FASP User Guide

Chunsheng Feng, Xiaozhe Hu, Zheng Li, Jinchao Xu, Chen-Song Zhang, Hongxuan Zhang, Ludmil Zikatanov

Contents

C	Contents						
1	Inti	roduction	3				
	1.1	General description	3				
	1.2	Roadmap: from basics to complex applications	4				
	1.3	How to use this guide	4				
	1.4	How to obtain FASP	4				
	1.5	Building and installing the FASP library and examples	6				
	1.6	Linking your own project with FASP	11				
2	A b	A brief tutorial					
	2.1	Example 1: An AMG solver for the Poisson equation	15				
	2.2	Example 2: Conjugate gradient without preconditioning	21				
	2.3	Example 3: Conjugate gradient with preconditioning	24				
	2.4	Example 4: An GMG solver for the Poisson equation	29				
	2.5	Example 5: Block ILU preconditioner	32				
	2.6	How to change parameters for solvers/preconditioners	35				
3	Dat	Data structures and basic usage					
	3.1	Vectors and sparse matrices	41				
	3.2	Block sparse matrices	46				
	3.3	I/O subroutines for sparse matrices	48				
	3.4	Sparse matrix-vector multiplication	51				
	3.5	Iterative methods	52				
	3.6	Algebraic multigrid	54				
4	Mo	re advanced features	59				
	4.1	An OpenMP example	59				
	4.2	Predefined constants	60				

2	CONTENTS
4.3	Debugging and how to enable it
Bibliog	graphy 67

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 are:

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

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).

LICENSING: This software is free software distributed under the Lesser General Public License or LGPL, version 3.0 or any later versions. This software distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU Lesser General Public License http://www.gnu.org/licenses/ for more details.

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

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 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.

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

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:

```
"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

```
<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/
```

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.

```
"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.

FASP on Linux or Mac OS X

To build the FASP library for these operating systems. Open a terminal window, wehre 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).

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

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:

$ make config  # Configure the building environment
$ make config CC=gcc  # Configure with a specific C compiler
$ make config debug=yes  # Configure with compiler debug options ON
$ make config debug=all  # Configure with FASP internal debug options ON
$ 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")
                     # Install FASP library and header files
$ make install
# Remove the files installed by "make install"
$ make uninstall
                      # Generate function declarations automatically
$ make headers
$ make docs
                      # Generate the FASP documentation with Doxygen
$ make clean
                      # Remove obj files but retain configuration options
$ make distclean
                     # Remove build directory and cleans test & tutorial
$ make version
                      # Show version information
$ make help
                      # Show this screen
```

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 2008 (VS08) distribution and a VS10 distribution of FASP for Windows users. For example, you can just open "faspsolver/vs08/faspsolver-vs08.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.

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.

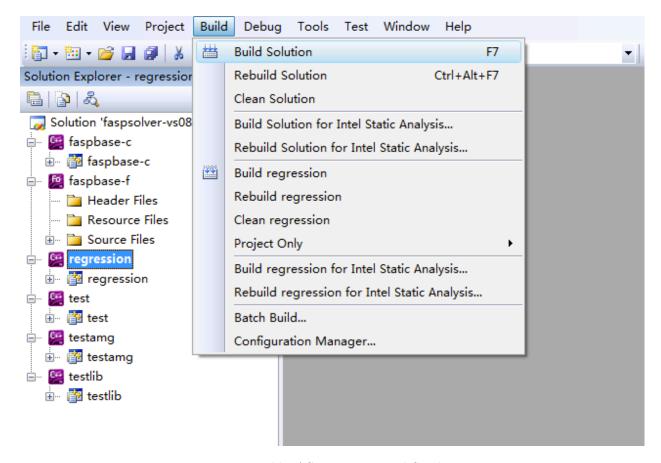


Figure 1.1: Build FASP using Visual Studio 2008.

If you are using other versions of Visual Studio (like VS05 or VS12), we advise NOT to convert the "VS08" 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

|--|

FASP	FAST AUXILIARY SPACE PRECONDITION Installation script	IING
Quit Config Install HTML docs	s Headers Uninstall	Help
Verbose output ?	Yes O No	
Build shared library ?	Yes O No	
Use Doxygen GUI (if found)?	Yes No	
Build with OpenMP support ?	Yes No	
Build with UMFPACK support ?	Yes O No	
Build type	Oebug Release	
The Debug build type assumes -g as a cortype assumes -O3 flag. Aditional compiler below.		
C flags		
F flags		
CXX flags		
Specify the path to SUITESPARSE (option use specific UMFPACK).	nal, use it when you want to	
SUITESPARSE		

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

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".

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):

```
8
9
   fasp_prefix = not-defined-yet
10
11 | fasp_library = not-defined-yet
12 CC = not-defined-yet
13 FC = not-defined-yet
   CXX = not-defined-yet
14
15
16
   # include the configuration written by CMake at config time if found
17
   sinclude ../Config.mk
18
19
   ifeq ($(fasp_prefix),not-defined-yet)
20
       fasp_prefix = ...
21
   ifeq ($(fasp_library), not-defined-yet)
22
       fasp_library = libfasp.a
24
   endif
   ifeq ($(CC),not-defined-yet)
25
26
      CC=gcc
27
   endif
   ifeq ($(FC),not-defined-yet)
28
29
      FC=gfortran
30
   \texttt{ifeq } (\$(\texttt{CXX}), \texttt{not-defined-yet})
31
32
     CXX=g++
33
   endif
34
   CFLAGS=-I$(fasp_prefix)/include
35
   CFLAGS+=-03
36
   FFLAGS=-I$(fasp_prefix)/include
37
   FFLAGS+=-03
38
   LINKER = $(FC) # because of linking with Fortran files
39
40
   LFLAGS = -L\$(fasp\_prefix)/lib - lfasp
   fasp_lib_file=$(fasp_prefix)/lib/$(fasp_library)
41
42
   examples = poisson-amg-c.ex poisson-its-c.ex poisson-pcg-c.ex \
43
              poisson-gmg-c.ex spe01-its-c.ex \
44
              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
49
   .PHONY: all clean
50
   all:
           $(examples_c) $(examples_f)
51
52
53
   %-c.ex: main/%.c $(fasp_lib_file)
54
       @\$(CC) -c \$(CFLAGS) -o main/\$@.o \$<
55
       @$(LINKER) -o $@ main/$@.o $(LFLAGS)
56
       @echo 'Building executable file $@'
57
   \%-f.ex: main/\%.f90 $(fasp_lib_file)
58
59
       @$(FC) -c $(FFLAGS) -o main/$@.o $<
       @$(FC) -o $@ main/$@.o $(LFLAGS)
```

```
@echo 'Building executable file $@'
61
62
63
    $(fasp_lib_file):
64
         (error\ The\ FASP\ library\ 0 is\ not\ found)
65
66
    clean:
        @-rm -f *.o main/*.o *~
67
68
69
    distclean: clean
         \texttt{@-rm} \ -f \ poisson-amg-c.ex \ poisson-its-c.ex \ poisson-pcg-c.ex \ \setminus
70
                       {\tt poisson-gmg-c.ex\ spe01-its-c.ex} \ \setminus
71
72
                     \verb"poisson-amg-f.ex" poisson-pcg-f.ex"
```

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
      \note AMG example for FASP: C version
7
8
    * Solving the Poisson equation (P1 FEM) with AMG
9
10
11
12
   #include "fasp.h"
13
   #include "fasp_functs.h"
14
15
16
    * \fn int main (int argc, const char * argv[])
17
    \ast \brief This is the main function for the first example.
18
19
    * \author Chensong Zhang
20
21
    * \date 12/21/2011
22
23
     * Modified by Chensong Zhang on 09/22/2012
24
   int main (int argc, const char * argv[])
25
26
   {
27
       input_param
                       inparam; // parameters from input files
                       amgparam; // parameters for AMG
28
       AMG_param
29
       printf("\n======="");
30
       printf("\n|| FASP: AMG example -- C version ||");
31
       printf("\n======\n\n");
32
33
       // Step O. Set parameters: We can use ini/amg.dat
34
       fasp_param_set(argc, argv, &inparam);
35
       fasp_param_init(&inparam, NULL, &amgparam, NULL, NULL);
36
37
       // Set local parameters using the input values
38
39
       const int print_level = inparam.print_level;
40
       // Step 1. Get stiffness matrix and right-hand side
41
       // Read A and b -- P1 FE discretization for Poisson. The location
42
       // of the data files is given in "ini/amg.dat".
43
       dCSRmat A;
44
45
       dvector b, x;
46
       char filename1[512], *datafile1;
47
       char filename2 [512], *datafile2;
48
49
       // Read the stiffness matrix from matFE.dat
50
       strncpy(filename1, inparam.workdir, 128);
51
       datafile1="csrmat_FE.dat"; strcat(filename1, datafile1);
52
53
       // Read the RHS from rhsFE.dat
54
       strncpy(filename2, inparam.workdir, 128);
       datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
55
56
       fasp_dcsrvec2_read(filename1, filename2,&A,&b);
```

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

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 12–13 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 35–36 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 44 defines a sparse matrix A in the compressed sparse row (CSR) format. Line 45 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 57 reads the matrix and the right-hand side from two disk files. Line 46–55 defines the filenames of them.
- Line 60–64 prints basic information of coefficient matrix, right-hand side, and solver parameters.
- Line 69–70 allocates memory for the solution vector x and set its initial value to be all zero.
- Line 72 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 75–77 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:
                                      1
AMG type:
                                      1
                                      1.00\,\mathrm{e}\!-\!06
AMG tolerance:
AMG max levels:
                                      20
                                      1
AMG cycle type:
AMG coarse solver type:
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 0.0068 seconds.
It Num | ||r||/||b|| |
                                  ||r||
                                              Conv. Factor
     0 \quad | \quad 1.0000000 \, \mathrm{e} \! + \! 00 \qquad | \quad 7.514358 \, \mathrm{e} \! + \! 00 \quad | \quad
                          | 7.403129 e - 02 |
     1 \mid 9.851978e-03
                                                      0.0099
     2 \mid 3.507451e-04
                              2.635624\,\mathrm{e}{-03}
                                                      0.0356
     3 \mid 1.764023 e - 05
                          1.325550e-04
                                                     0.0503
     4 \mid 8.820794 e - 07 \mid 6.628261 e - 06 \mid
                                                     0.0500
Number of iterations = 4 with relative residual 8.820794e-07.
AMG solve costs 0.0017 seconds.
AMG totally costs 0.0091\ \text{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
   !> \brief The first test example for FASP: using AMG to solve
           the discrete Poisson equation from P1 finite element.
   !>
3
            F90 version.
4
   !>
   !>
6
   !> \note AMG example for FASP: F90 version
   !>
7
   !> Solving the Poisson equation (P1 FEM) with AMG
9
   !> \author Chensong Zhang
10
11
   !> \date 12/21/2011
12
13
   program test
14
15
     implicit none
16
```

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

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

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).

