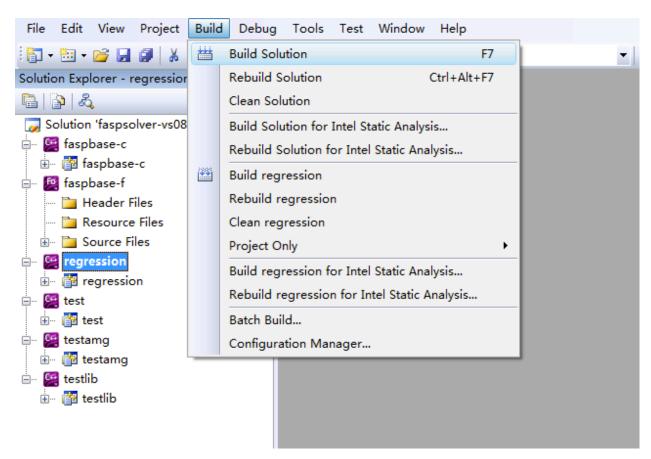


Figure 1.1: Build FASP using Visual Studio 2010.

You need a C/C++ complier and the Visual Studio to build FASP. For example, the build can be accomplished using either Microsoft Visual C++ or Intel C compiler.

If you are using other versions of Visual Studio (like VS05 or VS12), we advise NOT to convert the "VS10" files to your newer VS version automatically because the FASP source files might be removed by the Visual Studio. In such a case, we recommend that you create your own version to build all the libraries and test programs.

If you need to build a VS FASP yourself, you need to create 5 projects:

- 1. "faspbase-c" contains all the ".c" and ".inl" files in the directory "./base/src/". You should add "./base/include" in Additional Directories. This project contains the core subroutines of faspsolver.
- 2. "faspbase-f" contains all the ".f" files in "./base/extra/sparsekit".
- 3. "testlib" contains all the ".c" files in "./test/src/". You should add "./test/include" in Additional Directories.
- 4. "test" is an executing program for test purpose in FASP. The source file is "./test/main/test.c".
- 5. "regression" is another executing program, which contains several methods to test the problems. The source file is "./test/main/regression.c".

NOTE: If you are using Visual C++, all the C files should be compiled as C++ code (by using the /TP compiling option).

After a successful build on VS, you will have two static libraries named "faspbase-c-vs08.lib" and "faspbase-f-vs08.lib". You can use the "lib" command to wrap them together as one single file (e.g. FASP.lib) for better portability. For example:

```
C:\FASP> lib /ltcg /out:FASP.lib faspbase-c-vs08.lib faspbase-f-vs08.lib
```

Using a TCL based GUI for installation

For users who like more a GUI based installation, we provide a simple TCL Graphical User Interface (GUI) for building the FASP library. On a machine running Linux or Mac OS X with Tcl/Tk installed, you may invoke the GUI by typing

```
$ wish FASP_install.tcl
```

If all is OK, you should see on your screen the FASP window as shown in Figure 1.2. The rest of the building process is more or less straightforward: After choosing appropriate parameters, click "Config" first, followed by clicking "Install".

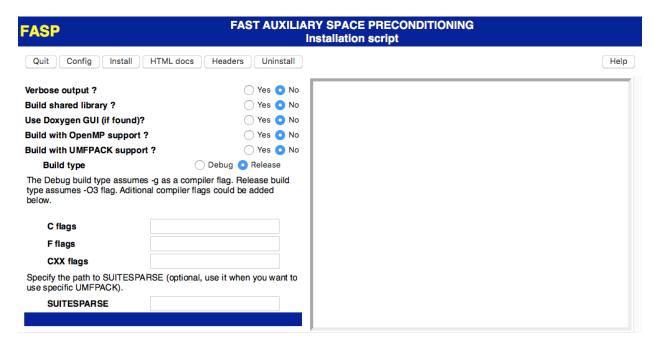


Figure 1.2: Install FASP using the TCL GUI on Mac OS X El Capitan.

External libraries

There are a few *optional* external libraries that you might want to use, including memory allocation routines, direct solvers, ILU methods, discretization packages, etc. FASP has interfaces to several of them, for example, FASP can be linked to use UMFPack, SuperLU, MUMPS, SparseKit, dlmalloc.

1.6 Linking your own project with FASP

The FASP distribution comes with two "local" Makefile(s) in the sub-directories for "test" and "tutorial", namely, \$(faspsolver)/test/Makefile and \$(faspsolver)/tutorial/Makefile. These two makefiles can be used to build the FASP tests and tutorial examples. They use minimal information about the library built. For convenience, at configuration time, such information is stored in \$(faspsolver)/Config.mk file for later use. A typical contents of such file is given below:

The variables defined in this file can also be set directly in \$(faspsolver)/test/Makefile, \$(faspsolver)/tutorial/Makefile, or, in your own Makefile. An external project can be compiled and linked with FASP by following the rules set in \$(faspsolver)/tutorial/Makefile (included below):

```
2
   # Fast Auxiliary Space Preconditioners (FASP)
3
  4
  # Makefile for building the tutorial executables. If the file
   # ../Config.mk exists it will take the values of configuration
6
   # variables from there. Otherwise, they have to be user supplied below.
   8
9
10
  fasp_prefix = not-defined-yet
11 | fasp_library = not-defined-yet
12 CC = not-defined-yet
13 | FC = not-defined-yet
   \mathtt{CXX} = \mathtt{not-defined-yet}
14
15
  # include the configuration written by CMake at config time if found
16
  sinclude ../Config.mk
17
18
  ifeq ($(fasp_prefix),not-defined-yet)
19
20
      fasp_prefix = ...
21
  ifeq ($(fasp_library), not-defined-yet)
22
23
      fasp_library = libfasp.a
^{24}
  ifeq ($(CC),not-defined-yet)
25
26
     CC=gcc
27
  ifeq ($(FC),not-defined-yet)
28
29
     FC=gfortran
  endif
31
  ifeq ($(CXX),not-defined-yet)
     CXX=g++
32
33
  endif
34
  CFLAGS=-I$(fasp_prefix)/include
35
36
  CFLAGS+=-03
37 | FFLAGS=-I$(fasp_prefix)/include
38
  FFLAGS+=-03
  LINKER = \$(FC) # because of linking with Fortran files
39
  LFLAGS = -L\$(fasp\_prefix)/lib - lfasp
41 | fasp_lib_file=$(fasp_prefix)/lib/$(fasp_library)
```

```
42
43
   examples = poisson-amg-c.ex poisson-its-c.ex poisson-pcg-c.ex \
44
               poisson-gmg-c.ex spe01-its-c.ex \
               poisson-amg-f.ex poisson-pcg-f.ex
45
   examples_f = $(filter %-f.ex,$(examples))
46
    examples_c = $(filter-out %-f.ex,$(examples))
47
48
   .PHONY: all clean
49
50
            $(examples_c) $(examples_f)
51
52
   %-c.ex: main/%.c $(fasp_lib_file)
53
54
        @$(CC) -c $(CFLAGS) -o main/$@.o $<
        @$(LINKER) -o $@ main/$@.o $(LFLAGS)
55
        @echo 'Building executable file $@'
56
57
   \%-f.ex: main/\%.f90 $(fasp_lib_file)
58
        @$(FC) -c $(FFLAGS) -o main/$@.o $<
59
60
        @$(FC) -o $@ main/$@.o $(LFLAGS)
61
        @echo 'Building executable file $@'
62
   $(fasp_lib_file):
63
        $(error The FASP library $0 is not found)
64
65
66
67
        Q-rm -f *.o main/*.o *
68
   distclean: clean
69
70
        @-rm -f poisson-amg-c.ex poisson-its-c.ex poisson-pcg-c.ex 
                    {\tt poisson-gmg-c.ex\ spe01-its-c.ex}\ \setminus
71
                    poisson-amg-f.ex poisson-pcg-f.ex
72
```

Chapter 2

A brief tutorial

In this chapter, we discuss several simple examples included with this FASP distribution and demonstrating how to use the FASP package for solving linear systems. We read the matrices from disk files (the files are also included in the FASP distribution). All the examples in this section can be found inside "faspsolver/tutorial/".

After you successfully build FASP (see §1.5), just go to the "faspsolver/tutorial/" directory and the tutorial examples should be ready to run.

In this section we mainly discuss the C version of these examples; the FASP distribution also includes F90 versions of some of the examples.

In the description below, we display a typical output from runs of each of the examples. Note that the actual output depends on the solver parameters, and, on your computer it may be different than what you see here.

2.1 Example 1: An AMG solver for the Poisson equation

The first example is a standard one: We read a symmetric positive definite matrix A and right-hand side b from harddisk and then we solve Ax = b using the classical AMG method [2, 13, 14]; see §3.6. In this example the matrix A included with the FASP distribution corresponds to a discretization with continuous piecewise linear finite elements of the Poisson equation

$$-\Delta u = f$$

(with the Dirichlet boundary conditions) on a triangulation of a bounded domain Ω .

```
/*! \file poisson-amg.c

*

* \brief The first test example for FASP: using AMG to solve

the discrete Poisson equation from P1 finite element.
```

```
5
              C version.
6
7
    * \note Solving the Poisson equation (P1 FEM) with AMG: C version
8
9
    * Copyright (C) 2011--2017 by the FASP team. All rights reserved.
10
    * Released under the terms of the GNU Lesser General Public License 3.0 or later.
11
12
13
14
   #include "fasp.h"
15
16
   #include "fasp_functs.h"
17
18
   * \fn int main (int argc, const char * argv[])
19
20
21
    * \brief This is the main function for the first example.
22
23
     * \author Chensong Zhang
    * \date 12/21/2011
24
25
26
    * Modified by Chensong Zhang on 09/22/2012
27
   int main (int argc, const char * argv[])
28
29
                       inparam; // parameters from input files
30
       input_param
                       amgparam; // parameters for AMG
31
       AMG_param
32
       printf("\n=========");
33
       printf("\n|| FASP: AMG example -- C version ||");
34
       printf("\n======\n\n");
35
36
37
       // Step O. Set parameters: We can use ini/amg.dat
       fasp_param_set(argc, argv, &inparam);
38
39
       fasp_param_init(&inparam, NULL, &amgparam, NULL, NULL);
40
       // Set local parameters using the input values
41
       const int print_level = inparam.print_level;
42
43
44
       // Step 1. Get stiffness matrix and right-hand side
       // Read A and b -- P1 FE discretization for Poisson. The location
45
46
       // of the data files is given in "ini/amg.dat".
47
       dCSRmat A;
       dvector b, x;
48
49
       char filename1[512], *datafile1;
50
       char filename2[512], *datafile2;
51
52
       // Read the stiffness matrix from matFE.dat
53
       strncpy(filename1, inparam.workdir, 128);
54
       datafile1="csrmat_FE.dat"; strcat(filename1, datafile1);
55
       // Read the RHS from rhsFE.dat
56
       strncpy(filename2, inparam.workdir, 128);
```

```
datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
58
59
        fasp_dcsrvec2_read(filename1, filename2, &A, &b);
60
61
        // Step 2. Print problem size and AMG parameters
62
        if (print_level>PRINT_NONE) {
63
            printf("A: m = %d, n = %d, nnz = %d\n", A.row, A.col, A.nnz);
64
            printf("b: n = %d\n", b.row);
65
66
            fasp_param_amg_print(&amgparam);
67
        }
68
69
        // Step 3. Solve the system with AMG as an iterative solver
70
        // Set the initial guess to be zero and then solve it
        // with AMG method as an iterative procedure
71
72
        fasp_dvec_alloc(A.row, &x);
73
        fasp_dvec_set(A.row, &x, 0.0);
74
        fasp\_solver\_amg(\&A, \&b, \&x, \&amgparam);
75
76
        // Step 4. Clean up memory
77
        fasp_dcsr_free(\&A);
78
79
        fasp_dvec_free(&b);
        fasp_dvec_free(&x);
80
81
        return FASP_SUCCESS;
82
83
84
85
                End of File
86
87
```

Since this is the first example, we will explain it in some detail:

- Line 1 tells the Doxygen documentation system¹ that the filename is "poisson-amg.c". Line 3-5 tells the Doxygen what is the purpose of this file (function).
- Line 15–16 includes the main FASP header file "fasp.h" and FASP function declarations header "fasp_functs.h". These two headers shall be included in all files that requires FASP subroutines. Please also be noted that the function declarations in "fasp_functs.h" are automatically generated from the source files by an awk script and we do not recommend modifying this file, since your changes may be lost.
- Line 38–39 sets solver parameters using the default parameters or from the command line options; see more discussions in §2.6. In the "tutorial/ini/amg.dat" file, we can set the location of the data files, type of solvers, maximal number of iteration numbers, convergence tolerance, and many other parameters for iterative solvers.

¹Doxygen http://www.doxygen.org is a useful tool for generating documentation from annotated sources. We use it in FASP development.

- Line 47 defines a sparse matrix A in the compressed sparse row (CSR) format. Line 48 defines two vectors: the right-hand side b and the numerical solution x. We refer to §3.1 for definitions of vectors and general sparse matrices.
- Line 60 reads the matrix and the right-hand side from two disk files. Line 54–58 defines the filenames of them.
- Line 60–64 prints basic information of coefficient matrix, right-hand side, and solver parameters.
- Line 72–73 allocates memory for the solution vector x and set its initial value to be all zero.
- Line 75 solves Ax = b using the AMG method. Type of the AMG method and other parameters have been given in "amgparam" at Line 36; see §3.6.
- Line 78–80 frees up memory allocated for A, b, and x.

