FASP User Guide

FASP Developer Team

Version 1.8.1

Contents

Chapter 1

Introduction

1.1 General description

The Fast Auxiliary Space Preconditioning (FASP) package provides C source files[1] to build a library of iterative solvers and preconditioners for the solution of large scale linear systems of equations. The components of the base FASP 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.

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,

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[1]The C code is in the C99 standard.

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; $H(\text{curl})/H(\text{div})$ 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-Seglman models; black-oil model in reservoir simulation; 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 manual[2] 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

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.

Downloading from SourceForge

The most updated version of FASP can be downloaded directly from

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

<div align="center">

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

</div>

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

<div align="center">

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

</div>

There are also many other third-party clients which provides Hg services, for example: EasyMercurial[5] (cross platform) and SourceTree[6] (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 book[7]. 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 pause[8], you should have obtained "*faspsolver*" in your current directory successfully. If you have already cloned the repository before, you can just pull a new version and update your local version with it: Go to your local "*faspsolver*" directory and then

```
"Pull a new version from BitBucket"
```

---

[3] Official website: https://bitbucket.org/
[4] Official website: http://mercurial.selenic.com/
[5] Official website: http://easyhg.org
[6] Official website: http://www.sourcetreeapp.com
[7] The hgbook, http://hgbook.red-bean.com/
[8] In 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.

```
$ hg pull

"Update you local version to the new version"
$ hg update
```

Windows OS

If you are using Windows, you may want to install TortoiseHg[9]. 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

<p align="center">https://faspusers@bitbucket.org/fasp/faspsovler</p>

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: (1) go to the "faspsolver" directory; (2) modify the "*FASP.mk.example*" file to math your system and save it as "FASP.mk"; (3) then execute:

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

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

In order to be sure that everything went all right, you can go to the "faspsolver/test" directory and try to run a test problem as follows:

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

---

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

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                   # Compile the library (after "make config")
$ make install           # install FASP libraries and related files
$ make uninstall         # Remove installed files by "make install"
$ make headers           # Generate function declarations automatically
$ make docs              # Generate the FASP documentation with Doxygen
$ make clean             # Remove obj files but retain configuration options
$ make distclean         # Clean and completely removes the build directory
$ make version           # Show version information
$ make help              # Show this screen
===================================================
```

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.
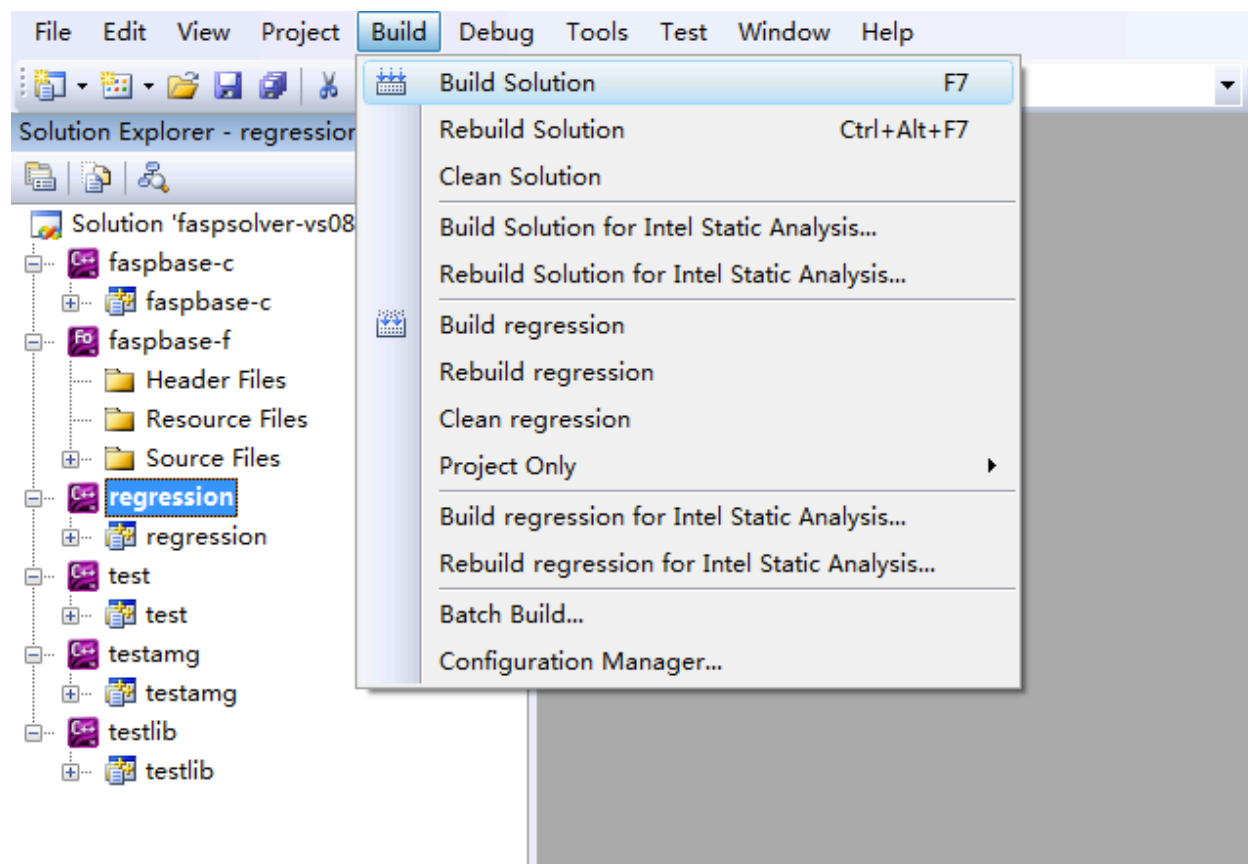
Figure 1.1: Build FASP using Visual Studio 2008.

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

If you are using other versions of Visual Studio (like VS05 or VS12), we advise NOT to convert the "VS08" files to your VS version because the FASP source files might be removed by the Visual Studio automatically. In such case, we recommend that you create your own version to build all the libraries and test programs.

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

1. "faspbase-c" contains all the ".c" and ".inl" files in the directory "./base/src/". You should add "./base/include" in Additional Directories. This project contains the core subroutines of faspsolver.

2. "faspbase-f" contains all the ".f" files in "./base/extra/sparsekit".

3. "testlib" contains all the ".c" files in "./test/src/". You should add "./test/include" in Additional Directories.

4. "test" is an executing program for test purpose in FASP. The source file is "./test/main/test.c".

5. "regression" is another executing program, which contains several methods to test the problems. The source file is "./test/main/regression.c".

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

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

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

Using a TCL based GUI for installation

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