```
/*! \file poisson-its.c
1
2
    * \brief The second test example for FASP: using ITS to solve
3
              the discrete Poisson equation from P1 finite element.
4
    * \note ITS example for FASP: C version
5
6
       Solving the Poisson equation (P1 FEM) with iterative methods
7
8
9
   #include "fasp.h"
10
   #include "fasp_functs.h"
11
12
13
    * \fn int main (int argc, const char * argv[])
14
15
16
    * \brief This is the main function for the second example.
17
    * \author Feiteng Huang
18
    * \date 04/13/2012
19
20
    * Modified by Chensong Zhang on 09/22/2012
21
22
   int main (int argc, const char * argv[])
24
                             inparam; // parameters from input files
25
       input_param
                             itparam; // parameters for itsolver
26
27
       printf("\n======="");
28
       printf("\n|\ FASP: ITS example -- C version |\");
29
30
       printf("\n======\n\n");
31
       // Step 0. Set parameters: We can use ini/its.dat
32
33
       fasp_param_set(argc, argv, &inparam);
34
       {\tt fasp\_param\_init}(\&{\tt inparam}\;,\;\&{\tt itparam}\;,\;\;{\tt NULL}\;,\;\;{\tt NULL}\;,\;\;{\tt NULL}\;)\;;
```

```
35
36
        // Set local parameters
        const int print_level = inparam.print_level;
37
38
        // Step 1. Get stiffness matrix and right-hand side
39
        // Read A and b -- P1 FE discretization for Poisson. The location
40
        // of the data files is given in "ini/its.dat".
41
42
        dCSRmat A;
43
        dvector b, x;
44
        char filename1[512], *datafile1;
        {\tt char filename2} \, [\, 5\, 1\, 2\, ] \; , \;\; *{\tt datafile2} \; ;
45
46
        // Read the stiffness matrix from matFE.dat
47
        strncpy(filename1, inparam.workdir, 128);
48
        datafile1="csrmat_FE.dat"; strcat(filename1,datafile1);
49
50
        // Read the RHS from rhsFE.dat
51
        strncpy(filename2, inparam.workdir, 128);
52
        datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
53
54
        fasp_dcsrvec2_read(filename1, filename2, &A, &b);
55
56
57
        // Step 2. Print problem size and ITS parameters
        if (print_level>PRINT_NONE) {
58
            printf("A: m = %d, n = %d, nnz = %d\n", A.row, A.col, A.nnz);
59
            printf("b: n = %d\n", b.row);
60
            fasp_param_solver_print(&itparam);
61
        }
62
63
        // Step 3. Solve the system with ITS as an iterative solver
64
        // Set the initial guess to be zero and then solve it using standard
65
        // iterative methods, without applying any preconditioners
66
67
        fasp_dvec_alloc(A.row, &x);
        fasp_dvec_set(A.row,&x,0.0);
68
69
        {\tt fasp\_solver\_dcsr\_itsolver(\&A\,,\,\&b\,,\,\&x\,,\,\,NULL\,,\,\,\&itparam\,)\,;}
70
71
        // Step 4. Clean up memory
72
        fasp_dcsr_free(\&A);
73
        fasp_dvec_free(&b);
74
75
        fasp_dvec_free(&x);
76
77
        return FASP_SUCCESS;
78
79
80
   /*----*/
81
               End of File
   /*----*/
```

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

• Line 67–68 allocates memory for the solution vector x and set its initial value to be all zero.

• Line 70 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...
A: m = 3969, n = 3969, nnz = 27281
b: n = 3969
          Parameters in itsolver_param
Solver print level:
                                                   2
Solver type:
                                                   1
Solver precond type:
                                                   2
Solver max num of iter:
                                                   500
                                                   1.00\,\mathrm{e}\!-\!06
Solver tolerance:
Solver stopping type:
                                                   1
Calling PCG solver (CSR) ...
It Num
                ||r||/||b||
                                              ||r||
                                                                  Conv. Factor
       0 |
            1.0000000e+00
                                         7.514358 e+00
             5.078029\,\mathrm{e}{-01}
                                                                       0.5078
       1 |
                                         3.815813\,\mathrm{e}{+00}
             3.728856\,\mathrm{e}\!-\!01
                                         2.801996\,\mathrm{e}{+00}
                                                                       0.7343
       2 \mid
       3 |
              3.359470\,\mathrm{e}\!-\!01
                                         2.524426\,\mathrm{e}{+00}
                                                                       0.9009
              2.590574\,\mathrm{e}\!-\!01
                                         1.946650\,\mathrm{e}{+00}
                                                                       0.7711
              2.380797 \, \mathrm{e}\!-\!01
                                         1.789016\,\mathrm{e}{+00}
                                                                       0.9190
       5
             1.992579\,\mathrm{e}\!-\!01
                                                                       0.8369
       6
                                         1.497295\,\mathrm{e}{+00}
       7
             1.847971\,\mathrm{e}\!-\!01
                                         1.388631\,\mathrm{e}{+00}
                                                                       0.9274
       8
             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 e - 01
                                         1.025661\,\mathrm{e}{+00}
                                                                       0.9019
      11
              1.283425\,\mathrm{e}{-01}
                                         9.644117e-01
                                                                       0.9403
             1.179652 \, \mathrm{e}{-01}
                                         8.864327 \, \mathrm{e}{-01}
     12
                                                                       0.9191
     13 |
             1.115146\,\mathrm{e}\!-\!01
                                         8.379605\,\mathrm{e}{-01}
                                                                       0.9453
             1.038726\,\mathrm{e}\!-\!01
                                         7.805360\,\mathrm{e}{-01}
                                                                       0.9315
     15 |
              9.863412\,\mathrm{e}\!-\!02
                                         7.411721\,\mathrm{e}\!-\!01
                                                                       0.9496
     16
              9.277360\,\mathrm{e}\!-\!02
                                         6.971341\,\mathrm{e}{-01}
                                                                       0.9406
      17
              8.842679\,\mathrm{e}\!-\!02
                                         6.644706\,\mathrm{e}\!-\!01
                                                                       0.9531
      18 \ | \ 8.378399 \, \mathrm{e}{-02}
                                       6.295829\,\mathrm{e}{-01}
                                                                       0.9475
```

```
19
          8.011023\,\mathrm{e}\!-\!02
                                         6.019770\,\mathrm{e}{-01}
                                                                             0.9562
20
          7.633221\,\mathrm{e}\!-\!02
                                         5.735875 e - 01
                                                                             0.9528
21
          7.317756\,\mathrm{e}\!-\!02
                                         5.498824 e - 01
                                                                             0.9587
22 - 1
          7.003292 e - 02
                                         5.262524\,\mathrm{e}\!-\!01
                                                                             0.9570
23 |
          6.728610\,\mathrm{e}\!-\!02
                                         5.056119\,\mathrm{e}\!-\!01
                                                                             0.9608
          6.461736\,\mathrm{e}\!-\!02
                                         4.855580\,\mathrm{e}{-01}
24
                                                                             0.9603
          6.219614\,\mathrm{e}\!-\!02
                                         4.673640\,\mathrm{e}{-01}
25 | 1
                                                                             0.9625
                                         4.500557\,\mathrm{e}{-01}
26 |
         5.989276\,\mathrm{e}\!-\!02
                                                                             0.9630
          5.773520\,\mathrm{e}\!-\!02
                                         4.338429\,\mathrm{e}\!-\!01
                                                                             0.9640
28 |
          5.571758\,\mathrm{e}\!-\!02
                                         4.186818 \, \mathrm{e}\!-\!01
                                                                             0.9651
29
          5.377630\,\mathrm{e}\!-\!02
                                         4.040944 \, \mathrm{e}{-01}
                                                                             0.9652
30 |
          5.198586 e - 02
                                         3.906404 e - 01
                                                                             0.9667
31
          5.022413e-02
                                         3.774021e-01
                                                                             0.9661
32 |
          4.861699\,\mathrm{e}\!-\!02
                                         3.653255\,\mathrm{e}\!-\!01
                                                                             0.9680
33
          4.700598e-02
                                         3.532197e-01
                                                                             0.9669
34
          4.554874e-02
                                         3.422696 \, \mathrm{e}{-01}
                                                                             0.9690
35 L
          4.406559 \, \mathrm{e}{-02}
                                         3.311246\,\mathrm{e}\!-\!01
                                                                             0.9674
          4.273253\,\mathrm{e}\!-\!02
                                         3.211075\,\mathrm{e}{-01}
36
                                                                             0.9697
37
          4.135901\,\mathrm{e}\!-\!02
                                          3.107864\,\mathrm{e}\!-\!01
                                                                             0.9679
38
          4.013076\,\mathrm{e}\!-\!02
                                         3.015569e-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\,\mathrm{e}{-01}
                                                                             0.9741
42
          3.648645\,\mathrm{e}\!-\!02
                                         2.741722\,\mathrm{e}\!-\!01
                                                                             0.9919
43
          3.725368\,\mathrm{e}\!-\!02
                                         2.799375\,\mathrm{e}\!-\!01
                                                                             1.0210
          3.922957\,\mathrm{e}\!-\!02
44
                                          2.947850\,\mathrm{e}\!-\!01
                                                                             1.0530
45
          4.003513\,\mathrm{e}\!-\!02
                                         3.008383e-01
                                                                             1.0205
46
          3.683219\,\mathrm{e}{-02}
                                         2.767703 e - 01
                                                                             0.9200
47
          3.161285\,\mathrm{e}\!-\!02
                                         2.375503\,\mathrm{e}\!-\!01
                                                                             0.8583
          2.944107e-02
                                          2.212307e-01
48
                                                                             0.9313
49
          2.961834\,\mathrm{e}\!-\!02
                                          2.225628\,\mathrm{e}\!-\!01
                                                                             1.0060
                                                                             0.9366
50
          2.774118\,\mathrm{e}\!-\!02
                                          2.084571 \, \mathrm{e}{-01}
```