To run this example, type:

```
$ ./poisson-amg-c.ex
```

A sample output is listed as follows:

```
\Pi
     FASP: AMG example -- C version
                                          fasp_dcsrvec2_read: reading file ../data/csrmat_FE.dat...
fasp_dcsrvec2_read: reading file ../data/rhs_FE.dat...
A: m = 3969, n = 3969, nnz = 27281
\mathtt{b}:\ \mathtt{n}\ =\ 3969
       Parameters in AMG_param
AMG print level:
                                      2
AMG max num of iter:
                                      100
AMG type:
                                      1
                                      1.00\,\mathrm{e}\!-\!06
AMG tolerance:
AMG max levels:
                                      20
                                      1
AMG cycle type:
AMG coarse solver type:
                                      0
AMG scaling of coarse correction:
AMG smoother type:
AMG smoother order:
AMG num of presmoothing:
AMG num of postsmoothing:
                                      1
AMG coarsening type:
                                      1
AMG interpolation type:
                                      1
AMG dof on coarsest grid:
```

```
0.3000
AMG strong threshold:
AMG truncation threshold:
                                 0.2000
AMG max row sum:
                                   0.9000
AMG aggressive levels:
AMG aggressive path:
Calling classical AMG ...
 Level Num of rows Num of nonzeros Avg. NNZ / row
    0
             3969
                               27281
                                               6.87
              1985
                               28523
                                               14.37
   1
    2
              541
                                7951
                                               14.70
              141
                                1803
                                              12.79
 Grid complexity = 1.672 | Operator complexity = 2.403
Classical AMG setup costs 0.0047\ \mathrm{seconds} .
It Num | ||r||/||b|| |
                              ||r|| | Conv. Factor
    0 \mid 1.0000000 \, e{+00} \mid 7.514358 \, e{+00} \mid
    1 \mid 9.851978 \, e{-03} \mid 7.403129 \, e{-02} \mid
                                                0.0099
                        | 2.635624e-03 |
    2 \mid 3.507451e-04
                                                0.0356
    3 \mid 1.764023 e - 05 \mid 1.325550 e - 04 \mid
                                               0.0503
                                              0.0500
    4 \mid 8.820794 e - 07 \mid 6.628261 e - 06 \mid
Number of iterations = 4 with relative residual 8.820794e-07.
AMG solve costs 0.0015 seconds.
AMG totally costs 0.0066 seconds.
```

We also provide a Fortran 90 example, which does the same thing as this C code except it gives less output, in "tutorial/main/poisson-amg.f90". Users who would like to call FASP solver from a Fortran based application can see how to do this example.

```
!> \file poisson-amg.f90
1
   !> \brief The first test example for FASP: using AMG to solve
       the discrete Poisson equation from P1 finite element.
4
   ! >
  ! >
            F90 version.
6
   ! >
   !> \note Solving the Poisson equation (P1 FEM) with AMG: F90 version
7
   !>
9
   !> Copyright (C) 2011--2017 by the FASP team. All rights reserved.
10
   !> Released under the terms of the GNU Lesser General Public License 3.0 or later.
11
12
13
14
  program test
15
16
   implicit none
```

```
17
18
     double precision, dimension(:), allocatable :: u, b, a
                     dimension(:), allocatable :: ia, ja
19
     integer,
20
                    :: iufile, n, nnz, i, prt_lvl, maxit
21
     double precision :: tol
22
23
     print*, ""
24
     25
     write(*,"(A)") "|| FASP: AMG example -- F90 version ||"
26
     write(*,"(A)") "-----"
27
     print*, ""
28
29
30
     ! Step 0: user defined variables
     prt_lvl = 3
31
     maxit = 100
32
33
     tol = 1.0d-6
     iufile = 1
34
35
36
     ! Step 1: read A and b
37
38
     !===> Read data A from file
     open(unit=iufile,file='../data/csrmat_FE.dat')
39
40
     read(iufile,*) n
41
42
     allocate(ia(1:n+1))
     read(iufile,*) (ia(i),i=1,n+1)
43
44
45
     nnz=ia(n+1)-ia(1)
     allocate(ja(1:nnz),a(1:nnz))
46
     read(iufile,*) (ja(i),i=1,nnz)
47
     read(iufile,*) (a(i),i=1,nnz)
48
49
     close(iufile)
50
51
     !===> Read data b from file
52
     open(unit=iufile,file='../data/rhs_FE.dat')
53
54
55
     read(iufile,*) n
     allocate(b(1:n))
56
57
     read(iufile,*)(b(i),i=1,n)
58
     close(iufile)
59
60
     !===> Shift the index to start from 0 (for C routines)
61
62
     forall (i=1:n+1) ia(i)=ia(i)-1
63
     forall (i=1:nnz) ja(i)=ja(i)-1
64
65
     ! Step 2: Solve the system
66
     !===> Initial guess
67
68
     allocate(u(1:n))
    u=0.0d0
```

```
70
    call fasp_fwrapper_amg(n,nnz,ia,ja,a,b,u,tol,maxit,prt_lvl)
71
72
    ! Step 3: Clean up memory
    deallocate(ia,ja,a)
73
    deallocate(b,u)
74
75
76
  end program test
77
  !/*----*/
78
         End of File
79
  !/*----*/
80
```

2.2 Example 2: Conjugate gradient without preconditioning

In the second example, we modify the previous example slightly and solve the Poisson equation using iterative methods (here by default we use the Conjugate Gradient method without preconditioning).

```
1
   /*! \file poisson-its.c
2
3
      \brief The second test example for FASP: using ITS to solve
              the discrete Poisson equation from P1 finite element.
4
5
    * \note Solving the Poisson equation (P1 FEM) with iterative methods: C version
6
7
8
    * Copyright (C) 2012--2017 by the FASP team. All rights reserved.
10
    * Released under the terms of the GNU Lesser General Public License 3.0 or later.
11
12
13
   #include "fasp.h"
14
   #include "fasp_functs.h"
16
17
   * \fn int main (int argc, const char * argv[])
18
19
20
    * \brief This is the main function for the second example.
21
22
    * \author Feiteng Huang
23
    * \date 04/13/2012
24
    * Modified by Chensong Zhang on 09/22/2012
25
26
   int main (int argc, const char * argv[])
27
28
29
       input_param
                     inparam; // parameters from input files
30
       ITS_param
                     itparam; // parameters for itsolver
31
       printf("\n======="");
32
       printf("\n|| FASP: ITS example -- C version ||");
33
```

```
printf("\n======\n\n");
34
35
       // Step O. Set parameters: We can use ini/its.dat
36
       fasp_param_set(argc, argv, &inparam);
37
       fasp_param_init(&inparam, &itparam, NULL, NULL, NULL);
38
39
       // Set local parameters
40
41
       const int print_level = inparam.print_level;
42
43
       // Step 1. Get stiffness matrix and right-hand side
       // Read A and b -- P1 FE discretization for Poisson. The location
44
45
       // of the data files is given in "ini/its.dat".
       dCSRmat A:
46
       dvector b, x;
47
       char filename1 [512], *datafile1;
48
       char filename2[512], *datafile2;
49
50
       // Read the stiffness matrix from matFE.dat
51
52
       strncpy(filename1, inparam.workdir, 128);
       datafile1="csrmat_FE.dat"; strcat(filename1, datafile1);
53
54
55
       // Read the RHS from rhsFE.dat
56
       strncpy(filename2, inparam.workdir, 128);
       datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
57
58
       fasp_dcsrvec2_read(filename1, filename2, &A, &b);
59
60
       // Step 2. Print problem size and ITS parameters
61
       if (print_level>PRINT_NONE) {
62
           printf("A: m = %d, n = %d, nnz = %d \ n", A.row, A.col, A.nnz);
63
           printf("b: n = %d n", b.row);
64
65
           fasp_param_solver_print(&itparam);
66
       }
67
       // Step 3. Solve the system with ITS as an iterative solver
68
       // Set the initial guess to be zero and then solve it using standard
69
       // iterative methods, without applying any preconditioners
70
       fasp_dvec_alloc(A.row, &x);
71
72
       fasp_dvec_set(A.row, &x, 0.0);
73
74
       fasp_solver_dcsr_itsolver(&A, &b, &x, NULL, &itparam);
75
       // Step 4. Clean up memory
76
       fasp_dcsr_free(&A);
77
78
       fasp_dvec_free(&b);
79
       fasp_dvec_free(&x);
80
81
       return FASP_SUCCESS;
82
   }
83
   /*----*/
84
           End of File
85
   /*----*/
```

This example is very similar to the first example and we briefly explain the differences:

- Line 71-72 allocates memory for the solution vector x and set its initial value to be all zero.
- Line 74 solves Ax = b using the general interface for Krylov subspace methods. Type the iterative method and other parameters have been specified in "itparam"; see §3.5 for details.

To run this example, we can simply type:

```
$ ./poisson-its-c.ex
```

A sample output is as follows:

```
FASP: ITS example -- C version
                                                    fasp_dcsrvec2_read: reading file ../data/csrmat_FE.dat...
fasp_dcsrvec2_read: reading file ../data/rhs_FE.dat...
{\tt A: \ m = 3969, \ n = 3969, \ nnz = 27281}
b: n = 3969
          Parameters in ITS_param
                                                2
Solver print level:
Solver type:
                                                1
                                                2
Solver precond type:
Solver max num of iter:
                                                500
Solver tolerance:
                                                1.00 \, \mathrm{e}{-06}
Solver stopping type:
Calling CG solver (CSR) \dots
It Num
               ||r||/||b||
                                           ||r||
                                                              Conv. Factor
      0 |
             1.0000000 \, \mathrm{e}{+00}
                                      7.514358\,\mathrm{e}{+00}
            5.078029\,\mathrm{e}\!-\!01
      1 |
                                      3.815813\,\mathrm{e}{+00}
                                                                  0.5078
            3.728856\,\mathrm{e}\!-\!01
                                      2.801996\,\mathrm{e}{+00}
                                                                  0.7343
      3 |
             3.359470\,\mathrm{e}{-01}
                                      2.524426\,\mathrm{e}{+00}
                                                                  0.9009
             2.590574\,\mathrm{e}\!-\!01
                                                                  0.7711
      4
                                      1.946650 \, e{+00}
             2.380797\,\mathrm{e}\!-\!01
                                      1.789016e+00
                                                                  0.9190
      6
             1.992579 e - 01
                                      1.497295 e + 00
                                                                  0.8369
             1.847971 \, \mathrm{e}{-01}
      7 |
                                      1.388631e+00
                                                                  0.9274
             1.619777 \, \mathrm{e}{-01}
                                      1.217158 e+00
                                                                  0.8765
      9 |
             1.513446\,\mathrm{e}\!-\!01
                                      1.137257e+00
                                                                  0.9344
     10
             1.364935 \, \mathrm{e}{\,-01}
                                      1.025661 e+00
                                                                  0.9019
     11 |
             1.283425\,\mathrm{e}\!-\!01
                                      9.644117\,\mathrm{e}{-01}
                                                                  0.9403
     12
             1.179652\,\mathrm{e}\!-\!01
                                       8.864327\,\mathrm{e}{-01}
                                                                  0.9191
     13 \mid 1.115146e-01
                                  | 8.379605e-01
                                                                  0.9453
```

```
14
         1.038726\,\mathrm{e}\!-\!01
                                         7.805360\,\mathrm{e}{-01}
                                                                            0.9315
          9.863412 e - 02
                                         7.411721\,\mathrm{e}{-01}
                                                                            0.9496
16
          9.277360 e - 02
                                         6.971341 e - 01
                                                                            0.9406
                                         6.644706 \, \mathrm{e}{-01}
17
          8.842679\,\mathrm{e}\!-\!02
                                                                            0.9531
18
          8.378399\,\mathrm{e}\!-\!02
                                         6.295829\,\mathrm{e}\!-\!01
                                                                            0.9475
          8.011023\,\mathrm{e}{-02}
19
                                         6.019770\,\mathrm{e}{-01}
                                                                            0.9562
          7.633221\,\mathrm{e}\!-\!02
20
                                         5.735875\,\mathrm{e}\!-\!01
                                                                            0.9528
21 |
         7.317756\,\mathrm{e}\!-\!02
                                         5.498824\,\mathrm{e}{-01}
                                                                            0.9587
22 |
          7.003292\,\mathrm{e}\!-\!02
                                         5.262524\,\mathrm{e}\!-\!01
                                                                            0.9570
23 |
          6.728610\,\mathrm{e}\!-\!02
                                         5.056119\,\mathrm{e}{-01}
                                                                            0.9608
24
          6.461736\,\mathrm{e}\!-\!02
                                         4.855580\,\mathrm{e}\!-\!01
                                                                            0.9603
25 |
          6.219614e-02
                                         4.673640\,\mathrm{e}{-01}
                                                                            0.9625
26
          5.989276 e - 02
                                         4.500557e - 01
                                                                            0.9630
27
          5.773520\,\mathrm{e}{-02}
                                         4.338429\,\mathrm{e}\!-\!01
                                                                            0.9640
28
          5.571758e-02
                                         4.186818 e - 01
                                                                            0.9651
                                         4.040944e\!-\!01
                                                                            0.9652
29
          5.377630 e - 02
30
          5.198586\,\mathrm{e}\!-\!02
                                         3.906404 e - 01
                                                                            0.9667
          5.022413\,\mathrm{e}\!-\!02
                                         3.774021\,\mathrm{e}{-01}
31
                                                                            0.9661
32
          4.861699\,\mathrm{e}\!-\!02
                                         3.653255\,\mathrm{e}\!-\!01
                                                                            0.9680
33
          4.700598e-02
                                         3.532197e-01
                                                                            0.9669
          4.554874 \, \mathrm{e}\!-\!02
                                         3.422696\,\mathrm{e}\!-\!01
                                                                            0.9690
34
         4.406559 \, \mathrm{e}{-02}
                                         3.311246\,\mathrm{e}{-01}
                                                                            0.9674
36 |
          4.273253\,\mathrm{e}\!-\!02
                                         3.211075\,\mathrm{e}{-01}
                                                                            0.9697
          4.135901\,\mathrm{e}\!-\!02
                                         3.107864\,\mathrm{e}\!-\!01
37 |
                                                                            0.9679
38
          4.013076\,\mathrm{e}\!-\!02
                                         3.015569\,\mathrm{e}\!-\!01
                                                                            0.9703
39
          3.885861\,\mathrm{e}\!-\!02
                                         2.919975\,\mathrm{e}\!-\!01
                                                                            0.9683
40
          3.776252\,\mathrm{e}\!-\!02
                                         2.837611 \, \mathrm{e}{-01}
                                                                            0.9718
41
          3.678565 e - 02
                                         2.764205 e - 01
                                                                            0.9741
          3.648645\,\mathrm{e}{-02}
                                         2.741722\,\mathrm{e}\!-\!01
                                                                            0.9919
42
          3.725368 e - 02
                                         2.799375 e - 01
43
                                                                            1.0210
44
          3.922957\,\mathrm{e}\!-\!02
                                         2.947850\,\mathrm{e}\!-\!01
                                                                            1.0530
          4.003513\,\mathrm{e}\!-\!02
45
                                         3.008383 e - 01
                                                                            1.0205
46
          3.683219 e - 02
                                         2.767703\,\mathrm{e}\!-\!01
                                                                            0.9200
          3.161285\,\mathrm{e}\!-\!02
47
                                         2.375503\,\mathrm{e}\!-\!01
                                                                            0.8583
48
          2.944107\,\mathrm{e}\!-\!02
                                         2.212307\,\mathrm{e}{-01}
                                                                            0.9313
49
          2.961834 e - 02
                                         2.225628\,\mathrm{e}\!-\!01
                                                                            1.0060
          2.774118e-02
                                         2.084571 \, \mathrm{e}{-01}
                                                                            0.9366
50
```

2.3 Example 3: Conjugate gradient with preconditioning

This example is a bit more involved and is a modification of the previous one. In this example, we wish to demonstrate how to use a the FASP library and run a preconditioned conjugate gradient (PCG) method.

```
/*! \file poisson-pcg.c

*

* \brief The third test example for FASP: using PCG to solve

the discrete Poisson equation from P1 finite element.

c version.