```
$ wish FASP_install.tcl
```

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

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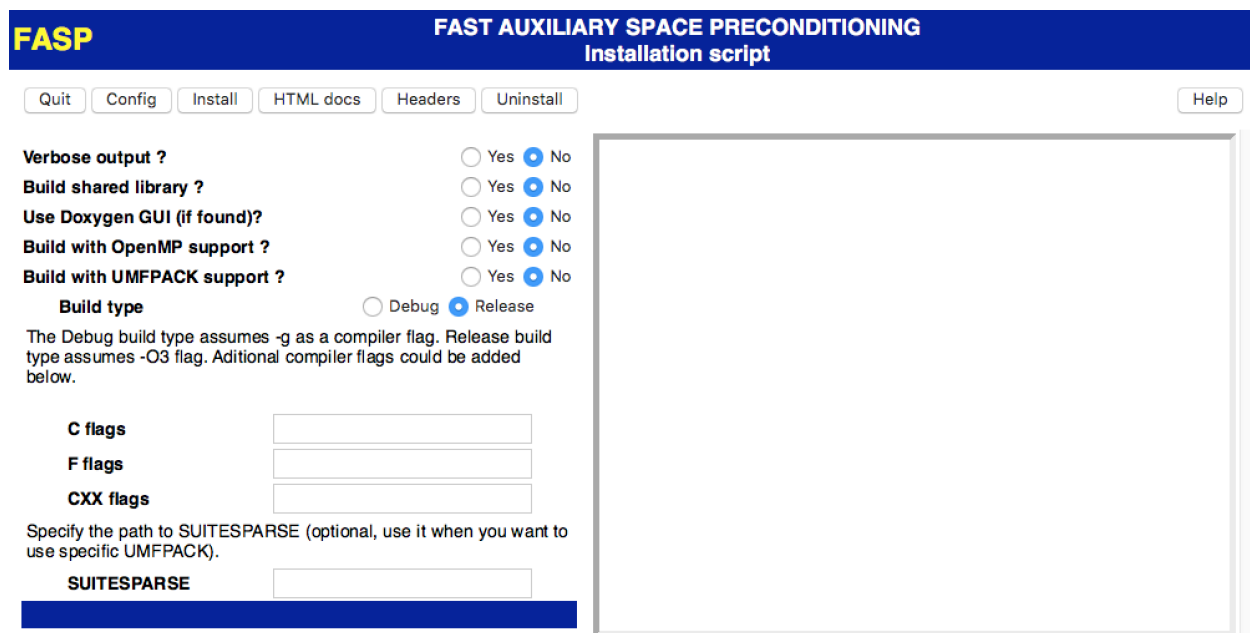
Figure 1.2: Install FASP using the TCL GUI on Mac OS X El Capitan.

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 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 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 from disk a symmetric positive definite matrix A and right-hand side b then we solve $Ax = b$ using the classical AMG method [2, 13, 14]; see §3.7. 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.

```
1  /*! \file poisson-amg.c
2   *
3   *  \brief The first test example for FASP: using AMG to solve
4   *         the discrete Poisson equation from P1 finite element.
```

```
 5   *          C version.
 6   *
 7   *   \note   AMG example for FASP: C version
 8   *
 9   *   Solving the Poisson equation (P1 FEM) with AMG
10   */
11
12  #include "fasp.h"
13  #include "fasp_functs.h"
14
15  /**
16   * \fn int main (int argc, const char * argv[])
17   *
18   * \brief This is the main function for the first example.
19   *
20   * \author Chensong Zhang
21   * \date    12/21/2011
22   *
23   * Modified by Chensong Zhang on 09/22/2012
24   */
25  int main (int argc, const char * argv[])
26  {
27      input_param      inparam;  // parameters from input files
28      AMG_param        amgparam; // parameters for AMG
29
30      printf("\n=======================================");
31      printf("\n||   FASP: AMG example -- C version    ||");
32      printf("\n=======================================\n\n");
33
34      // Step 0. Set parameters: We can use ini/amg.dat
35      fasp_param_set(argc, argv, &inparam);
36      fasp_param_init(&inparam, NULL, &amgparam, NULL, NULL);
37
38      // Set local parameters using the input values
39      const int print_level = inparam.print_level;
40
41      // Step 1. Get stiffness matrix and right-hand side
42      // Read A and b -- P1 FE discretization for Poisson. The location
43      // of the data files is given in "ini/amg.dat".
44      dCSRmat A;
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);
55      datafile2="rhs_FE.dat"; strcat(filename2,datafile2);
56
57      fasp_dcsrvec2_read(filename1,filename2,&A,&b);
```

```
58
59        // Step 2. Print problem size and AMG 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            fasp_param_amg_print(&amgparam);
64        }
65
66        // Step 3. Solve the system with AMG as an iterative solver
67        // Set the initial guess to be zero and then solve it
68        // with AMG method as an iterative procedure
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
74        // Step 4. Clean up memory
75        fasp_dcsr_free(&A);
76        fasp_dvec_free(&b);
77        fasp_dvec_free(&x);
78
79        return FASP_SUCCESS;
80    }
81
82   /*---------------------------------*/
83   /*--        End of File         --*/
84   /*---------------------------------*/
```

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

- Line 1 tells the Doxygen documentation system 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 §2.4. 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.

- 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 49–58 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 §3.7.

- 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 as follows:

```
=====================================
||    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
b: n = 3969


        Parameters in AMG_param
_____

AMG print level:                 2
AMG max num of iter:             1
AMG type:                        1
AMG tolerance:                   1.00e−06
AMG max levels:                  20
AMG cycle type:                  1
AMG coarse solver type:          0
AMG scaling of coarse correction: 0
AMG smoother type:               2
AMG smoother order:              1
AMG num of presmoothing:         1
AMG num of postsmoothing:        1
AMG coarsening type:             1
AMG interpolation type:          1
AMG dof on coarsest grid:        500
AMG strong threshold:            0.3000
AMG truncation threshold:        0.2000
AMG max row sum:                 0.9000
AMG aggressive levels:           0
AMG aggressive path:             1
```

```
_____


Calling classical AMG ...
_____

  Level    Num of rows    Num of nonzeros    Avg. NNZ / row
_____

    0            3969              27281             6.87
    1            1985              28523            14.37
    2             541               7951            14.70
    3             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 |   1.000000e+00   |   7.514358e+00   |      -.--
    1 |   9.851978e-03   |   7.403129e-02   |     0.0099
    2 |   3.507451e-04   |   2.635624e-03   |     0.0356
    3 |   1.764023e-05   |   1.325550e-04   |     0.0503
    4 |   8.820794e-07   |   6.628261e-06   |     0.0500
Number of iterations = 4 with relative residual 8.820794e-07.
AMG solve costs 0.0017 seconds.
AMG totally costs 0.0091 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.

```fortran
!> \file poisson-amg.f90
!> \brief The first test example for FASP: using AMG to solve
!>        the discrete Poisson equation from P1 finite element.
!>        F90 version.
!>
!> \note  AMG example for FASP: F90 version
!>
!> Solving the Poisson equation (P1 FEM) with AMG
!>
!> \author Chensong Zhang
!> \date   12/21/2011

program test

  implicit none

  double precision, dimension(:), allocatable :: u, b, a
  integer,          dimension(:), allocatable :: ia, ja

  integer          :: iufile, n, nnz, i, prt_lvl, maxit
  double precision :: tol
```

```fortran
22
23     print *, ""
24     write(*,"(A)") "======================================="
25     write(*,"(A)") "||   FASP: AMG example -- F90 version   ||"
26     write(*,"(A)") "======================================="
27     print *, ""
28
29     ! Step 0: user defined variables
30     prt_lvl = 3
31     maxit = 100
32     tol = 1.0d-6
33     iufile = 1
34
35     ! Step 1: read A and b
36
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     read(iufile,*) (ia(i),i=1,n+1)
43
44     nnz=ia(n+1)-ia(1)
45     allocate(ja(1:nnz),a(1:nnz))
46     read(iufile,*) (ja(i),i=1,nnz)
47     read(iufile,*) (a(i),i=1,nnz)
48
49     close(iufile)
50
51     !===> Read data b from file
52     open(unit=iufile,file='../data/rhs_FE.dat')
53
54     read(iufile,*) n
55     allocate(b(1:n))
56     read(iufile,*) (b(i),i=1,n)
57
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     ! Step 2: Solve the system
65
66     !===> Initial guess
67     allocate(u(1:n))
68     u=0.0d0
69     call fasp_fwrapper_amg(n,nnz,ia,ja,a,b,u,tol,maxit,prt_lvl)
70
71     ! Step 3: Clean up memory
72     deallocate(ia,ja,a)
73     deallocate(b,u)
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).