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
1
       \brief The third test example for FASP: using PCG to solve
2
3
              the discrete Poisson equation from P1 finite element.
4
              C version.
5
6
       \note PCG example for FASP: C version
7
8
       Solving the Poisson equation (P1 FEM) with PCG methods
9
    */
   #include "fasp.h"
```

```
12
   #include "fasp_functs.h"
13
14
    * \fn int main (int argc, const char * argv[])
15
16
     * \brief This is the main function for the third example.
17
18
19
    * \author Feiteng Huang
20
     * \date 05/17/2012
21
     * Modified by Chensong Zhang on 09/22/2012
22
23
24
   int main (int argc, const char * argv[])
25
   {
                             inparam; // parameters from input files
26
        input_param
                            itparam; // parameters for itsolver
27
        itsolver_param
        AMG_param
                             amgparam; // parameters for AMG
28
        ILU_param
                              iluparam; // parameters for ILU
29
30
        printf("\n========");
31
        printf("\n|| FASP: PCG example -- C version ||");
32
33
        printf("\n======\n\n");
34
        // Step 0. Set parameters: We can use ini/pcg.dat
35
        fasp_param_set(argc, argv, &inparam);
36
        fasp_param_init(&inparam, &itparam, &amgparam, &iluparam, NULL);
37
38
        // Set local parameters
39
        const SHORT print_level = itparam.print_level;
40
        const SHORT pc_type = itparam.precond_type;
41
        const SHORT stop_type = itparam.stop_type;
42
        const INT maxit
43
                                = itparam.maxit;
44
        const REAL tol
                                = itparam.tol;
45
        // Step 1. Get stiffness matrix and right-hand side
46
        // Read A and b -- P1 FE discretization for Poisson. The location
47
        // of the data files is given in "ini/pcg.dat".
48
        dCSRmat A;
49
        dvector b, x;
50
        \begin{array}{ll} \textbf{char} & \texttt{filename1} \left[ \, 5 \, 1 \, 2 \, \right] \, , & * \, \texttt{datafile1} \, ; \end{array}
51
52
        char filename2[512], *datafile2;
53
        // Read the stiffness matrix from matFE.dat
54
        strncpy(filename1, inparam.workdir, 128);
55
56
        datafile1="csrmat_FE.dat"; strcat(filename1,datafile1);
57
58
        // Read the RHS from rhsFE.dat
59
        strncpy(filename2, inparam.workdir, 128);
60
        datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
61
        fasp_dcsrvec2_read(filename1,filename2,&A,&b);
62
63
       // Step 2. Print problem size and PCG parameters
```

```
if (print_level>PRINT_NONE) {
65
66
            printf("A: m = %d, n = %d, nnz = %d n", A.row, A.col, A.nnz);
67
            printf("b: n = \frac{d}{n}, b.row);
            {\tt fasp\_param\_solver\_print}(\& {\tt itparam}) \; ;
68
69
70
        // Setp 3. Setup preconditioner
71
        // Preconditioner type is determined by pc_type
72
73
        precond *pc = fasp_precond_setup(pc_type, &amgparam, &iluparam, &A);
74
        // Step 4. Solve the system with PCG as an iterative solver
75
76
        // Set the initial guess to be zero and then solve it using PCG solver
77
        // Note that we call PCG interface directly. There is another way which
        // calls the abstract iterative method interface; see possion-its.c for
78
79
        // more details.
        fasp_dvec_alloc(A.row, &x);
80
        fasp_dvec_set(A.row, &x, 0.0);
81
82
        fasp_solver_dcsr_pcg(&A, &b, &x, pc, tol, maxit, stop_type, print_level);
83
84
        // Step 5. Clean up memory
85
86
        if (pc_type!=PREC_NULL) fasp_mem_free(pc->data);
87
        fasp_dcsr_free(&A);
        {\tt fasp\_dvec\_free}(\&{\tt b})\,;
88
        fasp_dvec_free(&x);
89
90
        return FASP_SUCCESS;
91
92
93
94
                End of File
95
         ----*/
```

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

- Line 36–37 sets default parameters. In this example, we need parameters for iterative methods, AMG preconditioner, and ILU preconditioner.
- Line 73 sets up the desired preconditioner and prepare it for the preconditioned iterative methods.
- Line 83 calls PCG to solve Ax = b. One can also call the general iterative method interface as in the previous example.
- Line 86 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):

```
\Pi
     FASP: PCG 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
b: n = 3969
       Parameters in itsolver_param
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 nonzeros
                                               Avg. NNZ / row
  Level
           Num of rows
                 3969
                                    27281
    0
                                                      6.87
                1985
                                    28523
                                                     14.37
    1
    2
                 541
                                     7951
                                                     14.70
    3
                  141
                                     1803
                                                     12.79
  Grid complexity = 1.672 | Operator complexity = 2.403
Classical AMG setup costs 0.0042\ \text{seconds} .
It Num |
            ||r||/||b|| |
                                   ||r||
                                                | Conv. Factor
     0 \mid 1.000000e+00
                               7.514358e+00
     1 |
          1.156153\,\mathrm{e}\!-\!02
                               8.687750\,\mathrm{e}{-02}
                                                       0.0116
                                                       0.0270
          3.127181 \, \mathrm{e}{-04}
                               2.349876\,\mathrm{e}{-03}
     3 \mid 4.813471 e - 06
                                                       0.0154
                               3.617014 \, \mathrm{e}{-05}
     4 \mid 5.312526 \, e{-08}
                            3.992022e-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
!> \brief The third test example for FASP: using PCG to solve
!> the discrete Poisson equation from P1 finite element.
!> F90 version.
```

```
5 !>
   !> \note PCG example for FASP: F90 version
7 !>
8 !> Solving the Poisson equation (P1 FEM) with PCG method.
   !>
9
   !> \author Chensong Zhang
10
   !> \date 12/21/2011
11
12
13
   program test
14
     implicit none
15
16
17
     \  \, double \  \, precision \, , \  \, dimension \, (:) \, , \  \, allocatable \  \, :: \  \, u \, , b \, \,
     \  \  \, double\  \  precision \, , \  \, dimension \, (:) \; , \  \, allocatable \; :: \; a
18
                      dimension(:), allocatable :: ia,ja
19
     integer,
20
21
     integer
                     :: iufile, n, nnz, i, prt_lvl, maxit
     double precision :: tol
22
23
24
     print*, ""
     25
26
     write(*,"(A)") "|| FASP: PCG example -- F90 version ||"
     27
28
     print*, ""
29
30
     ! Step 0: user defined variables
     prt_lvl = 3
31
     {\tt maxit} = 500
32
33
     tol = 1.0d-6
     iufile = 1
34
35
36
     ! Step 1: read A and b
37
     !===> Read data A from file
38
     open(unit=iufile,file='../data/csrmat_FE.dat')
39
40
     read(iufile,*) n
41
     allocate(ia(1:n+1))
42
43
     read(iufile,*) (ia(i),i=1,n+1)
44
45
     nnz=ia(n+1)-ia(1)
46
     allocate(ja(1:nnz),a(1:nnz))
     read(iufile,*) (ja(i),i=1,nnz)
47
     read(iufile,*) (a(i),i=1,nnz)
48
49
50
     close(iufile)
51
52
     !===> Read data b from file
53
     open(unit=iufile,file='../data/rhs_FE.dat')
54
     read(iufile,*) n
55
56
     allocate(b(1:n))
    read(iufile,*) (b(i),i=1,n)
```

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

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:

```
1
   /*! \file poisson-gmg.c
2
3
       \brief The fourth test example for FASP: using GMG to solve
              the discrete Poisson equation from five-point finite
4
5
              difference stencil. C version.
6
7
    * \note GMG example for FASP: C version
8
       Solving the Poisson equation (FDM) with GMG
9
10
11
   #include <time.h>
12
   #include <math.h>
13
14
   #include "fasp.h"
15
   #include "fasp_functs.h"
16
17
18
   const REAL pi = 3.14159265;
19
20
    * \fn static REAL f2d(INT i, INT j, INT nx, INT ny)
21
22
    * \brief Setting f in Poisson equation, where
23
            f = sin(pi x)*sin(pi y)
24
25
                   i-th position in x direction
26
     * \param i
                   j-th position in y direction
     * \param j
27
     * \param nx
                    Number of grids in x direction
28
                    Number of grids in y direction
29
     * \param ny
30
31
     * \author Ziteng Wang
32
     * \date 06/07/2013
33
    */
34
   static REAL f2d (INT i,
35
                     INT j,
36
                     INT nx,
```

```
INT ny)
37
38
    {
        return sin(pi *(((REAL) j)/((REAL) ny)))
39
              *sin(pi *(((REAL) i)/((REAL) nx)));
40
41
42
43
    * \fn static REAL L2NormError2d(REAL *u, INT nx, INT ny)
44
45
     * \brief Computing Discretization Error, where exact solution
46
              u = \sin(pi x)*\sin(pi y)/(2*pi*pi)
47
48
49
     * \param u
                    Vector of DOFs
                    Number of grids in x direction
50
     * \param nx
     * \param ny Number of grids in y direction
51
52
     * \author Ziteng Wang
53
    * \date 06/07/2013
54
55
    static REAL L2NormError2d (REAL *u,
56
                                 INT nx,
57
58
                                 INT ny)
59
        const REAL h = 1.0/nx;
60
        REAL 12norm = 0.0, uexact;
61
62
        INT i, j;
63
        for (i = 1; i < ny; i++) {
64
            for (j = 1; j < nx; j++)
65
                 uexact = sin(pi*i*h)*sin(pi*j*h)/(pi*pi*2.0);
66
                 12 \texttt{norm} += \texttt{pow}((\texttt{u}[\texttt{i}*(\texttt{nx}+1)+\texttt{j}] - \texttt{uexact}), 2);
67
68
69
        }
70
71
        return sqrt(12norm*h*h);
72
    }
73
74
75
    * \brief An example of GMG method using Full Multigrid cycle
76
77
    * \author Chensong Zhang
78
     * \date 10/12/2015
79
    * \note Number of grids of nx = ny should be equal to 2^maxlevel.
80
81
82
    int main (int argc, const char *argv[])
83
84
        const REAL rtol = 1.0e-6;
85
        const INT prtlvl = PRINT_MORE;
86
        INT
                   i, j, k, nx, maxlevel;
87
        REAL
                   *u, *b, h, error0;
88
89
```