*
```

```
* \note Solving the Poisson equation (P1 FEM) with PCG: C version
7
8
9
     * Copyright (C) 2012--2017 by the FASP team. All rights reserved.
10
    * Released under the terms of the GNU Lesser General Public License 3.0 or later.
11
12
13
14
15
   #include "fasp.h"
16
   #include "fasp_functs.h"
17
18
19
    * \fn int main (int argc, const char * argv[])
20
    * \brief This is the main function for the third example.
21
22
    * \author Feiteng Huang
23
    * \date 05/17/2012
24
25
    * Modified by Chensong Zhang on 09/22/2012
26
27
28
   int main (int argc, const char * argv[])
29
                        inparam; // parameters from input files
30
        input_param
                        itparam; // parameters for itsolver
31
        ITS_param
                        amgparam; // parameters for AMG
32
        AMG_param
        ILU_param
                        iluparam; // parameters for ILU
33
34
        printf("\n=========");
35
        printf("\n|| FASP: PCG example -- C version ||");
36
        printf("\n======\n\n");
37
38
39
        // Step O. Set parameters: We can use ini/pcg.dat
        fasp_param_set(argc, argv, &inparam);
40
41
        fasp_param_init(&inparam, &itparam, &amgparam, &iluparam, NULL);
42
        // Set local parameters
43
        const SHORT print_level = itparam.print_level;
44
        const SHORT pc_type = itparam.precond_type;
45
        const SHORT stop_type = itparam.stop_type;
46
47
        const INT maxit
                             = itparam.maxit;
48
        const REAL tol
                               = itparam.tol;
49
        // Step 1. Get stiffness matrix and right-hand side
50
        // Read A and b -- P1 FE discretization for Poisson. The location
51
52
        // of the data files is given in "ini/pcg.dat".
53
        dCSRmat A;
54
        dvector b, x;
55
        char filename1[512], *datafile1;
56
        \begin{array}{ll} \textbf{char} & \texttt{filename2} \left[ \, 5 \, 1 \, 2 \, \right] \, , & * \, \texttt{datafile2} \, ; \end{array}
57
        // Read the stiffness matrix from matFE.dat
58
59
        strncpy(filename1, inparam.workdir, 128);
```

```
datafile1="csrmat_FE.dat"; strcat(filename1, datafile1);
60
61
         // Read the RHS from rhsFE.dat
62
         strncpy(filename2, inparam.workdir, 128);
63
         datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
64
65
         {\tt fasp\_dcsrvec2\_read} \, (\, {\tt filename1} \, , \, \, \, {\tt filename2} \, , \, \, \, \& \! A \, , \, \, \& b \, ) \, ; \\
66
67
68
         // Step 2. Print problem size and PCG parameters
69
         if (print_level>PRINT_NONE) {
             printf("A: m = %d, n = %d, nnz = %d n", A.row, A.col, A.nnz);
70
71
             printf("b: n = \frac{d}{n}, b.row);
72
             fasp_param_solver_print(&itparam);
        }
73
74
        // Setp 3. Setup preconditioner
75
         // Preconditioner type is determined by pc_type
76
         {\tt precond *pc = fasp\_precond\_setup(pc\_type\,, \,\,\&amgparam\,, \,\,\&iluparam\,, \,\,\&A)\,;}
77
78
         // Step 4. Solve the system with PCG as an iterative solver
79
        // Set the initial guess to be zero and then solve it using PCG solver
80
81
        // Note that we call PCG interface directly. There is another way which
        // calls the abstract iterative method interface; see possion-its.c for
82
         // more details.
83
         fasp_dvec_alloc(A.row, &x);
84
         fasp_dvec_set(A.row, &x, 0.0);
85
86
         fasp_solver_dcsr_pcg(&A, &b, &x, pc, tol, maxit, stop_type, print_level);
87
88
         // Step 5. Clean up memory
89
         if (pc_type!=PREC_NULL) fasp_mem_free(pc->data);
90
         fasp_dcsr_free(&A);
91
92
         fasp_dvec_free(&b);
        fasp_dvec_free(&x);
93
94
         return FASP_SUCCESS;
95
96
97
98
                 End of File
99
          ----*/
100
```

This example is very similar to the first example, and the details are as follows.

- Line 40–41 sets default parameters. In this example, we need parameters for iterative methods, AMG preconditioner, and ILU preconditioner.
- Line 77 sets up the desired preconditioner and prepare it for the preconditioned iterative methods.
- Line 87 calls PCG to solve Ax = b. One can also call the general iterative method interface as in the previous example.

• Line 90 cleans up auxiliary data associated with the preconditioner in use if necessary.

To run this example, we can simply type:

```
$ ./poisson-pcg-c.ex
```

A sample output is given as follows (note that the actual output depends on the solver parameters and might be different than what you see here):

```
\prod
     FASP: PCG example -- C version
                                               \Pi
fasp_dcsrvec2_read: reading file ../data/csrmat_FE.dat...
fasp_dcsrvec2_read: reading file ../data/rhs_FE.dat...
A: m = 3969, n = 3969, nnz = 27281
\mathtt{b:} \ \mathtt{n} = 3969
        Parameters in ITS_param
                                           2
Solver print level:
Solver type:
                                           1
Solver precond type:
                                           2
Solver max num of iter:
                                           500
Solver tolerance:
                                           1.00\,\mathrm{e}\!-\!06
Solver stopping type:
          Num of rows Num of nonzeros Avg. NNZ / row
  Level
    0
                  3969
                                       27281
                                                           6.87
    1
                  1985
                                                         14.37
                                       28523
    2
                   541
                                        7951
                                                         14.70
                   141
                                        1803
                                                          12.79
  Grid complexity = 1.672 | Operator complexity = 2.403
Classical AMG setup costs 0.0044 seconds.
It Num |
             ||r||/||b||
                                      ||r||
                                                   | Conv. Factor
      0 |
           1.0000000 e+00
                                  7.514358 e+00
                             8.687750 \,\mathrm{e}{-02}
      1 |
           1.156153\,\mathrm{e}\!-\!02
                                                           0.0116
                                  2.349876\,\mathrm{e}{-03}
           3.127181 \, \mathrm{e} \! - \! 04
                                                           0.0270
           4.813471 \, \mathrm{e}\!-\!06
                                  3.617014 \, \mathrm{e}{-05}
      3 |
                                                           0.0154
      4
            5.312526\,\mathrm{e}\!-\!08
                                  3.992022\,\mathrm{e}\!-\!07
                                                           0.0110
Number of iterations = 4 with relative residual 5.312526\,\mathrm{e}-08.
```

We also provide a Fortran 90 example, which does the same thing as this C code except it gives less output, in "tutorial/main/poisson-pcg.f90". Users who would like to call FASP solver

from a Fortran based application can see how to do this example.

```
!> \file poisson-pcg.f90
   !>
2
   !> \brief The third test example for FASP: using PCG to solve
          the discrete Poisson equation from P1 finite element.
   !>
   ! >
           F90 version.
5
   !>
   !> \note Solving the Poisson equation (P1 FEM) with PCG: F90 version
7
   !>
8
   !>-----
9
   !> Copyright (C) 2012--2017 by the FASP team. All rights reserved.
10
   !> Released under the terms of the GNU Lesser General Public License 3.0 or later.
11
12
13
   program test
14
15
16
    implicit none
17
     \  \  \, double\ precision\,,\ dimension\,(:)\,,\ allocatable\ ::\ u\,,b
18
19
     double precision, dimension(:), allocatable :: a
                    dimension(:), allocatable :: ia,ja
20
     integer,
21
                   :: iufile, n, nnz, i, prt_lvl, maxit
22
23
     double precision :: tol
24
     print*, ""
25
26
     write(*,"(A)") "|| FASP: PCG example -- F90 version ||"
27
     28
     print*, ""
29
30
31
     ! Step 0: user defined variables
     prt_lvl = 3
32
     maxit = 500
33
     tol = 1.0d-6
34
     iufile = 1
35
36
37
     ! Step 1: read A and b
38
     !===> Read data A from file
39
     open(unit=iufile,file='../data/csrmat_FE.dat')
40
41
     read(iufile,*) n
42
     allocate(ia(1:n+1))
43
     read(iufile,*) (ia(i),i=1,n+1)
44
45
46
     nnz=ia(n+1)-ia(1)
47
     allocate(ja(1:nnz),a(1:nnz))
     read(iufile,*) (ja(i),i=1,nnz)
48
49
     read(iufile,*) (a(i),i=1,nnz)
50
    close(iufile)
51
```

```
52
53
     !===> Read data b from file
     open(unit=iufile,file='../data/rhs_FE.dat')
54
55
     read(iufile,*) n
56
     allocate(b(1:n))
57
     read(iufile,*) (b(i),i=1,n)
58
59
60
     close(iufile)
61
     !===> Shift the index to start from 0 (for C routines)
62
63
     forall (i=1:n+1) ia(i)=ia(i)-1
64
     forall (i=1:nnz) ja(i)=ja(i)-1
65
66
     ! Step 2: Solve the system
67
     !===> Initial guess
68
     allocate(u(1:n))
69
70
     u=0.0d0
     call fasp_fwrapper_krylov_amg(n,nnz,ia,ja,a,b,u,tol,maxit,prt_lvl);
71
72
73
     ! Step 3: Clean up memory
     deallocate(ia,ja,a)
74
     deallocate(b,u)
75
76
   end program test
77
78
   !/*----*/
79
           End of File --*/
80
81
```

2.4 Example 4: An GMG solver for the Poisson equation

The geometric multigrid method (GMG) is one of the most efficient solving techniques for discrete algebraic systems arising from many types of partial differential equations [1, 16]. GMG utilizes a hierarchy of grids or discretizations and reduces the error at a number of frequencies simultaneously. Because of its plausible linear complexity—i.e., the low computational cost of solving a linear system with N unknowns is O(N)—the GMG method is one of the most popular Poisson solvers. Although the GMG's applicability is limited as it requires explicit information on the hierarchy of the discrete system, when it can be applied, GMG is far more efficient than its algebraic version, the algebraic multigrid (AMG) method.

We now give a simple example on calling the geometric multigrid for solving the Poisson's equation in 2D (discretized by the standard five-point finite difference stencil). Consider the Poisson equation

$$\begin{cases}
-\Delta u &= f & \text{in } \Omega \\
u &= 0 & \text{on } \partial\Omega,
\end{cases}$$

where $\Omega = (0,1)^2 \subset \mathbb{R}^2$. The main reason why we choose this simplest possible setting is to emphasize that, even for a simple problem, the new heterogeneous architectures present challenges for numerical implementation. Another reason is to allow us to use explicit stencils and to avoid the bottleneck of sparse matrix-vector production. The standard central finite difference method is applied to discretize the Poisson's equation. In other words, the Laplace operator is discretized by the classical second-order central difference scheme. After discretization, we end up with a system of linear equations:

$$\mathbf{A}\vec{u} = \vec{f}.$$

We use the five-point central difference scheme in 2D. Consider a uniform square mesh of $\Omega = [0, 1]^2$ with size $h = \frac{1}{n}$ and in which $x_i = ih$, $y_j = jh$ (i, j = 0, 1, ..., n). Let $u_{i,j}$ be the numerical approximation of $u(x_i, y_j)$. The five-point central difference scheme for solving the Poisson's equation in 2D can be written as follows:

$$-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i+1,j} - u_{i,j+1} = h^2 f(x_i, y_j) \qquad i, j = 1, 2, \dots, n-1.$$