```c
1    /*! \file poisson-its.c
2     *  \brief The second test example for FASP: using ITS to solve
3     *          the discrete Poisson equation from P1 finite element.
4     *
5     *  \note  ITS example for FASP: C version
6     *
7     *  Solving the Poisson equation (P1 FEM) with iterative methods
8     */
9
10   #include "fasp.h"
11   #include "fasp_functs.h"
12
13   /**
14    * \fn int main (int argc, const char * argv[])
15    *
16    * \brief This is the main function for the second example.
17    *
18    * \author Feiteng Huang
19    * \date   04/13/2012
20    *
21    * Modified by Chensong Zhang on 09/22/2012
22    */
23   int main (int argc, const char * argv[])
24   {
25       input_param           inparam;  // parameters from input files
26       itsolver_param        itparam;  // parameters for itsolver
27
28       printf("\n=======================================");
29       printf("\n||   FASP: ITS example -- C version   ||");
30       printf("\n=======================================\n\n");
31
32       // Step 0. Set parameters: We can use ini/its.dat
33       fasp_param_set(argc, argv, &inparam);
34       fasp_param_init(&inparam, &itparam, NULL, NULL, NULL);
35
36       // Set local parameters
37       const int print_level = inparam.print_level;
38
39       // Step 1. Get stiffness matrix and right-hand side
```

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

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
Solver tolerance:                 1.00e−06
Solver stopping type:             1
─────────────────────────────────────────────────


Calling PCG solver (CSR) ...
─────────────────────────────────────────────────
It Num |    ||r||/||b||    |       ||r||      |   Conv. Factor
─────────────────────────────────────────────────
      0 |   1.000000e+00   |   7.514358e+00   |     −.−−
      1 |   5.078029e−01   |   3.815813e+00   |    0.5078
      2 |   3.728856e−01   |   2.801996e+00   |    0.7343
      3 |   3.359470e−01   |   2.524426e+00   |    0.9009
      4 |   2.590574e−01   |   1.946650e+00   |    0.7711
      5 |   2.380797e−01   |   1.789016e+00   |    0.9190
      6 |   1.992579e−01   |   1.497295e+00   |    0.8369
      7 |   1.847971e−01   |   1.388631e+00   |    0.9274
      8 |   1.619777e−01   |   1.217158e+00   |    0.8765
      9 |   1.513446e−01   |   1.137257e+00   |    0.9344
     10 |   1.364935e−01   |   1.025661e+00   |    0.9019
     11 |   1.283425e−01   |   9.644117e−01   |    0.9403
     12 |   1.179652e−01   |   8.864327e−01   |    0.9191
     13 |   1.115146e−01   |   8.379605e−01   |    0.9453
     14 |   1.038726e−01   |   7.805360e−01   |    0.9315
     15 |   9.863412e−02   |   7.411721e−01   |    0.9496
     16 |   9.277360e−02   |   6.971341e−01   |    0.9406
     17 |   8.842679e−02   |   6.644706e−01   |    0.9531
     18 |   8.378399e−02   |   6.295829e−01   |    0.9475
     19 |   8.011023e−02   |   6.019770e−01   |    0.9562
     20 |   7.633221e−02   |   5.735875e−01   |    0.9528
     21 |   7.317756e−02   |   5.498824e−01   |    0.9587
     22 |   7.003292e−02   |   5.262524e−01   |    0.9570
     23 |   6.728610e−02   |   5.056119e−01   |    0.9608
```

```
24  |   6.461736e−02   |   4.855580e−01   |     0.9603
25  |   6.219614e−02   |   4.673640e−01   |     0.9625
26  |   5.989276e−02   |   4.500557e−01   |     0.9630
27  |   5.773520e−02   |   4.338429e−01   |     0.9640
28  |   5.571758e−02   |   4.186818e−01   |     0.9651
29  |   5.377630e−02   |   4.040944e−01   |     0.9652
30  |   5.198586e−02   |   3.906404e−01   |     0.9667
31  |   5.022413e−02   |   3.774021e−01   |     0.9661
32  |   4.861699e−02   |   3.653255e−01   |     0.9680
33  |   4.700598e−02   |   3.532197e−01   |     0.9669
34  |   4.554874e−02   |   3.422696e−01   |     0.9690
35  |   4.406559e−02   |   3.311246e−01   |     0.9674
36  |   4.273253e−02   |   3.211075e−01   |     0.9697
37  |   4.135901e−02   |   3.107864e−01   |     0.9679
38  |   4.013076e−02   |   3.015569e−01   |     0.9703
39  |   3.885861e−02   |   2.919975e−01   |     0.9683
40  |   3.776252e−02   |   2.837611e−01   |     0.9718
41  |   3.678565e−02   |   2.764205e−01   |     0.9741
42  |   3.648645e−02   |   2.741722e−01   |     0.9919
43  |   3.725368e−02   |   2.799375e−01   |     1.0210
44  |   3.922957e−02   |   2.947850e−01   |     1.0530
45  |   4.003513e−02   |   3.008383e−01   |     1.0205
46  |   3.683219e−02   |   2.767703e−01   |     0.9200
47  |   3.161285e−02   |   2.375503e−01   |     0.8583
48  |   2.944107e−02   |   2.212307e−01   |     0.9313
49  |   2.961834e−02   |   2.225628e−01   |     1.0060
50  |   2.774118e−02   |   2.084571e−01   |     0.9366
```