```
// Step O. Set number of levels for GMG
90
91
         printf("Enter the desired number of levels:
92
         scanf("%d", &maxlevel);
93
         // Step 1. Compute right-hand side b and set approximate solution u
94
         nx = (int) pow(2.0, maxlevel);
95
        h = 1.0/((REAL) nx);
96
97
98
         u = (REAL *) malloc((nx+1)*(nx+1)*sizeof(REAL));
99
        fasp_array_set((nx+1)*(nx+1), u, 0.0);
100
101
         b = (REAL *) malloc((nx+1)*(nx+1)*sizeof(REAL));
102
         for (i = 0; i \le nx; i++) {
             for (j = 0; j \le nx; j++) {
103
104
                 b[j*(nx+1)+i] = h*h*f2d(i, j, nx, nx);
105
106
        }
107
         // Step 2. Solve the Poisson system in 2D with full Multigrid cycle
108
        \verb|fasp_poisson_fgmg_2D| (u, b, nx, nx, maxlevel, rtol, prtlvl); \\
109
110
111
         // Step 3. Compute error in L2 norm
        error0 = L2NormError2d(u, nx, nx);
112
113
         printf("L2 error ||u-u'|| = %e\n", error0);
114
115
116
        // Step 4. Clean up memory
117
        free(u);
        free(b);
118
119
120
         return FASP_SUCCESS;
121
    }
122
123
124
               End of File
    /*----*/
125
```

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
    * \brief The fifth test example for FASP: using ITS_BSR to solve
```

```
3
              the Jacobian equation from reservoir simulation benchmark
4
              problem SPE01.
5
    * \note ITS_BSR example for FASP: C version
6
7
    * Solving the Society of Petroleum Engineers SPE01 benchmark problem
8
    * with Block ILU preconditioned Krylov methods
9
10
11
   #include "fasp.h"
12
   #include "fasp_functs.h"
13
14
15
16
    * \fn int main (int argc, const char * argv[])
17
    * \brief This is the main function for the fourth example.
18
19
    * \author Feiteng Huang, Chensong Zhang
20
21
    * \date
             05/22/2012
22
    * Modified by Chensong Zhang on 09/22/2012
23
^{24}
   int main (int argc, const char * argv[])
25
26
                            inparam; // parameters from input files
^{27}
       input_param
                            itparam; // parameters for itsolver
28
       itsolver_param
       ILU_param
                            iluparam; // parameters for ILU
29
30
       printf("\n======="");
31
       printf("\n|| FASP: SPE01 -- ITS BSR version ||");
32
       printf("\n======\n\n");
33
34
35
       // Step O. Set parameters: We can ini/its_bsr.dat
       fasp_param_set(argc, argv, &inparam);
36
37
       fasp_param_init(&inparam, &itparam, NULL, &iluparam, NULL);
38
       // Set local parameters
39
       const int print_level = inparam.print_level;
40
41
42
       // Step 1. Get stiffness matrix and right-hand side
       // Read A and b -- P1 FE discretization for Poisson. The location
43
44
       // of the data files is given in "its.dat".
45
       dBSRmat A;
       dvector b, x;
46
47
       char filename1[512], *datafile1;
48
       char filename2[512], *datafile2;
49
50
       // Read the stiffness matrix from bsrmat_SPE01.dat
51
       strncpy(filename1, inparam.workdir, 128);
52
       datafile1="bsrmat_SPE01.dat"; strcat(filename1,datafile1);
       fasp_dbsr_read(filename1, &A);
53
54
      // Read the RHS from rhs_SPE01.dat
```

```
strncpy(filename2, inparam.workdir, 128);
56
        datafile2="rhs_SPE01.dat"; strcat(filename2,datafile2);
57
        fasp_dvec_read(filename2, &b);
58
59
        // Step 2. Print problem size and ITS_bsr parameters
60
        if (print_level>PRINT_NONE) {
61
             printf("A: m = %d, n = %d, nnz = %d\n", A.ROW, A.COL, A.NNZ);
62
             printf("b: n = %d\n", b.row);
63
64
             fasp_param_solver_print(&itparam);
65
             fasp_param_ilu_print(&iluparam);
        }
66
67
        // Step 3. Solve the system with ITS_BSR as an iterative solver
68
        // Set the initial guess to be zero and then solve it using standard
69
70
        // iterative methods, without applying any preconditioners
71
        fasp_dvec_alloc(b.row, &x);
        \mathtt{fasp\_dvec\_set}\,(\,\mathtt{b}\,.\,\mathtt{row}\,,\&\,\mathtt{x}\,,0\,.\,0\,)\;;
72
73
        itparam.itsolver_type = SOLVER_GMRES;
74
        \verb|fasp_solver_dbsr_krylov_ilu| (\&A , \&b , \&x , \&itparam , \&iluparam); \\
75
76
77
        // Step 4. Clean up memory
        fasp_dbsr_free(\&A);
78
        {\tt fasp\_dvec\_free}(\&{\tt b})\,;
79
80
        fasp_dvec_free(&x);
81
        return FASP_SUCCESS;
82
83
    }
84
85
86
                End of File
    /*----*/
87
```

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 itsolver_param
Solver print level:
                                    2
Solver type:
                                    1
                                    2
Solver precond type:
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:
ILU relaxation factor:
                                           0.0000
ILU drop tolerance:
                                           1.00\,\mathrm{e}\!-\!03
ILU permutation tolerance:
                                           0.00e+00
BSR ILU(0) setup costs 0.000202 seconds.
Calling GMRES solver (BSR) ...
It Num |
             ||r||/||b||
                                      ||r||
                                                       Conv. Factor
          1.0000000 e+00
                                  8.207069\,\mathrm{e}{+03}
      0 |
      1 \mid 9.999991 e-01
                                  8.207062\,\mathrm{e}{+03}
                                                           1.0000
      2 \mid 9.991891e-01
                                 8.200415 e+03
                                                           0.9992
      3 \mid 9.984917e-01
                                  8.194691 e+03
                                                           0.9993
      4
            9.581382\,\mathrm{e}\!-\!01
                                  7.863507e+03
                                                           0.9596
      5
           9.387736\,\mathrm{e}\!-\!01
                                  7.704580\,\mathrm{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
                              7.034036e+03
                                                           0.9555
                              | 4.357360 e+03
           5.309276 \, \mathrm{e}{-01}
      9 |
                                                           0.6195
     10
           1.462587 \, \mathrm{e}{-01}
                                  1.200355\,\mathrm{e}{+03}
                                                           0.2755
            3.520599 e - 02
                                  2.889380 e+02
                                                           0.2407
                             6.966349\,e+01
    12 |
           8.488230\,\mathrm{e}{-03}
                                                           0.2411
    13 \mid 2.019708 e - 03
                             1.657588 e+01
                                                           0.2379
                             3.713630 e+00
    14 \mid 4.524916e-04
                                                           0.2240
           9.670973\,\mathrm{e}{-05}
                             7.937035e-01
                                                           0.2137
    16
           1.970931 \, \mathrm{e}{-05}
                             | 1.617557 e - 01
                                                           0.2038
    17 |
            3.905034 \, \mathrm{e}{-06}
                                  3.204889\,\mathrm{e}{-02}
                                                           0.1981
           8.553378\,\mathrm{e}\!-\!07
                                  7.019817\,\mathrm{e}{-03}
                                                           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
3 \% lines starting with \% are comments
                                                      %
4\ \% must have spaces around the equal sign "="
6
   workdir = ../data/
                           \% work directory, no more than 128 characters
   print_level = 3
8
                           \% How much information to print out
9
10
                                                      %
11
   \% parameters for multilevel iteration
12
13
14
    AMG_type
                              = C
                                        \% C classic AMG
15
                                        \% SA smoothed aggregation
                                        \% UA unsmoothed aggregation
16
17
   AMG_cycle_type
                              = v
                                        \% V V-cycle | W W-cycle
                                        \% A AMLI-cycle | NA Nonlinear AMLI-cycleA
18
   AMG_tol
                                        \% tolerance for AMG
                              = 1e-8
19
                                        \% number of AMG iterations
20
   {\tt AMG\_maxit}
                              = 100
    AMG_levels
                              = 20
                                        \% max number of levels
21
                             = 500
                                        \% max number of coarse degrees of freedom
22
   AMG_coarse_dof
   \begin{array}{lll} {\tt AMG\_coarse\_scaling} & = & {\tt OFF} \\ {\tt AMG\_amli\_degree} & = & 2 \end{array}
                                        \% switch of scaling of the coarse grid correction
23
                                        \% degree of the polynomial used by AMLI cycle
   AMG_nl_amli_krylov_type = 6
                                        % Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCG
25
26
27
                                                      -%
   \% parameters for AMG smoothing
                                                      %
28
                                                      -%
29
30
                                        % GS | JACOBI | SGS
31
   AMG_smoother
                              = GS
                                        \% SOR | SSOR | GSOR | SGSOR | POLY
32
   AMG_ILU_levels
                              = 0
                                        \% number of levels using ILU smoother
33
                              = 0
    AMG_Schwarz_levels
                                        \% number of levels using Schwarz smoother
34
   AMG_relaxation
                              = 1.1
                                        \% relaxation parameter for SOR smoother
35
                                        \% degree of the polynomial smoother
   AMG_polynomial_degree
                              = 3
36
   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
44
                              = 1
                                        \% 1 Modified RS
45
                                        \% 3 Compatible Relaxation
                                        \% 4 Aggressive
46
47
    AMG_interpolation_type
                              = 1
                                        \% 1 Direct | 2 Standard | 3 Energy-min
    AMG\_strong\_threshold = 0.6 % Strong threshold
```