The sample code for this solver can be found in "tutorial/main/poisson-gmg.c" and a piece of the source code is listed as follows:

```
/*! \file poisson-gmg.c
1
2
       \brief The fourth test example for FASP: using GMG to solve
3
4
               the discrete Poisson equation from five-point finite
               difference stencil. C version.
5
6
       \note Solving the Poisson equation (FDM) with GMG: C version
7
8
9
10
11
       Copyright (C) 2013--2017 by the FASP team. All rights reserved.
12
       Released under the terms of the GNU Lesser General Public License 3.0 or later.
13
14
15
   #include <time.h>
16
   #include <math.h>
17
18
   #include "fasp.h"
19
   #include "fasp_functs.h"
20
21
   const REAL pi = 3.14159265;
22
23
24
25
    * \fn static REAL f2d(INT i, INT j, INT nx, INT ny)
26
    * \brief Setting f in Poisson equation, where
27
28
             f = sin(pi x)*sin(pi y)
29
```

```
* \param i i-th position in x direction
30
31
    * \param j
                  j-th position in y direction
32
    * \param nx Number of grids in x direction
    * \param ny Number of grids in y direction
33
34
    * \author Ziteng Wang
35
    * \date 06/07/2013
36
37
38
   static REAL f2d (INT i,
39
                    INT j,
                    INT nx,
40
41
                    INT ny)
42
       return sin(pi *(((REAL) j)/((REAL) ny)))
43
             *sin(pi *(((REAL) i)/((REAL) nx)));
44
45
   }
46
47
48
    * \fn static REAL L2NormError2d(REAL *u, INT nx, INT ny)
49
    * \brief Computing Discretization Error, where exact solution
50
51
           u = \sin(pi x)*\sin(pi y)/(2*pi*pi)
52
                   Vector of DOFs
    * \param u
53
                 Number of grids in x direction
54
    * \param nx
     * \param ny
                    Number of grids in y direction
55
56
    * \author Ziteng Wang
57
    * \date 06/07/2013
58
59
   static REAL L2NormError2d (REAL *u,
60
61
                               INT nx,
62
                               INT ny)
63
   {
64
       const REAL h = 1.0/nx;
       REAL 12norm = 0.0, uexact;
65
66
       INT i, j;
67
       for (i = 1; i < ny; i++) {
68
69
           for (j = 1; j < nx; j++)
70
                uexact = sin(pi*i*h)*sin(pi*j*h)/(pi*pi*2.0);
71
               12 norm += pow((u[i*(nx+1)+j] - uexact), 2);
72
           }
       }
73
74
75
       return sqrt(12norm*h*h);
76
   }
77
78
79
   * \brief An example of GMG method using Full Multigrid cycle
80
81
    * \author Chensong Zhang
    * \date 10/12/2015
```

```
83
 84
      * \note
                Number of grids of nx = ny should be equal to 2^maxlevel.
 85
    int main (int argc, const char *argv[])
 86
 87
         const REAL rtol = 1.0e-6;
 88
         const INT prtlvl = PRINT_MORE;
 89
90
 91
         INT
                     i, j, nx, maxlevel;
                    *u, *b, h, error0;
92
         REAL
93
         // Step O. Set number of levels for GMG
94
         printf("Enter the desired number of levels: ");
95
         if ( scanf("%d", \&maxlevel) > 1 ) {
96
              printf("### ERROR: Did not get a valid input !!!\n");
97
             return ERROR_INPUT_PAR;
98
99
         }
100
101
         // Step 1. Compute right-hand side b and set approximate solution u
102
         nx = (int) pow(2.0, maxlevel);
         h = 1.0/((REAL) nx);
103
104
         u = (REAL *)malloc((nx+1)*(nx+1)*sizeof(REAL));
105
         \texttt{fasp\_darray\_set}\left(\left(\,\texttt{nx}\!+\!1\right)\!*\!\left(\,\texttt{nx}\!+\!1\right),\ \texttt{u}\,,\ 0.0\,\right);
106
107
         b = (REAL *)malloc((nx+1)*(nx+1)*sizeof(REAL));
108
         for (i = 0; i \le nx; i++) {
109
              for (j = 0; j \le nx; j++) {
110
111
                  b[j*(nx+1)+i] = h*h*f2d(i, j, nx, nx);
112
         }
113
114
115
         // Step 2. Solve the Poisson system in 2D with full Multigrid cycle
         {\tt fasp\_poisson\_fgmg2d} \, (u\,,\ b\,,\ nx\,,\ nx\,,\ maxlevel\,,\ rtol\,,\ prtlvl\,)\,;
116
117
         // Step 3. Compute error in L2 norm
118
         error0 = L2NormError2d(u, nx, nx);
119
120
121
         printf("L2 error ||u-u'|| = %e\n", error0);
122
123
         // Step 4. Clean up memory
124
         free(u);
125
         free(b);
126
127
         return FASP_SUCCESS;
128
     }
129
     /*----*/
130
131
     /*--
                End of File
132
```

2.5 Example 5: Block ILU preconditioner

We now show a simple example for calling iterative solvers in BSR format. The test example is from a test problem given by the Society of Petroleum Engineers (SPE01 Benchmark) using a fully implicit black-oil simulator at certain time step. The test matrix is the Jacobian matrix from the Newton linearization and is stored as a BSR matrix (see §3.2 for details).

The sample code for this solver can be found in "tutorial/main/spe01-its.c" and a piece of the source code is listed as follows:

```
/*! \file spe01-its.c
1
2
3
       \brief The fifth test example for FASP: using ITS_BSR to solve
4
              the Jacobian equation from reservoir simulation benchmark
5
              problem SPE01.
6
7
       \note ITS_BSR example for FASP: C version
8
      Solving the Society of Petroleum Engineers SPE01 benchmark problem
9
10
       with Block ILU preconditioned Krylov methods
11
12
      Copyright (C) 2012--2017 by the FASP team. All rights reserved.
13
       Released under the terms of the GNU Lesser General Public License 3.0 or later.
14
15
16
17
   #include "fasp.h"
18
   #include "fasp_functs.h"
19
20
21
    * \fn int main (int argc, const char * argv[])
22
23
    * \brief This is the main function for the fourth example.
24
25
    * \author Feiteng Huang, Chensong Zhang
^{26}
27
    * \date 05/22/2012
28
    * Modified by Chensong Zhang on 09/22/2012
29
30
   int main (int argc, const char * argv[])
31
32
                       inparam; // parameters from input files
33
       input_param
                       itparam;
                                // parameters for itsolver
34
       ITS_param
       ILU_param
                       iluparam; // parameters for ILU
35
36
       printf("\n======="");
37
38
       printf("\n||
                    FASP: SPE01 -- ITS BSR version ||");
       printf("\n======\n\n");
39
40
41
       // Step O. Set parameters: We can ini/its_bsr.dat
```

```
42
        fasp_param_set(argc, argv, &inparam);
43
        fasp_param_init(&inparam, &itparam, NULL, &iluparam, NULL);
44
        // Set local parameters
45
        const int print_level = inparam.print_level;
46
47
        // Step 1. Get stiffness matrix and right-hand side
48
        // Read A and b -- P1 FE discretization for Poisson. The location
49
50
        // of the data files is given in "its.dat".
51
        dBSRmat A;
        dvector b, x;
52
53
        char filename1[512], *datafile1;
        char filename2[512], *datafile2;
54
55
        // Read the stiffness matrix from bsrmat_SPE01.dat
56
        strncpy(filename1, inparam.workdir, 128);
57
        datafile1="bsrmat_SPE01.dat"; strcat(filename1, datafile1);
58
        fasp_dbsr_read(filename1, &A);
59
60
        // Read the RHS from rhs_SPE01.dat
61
        strncpy(filename2, inparam.workdir, 128);
62
63
        datafile2="rhs_SPE01.dat"; strcat(filename2, datafile2);
64
        fasp_dvec_read(filename2, &b);
65
        // Step 2. Print problem size and ITS_bsr parameters
66
        if (print_level>PRINT_NONE) {
67
            printf("A: m = %d, n = %d, nnz = %d \ n", A.ROW, A.COL, A.NNZ);
68
            printf("b: n = %d\n", b.row);
69
            fasp_param_solver_print(&itparam);
70
            fasp_param_ilu_print(&iluparam);
71
        }
72
73
74
        // Step 3. Solve the system with ITS_BSR as an iterative solver
        // Set the initial guess to be zero and then solve it using standard
75
76
        // iterative methods, without applying any preconditioners
77
        fasp_dvec_alloc(b.row, &x);
        \texttt{fasp\_dvec\_set} \left( \texttt{b.row} \,, \,\, \&x \,, \,\, \, 0.0 \right);
78
79
        itparam.itsolver_type = SOLVER_GMRES;
80
        fasp_solver_dbsr_krylov_ilu(&A, &b, &x, &itparam, &iluparam);
81
82
83
        // Step 4. Clean up memory
84
        fasp_dbsr_free(\&A);
        fasp_dvec_free(&b);
85
        fasp_dvec_free(&x);
86
87
88
        return FASP_SUCCESS;
89
   }
90
91
              End of File
92
    /*----*/
```

A sample output is given as follows (note that the actual output depends on the solver parameters and might be different than what you see here):

```
FASP: SPE01 — ITS BSR version
                                          fasp_dbsr_read: reading file ../data/bsrmat_SPE01.dat...
fasp_dvec_read: reading file ../data/rhs_SPE01.dat...
A: m = 302, n = 302, nnz = 1788
b: n = 906
       Parameters in ITS_param
Solver print level:
                                      2
Solver type:
                                      1
Solver precond type:
                                      2
Solver max num of iter:
                                      500
Solver tolerance:
                                      1.00\,\mathrm{e}\!-\!06
Solver stopping type:
       Parameters in ILU_param
                                      2
ILU print level:
ILU type:
                                      1
ILU level of fill-in:
                                      0
ILU relaxation factor:
                                      0.0000
ILU drop tolerance:
                                      1.00\,\mathrm{e}\!-\!03
ILU permutation tolerance:
                                      0.00\,\mathrm{e}{+00}
BSR ILU(0) setup costs 0.000228 seconds.
Calling GMRES solver (BSR) ...
It Num
            ||r||/||b||
                                  ||r||
                                                 Conv. Factor
                           8.207069e+03
     0 \mid 1.000000e+00
     1 \mid 9.999991e-01
                           8.207062e+03
                                                    1.0000
                           8.200415e+03
     2 \mid 9.991891e-01
                                                    0.9992
     3 \mid 9.984917e-01
                              8.194691e+03
                                                    0.9993
     4 \mid 9.581382 e - 01
                              7.863507e+03
                                                     0.9596
          9.387736\,\mathrm{e}\!-\!01
                              7.704580 \, e{+03}
                                                    0.9798
     6 \mid 8.996932e-01
                              7.383844 e+03
                                                    0.9584
     7 \mid 8.970099e-01
                         7.361822e+03
                                                    0.9970
     8 \mid 8.570704e-01
                         7.034036 e+03
                                                    0.9555
     9 \mid 5.309276e-01
                         | 4.357360 e+03
                                                    0.6195
    10 \mid 1.462587 e - 01
                              1.200355 e+03
                                                    0.2755
    11 \mid 3.520599e-02
                              2.889380\,\mathrm{e}{+02}
                                                    0.2407
    12 \mid 8.488230 \, e{-03}
                          6.966349e+01
                                                    0.2411
```

```
13 \mid 2.019708e-03
                                1.657588e+01
                                                                 0.2379
            4.524916\,\mathrm{e}\!-\!04
                                     3.713630\,\mathrm{e}{+00}
                                                                 0.2240
             9.670973 e - 05
                                     7.937035 \, e{-01}
                                                                 0.2137
             1.970931 e - 05
                                     1.617557e-01
                                                                 0.2038
     17
             3.905034\,\mathrm{e}\!-\!06
                                     3.204889\,\mathrm{e}\!-\!02
                                                                 0.1981
                                     7.019817 \, \mathrm{e}{-03}
             8.553378\,\mathrm{e}\!-\!07
                                                                 0.2190
Number of iterations = 18 with relative residual 8.553446\,\mathrm{e}{-07}.
Iterative method costs 0.0009 seconds.
{\tt ILUk\_Krylov} method totally costs 0.0009 seconds.
```

2.6 How to change parameters for solvers/preconditioners

In the previous examples, we have seen how to use the default parameters in FASP. In this section we discuss changing such parameters by reading them from a disk file or from the command line. An example of parameter initialization file is found in the FASP tutorial directory and is named "tutorial/ini/amg.dat".

```
$ ./poisson-amg-c.ex -ini ini/amg.dat
```

We take "tutorial/ini/amg.dat" as an example:

```
-%
   \% input parameters
                                                     %
2
                                                    %
   |\%| lines starting with \% are comments
   |\% must have spaces around the equal sign "="
                                                    %
6
   workdir = ../data/
                          \% work directory, no more than 128 characters
                          \% How much information to print out
8
   print_level = 3
                                                    -%
10
   \% parameters for multilevel iteration
                                                    %
11
12
13
                                       \% C classic AMG
14
   AMG_type
                                       \% SA smoothed aggregation
15
                                       \% UA unsmoothed aggregation
16
                             = v
                                       \% V V-cycle | W W-cycle
17
   AMG_cycle_type
                                       \% A AMLI-cycle | NA Nonlinear AMLI-cycleA
18
   AMG_tol
                                       \% tolerance for AMG
19
                             = 1e-8
                                       \% number of AMG iterations
20
   AMG_maxit
                             = 100
21
   AMG_levels
                             = 20
                                       \% max number of levels
                             = 500
                                       \% max number of coarse degrees of freedom
22
   AMG_coarse_dof
   AMG_coarse_scaling
                             = 0FF
                                       \% switch of scaling of the coarse grid correction
   AMG_amli_degree
                             = 2
                                       \% degree of the polynomial used by AMLI cycle
25
   AMG_nl_amli_krylov_type = 6
                                       \% Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCG
26
27
   |\% parameters for AMG smoothing
                                                     %
```

```
29
30
31
   AMG_smoother
                             = GS
                                       % GS | JACOBI | SGS
                                       \% SOR | SSOR | GSOR | SGSOR | POLY
32
   AMG_ILU_levels
                             = 0
                                       \% number of levels using ILU smoother
33
                                       \% number of levels using Schwarz smoother
34
   AMG_SWZ_levels
                             = 0
                                       \% relaxation parameter for SOR smoother
35
   AMG_relaxation
                             = 1.1
                                       \% degree of the polynomial smoother
36
   AMG_polynomial_degree
                             = 3
37
   AMG_presmooth_iter
                             = 2
                                       \% number of presmoothing sweeps
   AMG_postsmooth_iter
                             = 2
                                       \% number of postsmoothing sweeps
38
39
40
                                                    -%
   \% parameters for classical AMG SETUP
                                                    %
41
                                                    -%
42
43
   AMG_coarsening_type
                                       \% 1 Modified RS
44
                             = 1
                                       \% 3 Compatible Relaxation
45
                                       \% 4 Aggressive
46
   AMG_interpolation_type
                             = 1
                                       \% 1 Direct | 2 Standard | 3 Energy-min
47
   AMG\_strong\_threshold = 0.6
                                       \% Strong threshold
48
   {\tt AMG\_truncation\_threshold} \ = \ 0.4
                                       \% Truncation threshold
49
   AMG_max_row_sum
                             = 0.9
                                       \% Max row sum
51
                                                    -%
52
   \% parameters for aggregation-type AMG SETUP
                                                    %
53
54
55
                             = 0.08
                                       % Strong coupled threshold
56
   AMG_strong_coupled
                             = 20
                                       \% Max size of aggregations
57
   AMG_max_aggregation
                             = 0.67
                                       \% Smoothing factor for tentative prolongation
   AMG_tentative_smooth
58
                                       \% Switch for filtered matrix for smoothing
                             = OFF
59
   AMG_smooth_filter
```

We now briefly discuss the parameters above: This example is very similar to the first example and we now briefly explain it:

- Line 7 sets the working directory, which should contain data files for the matrices (and right-hand side vectors when necessary).
- Line 8 sets the level of output for FASP routines. It should range from 0 to 10 with 0 means no output and 10 means output everything possible.
- Line 14–25 sets the basic parameters for multilevel iterations. For example, type of AMG, type of multilevel cycles, number of maximal levels, etc.
- Line 31–38 sets the type of smoothers, number of smoothing sweeps, etc.
- Line 44–50 sets the parameters for the setup phase of the classical AMG method (§3.6).
- Line 56–59 gives the parameters for the setup phase of the aggregation-base AMG methods (§3.6).