```
\% Truncation threshold
   AMG\_truncation\_threshold = 0.4
49
   AMG_max_row_sum
                     = 0.9
                                      \% Max row sum
50
51
52
   \% parameters for aggregation-type AMG SETUP
53
54
55
                            = 0.08
                                     \% Strong coupled threshold
56
   AMG_strong_coupled
57
   AMG_max_aggregation
                            = 20
                                      \% Max size of aggregations
   AMG_tentative_smooth
                            = 0.67
                                      \% Smoothing factor for tentative prolongation
58
   AMG_smooth_filter
                             = OFF
                                      \% Switch for filtered matrix for smoothing
59
```

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

```
AMG print level:
                                    3
AMG max num of iter:
                                     100
                           2\\1.0\\20
AMG type:
                                    1.00\,\mathrm{e}\!-\!08
AMG tolerance:
AMG max levels:
AMG cycle type:
{\tt AMG \ coarse \ solver \ type:} \qquad \qquad 0
AMG scaling of coarse correction: 0
AMG smoother type:
AMG smoother order:
AMG num of presmoothing:
AMG num of postsmoothing:
Aggregation type:
Aggregation number of pairs: 2
Aggregation quality bound: 8.00
Calling SA AMG \dots
```

Level	Num of rows	Num of nonzeros	Avg. NNZ / row
0	3969	27281	6.87
1	541	6531	12.07
2	41	421	10.27

Grid complexity = 1.147 | Operator complexity = 1.255

Smoothed aggregation setup costs $0.0028\ \mbox{seconds}.$

Ιt	Num	r / b		r		Conv. Factor
	0	1.000000e+00		7.514358e+00		
	1	$4.345463\mathrm{e}\!-\!02$		$3.265336\mathrm{e}\!-\!01$		0.0435
	2	$8.041967\mathrm{e}{-03}$	İ	$6.043022\mathrm{e}\!-\!02$	ĺ	0.1851
	3	$3.808810\mathrm{e}{-03}$	i	$2.862076\mathrm{e}{-02}$	i	0.4736
	4	$1.838990\mathrm{e}{-03}$	i	$1.381883\mathrm{e}{-02}$	i	0.4828
	5	$8.675952\mathrm{e}{-04}$	i	$6.519421\mathrm{e}{-03}$	i	0.4718
	6	$4.089274\mathrm{e}{-04}$	i	3.072827 e - 03	i	0.4713
	7	$1.939823\mathrm{e}{-04}$	i	$1.457653 \mathrm{e}{-03}$	i	0.4744
	8	$9.276723\mathrm{e}{-05}$	i	$6.970862 \mathrm{e}{-04}$	i	0.4782
	9	$4.471799 e{-05}$	i	$3.360270\mathrm{e}{-04}$	i	0.4820
	10	$2.171249\mathrm{e}{-05}$	i	$1.631554 \mathrm{e}{-04}$	i	0.4855
	11	1.060934e-05	i	$7.972239\mathrm{e}{-05}$	i	0.4886
	12	$5.212246\mathrm{e}{-06}$	i	3.916668 e - 05		0.4913
	13	2.572464e-06		1.933042e-05		0.4935
	14	1.274466e-06		9.576797e-06		0.4954
	'	6.333891e-07		4.759512e-06		0.4934 0.4970
	15					
	16	$3.155926\mathrm{e}{-07}$		2.371476e-06		0.4983
	17	1.575755e-07		$1.184079\mathrm{e}{-06}$		0.4993
	18	$7.881043\mathrm{e}{-08}$		$5.922098 \mathrm{e}{-07}$		0.5001
	19	3.947044e -08		$2.965950\mathrm{e}{-07}$		0.5008

You can compare this with the sample results in §2.1.

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

```
\Pi
     FASP: AMG example -- C version
                                           FASP command line options:
                      [CharValue] : Ini file name
 -ini
                      [IntValue] : Print level
 -\mathtt{print}
                      [IntValue] : Output to screen or a log file
 -output
                      [IntValue] : Solver type
 -\mathtt{solver}
                      [IntValue] : Preconditioner type
  -precond
                      [IntValue] : Max number of iterations
  -\mathtt{maxit}
                      [RealValue] : Tolerance for iterative solvers
 -\mathtt{tol}
                    [IntValue] : Max number of AMG iterations
 -\mathtt{amgmaxit}
 -\mathtt{amgtol}
                     [RealValue] : Tolerance for AMG methods
 -\mathtt{amgtype}
                      [IntValue] : AMG type
 -{\tt amgcycle}
                      [IntValue] : AMG cycle type
                      [IntValue] : AMG coarsening type
  -amgcoarsening
 -{\tt amginterpolation} \ \ [\, {\tt IntValue} \,] \quad : \ {\tt AMG} \ \ {\tt interpolation} \ \ {\tt type}
 -{\tt amgsmoother}
                    [IntValue] : AMG smoother type
                      [RealValue] : AMG strong threshold
 -{\tt amgsthreshold}
 -amgscoupled
                      [RealValue] : AMG strong coupled threshold
                                    : Brief help messages
 -help
```

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:

```
./{	t 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.

```
330
331
      * \struct dvector
332
333
       \brief Vector with n entries of REAL type
334
335
    typedef struct dvector{
336
         //! number of rows
337
         INT row;
338
339
         //! actual vector entries
341
         REAL *val;
```

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.

```
192
193
     * \struct dCOOmat
194
     * \brief Sparse matrix of REAL type in COO (or IJ) format
195
196
197
      * Coordinate Format (I,J,A)
198
     * \note The starting index of A is 0.
199
     st \note Change I to rowind, J to colind. To avoid with complex.h confliction on I.
200
201
    typedef struct dCOOmat{
202
203
         //! row number of matrix A, m
204
        INT row;
205
206
         //! column of matrix A, n
207
208
         INT col;
209
210
         //! number of nonzero entries
211
         INT nnz;
212
213
         //! integer array of row indices, the size is nnz
214
         INT *rowind;
215
216
         //! integer array of column indices, the size is nnz
217
         INT *colind;
218
219
         //! nonzero entries of A
220
         REAL *val;
```

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:

```
132
133
134
      * \struct dCSRmat
      * \brief Sparse matrix of REAL type in CSR format
135
136
137
      * CSR Format (IA, JA, A) in REAL
138
139
      * \note The starting index of A is 0.
140
141
    typedef struct dCSRmat{
142
```

```
143
         //! row number of matrix A, m
144
         INT row;
145
         //! column of matrix A, n
146
         INT col;
147
148
         //! number of nonzero entries
149
150
         INT nnz;
151
         //! integer array of row pointers, the size is m+1
152
         INT *IA;
153
154
         //! integer array of column indexes, the size is nnz
155
156
157
158
         //! nonzero entries of A
159
         REAL *val:
```

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.

```
253
254
255
      * \struct dCSRLmat
256
      * \brief Sparse matrix of REAL type in CSRL format
257
    typedef struct dCSRLmat{
258
259
         //! number of rows
260
         INT row;
261
262
263
         //! number of cols
264
         INT col;
265
266
         //! number of nonzero entries
```

```
267
         INT nnz;
268
269
         //! number of different values in i-th row, i=0:nrows-1
         INT dif:
270
271
         //! nz_diff[i]: the i-th different value in 'nzrow'
272
         INT *nz_diff;
273
274
275
         //! row index of the matrix (length-grouped): rows with same nnz are together
276
277
         //! j in {start[i],...,start[i+1]-1} means nz_diff[i] nnz in index[j]-row
278
279
         INT *start;
280
         //! column indices of all the nonzeros
281
282
         INT *ja;
283
         //! values of all the nonzero entries
284
         REAL *val;
285
```

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.

```
33
34
35
    * \struct dBSRmat
     * \brief Block sparse row storage matrix of REAL type
36
37
    * \note This data structure is adapted from the Intel MKL library. Refer to:
38
    * http://software.intel.com/sites/products/documentation/hpc/mkl/lin/index.htm
39
40
     st \note Some of the following entries are capitalized to stress that they are
41
             for blocks!
42
43
   typedef struct dBSRmat {
44
45
        //! number of rows of sub-blocks in matrix A, M
46
47
       INT ROW;
48
49
        //! number of cols of sub-blocks in matrix A, N
50
        INT COL:
51
52
       //! number of nonzero sub-blocks in matrix A, NNZ
53
       INT NNZ;
54
        //! dimension of each sub-block
55
56
        INT nb; // NOTE: for the moment, allow nb*nb full block
57
        //! storage manner for each sub-block
58
        INT storage_manner; // 0: row-major order, 1: column-major order
59
60
        //! A real array that contains the elements of the non-zero blocks of
61
        //! a sparse matrix. The elements are stored block-by-block in row major
62
        //! order. A non-zero block is the block that contains at least one non-zero
63
       //! element. All elements of non-zero blocks are stored, even if some of
64
        //! them is equal to zero. Within each nonzero block elements are stored
65
        //! in row-major order and the size is (NNZ*nb*nb).
66
       REAL *val:
67
68
        //! integer array of row pointers, the size is ROW+1
69
       INT *IA;
70
71
        //! Element i of the integer array columns is the number of the column in the
72
73
        //! block matrix that contains the i-th non-zero block. The size is NNZ.
        INT *JA;
74
```

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) CSR Block format

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

```
77
78
79
     * \struct block_dCSRmat
       \brief Block REAL CSR matrix format
81
       \note The starting index of A is 0.
82
83
    typedef struct block_dCSRmat {
84
85
86
        //! row number of blocks in A, m
87
        INT brow;
88
        //! column number of blocks A, n
89
        INT bcol;
90
91
92
        //! blocks of dCSRmat, point to blocks[brow][bcol]
        dCSRmat **blocks;
```

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/io.c" and we list the available functions as follows:

```
834 /*----- In file: io.c -----*/
```

```
835
836
    void fasp_dcsrvec1_read (const char *filename,
                               dCSRmat *A,
837
                               dvector *b);
838
839
    void fasp_dcsrvec2_read (const char *filemat,
840
                               const char *filerhs,
841
                               dCSRmat *A,
842
843
                               dvector *b );
844
    void fasp_dcsr_read (const char *filename,
845
846
                           dCSRmat *A);
847
848
    void fasp_dcoo_read (const char *filename,
                           dCSRmat *A);
849
850
851
    void fasp_dcoo1_read (const char *filename,
                            dCOOmat *A);
852
853
854
    void fasp_dcoo_shift_read (const char *filename,
                                 dCSRmat *A);
855
856
    void fasp_dmtx_read (const char *filename,
857
                           dCSRmat *A);
858
859
860
    void fasp_dmtxsym_read (const char *filename,
                              dCSRmat *A);
861
862
863
    void fasp_dstr_read (const char *filename,
864
                           dSTRmat *A);
865
    void fasp_dbsr_read (const char *filename,
866
867
                           dBSRmat *A);
868
    void fasp_dvecind_read (const char *filename,
869
870
                              dvector *b);
871
    void fasp_dvec_read (const char *filename,
872
873
                           dvector *b);
874
875
    void fasp_ivecind_read (const char *filename,
876
                             ivector *b);
877
878
    void fasp_ivec_read (const char *filename,
879
                           ivector *b);
880
881
    void fasp_dcsrvec1_write (const char *filename,
882
                                dCSRmat *A,
883
                                dvector *b);
884
    void fasp_dcsrvec2_write (const char *filemat,
885
886
                                const char *filerhs,
887
                               dCSRmat *A,
```

```
dvector *b );
888
889
890
    void fasp_dcoo_write (const char *filename,
                            dCSRmat *A);
891
892
    void fasp_dstr_write (const char *filename,
893
894
                            dSTRmat *A);
895
896
    void fasp_dbsr_write (const char *filename,
897
                            dBSRmat *A);
898
    void fasp_dvec_write (const char *filename,
899
900
                            dvector *vec);
901
    void fasp_dvecind_write (const char *filename,
902
                               dvector *vec);
903
904
    void fasp_ivec_write (const char *filename,
905
906
                            ivector *vec);
907
908
    void fasp_dvec_print (INT n,
909
                            dvector *u);
910
    void fasp_ivec_print (INT n,
911
912
                            ivector *u);
913
    void fasp_dcsr_print (dCSRmat *A);
914
915
916
    void fasp_dcoo_print (dCOOmat *A);
917
    void fasp_dbsr_print (dBSRmat *A);
918
919
920
    void fasp_dbsr_write_coo (const char *filename,
                                const dBSRmat *A);
921
922
923
    void fasp_dcsr_write_coo (const char *filename,
                                const dCSRmat *A);
924
925
926
    void fasp_dstr_print (dSTRmat *A);
927
928
    void fasp_matrix_read (const char *filename,
929
                             void *A);
930
931
    void fasp_matrix_read_bin (const char *filename,
932
                                 void *A);
933
    void fasp_matrix_write (const char *filename,
934
935
                              void *A,
936
                              INT flag);
937
    void fasp_vector_read (const char *filerhs,
938
939
                             void *b);
940
```

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
      * \brief Matrix-vector multiplication y = A*x
 4
 5
      * \param A Pointer to dCSRmat matrix A
 6
      * \param x Pointer to array x
 7
      * \param y Pointer to array y
10
      * \author Chensong Zhang
      * \date 07/01/2009
11
12
    void fasp_blas_dcsr_mxv (dCSRmat *A,
13
                                      REAL *x,
14
                                      REAL *y)
15
16
    {
          const INT
                        m = A \rightarrow row;
17
18
          const INT *ia = A->IA, *ja = A->JA;
          const REAL *aj = A->val;
19
20
          INT i, k, beg, end;
21
22
          register REAL tmp;
23
          for (i=0; i< m; ++i) {
24
25
               tmp = 0.0;
               {\tt beg} \, = \, {\tt ia} \, [\, {\tt i} \, ] \, ; \  \, {\tt end} \, = \, {\tt ia} \, [\, {\tt i} \, + 1 \, ] \, ;
26
               \label{eq:for} \mbox{for } ( \mbox{ $k$=$beg}; \mbox{ $k$<$end}; \mbox{ $+\!\!\!+$k} ) \mbox{ $tmp$ $+\!\!\!=$ aj[k]*x[ja[k]];}
27
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 notice the abstract interface for the iterative methods. The following code segment is taken from "base/src/itsolver_csr.c":

```
20
    * \fn INT fasp_solver_dcsr_itsolver (dCSRmat *A, dvector *b, dvector *x,
21
                                           precond *pc, itsolver_param *itparam)
22
23
      \brief Solve Ax=b by preconditioned Krylov methods for CSR matrices
24
25
26
     * \param A
                       Pointer to the coeff matrix in dCSRmat format
27
     * \param b
                       Pointer to the right hand side in dvector format
                       Pointer to the approx solution in dvector format
28
     * \param x
     * \param pc
                       Pointer to the preconditioning action
29
30
      \param itparam Pointer to parameters for iterative solvers
31
32
                       Iteration number if converges; ERROR otherwise.
    * \return
33
     * \author Chensong Zhang
34
    * \date 09/25/2009
35
36
      \note This is an abstract interface for iterative methods.
37
38
39
   INT fasp_solver_dcsr_itsolver (dCSRmat *A,
40
                                    dvector *b,
41
                                    dvector *x,
42
                                    precond *pc.
43
                                    itsolver_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
ILU_data LU;
if ((status = fasp_ilu_dcsr_setup(A,&LU,iluparam)) < 0 ) goto FINISHED;
```

```
466
467
         // check iludata
468
         if ( (status = fasp_mem_iludata_check(&LU)) < 0 ) goto FINISHED;</pre>
469
         // set preconditioner
470
471
         precond pc;
472
         pc.data = \&LU;
473
         pc.fct = fasp_precond_ilu;
474
475
         // call iterative solver
         status = fasp_solver_dcsr_itsolver(A,b,x,&pc,itparam);
476
```

Now we explain this code segment a little bit:

- Line 463–465 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 471–473 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 476 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 itsolver_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 */
} itsolver_param; /**< Parameters for iterative solvers */</pre>
```

Possible "itsolver_type" includes:

```
/**

* \brief Definition of solver types for iterative methods

*/

#define SOLVER.DEFAULT

0 /**< Use default solver in FASP */
```

```
#define SOLVER_CG
#define SOLVER_BiCGstab
                                  1 /**< Conjugate Gradient */</pre>
                                  2 /**< Bi-Conjugate Gradient Stabilized */</pre>
#define SOLVER_MinRes
                                   3 /**< Minimal Residual */</pre>
#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
#define SOLVER_GCR
                                  7 /** Generalized Conjugate Gradient */
                                  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_SCMRES 14 /**< CMRes with safety net */
#define SOLVER_SGMRES
                                 14 /**< GMRes with safety net */
#define SOLVER_SVGMRES
                               14 /**< GMRes with safety net */
15 /**< Variable-restart GMRES with safety net */
#define SOLVER.SVFGMRES 16 /**< Variable-restart FGMRES define SOLVER.SGCG 17 /**< GCG with safety net */
                                 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/amg.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).

```
42
       const SHORT max_levels = param->max_levels;
43
       const SHORT prtlvl = param->print_level;
       const SHORT amg_type = param->AMG_type;
44
       const SHORT cycle_type = param->cycle_type;
45
                    nnz = A->nnz, m = A->row, n = A->col;
46
       const INT
47
       // local variables
48
       SHORT status;
49
50
       AMG_data *
                  mgl = fasp_amg_data_create(max_levels);
51
       REAL
                  AMG_start, AMG_end;
52
   #if DEBUG_MODE > 0
53
54
       printf("### DEBUG: %s ..... [Start]\n", __FUNCTION__);
   #endif
```

```
56
57
         if ( prtlvl > PRINT_NONE ) fasp_gettime(&AMG_start);
58
         // check matrix data
59
         if ( m != n ) {
60
              printf("### ERROR: A is not a square matrix!\n");
61
              fasp_chkerr(ERROR_MAT_SIZE, __FUNCTION__);
62
         }
63
64
         if ( nnz \ll 0 ) {
65
              printf("### ERROR: A has no nonzero entries!\n");
66
67
              fasp_chkerr(ERROR_MAT_SIZE, __FUNCTION__);
68
         }
69
         // Step 0: initialize mgl[0] with A, b and x
70
         mgl[0].A = fasp_dcsr_create(m, n, nnz);
71
         {\tt fasp\_dcsr\_cp}\left({\tt A}\,,\,\,\&{\tt mgl}\left[\,0\,\right].\,{\tt A}\,\right);
72
73
74
         mgl[0].b = fasp_dvec_create(n);
         fasp_dvec_cp(b, \&mgl[0].b);
75
76
77
         mgl[0].x = fasp_dvec_create(n);
78
         fasp_dvec_cp(x, \&mgl[0].x);
79
         // Step 1: AMG setup phase
80
         switch (amg_type) {
81
82
              case SA_AMG: // Smoothed Aggregation AMG setup
83
                   if ( prtlvl > PRINT_NONE ) printf("\nCalling SA AMG ...\n");
84
                   {\tt status} \ = \ {\tt fasp\_amg\_setup\_sa(mgl\,, param)} \, ; \ \ {\tt break} \, ;
85
86
              case UA_AMG: // Unsmoothed Aggregation AMG setup
87
                   if ( prtlvl > PRINT_NONE ) printf("\nCalling UA AMG ...\n");
88
                   status = fasp_amg_setup_ua(mgl, param); break;
89
90
              default: // Classical AMG setup
91
                   if ( prtlvl > PRINT_NONE ) printf("\nCalling classical AMG ...\n");
92
                   {\tt status} \ = \ {\tt fasp\_amg\_setup\_rs} \, (\, {\tt mgl} \, \, , \  \, {\tt param} \, ) \, ;
93
94
         }
95
96
97
         // Step 2: AMG solve phase
         if ( status == FASP_SUCCESS ) { // call a multilevel cycle
98
99
100
              switch (cycle_type) {
101
102
                   case AMLI_CYCLE: // AMLI-cycle
103
                       fasp_amg_solve_amli(mgl, param); break;
104
                   case NL_AMLI_CYCLE: // Nonlinear AMLI-cycle
105
                       fasp_amg_solve_nl_amli(mgl, param); break;
106
107
108
                   default: // V,W-cycles (determined by param)
```

```
109
                      fasp_amg_solve(mgl, param); break;
110
111
             }
112
             fasp_dvec_cp(\&mgl[0].x, x);
113
114
         }
115
116
117
         else { // call a backup solver
118
             if ( prtlvl > PRINT_MIN ) {
119
120
                  printf("### WARNING: AMG setup failed!\n");
121
                  printf("### WARNING: Use a backup solver instead.\n");
             }
122
123
             fasp_solver_dcsr_spgmres (A, b, x, NULL, param->tol, param->maxit,
124
                                          20, 1, prtlv1);
125
126
```