You can do a very simple experiment—Simply change the AMG type from the classical AMG to smoothed aggregation AMG by revise Line 14 to:

```
AMG_type = SA
```

Then you run "poisson-amg-c.ex" one more time and will get

```
fasp_dcsrvec2_read: reading file ../data/csrmat_FE.dat...
fasp_dcsrvec2_read: reading file ../data/rhs_FE.dat...
A: m = 3969, n = 3969, nnz = 27281
b: n = 3969
       {\tt Parameters \ in \ AMG\_param}
AMG print level:
                                    3
AMG max num of iter:
                                   100
AMG type:
                                    2
AMG tolerance:
                                   1.00\,\mathrm{e}\!-\!08
AMG max levels:
                                   20
AMG cycle type:
                                   1
AMG coarse solver type:
AMG scaling of coarse correction:
AMG smoother type:
AMG smoother order:
AMG num of presmoothing:
AMG num of postsmoothing:
Aggregation type:
Aggregation number of pairs:
Aggregation quality bound:
                                   8.00
Calling SA AMG \dots
  Level
         Num of rows Num of nonzeros Avg. NNZ / row
               3969
                                 27281
    0
                                                 6.87
                541
                                  6531
                                                12.07
    1
                 41
                                  421
                                                10.27
 Grid complexity = 1.147 | Operator complexity = 1.255
Smoothed aggregation setup costs 0.0032 seconds.
                               ||r||
It Num
           ||r||/||b|| |
                                           Conv. Factor
     0 |
         1.0000000 \, \mathrm{e}{+00}
                            7.514358\,\mathrm{e}{+00}
                        3.265336e-01
     1 \mid 4.345463e-02
                                                 0.0435
```

```
2 \mid 8.041967e-03
                             6.043022e-02
                                                        0.1851
     3 \mid 3.808810 e - 03
                                2.862076\,\mathrm{e}{-02}
                                                        0.4736
     4 \mid 1.838990 e - 03
                                1.381883 \, \mathrm{e}{-02}
                                                        0.4828
     5 \mid 8.675952e-04
                               6.519421 \, \mathrm{e}{-03}
                                                        0.4718
     6 \mid 4.089274 e - 04
                            3.072827e-03
                                                        0.4713
          1.939823\,\mathrm{e}{-04}
                           1.457653 e-03
     7
                                                       0.4744
     8 \mid 9.276723 e - 05
                           | 6.970862 e - 04 |
                                                       0.4782
                           | 3.360270 e - 04 |
     9 \mid 4.471799e-05
                                                       0.4820
                           | 1.631554 e - 04 |
    10 \mid 2.171249 e - 05
                                                       0.4855
    11 \mid 1.060934e-05
                           | 7.972239 e - 05 |
                                                       0.4886
                           | 3.916668 e - 05 |
    12 \mid 5.212246 \, e{-06}
                                                       0.4913
    13 \mid 2.572464 e - 06
                                1.933042 e - 05
                                                       0.4935
                           | 9.576797 e - 06
    14 \mid 1.274466 e-06
                                                       0.4954
    15 \mid 6.333891e-07
                           4.759512e-06
                                                       0.4970
    16 \mid 3.155926e-07
                           2.371476 e-06
                                                       0.4983
                           1.184079e-06
    17 \mid 1.575755e-07
                                                       0.4993
    18 \mid 7.881043 e - 08
                           5.922098e-07
                                                        0.5001
    19 \mid 3.947044e-08
                             2.965950e-07
                                                        0.5008
    20 |
          1.978978\,\mathrm{e}\!-\!08
                                1.487075\,\mathrm{e}{-07}
                                                       0.5014
    21 \mid 9.931176 e - 09 \mid 7.462641 e - 08 \mid
                                                       0.5018
Number of iterations = 21 with relative residual 9.931176\,\mathrm{e}-09.
AMG solve costs 0.0061\ \text{seconds}\,.
AMG totally costs 0.0098 seconds.
```

You can compare this with the results in §2.1.

Similarly, you can solve the same problem using pairwise unsmoothed aggregation AMG preconditioned conjugated gradient method by calling

```
$ ./poisson-pcg-c.ex -ini ini/amg_ua.dat
```

and it will yield the following result:

```
{\tt FASP:\ PCG\ example\ -\!-\ C\ version}
                                               \Pi
{\tt fasp\_dcsrvec2\_read: reading file } \dots / \, {\tt data/csrmat\_FE.dat} \dots
{\tt fasp\_dcsrvec2\_read: reading file } \dots / \, {\tt data/rhs\_FE.dat} \dots
A: m = 3969, n = 3969, nnz = 27281
b: n = 3969
        Parameters in ITS_param
Solver print level:
                                           3
Solver type:
                                           1
Solver precond type:
                                           2
Solver max num of iter:
                                          1000
Solver tolerance:
                                           1.00\,\mathrm{e}\!-\!06
Solver stopping type:
                                           1
```

Level	Num of rows	Num of nonzeros	Avg. NNZ / row
0	3969	27281	6.87
1	1059	7169	6.77
2	286	1884	6.59
3	71	431	6.07
Grid co	emplexity = 1.3	57 Operator com	plexity = 1.348
Unsmoothe	d aggregation	setup costs 0.0016	seconds.
It Num	r / b		Conv. Factor
0	1.000000e+00	7.514358e+00	
1	$5.078363\mathrm{e}\!-\!01$	3.816064 e+00	0.5078
2	$8.526434\mathrm{e}\!-\!02$	$ 6.407068 \mathrm{e} \! - \! 01$	0.1679
3	$3.081067\mathrm{e}\!-\!02$	$ 2.315224\mathrm{e}{-01}$	0.3614
4	$7.522033\mathrm{e}\!-\!03$	$ 5.652325\mathrm{e}{-02}$	0.2441
5	$1.997295\mathrm{e}\!-\!03$	$ 1.500839 \mathrm{e}{-02}$	0.2655
6	$5.914181\mathrm{e}\!-\!04$	$ 4.444127\mathrm{e}{-03}$	0.2961
7	$1.498444\mathrm{e}\!-\!04$	$ 1.125985\mathrm{e}{-03}$	0.2534
8	$4.380269\mathrm{e}\!-\!05$	3.291491 e - 04	0.2923
9	$1.120054\mathrm{e}\!-\!05$	8.416489 e - 05	0.2557
10	$2.772669\mathrm{e}\!-\!06$	$ 2.083482 \mathrm{e}{-05}$	0.2475
11	$8.491093\mathrm{e}\!-\!07$	$ 6.380511\mathrm{e}\!-\!06$	0.3062
Number of	iterations =	11 with relative re	sidual 8.491093e

The input parameters allowed in FASP are not limited to the ones listed in this example. A list of possible iterative methods and preconditioners can be found in "base/include/fasp_const.h"; see §4.2. For more parameters and their ranges, we refer to the FASP Reference Manual.

Using "-ini [FILE]" is just one example of allowed command line option. To find out more what command line options are acceptable, you can type in a terminal window:

```
$ ./poisson-amg-c.ex -help
```

which will give you something like

```
-\mathtt{precond}
            [IntValue] : Preconditioner type
-\mathtt{maxit}
                  [IntValue] : Max number of iterations
-tol
                  [RealValue] : Tolerance for iterative solvers
-to1
-amgmaxit
                 [IntValue] : Max number of AMG iterations
[RealValue] : Tolerance for AMG methods
-{\tt amgtol}
-amgcoarsening [IntValue] : AMG coarsening type
-amginterpolation [IntValue] : AMG interpolation type
-amgsmoother [IntValue] : AMG smoother type
-amgsthreshold [RealValue] : AMG strong threshold
-{\tt amgscoupled} \qquad \qquad [\,{\tt RealValue}\,] \;\; : \;\; {\tt AMG} \;\; {\tt strong} \;\; {\tt coupled} \;\; {\tt threshold}
-\mathtt{help}
                         : Brief help messages
```

For example, in order to the change the AMG type to the smoothed aggregation (SA) used by the preconditioner for PCG, you can also use the command line options:

```
./poisson-amg-c.ex -amgtype 2 -amgmaxit 100
```

Here we only changed two parameters from the default setting without changing anything else. So it might not give the same output as in the previous example.

Chapter 3

Data structures and basic usage

In this chapter, we discuss the basic data structures and the important building blocks which are useful for constructing auxiliary space preconditioners for systems of PDEs in Chapter 4. In particular, we will discuss vectors, sparse matrices, iterative methods, and multigrid methods.

3.1 Vectors and sparse matrices

The data structures most often used for implementing iterative methods are sparse matrices and vectors. In this section, we first discuss the data structures for vectors and matrices in FASP; and then we discuss BLAS operations for sparse matrices. The definitions can be found in "base/include/fasp.h".

Vectors

The data structure for vectors is very simple. It only contains the length of the vector and an array which contains the entries of this vector.

```
337
      * \struct dvector
338
339
      * \brief Vector with n entries of REAL type
340
341
    typedef struct dvector{
342
343
         //! number of rows
344
         INT row;
345
         //! actual vector entries
346
347
         REAL *val;
348
    } dvector; /**< Vector of REAL type */
```

Sparse matrices

On the other hand, sparse matrices for PDE applications are very complicated. It depends on the particular applications, discretization methods, as well as solution algorithms. In FASP, there are several types of sparse matrices, COO, CSR, CSRL, BSR, and CSR Block, etc. The presentation closely follows ideas from Pissanetzky [12].

In this section, we use the following sparse matrix as an example to explain different formats for sparse matrices:

Example 3.1.1 Consider the following 4×5 matrix with 12 non-zero entries

$$\left(\begin{array}{cccccc}
1 & 1.5 & 0 & 0 & 12 \\
0 & 1 & 6 & 7 & 1 \\
3 & 0 & 6 & 0 & 0 \\
1 & 0 & 2 & 0 & 5
\end{array}\right)$$

(i) COO format

The coordinate (COO) format or IJ format is the simplest sparse matrix format.

```
/**
199
200
     * \struct dCOOmat
     * \brief Sparse matrix of REAL type in COO (or IJ) format
201
202
203
      * Coordinate Format (I,J,A)
204
      * \note The starting index of A is 0.
205
      st \note Change I to rowind, J to colind. To avoid with complex.h confliction on I.
206
207
208
    typedef struct dCOOmat{
209
         //! row number of matrix A, m
210
         INT row;
211
212
         //! column of matrix A, n
213
         INT col;
214
215
216
         //! number of nonzero entries
217
         INT nnz;
218
         //! integer array of row indices, the size is nnz
219
220
221
222
         //! integer array of column indices, the size is nnz
223
         INT *colind;
224
225
         //! nonzero entries of A
226
         REAL *val;
227
```

```
228 } dCOOmat; /**< Sparse matrix of REAL type in COO format */
```

So it clear that the sparse matrix in Example 3.1.1 in COO format is stored as:

```
row = 4
col = 5
nnz = 12

I J val

0 0 1.0
0 1 1.5
0 4 12.0
1 1 1.0
1 2 6.0
1 3 7.0
1 4 1.0
......
```

Although the COO format is easy to understand or use, it wastes storage space and has little advantages in sparse BLAS operations.

NOTE: In FASP, the indices always start from 0, instead of from 1. This is often the source of problems related to vectors and matrices.

(ii) CSR format

The most commonly used data structure for sparse matrices nowadays is probably the so-called compressed sparse row (CSR) format, according to Saad [15]. The compressed row storage format of a matrix $A \in \mathbb{R}^{n \times m}$ (n rows and m columns) consists of three arrays, as follows:

- 1. An integer array of row pointers of size n+1;
- 2. An integer array of column indexes of size nnz;
- 3. An array of actual matrix entries.

In FASP, we define:

```
/**

* \struct dCSRmat

* \brief Sparse matrix of REAL type in CSR format

* \brief Sparse matrix of REAL type in CSR format

* CSR Format (IA, JA, A) in REAL

* \ * \note The starting index of A is 0.

*/

typedef struct dCSRmat {
```

```
148
149
         //! row number of matrix A, m
150
151
         //! column of matrix A, n
152
153
154
155
         //! number of nonzero entries
156
157
         //! integer array of row pointers, the size is m+1
158
159
         INT *IA;
160
         //! integer array of column indexes, the size is nnz
161
162
163
164
         //! nonzero entries of A
         REAL *val;
165
166
    } dCSRmat; /**< Sparse matrix of REAL type in CSR format */
167
```

The matrix (only nonzero elements) is stored in the array val row after row, in a way that i-th row begins at val(IA(i)) and ends at val(IA(i+1)-1). In the same way, JA(IA(i)) to JA(IA(i+1)-1) will contain the column indexes of the non-zeros in row i. Thus IA is of size n+1 (number of rows in val plus one), JA and val are of size equal to the number of non-zeroes. The total number of non-zeroes is equal to IA(n+1)-1.

NOTE: When the sparse matrix A is a boolean (i.e. all entries are either 0 or 1), the actual non-zeroes are not stored because it is understood that, if it is nonzero, it could only be 1 and there is no need to store it.

The matrix in Example 3.1.1 in CSR format is represented in the following way:

• IA is of size 5 and

$$IA = \parallel 0 \parallel 3 \parallel 7 \parallel 9 \parallel 12 \parallel$$

• JA is of size IA(5) - 1 = 12

• val is of the same size as JA and

$$val = || 1. || 1.5 || 12. || 1. || 7. || 6. || 1. || 3. || 6. || 2. || 5. || 1. ||$$

Here we use double vertical bars to separate rows and single vertical bars to separate values.

NOTE: The indices in JA and entries of val does NOT have to be ordered as seen in this example. Sometimes they are sorted in ascending order in each row. More often, the diagonal entries are stored in the first position in each row and the rest are sorted in ascending order.

Below is a "non-numeric" example.

Example 3.1.2 Consider the following sparse matrix:

$$\begin{pmatrix}
a_{11} & 0 & a_{13} & 0 \\
0 & a_{22} & a_{23} & a_{24} \\
0 & a_{32} & 0 & a_{34} \\
a_{41} & a_{42} & a_{43} & 0
\end{pmatrix}$$

For this matrix, we have that the number of non-zeros nnz = 10. Furthermore, the three arrays of in the CSR format are:

$$IA = \left\| \begin{array}{c|c} 0 & 2 & 5 & 7 \end{array} \right\|,$$

$$JA = \left\| \begin{array}{c|c} 0 & 2 & 1 \end{array} \right| \left. \begin{array}{c|c} 2 & 3 & 1 \end{array} \right| \left. \begin{array}{c|c} 3 & 0 \end{array} \right| \left. \begin{array}{c|c} 1 & 2 \end{array} \right|,$$

and

$$val = || a_{11} | a_{13} || a_{22} | a_{23} | a_{24} || a_{32} | a_{34} || a_{41} | a_{42} | a_{43} ||.$$

NOTE: The CSR format presents challenges to sparse matrix-vector product mainly because of the high cache missing rate due to indirect memory access and irregular access pattern. In order to reduce the cache missing rate, we introduce an improved data format, CSRL.

(iii) CSRL format

CSRL matrix format [10] groups rows with same number of nonzeros together and improves cache hitting rate.

```
260
261
     * \struct dCSRLmat
262
      * \brief Sparse matrix of REAL type in CSRL format
263
    typedef struct dCSRLmat{
264
265
         //! number of rows
266
         INT row:
267
268
269
         //! number of cols
270
         INT col;
271
272
         //! number of nonzero entries
273
         INT nnz;
```

```
274
275
         //! number of different values in i-th row, i=0:nrows-1
276
277
         //! nz_diff[i]: the i-th different value in 'nzrow'
278
         INT *nz_diff;
279
280
         //! row index of the matrix (length-grouped): rows with same nnz are together
281
282
         INT *index;
283
         //! j in {start[i],...,start[i+1]-1} means nz_diff[i] nnz in index[j]-row
284
285
         INT *start;
286
         //! column indices of all the nonzeros
287
288
         INT * ja;
289
         //! values of all the nonzero entries
290
         REAL *val;
291
292
      dCSRLmat; /**< Sparse matrix of REAL type in CSRL format */
293
```

3.2 Block sparse matrices

For PDE applications, we often need to solve systems of partial differential equations. Many iterative methods and preconditioners could take advantages of the structure of PDE systems and improve efficiency. So we often need to use semi-structured (block) sparse data structures to store the coefficient matrix arising from PDE systems.

Depending on different applications and different solving algorithms, we can use two types of block matrices: dBSRmat (or BSR Block Compressed Sparse Row) and block_dCSRmat (CSR Block or Block of CSR matrices).

For more details as well as other specialized block matrices, readers are referred to the header file "base/include/fasp_block.h".

As an example, we consider the following matrix, which have been used in §3.1 for the CSR format. We add structure to this matrix and divide it as a 2×2 block matrix:

Example 3.2.1

$$\begin{pmatrix}
a_{11} & 0 & a_{13} & 0 \\
0 & a_{22} & a_{23} & a_{24} \\
\hline
0 & a_{32} & 0 & a_{34} \\
a_{41} & a_{42} & a_{43} & 0
\end{pmatrix}$$

(i) BSR format

This format is a standard data structure for storing block sparse matrices which has been used by the Intel MKL library.

```
24
25
    * \struct dBSRmat
26
    * \brief Block sparse row storage matrix of REAL type
27
28
     st \note This data structure is adapted from the Intel MKL library. Refer to:
    * http://software.intel.com/sites/products/documentation/hpc/mkl/lin/index.htm
29
30
31
     st \note Some of the following entries are capitalized to stress that they are
32
            for blocks!
33
34
   typedef struct dBSRmat {
35
        //! number of rows of sub-blocks in matrix A, M
36
       INT ROW;
37
38
        //! number of cols of sub-blocks in matrix A, N
39
       INT COL:
40
41
       //! number of nonzero sub-blocks in matrix A, NNZ
42
43
44
        //! dimension of each sub-block
45
        INT nb; // NOTE: for the moment, allow nb*nb full block
46
47
        //! storage manner for each sub-block
48
       INT storage_manner; // 0: row-major order, 1: column-major order
49
50
51
        //! A real array that contains the elements of the non-zero blocks of
        //! a sparse matrix. The elements are stored block-by-block in row major
52
       //! order. A non-zero block is the block that contains at least one non-zero
53
54
       //! element. All elements of non-zero blocks are stored, even if some of
55
       //! them is equal to zero. Within each nonzero block elements are stored
       //! in row-major order and the size is (NNZ*nb*nb).
56
       REAL *val;
57
58
       //! integer array of row pointers, the size is ROW+1
59
60
61
62
       //! Element i of the integer array columns is the number of the column in the
        //! block matrix that contains the i-th non-zero block. The size is NNZ.
63
64
        INT *JA;
65
   } dBSRmat; /**< Matrix of REAL type in BSR format */
```

For the matrix in Example 3.2.1, we have that the number of block rows ROW = 2, the number of block columns COL = 2, and the number of block nonzeros NNZ = 4. The block size is nb = 2.

We can choose different storage manners for storing the small blocks. Suppose that we set it to be 0, i.e. row-major format. Then the three arrays of in the BSR format are:

$$IA = \parallel 0 \parallel 8 \parallel 16 \parallel,$$

 $JA = \parallel 0 \mid 1 \parallel 0 \mid 1 \parallel,$

and

$$val = || a_{11} | 0 | 0 | a_{22} || a_{13} | 0 | a_{23} | a_{24} ||$$
$$|| 0 | a_{32} | a_{41} | a_{42} || 0 | a_{34} | a_{43} | 0 ||.$$

We immediately notice that this format might be not be the best choice for this particular matrix due to all the blocks are nonzero blocks, i.e., contain nonzero entries. However, for PDE applications, this does not usually happen.

(ii) BLC format

This format is simple and is derived from the dCSRmat data structure. The following definition explains itself.

```
68
69
     * \struct dBLCmat
70
      \brief Block REAL CSR matrix format
71
72
      \note The starting index of A is 0.
73
   typedef struct dBLCmat {
74
75
        //! row number of blocks in A, m
76
77
        INT brow;
78
79
        //! column number of blocks A, n
80
81
        //! blocks of dCSRmat, point to blocks[brow][bcol]
82
        dCSRmat **blocks;
83
84
   } dBLCmat; /**< Matrix of REAL type in Block CSR format */
85
```

3.3 I/O subroutines for sparse matrices

In FASP, we provided several functions for reading, writing, and printing different formats of sparse matrices in plain text or binary formats. These functions can be found in "base/src/BlaIO.c" and we list the available functions as follows:

```
void fasp_dcsrvec1_read (const char *filename,
468
469
                              dCSRmat
                                          *A,
470
                              dvector
                                          *b);
471
472
    void fasp_dcsrvec2_read (const char *filemat,
473
                              const char *filerhs,
474
                              dCSRmat
                                          *A.
475
                              dvector
                                          *b);
476
477
    void fasp_dcsr_read (const char *filename,
478
                          dCSRmat
479
480
    void fasp_dcoo_read (const char *filename,
481
                          dCSRmat
                                      *A);
482
    void fasp_dcoo1_read (const char *filename,
483
                           dC00mat
484
                                       *A);
485
486
    void fasp_dcoo_shift_read (const char *filename,
487
                                dCSRmat
488
    void fasp_dmtx_read (const char *filename,
489
490
                          dCSRmat
                                     *A);
491
492
    void fasp_dmtxsym_read (const char *filename,
493
                             dCSRmat
                                        *A);
494
    void fasp_dstr_read (const char *filename,
495
496
                          dSTRmat
497
    void fasp_dbsr_read (const char *filename,
498
499
                          dBSRmat
500
    void fasp_dvecind_read (const char *filename,
501
502
                             dvector
                                         *b);
503
504
    void fasp_dvec_read (const char *filename,
505
                          dvector
                                    *b);
506
507
    void fasp_ivecind_read (const char *filename,
508
                             ivector
                                         *b);
509
510
    void fasp_ivec_read (const char *filename,
511
                          ivector
                                      *b);
512
513
    void fasp_dcsrvec1_write (const char *filename,
514
                               dCSRmat
                                           *A.
515
                               dvector
                                           *b);
517
    void fasp_dcsrvec2_write (const char *filemat,
                               const char *filerhs,
518
519
                               dCSRmat
                                           *A,
520
                              dvector *b);
```

```
521
522
    void fasp_dcoo_write (const char *filename,
                           dCSRmat
523
                                       *A);
524
    void fasp_dstr_write (const char *filename,
525
526
527
528
    void fasp_dbsr_write (const char *filename,
529
                           dBSRmat *A);
530
    void fasp_dvec_write (const char *filename,
531
532
                           dvector *vec);
533
    void fasp_dvecind_write (const char *filename,
534
535
                             dvector
536
537
    void fasp_ivec_write (const char *filename,
                           ivector
538
                                       *vec);
539
540
    void fasp_dvec_print (const INT n,
                           dvector *u);
541
542
    void fasp_ivec_print (const INT n,
543
                           ivector *u);
544
545
    void fasp_dcsr_print (const dCSRmat *A);
546
547
    void fasp_dcoo_print (const dCOOmat *A);
548
549
    void fasp_dbsr_print (const dBSRmat *A);
550
551
    void fasp_dbsr_write_coo (const char *filename,
552
553
                              const dBSRmat *A);
554
555
    void fasp_dcsr_write_coo (const char *filename,
556
                              const dCSRmat *A);
557
    void fasp_dstr_print (const dSTRmat *A);
558
559
560
    void fasp_matrix_read (const char *filename,
561
                           void
562
    void fasp_matrix_read_bin (const char *filename,
563
564
                                void
                                           *A);
565
566
    void fasp_matrix_write (const char *filename,
567
                             void
568
                             const INT flag);
569
    void fasp_vector_read (const char *filerhs,
570
571
                            void
                                    *b);
572
    void fasp_vector_write (const char *filerhs,
```

NOTE: The above function declarations are taken from "base/include/fasp_functs.h". This header file is automatically generated based on the source codes. Users are discouraged from changing it by hand; their changes may be lost.

3.4 Sparse matrix-vector multiplication

The matrix-vector multiplication: y = Ax can be performed in the following simple way:

```
1
 2
     * \fn void fasp_blas_dcsr_mxv (dCSRmat *A, REAL *x, REAL *y)
 3
 4
      * \brief Matrix-vector multiplication y = A*x
 5
      * \param A Pointer to dCSRmat matrix A
 6
 7
      * \param x Pointer to array x
 8
      * \param y Pointer to array y
 9
     * \author Chensong Zhang
10
11
      * \date 07/01/2009
12
13
    void fasp_blas_dcsr_mxv (dCSRmat *A,
14
                                   REAL *x,
15
                                   REAL *y)
16
17
         const INT
                      \mathtt{m} = \mathtt{A} - \!\!\! > \!\!\! \mathtt{row} \; ;
18
         const INT *ia = A->IA, *ja = A->JA;
         \begin{array}{lll} {\tt const} & {\tt REAL} & {\tt *aj} & = & {\tt A-\!\!>\!\! val} \; ; \end{array}
19
20
         INT i, k, beg, end;
21
         register REAL tmp;
22
23
         for (i=0; i< m; ++i)
^{24}
25
              tmp = 0.0;
26
              beg = ia[i]; end = ia[i+1];
27
              for (k=beg; k<end; ++k) tmp += aj[k]*x[ja[k]];
28
              y[i] = tmp;
         }
29
30
```

This is only a simple example for sparse matrix-vector multiplication (SpMV) kernel. Since we need many types of sparse matrices, there are various of versions of SpMV for different data structures. See the Reference Manual for more details.

3.5 Iterative methods

In FASP, there are a couple of standard preconditioned iterative methods [15] implemented, including preconditioned CG, BiCGstab, GMRES, Variable Restarting GMRES, Flexible GMRES, etc. In this section, we use the CSR matrix format as example to introduce how to call these iterative methods. To learn more details, we refer to the Reference Manual.

We first show the abstract interface for the iterative methods. The following code segment is taken from "base/src/SolCSR.c":

```
37
     st \fn INT fasp_solver_dcsr_itsolver (dCSRmat stA, dvector stb, dvector stx,
38
                                            precond *pc, ITS_param *itparam)
39
40
      \brief Solve Ax=b by preconditioned Krylov methods for CSR matrices
41
42
43
      \note This is an abstract interface for iterative methods.
44
      \param A
45
                       Pointer to the coeff matrix in dCSRmat format
      \param b
                       Pointer to the right hand side in dvector format
46
47
      \param x
                       Pointer to the approx solution in dvector format
48
      \param pc
                       Pointer to the preconditioning action
     * \param itparam Pointer to parameters for iterative solvers
49
50
                       Iteration number if converges; ERROR otherwise.
51
     * \return
52
53
     * \author Chensong Zhang
      \date 09/25/2009
54
55
     * Modified by Chunsheng Feng on 03/04/2016: add VBiCGstab solver
56
57
58
   INT fasp_solver_dcsr_itsolver (dCSRmat
                                                *A,
59
                                    dvector
                                                *b.
60
                                    dvector
                                                *X,
61
                                    precond
                                                *pc.
62
                                    ITS_param *itparam)
```

The names of the input arguments explain themselves mostly and they are explained in the Reference Manual in detail.