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

- Line 42-45 reads some of the parameters from "AMG_param", which can be defined from a input file; see §2.6.
- Line 50–78 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 81–95 calls three different AMG setup methods, determined by "amg_type".
- Line 98–115 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.

```
-%
55
   \% parameters for multilevel iteration
                                                       %
56
57
   %
                                                       -%
58
   AMG_type
                               = C
                                         \% C classic AMG
59
60
                                         \% SA smoothed aggregation
61
                                         \% UA unsmoothed aggregation
62
   AMG_cycle_type
                               = V
                                         \% V V-cycle | W W-cycle
                                         \% A AMLI-cycle | NA Nonlinear AMLI-cycleA
63
64
    AMG_tol
                                        \% tolerance for AMG
   AMG_maxit
                                         \% number of AMG iterations
```

```
= 20
    AMG_levels
                                       \% max number of levels
    AMG_coarse_dof
                              = 500
                                       \% max number of coarse degrees of freedom
67
68
    AMG_coarse_solver
                              = 0
                                       \% coarsest solver: 0 iterative
                                       \% 31 SuperLU | 32 UMFPack | 33 MUMPS
69
                                       \% switch of scaling of the coarse grid correction
    AMG_coarse_scaling
                             = OFF
70
    AMG_amli_degree
                              = 2
                                       \% degree of the polynomial used by AMLI cycle
71
    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
78
    AMG_smoother
                              = GS
                                       \% GS | JACOBI | SGS SOR | SSOR |
                                       \% GSOR | SGSOR | POLY | L1DIAG | CG
79
    AMG_smooth_order
                                       \% NO: natural order | CF: CF order
80
                              = CF
    AMG_ILU_levels
                             = 0
                                       \% number of levels using ILU smoother
81
    AMG_Schwarz_levels
                             = 0
                                       \% number of levels using Schwarz smoother
82
    AMG_relaxation
                             = 1.0
                                       \% relaxation parameter for SOR smoother
83
    AMG_polynomial_degree
                              = 3
                                      \% degree of the polynomial smoother
                            \% degree of the polynomial smooth =1 % number of presmoothing sweeps =1 % number of postsmoothing sweeps
    AMG_presmooth_iter
85
    AMG_postsmooth_iter
86
87
88
    \% parameters for classical AMG SETUP
                                                     %
89
                                                     -%
90
91
                                       \% 1 Modified RS
                              = 1
92
    AMG_coarsening_type
                                       \% 3 Compatible Relaxation
93
                                       % 4 Aggressive
    AMG_interpolation_type = 1
                                       \% 1 Direct | 2 Standard | 3 Energy-min
95
    AMG\_strong\_threshold = 0.3
96
                                       \% Strong threshold
97
    AMG\_truncation\_threshold = 0.1
                                       \% Truncation threshold
                                       \% Max row sum
98
    AMG_max_row_sum
                             = 0.9
99
                                                    -%
100
    \% parameters for aggregation-type AMG SETUP
101
102
103
                             = 2
    AMG_aggregation_type
                                       \% 1 Matching | 2 VMB
104
105
    AMG_pair_number
                             = 2
                                       \% Number of pairs in matching
                            =0.08 % Strong coupled threshold
106
    AMG_strong_coupled
107
    AMG_max_aggregation
                            = 20
                                       \% Max size of aggregations
108
   AMG_tentative_smooth
                            = 0.67
                                       \% Smoothing factor for tentative prolongation
   AMG_smooth_filter
                             = OFF
                                       \% Switch for filtered matrix for smoothing
109
110 AMG_quality_bound
                              = 8.0
                                       \% quality of aggregation: 8.0~{
m symm} | 10.0~{
m 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 An OpenMP example

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
       \brief Definition of all kinds of messages, including error messages,
2
3
               solver types, etc.
4
       \note This is internal use only. Do NOT change.
5
6
7
       Created by Chensong Zhang on 03/20/2010.
8
9
       Modified by Chensong Zhang on 12/06/2011.
       Modified by Chensong Zhang on 12/25/2011.
10
       Modified by Chensong Zhang on 04/22/2012.
11
       Modified by Ludmil Zikatanov on 02/15/2013: CG -> SMOOTHER_CG.
12
       Modified by Chensong Zhang on 02/16/2013: GS -> SMOOTHER_GS, etc.
13
       Modified by Chensong Zhang on 04/09/2013\colon Add safe Krylov methods.
14
       Modified by Chensong Zhang on 09/22/2013: Clean up Doxygen.
15
     st Modified by Chensong Zhang on 09/17/2013: Filename changed from message.h.
16
17
18
19
    */
20
   #ifndef __FASP_MESSAGES__
                                       /*-- allow multiple inclusions --*/
21
22
   #define __FASP_MESSAGES__
23
24
    * \brief Definition of return status and error messages
25
26
   #define FASP_SUCCESS
                                    0 /**< return from function successfully */</pre>
```

```
#define ERROR_OPEN_FILE -10 /**< fail to open a file */
#define ERROR_WRONG_FILE -11 /**< input contains wrong format */</pre>
30 #define ERROR_WRONG_FILE
31 #define ERROR_INPUT_PAR
                              -13 /**< wrong input argument */
                                -14 /**< regression test fail */
32 #define ERROR_REGRESS
33 #define ERROR_MAT_SIZE
                                -15 /**< wrong problem size */
  #define ERROR_NUM_BLOCKS
                                -18 /**< wrong number of blocks */
34
  #define ERROR_MISC
35
                                -19 /**< other error */
  //---
36
   #define ERROR_ALLOC_MEM -20 /**< fail to allocate memory */
37
   #define ERROR_DATA_STRUCTURE -21 /**< problem with data structures */
38
   #define ERROR_DATA_ZERODIAG -22 /**< matrix has zero diagonal entries */
39
40
   #define ERROR_DUMMY_VAR -23 /**< unexpected input data */
41
   #define ERROR_AMG_INTERP_TYPE -30 /**< unknown interpolation type */
42
43 #define ERROR_AMG_SMOOTH_TYPE -31 /**< unknown smoother type */
44 #define ERROR_AMG_COARSE_TYPE -32 /**< unknown coarsening type */
45 #define ERROR_AMG_COARSEING -33 /**< coarsening step failed to complete */
46
   #define ERROR_SOLVER_TYPE -40 /**< unknown solver type */
47
   #define ERROR_SOLVER_PRECTYPE -41 /**< unknown precond type */
48
  #define ERROR_SOLVER_STAG -42 /**< solver stagnates */
   #define ERROR_SOLVER_SOLSTAG -43 /**< solver's solution is too small */
50
   #define ERROR_SOLVER_TOLSMALL -44 /**< solver's tolerance is too small */
51
   #define ERROR_SOLVER_ILUSETUP -45 /**< ILU setup error */</pre>
52
   #define ERROR_SOLVER_MISC -46 /**< misc solver error during run time */
53
   #define ERROR_SOLVER_MAXIT
                                -48 /**< maximal iteration number exceeded */
54
   #define ERROR_SOLVER_EXIT -49 /**< solver does not quit successfully */
55
  #define ERROR_QUAD_TYPE -60 /**< unknown quadrature type */
#define ERROR_QUAD_DIM -61 /**< unsupported quadrature dim */
57
58
   #define ERROR_LIC_TYPE -80 /**< wrong license type */
60
61
   #define ERROR_UNKNOWN -99 /**< an unknown error type */
62
63
64
    * \brief Definition of logic type
65
66
   #define TRUE
                                 1 /**< logic TRUE */
67
                                  0 /**< logic FALSE */
68
   #define FALSE
70
   * \brief Definition of switch
71
72
73
   #define ON
                                  1 /**< turn on certain parameter */</pre>
74
   #define OFF
                                  0 /**< turn off certain parameter */</pre>
75
76
77
   * \brief Print level for all subroutines -- not including DEBUG output
78
                        0 /**< silent: no printout at all */
   #define PRINT_NONE
79
```

```
81 #define PRINT_SOME 2 /**< some: print less important warnings */
 82 #define PRINT_MORE 4 /**< more: print some useful debug info */
 83 #define PRINT_MOST
                                         8 /**< most: maximal printouts, no files */
 84 #define PRINT_ALL
                                        10 /**< all: all printouts, including files */
 85
 86
     * \brief Definition of matrix format
 87
 88
    #define MAT_FREE
                              0 /**< matrix-iroc 1 /**< compressed sparse row */
 89
                                         0 /**< matrix-free format: only mxv action */</pre>
     #define MAT_CSR
 90
    #define MAT_BSR
                                         2 /**< block-wise compressed sparse row */</pre>
 91
                                         3 /**< structured sparse matrix */</pre>
     #define MAT_STR
 92
 93
     #define MAT_bCSR
                                         4 /**< block matrix of CSR */
                                         5 /**< block matrix of BSR for bordered systems */
    #define MAT_bBSR
 94
                                         6 /**< modified CSR to reduce cache missing */
 95 #define MAT_CSRL
                                   7 /**< symmetric CSR format */
 96 #define MAT_SymCSR
 97
 98
      * \brief Definition of solver types for iterative methods
 99
100
101 #define SOLVER_DEFAULT 0 /**< Use default solver in FASP */
102 //-----
103 #define SOLVER_CG
                                      1 /**< Conjugate Gradient */
2 /**< Bi-Conjugate Gradient Stabilized */</pre>
104 #define SOLVER_BiCGstab
     #define SOLVER_MinRes
                                         3 /**< Minimal Residual */
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_GCG / /** Generalized Conjugate Residual */
111 //-----
#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 16 /**< Variable-restart FGMRES with safety net */
#define SOLVER_SVFGMRES 16 /**< Variable-restart FGMRES with safety net */
#define SOLVER_SCGG 17 /**< GCG with safety net */
     //-----
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 /**< SuperLU Direct Solver */
                                 32 /**< UMFPack Direct Solver */
33 /**< MUMPS Direct Solver */
124 #define SOLVER_UMFPACK
125 #define SOLVER_MUMPS
126
127
128
     st \brief Definition of iterative solver stopping criteria types
                                       1 /**< relative residual ||r||/||b|| */
2 /**< relative B-residual ||r||_B/||b||_B */
130 #define STOP_REL_RES
     #define STOP_REL_PRECRES
131
     #define STOP_MOD_REL_RES
                                         3 /**< modified relative residual ||r||/||x|| */
132
133
```

```
134 /**
135
    * \brief Definition of preconditioner type for iterative methods
#define PREC_FMG

#define PREC_ILU

#define PREC_SCHWARZ

#define PREC_SCHWARZ
                                  0 /**< with no precond */
                                  1 /**< with diagonal precond */</pre>
                                  2 /**< with AMG precond */
                              3 /**< with full AMG precond */
                                  4 /**< with ILU precond */
#define PREC_SCHWARZ 5 /**< with Schwarz preconditioner */
145
     * \brief Type of ILU methods
146 */
                                  1 /**< ILUk */
147 #define ILUk
148 #define ILUt
                                  2 /**< ILUt */
149 #define ILUtp
                                  3 /**< ILUtp */
150
151 /**
152
    * \brief Type of Schwarz smoother
153 | */
#define SCHWARZ_FORWARD 1 /**< Forward ordering */
155 #define SCHWARZ_BACKWARD 2 /**< Backward ordering */
156 #define SCHWARZ_SYMMETRIC 3 /**< Symmetric smoother */
157
158
159
     * \brief Definition of AMG types
160 */
161 #define CLASSIC_AMG 1 /**< classic AMG */
161 #define SA_AMG
                                  2 /**< smoothed aggregation AMG */</pre>
                                  3 /**< unsmoothed aggregation AMG */</pre>
163 #define UA AMG
164
165
    st \brief Definition of aggregation types
166
167
    #define PAIRWISE
                                  1 /**< pairwise aggregation */</pre>
168
169 #define VMB
                                  2 /**< VMB aggregation */
170
171
172
     * \brief Definition of cycle types
173
    */
3 /**< AMLI-cycle */
177 #define NL_AMLI_CYCLE
                                  4 /** Nonlinear AMLI-cycle */
178
179 /**
180 | * \brief Definition of standard smoother types
181 */
182 #define SMOOTHER_JACOBI 1 /**< Jacobi smoother */
#define SMOOTHER_GS
                                  2 /**< Gauss-Seidel smoother */
184 #define SMOOTHER_SGS
                                  3 /**< Symmetric Gauss-Seidel smoother */</pre>
185 #define SMOOTHER_CG
                                  4 /**< CG as a smoother */
#define SMOOTHER_SOR 5 /**< SOR smoother */
```

```
#define SMOOTHER_SSOR 6 /**< SSOR smoother */
#define SMOOTHER_GSOR 7 /**< GS + SOR smoother */
                                 8 /**< SGS + SSOR smoother */
9 /**< Polynomial smoother */
189 #define SMOOTHER_SGSOR
190 #define SMOOTHER_POLY
191 #define SMOOTHER_L1DIAG 10 /**< L1 norm diagonal scaling smoother */
192
193 /**
194 * \brief Definition of coarsening types
                              1 /**< Classical */
2 /**< Classical, with positive offdiags */</pre>
196 #define COARSE_RS
197 #define COARSE_RSP
                                     3 /**< Compatible relaxation */</pre>
198 #define COARSE_CR
                                     4 /**< Aggressive coarsening */
199
    #define COARSE_AC
200 #define COARSE_MIS
                                     5 /**< Aggressive coarsening based on MIS */
201
203 | * \brief Definition of interpolation types
204 */
#define INTERP_DIR 1 /**< Direct interpolation */
206 #define INTERP_STD 2 /**< Standard interpolation 207 #define INTERP_ENG 3 /**< energy minimization int
                                     2 /**< Standard interpolation */</pre>
                                     3 /**< energy minimization interpolation */</pre>
208
209
    st \brief Type of vertices (DOFs) for coarsening
210
211
                                     -5 /**< Cannot fit in aggregates */
212 #define GOPT
213 #define UNPT
                                     -1 /**< Undetermined points */
214 #define FGPT
                                     0 /**< Fine grid points */
215 #define CGPT
                                     1 /**< Coarse grid points */</pre>
216 #define ISPT
                                     2 /**< Isolated points */
217
218 /**
    * \brief Definition of smoothing order
219
220 */
221 #define NO_ORDER
222 #define CF_ORDER
                                     0 /**< Natural order smoothing */</pre>
                                     1 /**< C/F order smoothing */</pre>
223
224
225
     * \brief Type of ordering for smoothers
226
227 #define USERDEFINED 0 /**< User defined order */
228 #define CPFIRST
                                     1 /**< C-points first order */
                                    -1 /**< F-points first order */
229 #define FPFIRST
                                    12 /**< Ascending order */
230 #define ASCEND
                                21 /**< Descending order */
231 #define DESCEND
232
233
234 * \brief Some global constants
#define BIGREAL 1e+20 /**< A large real number */
237 #define SMALLREAL 1e-20 /**< A small real number */
238 #define SMALLREAL2 1e-40 /**< An extractal
                                 1e-40 /**< An extremely small real number */
239 #define MAX_REFINE_LVL 20 /**< Maximal refinement level */
```

```
240
    #define MAX_AMG_LVL
                                   20 /**< Maximal AMG coarsening level */
241
    #define MIN_CDOF
                                   20 /**< Minimal number of coarsest variables */
242
    #define MIN_CRATE
                                  0.9 /**< Minimal coarsening ratio */
                                 20.0 /**< Maximal coarsening ratio */
    #define MAX_CRATE
243
    #define MAX_RESTART
                                   20 /**< Maximal restarting number */
244
    #define MAX_STAG
                                       /**< Maximal number of stagnation times */
245
    #define STAG_RATIO
                                       /** Stagnation tolerance = tol*STAGRATIO */
246
                                 1e-4
                                 2000 /**< Smallest size for OpenMP version */
    #define OPENMP_HOLDS
247
248
249
    #endif
                                       /* end if for __FASP_MESSAGES__ */
250
251
252
    /*--
                End of File
                                      --*/
253
```