We briefly discuss how to call this function; and, once you understand PCG, you can easily call other iterative methods.

```
// ILU setup for whole matrix
```

```
490
         ILU_data LU;
491
         if ( (status = fasp_ilu_dcsr_setup(A, &LU, iluparam)) < 0 ) goto FINISHED;
492
        // check iludata
493
         if ( (status = fasp_mem_iludata_check(&LU)) < 0 ) goto FINISHED;
494
495
496
        // set preconditioner
497
        precond pc;
498
        pc.data = \&LU;
499
        pc.fct = fasp_precond_ilu;
500
501
         // call iterative solver
502
         status = fasp_solver_dcsr_itsolver(A, b, x, &pc, itparam);
```

Now we explain this code segment a little bit:

- Line 490–491 performs the setup phase for ILU method. The particular type of ILU method is determined by "iluparam"; see §2.6. Line 7 performs a simple memory check for ILU.
- Line 497–499 defines the preconditioner data structure "pc", which contains two parts: one is the actual preconditioning action "pc.fct", the other is the auxiliary data which is needed to perform the preconditioning action "pc.data".
- Line 502 calls iterative methods. "A" is the matrix in dCSRmat format; "b" and "x" are the right-hand side and the solution vectors, respectively. Similar to ILU setup, the type of iterative methods is determined by "itparam".

Apparently, we should now explain the data structure "itparam".

```
/**
  * \struct ITS_param
  * \brief Parameters passed to iterative solvers
  */
typedef struct {

    SHORT itsolver_type; /**< solver type: see message.h */
    SHORT precond_type; /**< preconditioner type: see message.h */
    SHORT stop_type; /**< stopping criteria type */
    INT maxit; /**< max number of iterations */
    REAL tol; /**< convergence tolerance */
    INT restart; /**< number of steps for restarting: for GMRES etc */
    SHORT print_level; /**< print level: 0--10 */
} ITS_param; /**< Parameters for iterative solvers */</pre>
```

Possible "itsolver_type" includes:

```
/**
    * \brief Definition of solver types for iterative methods
```

```
*/
//-----
#define SOLVER_CG 1 /**< Conjugate Gradient */
#define SOLVER_BiCGstab
                                2 /**< Bi-Conjugate Gradient Stabilized */</pre>
#define SOLVER_VBiCGstab
                                 9 /**< VBi-Conjugate Gradient Stabilized */
#define SOLVER_MinRes
                                3 /**< Minimal Residual */
#define SOLVER_GMRES
                                4 /**< Generalized Minimal Residual */
#define SOLVER_VGMRES
                                5 /**< Variable Restarting GMRES */
#define SOLVER_VFGMRES
                               6 /**< Variable Restarting Flexible GMRES */
#define SOLVER_GCG 7 /**< Generalized Conjugate Gradient */
#define SOLVER_GCR 8 /**< Generalized Conjugate Residual */
#define SOLVER_SCG 11 /**< Conjugate Gradient with safety net */
#define SOLVER_SBiCGstab 12 /**< BiCGstab with safety net */
#define SOLVER_SMinRes 13 /**< MinRes with safety net */
#define SOLVER_SGMRES
                              14 /**< GMRes with safety net */
#define SOLVER_SVGMRES
                               15 /**< Variable-restart GMRES with safety net */
#define SOLVER.SVFGMRES
#define SOLVER.SGCG 16 /**< Variable-restart FGMRES
17 /**< GCG with safety net */</pre>
                               16 /**< Variable-restart FGMRES with safety net */
#define SOLVER.AMG 21 /**< AMG as an iterative solver */
#define SOLVER.FMG 22 /**< Full AMG as an solver */
```

3.6 Algebraic multigrid

The classical algebraic multigrid method [14] is an important component in many of our auxiliary space preconditioners. Because of its user-friendly and scalability, AMG becomes increasingly popular in scientific and engineering computing, especially when GMG is difficult or not possible to be applied. Various of new AMG techniques [17, 18, 4, 7, 5, 9, 6, 20, 3, 11, 8] have emerged in recent years.

The following code segment is part of "base/src/SolAMG.c" and it is a good example which shows how to call different AMG methods (classical AMG, smoothed aggregation, un-smoothed aggregation) and different multilevel iterative methods (V-cycle, W-cycle, AMLI-cycle, Nonlinear AMLI-cycle, etc).

```
void fasp_solver_amg (const dCSRmat *A,
46
47
                                    const dvector *b,
48
                                    dvector
                                                          *X,
49
                                    AMG_param
                                                          *param)
50
51
          const SHORT max_levels = param->max_levels;
52
          const SHORT prtlvl = param->print_level;
53
          \begin{array}{lll} {\tt const} & {\tt SHORT} & {\tt amg\_type} & = & {\tt param-}{\!>} {\tt AMG\_type} \; ; \end{array}
           {\color{red} \texttt{const}} \  \, \texttt{SHORT} \qquad \texttt{cycle\_type} \  \, = \, \texttt{param-}\!\!>\!\! \texttt{cycle\_type} \, \, ;
54
55
           const INT
                              nnz = A->nnz, m = A->row, n = A->col;
56
```

```
// local variables
57
58
         SHORT
                        status;
59
         AMG_data *
                         mgl = fasp_amg_data_create(max_levels);
         REAL
                         AMG_start, AMG_end;
60
61
     #if DEBUG_MODE > 0
62
         printf("### DEBUG: %s ..... [Start]\n", __FUNCTION__);
63
64
65
         if ( prtlvl > PRINT_NONE ) fasp_gettime(&AMG_start);
66
67
68
         // check matrix data
69
         fasp_check_dCSRmat(A);
70
         // Step 0: initialize mgl[0] with A, b and x
71
         mgl[0].A = fasp_dcsr_create(m, n, nnz);
72
         {\tt fasp\_dcsr\_cp}\left({\tt A}\,,\,\,\&{\tt mgl}\left[\,0\,\right].\,{\tt A}\,\right);
73
74
75
         mgl[0].b = fasp_dvec_create(n);
         fasp_dvec_cp(b, \&mgl[0].b);
76
77
78
         mgl[0].x = fasp_dvec_create(n);
79
         fasp_dvec_cp(x, \&mgl[0].x);
80
         // Step 1: AMG setup phase
81
         switch (amg_type) {
82
83
              case SA_AMG: // Smoothed Aggregation AMG setup
84
                  if ( prtlvl > PRINT_NONE ) printf("\nCalling SA AMG ...\n");
85
                  {\tt status} \ = \ {\tt fasp\_amg\_setup\_sa(mgl\,, param)} \, ; \ \ {\tt break} \, ;
86
87
              case UA_AMG: // Unsmoothed Aggregation AMG setup
88
89
                  if ( prtlvl > PRINT_NONE ) printf("\nCalling UA AMG ...\n");
                  status = fasp_amg_setup_ua(mgl, param); break;
90
91
              default: // Classical AMG setup
92
                  if ( prtlvl > PRINT_NONE ) printf("\nCalling classical AMG ...\n");
93
                  {\tt status} = {\tt fasp\_amg\_setup\_rs(mgl\,, param)}\,; \ {\tt break}\,;
94
95
         }
96
97
98
         // Step 2: AMG solve phase
         if ( status == FASP_SUCCESS ) { // call a multilevel cycle
99
100
101
              switch (cycle_type) {
102
103
                  case AMLI_CYCLE: // AMLI-cycle
104
                       fasp_amg_solve_amli(mgl, param); break;
105
106
                  case NL_AMLI_CYCLE: // Nonlinear AMLI-cycle
                       fasp_amg_solve_namli(mgl, param); break;
107
108
109
                  default: // V,W-cycles (determined by param)
```

```
110
                      fasp_amg_solve(mgl, param); break;
111
112
             }
113
             fasp_dvec_cp(\&mgl[0].x, x);
114
115
         }
116
117
118
         else { // call a backup solver
119
             if ( prtlvl > PRINT_MIN ) {
120
121
                  printf("### WARNING: AMG setup failed!\n");
122
                 printf("### WARNING: Use a backup solver instead!\n");
123
124
             fasp_solver_dcsr_spgmres (A, b, x, NULL, param->tol, param->maxit,
                                          20, 1, prtlv1);
125
126
         }
127
128
         // clean-up memory
129
         fasp_amg_data_free(mgl, param);
130
131
         // print out CPU time if needed
132
         if ( prtlvl > PRINT_NONE ) {
133
             fasp_gettime(\&AMG_end);
134
             print_cputime("AMG totally", AMG_end - AMG_start);
135
136
         }
137
     #if DEBUG_MODE > 0
138
         printf("### DEBUG: %s ..... [Finish]\n", __FUNCTION__);
139
    #endif
140
141
142
         return;
    }
143
```

The code above is very simple and we only wish to point out that:

- Line 51-54 reads some of the parameters from "AMG_param", which can be set in an input file; see §2.6.
- Line 72–79 initializes the "AMG_data" with a copy of the coefficient matrix, the right-hand side, and the initial solution (it will store the final solution eventually).
- Line 82–96 calls three different AMG setup methods, determined by "amg_type".
- Line 101–112 calls three different multilevel iterative methods, determined by "cycle_type".

Parameters for AMG

There are a couple of controlling parameters for algebraic multigrid methods in FASP. Basically, there are four types of parameters for AMG—They control multilevel iterations, smoothing, classical

AMG setup, and aggregation AMG setup. The following is a sample from "test/ini/input.dat" and a brief explanation of each parameter is given.

```
-%
                                                     %
56
    \% parameters for multilevel iteration
    %-
                                                     -%
57
58
                              = C
                                        \% C classic AMG
59
    AMG_type
                                        \% SA smoothed aggregation
60
                                        \% UA unsmoothed aggregation
61
62
    AMG_cycle_type
                                        % V V-cycle | W W-cycle
63
                                        % A AMLI-cycle | NA Nonlinear AMLI-cycleA
64
    AMG_tol
                              = 1e-6
                                        \% tolerance for AMG
                                        \% number of AMG iterations
    AMG_maxit
                              = 1
65
    AMG_levels
                              = 20
                                        \% max number of levels
66
67
    AMG_coarse_dof
                              = 500
                                        \% max number of coarse degrees of freedom
    AMG_coarse_solver
                              = 0
                                        \% coarsest solver: 0 iterative |
68
69
                                        \% 31 SuperLU | 32 UMFPack | 33 MUMPS
70
    AMG_coarse_scaling
                              = OFF
                                        \% switch of scaling of the coarse grid correction
71
    AMG_amli_degree
                              = 2
                                        \% degree of the polynomial used by AMLI cycle
    AMG_nl_amli_krylov_type = 6
                                        \% Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCG
72
73
                                                     -%
74
                                                     %
    \% parameters for AMG smoothing
75
76
                                                     -%
77
                                        \% GS | JACOBI | SGS SOR | SSOR |
                              = GS
78
    AMG_smoother
                                        \% GSOR | SGSOR | POLY | L1DIAG | CG
79
    AMG_smooth_order
                              = CF
                                        \% NO: natural order | CF: CF order
80
    AMG_ILU_levels
                              = 0
                                        \% number of levels using ILU smoother
81
    AMG_SWZ_levels
                              = 0
                                        \% number of levels using Schwarz smoother
82
83
    AMG_relaxation
                              = 1.0
                                        \% relaxation parameter for SOR smoother
    {\tt AMG\_polynomial\_degree}
                              = 3
                                        \% degree of the polynomial smoother
84
                                        \% number of presmoothing sweeps
    AMG_presmooth_iter
                              = 1
85
    AMG_postsmooth_iter
                              = 1
                                        \% number of postsmoothing sweeps
86
87
                                                     -%
88
                                                     %
89
    \% parameters for classical AMG SETUP
                                                     -%
90
91
                              = 1
                                        \% 1 Modified RS
92
    AMG_coarsening_type
                                        \% 2 Mofified RS for positive off-diags
93
                                        \% 3 Compatible Relaxation
94
                                        \% 4 Aggressive
95
96
    AMG_interpolation_type
                              = 1
                                        \% 1 Direct | 2 Standard | 3 Energy-min
97
    AMG_strong_threshold
                              = 0.3
                                        % Strong threshold
98
    {\tt AMG\_truncation\_threshold} = 0.1
                                        \% Truncation threshold
99
    AMG_max_row_sum
                              = 0.9
                                        \% Max row sum
100
101
                                                     -%
                                                     %
102
    \% parameters for aggregation—type AMG SETUP
```

```
104 |
105 AMG_aggregation_type = 2  % 1 Matching | 2 VMB
106 AMG_pair_number = 2  % Number of pairs in matching
107 AMG_strong_coupled = 0.08  % Strong coupled threshold
108 AMG_max_aggregation = 20  % Max size of aggregations
109 AMG_tentative_smooth = 0.67  % Smoothing factor for tentative prolongation
110 AMG_smooth_filter = 0FF  % Switch for filtered matrix for smoothing
111 AMG_quality_bound = 8.0  % quality of aggregation: 8.0 sysmm | 10.0 unsymm
```

NOTE: Here we can not discuss the details of these parameters as a full discussion requires more understand of the underlying algorithms which we have completely omitted. So to learn more about, we refer to the Reference Manual.

Chapter 4

More advanced features

In this chapter, we discuss a few more advanced features of FASP. We will discuss parallel versions of FASP and its build-in features for debugging purposes. These features will be helpful for people who would like to develop on the top of FASP. For users who only wish to call a few standard solvers, they can skip this chapter.

4.1 Enabling OpenMP

OpenMP¹ (Open Multiprocessing) is an API that supports multi-platform shared memory multi-processing programming in C, C++, and Fortran, on most processor architectures and operating systems. It consists of a set of compiler directives, library routines, and environment variables that influence run-time behavior. Some preliminary OpenMP support has been included since the very beginning of FASP. We consistently improves and expands OpenMP support as multiprocessor architectures become the dominant desktop computing environment.

NOTE: By default, OpenMP is disabled in FASP. In order to turn it on, you need to modify FASP.mk slightly as follows.

To enable OpenMP support in FASP, you can simply use the config option

```
$ make config openmp=yes
```

If you use OpenMP very often and do not want type in this extra command-line option, you need to uncomment one line in "FASP.mk". If you do not have "FASP.mk" file, just copy "FASP.mk.example" to "FASP.mk". Then set "openmp" to "yes" on line 44 "FASP.mk":

```
37 #
```

¹Official website: http://openmp.org/

```
# You may use multithread version after you enable OpenMP support. To
# setup the environment, you need
# >> export OMP_NUM_THREADS=4 (for bash)
# >> setenv OMP_NUM_THREADS 4 (for tcsh)
# If you want to compile with OpenMP support, uncomment the next line:
# # openmp=yes
# # openmp=yes
```

After you build FASP with "openmp=yes", OpenMP is turned on and the number of threads is determined by the environment variable OMP_NUM_THREADS. For example, to use 8 threads in sh/bash, you need to set:

```
$ export OMP_NUM_THREADS=8
```

4.2 Predefined constants

FASP has many predefined constants used in the source files. Using these macros makes the source codes more readable. These constants are defined in "base/include/fasp_const.h" and a printout of this file is below:

```
/*! \file fasp_const.h
1
2
       \brief Definition of all kinds of FASP constants, including error messages,
3
              solver types, etc.
4
5
6
      Copyright (C) 2009-2017 by the FASP team. All rights reserved.
7
    st Released under the terms of the GNU Lesser General Public License 3.0 or later.
8
9
10
       \warning This is for internal use only. Do NOT change!
11
12
    */
13
                                       /*-- allow multiple inclusions --*/
   #ifndef __FASP_CONST__
14
   #define __FASP_CONST__
15
16
17
   * \brief Definition of return status and error messages
18
19
   #define FASP_SUCCESS
20
                                  0 /**< return from function successfully */</pre>
21
22
   #define ERROR_OPEN_FILE
                                 -10 /**< fail to open a file */
23
   #define ERROR_WRONG_FILE
                                 -11 /**< input contains wrong format */
24
   #define ERROR_INPUT_PAR
                                 -13 /**< wrong input argument */
   #define ERROR_REGRESS
                                 -14 /**< regression test fail */
25
                                  -15 /**< wrong problem size */
   #define ERROR_MAT_SIZE
  #define ERROR_NUM_BLOCKS -18 /**< wrong number of blocks */
```

```
#define ERROR_MISC -19 /**< other error */
29
  //----
  |//
|#define ERROR_ALLOC_MEM -20 /**< fail to allocate memory */
30
31 #define ERROR_DATA_STRUCTURE -21 /**< problem with data structures */
32 #define ERROR_DATA_ZERODIAG -22 /**< matrix has zero diagonal entries */
   #define ERROR_DUMMY_VAR -23 /**< unexpected input data */
33
34
   #define ERROR_AMG_INTERP_TYPE -30 /**< unknown interpolation type */
35
   #define ERROR_AMG_SMOOTH_TYPE -31 /**< unknown smoother type */
37
   #define ERROR_AMG_COARSE_TYPE -32 /**< unknown coarsening type */
   #define ERROR_AMG_COARSEING -33 /**< coarsening step failed to complete */
38
39
   #define ERROR_SOLVER_TYPE -40 /**< unknown solver type */
40
   #define ERROR_SOLVER_PRECTYPE -41 /**< unknown precond type */
41
42 #define ERROR_SOLVER_STAG -42 /**< solver stagnates */
43 #define ERROR_SOLVER_SOLSTAG -43 /**< solver's solution is too small */
44 #define ERROR_SOLVER_TOLSMALL -44 /**< solver's tolerance is too small */
45 #define ERROR_SOLVER_ILUSETUP -45 /**< ILU setup error */
   #define ERROR_SOLVER_MISC -46 /**< misc solver error during run time */
   #define ERROR_SOLVER_MAXIT -48 /**< maximal iteration number exceeded */
47
   #define ERROR_SOLVER_EXIT -49 /**< solver does not quit successfully */
48
49
   #define ERROR_QUAD_TYPE -60 /**< unknown quadrature type */
#define ERROR_QUAD_DIM -61 /**< unsupported quadrature dim */
50
51
52
   //----
   #define ERROR_LIC_TYPE -80 /**< wrong license type */
53
54
   #define ERROR_UNKNOWN -99 /**< an unknown error type */
55
56
57
   * \brief Definition of logic type
58
59
60
   #define TRUE
                                  1 /**< logic TRUE */
   #define FALSE
                                   0 /**< logic FALSE */
61
62
63
   * \brief Definition of switch
64
65
   #define ON
                                   1 /**< turn on certain parameter */</pre>
66
   #define OFF
                                   0 /**< turn off certain parameter */</pre>
67
68
69
   * \brief Print level for all subroutines -- not including DEBUG output
70
71
72
   #define PRINT_NONE
                                  0 /**< silent: no printout at all */</pre>
73
   #define PRINT_MIN
                                   1 /**< quiet: print error, important warnings */</pre>
74 #define PRINT SOME
                                  2 /**< some: print less important warnings */</pre>
75
  #define PRINT_MORE
                                  4 /**< more: print some useful debug info */
76
   #define PRINT_MOST
                                  8 /**< most: maximal printouts, no files */
77 #define PRINT_ALL
                                 10 /**< all: all printouts, including files */
78
79
80 * \brief Definition of matrix format
```

```
**/
   #define MAT_FREE 0 /**< matrix-free format: only mxv action */
 83 //-----
                       1 /**< compressed sparse row */
 84 #define MAT CSR
                               2 /**< block-wise compressed sparse row */</pre>
 85 #define MAT_BSR
                               3 /**< structured sparse matrix */</pre>
 86 #define MAT_STR
   #define MAT_CSRL
                               6 /**< modified CSR to reduce cache missing */
 87
                             7 /**< symmetric CSR format */
 88
   #define MAT_SymCSR
   #define MAT_BLC
                                8 /**< block CSR matrix */
 90
   //----
        For bordered systems in reservoir simulation
 91
 92
 93
    #define MAT_bCSR
                    11 /**< block CSR/CSR matrix == 2*2 BLC matrix */
   #define MAT_bBSR
                               12 /**< block BSR/CSR matrix */
 94
   #define MAT_bSTR
                               13 /** block STR/CSR matrix */
 95
 96
 97
    * \brief Definition of solver types for iterative methods
 98
 99
    #define SOLVER_DEFAULT 0 /**< Use default solver in FASP */
100
101
#define SOLVER_CG 1 /**< Conjugate Gradient */
103 #define SOLVER_BiCGstab 2 /**< Bi-Conjugate Gradient Stabilized */
104 #define SOLVER_VBiCGstab 9 /**< VBi-Conjugate Gradient Stabilized */
    #define SOLVER_MinRes
                               3 /**< Minimal Residual */</pre>
105
                                4 /**< Generalized Minimal Residual */
    #define SOLVER_GMRES
                               5 /** Variable Restarting GMRES */
107 #define SOLVER_VGMRES
                               6 /**< Variable Restarting Flexible GMRES */
108 #define SOLVER_VFGMRES
109 #define SOLVER_GCG
                               7 /** Generalized Conjugate Gradient */
#define SOLVER_GCR 8 /**< Generalized Conjugate Residual */
111 //-----
//-----
119
    #define SOLVER_AMG 21 /**< AMG as an iterative solver */
#define SOLVER_FMG 22 /**< Full AMG as an solver */
120
   #define SOLVER_FMG
121
122 //----
#define SOLVER_SUPERLU 31 /**< Direct Solver: SuperLU */
124 #define SOLVER_UMFPACK
                              32 /** Direct Solver: UMFPack */
                              33 /**< Direct Solver: MUMPS */
125
    #define SOLVER_MUMPS
    #define SOLVER_PARDISO
126
                               34 /**< Direct Solver: PARDISO */
127
128
    st \brief Definition of iterative solver stopping criteria types
130 | */
131 #define STOP_REL_RES
                               1 /**< relative residual ||r||/||b|| */
    132
| #define STOP_MOD_REL_RES | 3 | /**< modified relative residual ||r||/||x|| */
```

```
134
135
136
    * \brief Definition of preconditioner type for iterative methods
137 */
                                      0 /**< with no precond */
138 #define PREC_NULL
139 #define PREC_DIAG
                                      1 /**< with diagonal precond */</pre>
#define PREC_DIAG

#define PREC_AMG

#define PREC_FMG

#define PREC_ILU
                                      2 /**< with AMG precond */
                                     3 /**< with full AMG precond */</pre>
                                      4 /**< with ILU precond */
#define PREC_SCHWARZ 5 /**< with Schwarz preconditioner */
144
145
146
    * \brief Type of ILU methods
147 */
                                      1 /**< ILUk */
148 #define ILUk
149 #define ILUt
                                      2 /**< ILUt */
150 #define ILUtp
                                      3 /**< ILUtp */
151
152
153
    * \brief Type of Schwarz smoother
154
#define SCHWARZ_FORWARD 1 /**< Forward ordering */
156 #define SCHWARZ_BACKWARD 2 /**< Backward ordering */
157 #define SCHWARZ_SYMMETRIC 3 /**< Symmetric smoother */
158
159
160
    * \brief Definition of AMG types
161 */
162 #define CLASSIC_AMG
                                     1 /**< classic AMG */
#define SA_AMG

#define UA AMG
                                      2 /**< smoothed aggregation AMG */</pre>
                                      3 /**< unsmoothed aggregation AMG */</pre>
164 #define UA_AMG
165
166
    *\ \brief Definition of aggregation types
167
168
#define PAIRWISE 1 /**< pairwise aggregation */
170 #define VMB
                                      2 /**< VMB aggregation */
171
172
173
     * \brief Definition of cycle types
174 */
#define V_CYCLE

#define W_CYCLE

#define AMLI_CYCLE

#define NL_AMLI_CYCLE
                                      1 /**< V-cycle */
                                      2 /**< W-cycle */
                                      3 /**< AMLI-cycle */
                                      4 /** Nonlinear AMLI-cycle */
179
180 /**
181 * \brief Definition of standard smoother types
#define SMOOTHER_GS 2 /**< Gauss-Seidel smoothe
185 #define SMOOTHER_SGS 3 /**< Symmetric Gauss-Seid
186 #define SMOOTHER_CG 4 /**< CG as a smoother */
                                      2 /**< Gauss-Seidel smoother */
                                      3 /**< Symmetric Gauss-Seidel smoother */</pre>
```

```
187 #define SMOOTHER_SOR 5 /**< SOR smoother */
#define SMOOTHER_SSOR 6 /**< SSOR smoother */
189 #define SMOOTHER_GSOR
                                 7 /**< GS + SOR smoother */
189 #define SMOOTHER_SGSOR
                                 8 /**< SGS + SSOR smoother */
9 /**< Polynomial smoother */
191 #define SMOOTHER_POLY
192 #define SMOOTHER_L1DIAG
                                10 /**< L1 norm diagonal scaling smoother */
193
194
   st \brief Definition of specialized smoother types
196
   #define SMOOTHER_BLKOIL 11 /**< Used in monolithic AMG for black-oil */
#define SMOOTHER_SPETEN 19 /**< Used in monolithic AMG for black-oil */
197
198
199
200
   * \brief Definition of coarsening types
201
203 #define COARSE RS
                                 1 /**< Classical */
204 #define COARSE_RSP
                                 2 /**< Classical, with positive offdiags */
                                 3 /**< Compatible relaxation */</pre>
205 #define COARSE_CR
206 #define COARSE_AC
                                 4 /**< Aggressive coarsening */
207 #define COARSE_MIS
                                 5 /**< Aggressive coarsening based on MIS */
208
209
    * \brief Definition of interpolation types
210
211
213 #define INTERP_STD
                                 2 /**< Standard interpolation */</pre>
214 #define INTERP_ENG
                                 3 /**< Energy minimization interpolation */</pre>
215 #define INTERP_EXT
                                 6 /**< Extended interpolation */
216
217 /**
    * \brief Type of vertices (DOFs) for coarsening
218
219
220 #define GOPT
                                 -5 /**< Cannot fit in aggregates */
                                 -1 /**< Undetermined points */
221 #define UNPT
222 #define FGPT
                                 0 /**< Fine grid points */</pre>
223 #define CGPT
                                 1 /**< Coarse grid points */
224 #define ISPT
                                 2 /**< Isolated points */
225
226
227 * \brief Definition of smoothing order
228 */
229 #define NO_ORDER
                                 0 /**< Natural order smoothing */</pre>
230 #define CF_ORDER
231 #define ILU_MC_OMP
                                 1 /**< C/F order smoothing */</pre>
                                 1 /**< Multi-colors Parallel smoothing */
232
233
234
   * \brief Type of ordering for smoothers
236 #define USERDEFINED
                                 0 /**< User defined order */</pre>
237 #define CPFIRST
                                 1 /**< C-points first order */</pre>
                                 -1 /**< F-points first order */
238 #define FPFIRST
239 #define ASCEND 12 /**< Ascending order */
```

```
240
    #define DESCEND
                                   21 /**< Descending order */
241
242
243
    * \brief Some global constants
244
245
    #define BIGREAL
                                1e+20 /**< A large real number */
                                       /**< A small real number */
    #define SMALLREAL
                                1e-20
246
    #define SMALLREAL2
247
                                1e-40 /**< An extremely small real number */
248
    #define MAX_REFINE_LVL
                                 20 /**< Maximal refinement level */
249
    #define MAX_AMG_LVL
                                   20 /**< Maximal AMG coarsening level */
    #define MIN_CDOF
                                   20 /**< Minimal number of coarsest variables */
250
251
    #define MIN_CRATE
                                  0.9 /**< Minimal coarsening ratio */
252
    #define MAX_CRATE
                                 20.0
                                       /**< Maximal coarsening ratio */
                                  20 /**< Maximal restarting number */
    #define MAX_RESTART
253
254
    #define MAX_STAG
                                   20 /**< Maximal number of stagnation times */
                                 1e-4 /**< Stagnation tolerance = tol*STAGRATIO */</pre>
255
    #define STAG_RATIO
    #define OPENMP_HOLDS
                                 2000 /**< Smallest size for OpenMP version */
256
257
258
    #endif
                                        /* end if for __FASP_CONST__ */
259
260
261
                End of File
262
```

4.3 Debugging and how to enable it

NOTE: The default FSP build is a RELEASE version (/03 or equivalent compiler options are enabled) and such version is compiled with optimization and no warnings are displayed during the build. How to build the FASP library with debugging enabled is described below.

There is a built-in debug feature which is intended to help developers and users to locate malfunctions and bugs in FASP (and hopefully fix them). In order to turn this feature on, you need to add the debug option during the config stage by

```
$ make config debug=all
```

When this debug feature is turned on, there will be a lot more information printed when you run FASP. If you just want to enable the debugging and warnings during the compile stage, you can do so by using

```
$ make config debug=yes
```

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