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
```

Bibliography

- J. Bramble. Multigrid methods, volume 294 of Pitman Research Notes in Mathematics Series. Longman Scientific & Technical, Harlow, 1993.
- [2] A. Brandt, S. McCormick, and J. Ruge. Algebraic multigrid (AMG) for automatic multigrid solution with application to geodetic computations, Report. Inst. Comp. Studies Colorado State Univ, 109:110, 1982.
- [3] J. Brannick and L. Zikatanov. Algebraic multigrid methods based on compatible relaxation and energy minimization. Lecture Notes in Computational Science and Engineering, 55:15, 2007.
- [4] M. Brezina, A. Cleary, R. Falgout, V. Henson, J. Jones, T. A. Manteuffel, S. F. McCormick, and J. W. Ruge. Algebraic multigrid based on element interpolation (AMGe). SIAM Journal on Scientific Computing, 22(5):1570–1592, 2000.
- [5] T. Chartier, R. Falgout, V. Henson, J. Jones, T. Manteuffel, S. McCormick, J. Ruge, and P. Vassilevski. Spectral AMGe (ρAMGe). SIAM J. Sci. Comput., 25(1):1–26, 2003.
- [6] R. Falgout and P. Vassilevski. On generalizing the algebraic multigrid framework. SIAM J. Numer. Anal., 42(4):1669–1693 (electronic), 2004.
- [7] V. Henson and P. Vassilevski. Element-free AMGe: general algorithms for computing interpolation weights in AMG. SIAM J. Sci. Comput., 23(2):629–650, 2001.
- [8] X. Hu, P. S. Vassilevski, and J. Xu. Comparative convergence analysis of nonlinear amli-cycle multigrid. SIAM J. Num. Anal, 51(2):1349-1369, 2013.
- [9] O. E. Livne. Coarsening by compatible relaxation. Numer. Linear Algebra Appl., 11(2-3):205-227, 2004.
- [10] J. Mellor-crummey and J. Garvin. Optimizing Sparse Matrix-Vector Product Computations Using Unroll and Jam. International Journal of High Performance Computing Applications, 18(2):225—-236, 2004.
- [11] A. Muresan and Y. Notay. Analysis of aggregation-based multigrid. SIAM Journal on Scientific Computing, 30(2):1082–1103, 2008.
- [12] S. Pissanetzky. Sparse matrix technology. Academic Press Inc. [Harcourt Brace Jovanovich Publishers], London, 1984.
- [13] J. Ruge and K. Stuben. Efficient solution of finite difference and finite element equations. In D. J. Paddon and H. Holstein, editors, Multigrid Methods for Integral and Differential Equations, volume 3, pages 169–212. Clarendon Press, 1985.
- [14] J. Ruge and K. Stüben. Algebraic multigrid. Multigrid methods, 3:73–130, 1987.
- [15] Y. Saad. Iterative methods for sparse linear systems. Society for Industrial and Applied Mathematics, Philadelphia, PA, second edition, 2003.

68 BIBLIOGRAPHY

[16] U. Trottenberg, C. Oosterlee, and A. Schüller. Multigrid. With contributions by A. Brandt, P. Oswald and K. Stuben, 2001.

- [17] P. Vaněk, J. Mandel, and M. Brezina. Algebraic multigrid by smoothed aggregation for second and fourth order elliptic problems. *Computing*, 56(3):179–196, 1996.
- [18] W. Wan, T. Chan, and B. Smith. An energy-minimizing interpolation for robust multigrid methods. SIAM Journal on Scientific Computing, 21(4):1632–1649, 2000.
- [19] J. Xu. Fast Poisson-Based Solvers for Linear and Nonlinear PDEs Jinchao Xu. In *Proceedings of the International Congress of Mathematicians*, pages 2886–2912, 2010.
- [20] J. Xu and L. Zikatanov. On an energy minimizing basis for algebraic multigrid methods. *Computing and Visualization in Science*, 7(3):121–127, 2004.