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 conjugate gradient (PCG) method.

```
1   /*! \file poisson-pcg.c
2    *  \brief The third test example for FASP: using PCG to solve
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    */
10
11  #include "fasp.h"
12  #include "fasp_functs.h"
13
14  /**
15   * \fn int main (int argc, const char * argv[])
16   *
```

```
17    * \brief This is the main function for the third example.
18    *
19    * \author Feiteng Huang
20    * \date   05/17/2012
21    *
22    * Modified by Chensong Zhang on 09/22/2012
23    */
24   int main (int argc, const char * argv[])
25   {
26       input_param         inparam;  // parameters from input files
27       itsolver_param      itparam;  // parameters for itsolver
28       AMG_param           amgparam; // parameters for AMG
29       ILU_param           iluparam; // parameters for ILU
30
31       printf("\n========================================");
32       printf("\n||   FASP: PCG example -- C version   ||");
33       printf("\n========================================\n\n");
34
35       // Step 0. Set parameters: We can use ini/pcg.dat
36       fasp_param_set(argc, argv, &inparam);
37       fasp_param_init(&inparam, &itparam, &amgparam, &iluparam, NULL);
38
39       // Set local parameters
40       const SHORT print_level = itparam.print_level;
41       const SHORT pc_type     = itparam.precond_type;
42       const SHORT stop_type   = itparam.stop_type;
43       const INT   maxit       = itparam.maxit;
44       const REAL  tol         = itparam.tol;
45
46       // Step 1. Get stiffness matrix and right-hand side
47       // Read A and b -- P1 FE discretization for Poisson. The location
48       // of the data files is given in "ini/pcg.dat".
49       dCSRmat A;
50       dvector b, x;
51       char filename1[512], *datafile1;
52       char filename2[512], *datafile2;
53
54       // Read the stiffness matrix from matFE.dat
55       strncpy(filename1,inparam.workdir,128);
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
62       fasp_dcsrvec2_read(filename1,filename2,&A,&b);
63
64       // Step 2. Print problem size and PCG parameters
65       if (print_level>PRINT_NONE) {
66           printf("A: m = %d, n = %d, nnz = %d\n", A.row, A.col, A.nnz);
67           printf("b: n = %d\n", b.row);
68           fasp_param_solver_print(&itparam);
69       }
```

```
70
71      // Setp 3. Setup preconditioner
72      // Preconditioner type is determined by pc_type
73      precond *pc = fasp_precond_setup(pc_type, &amgparam, &iluparam, &A);
74
75      // Step 4. Solve the system with PCG as an iterative solver
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
78      // calls the abstract iterative method interface; see possion-its.c for
79      // more details.
80      fasp_dvec_alloc(A.row, &x);
81      fasp_dvec_set(A.row, &x, 0.0);
82
83      fasp_solver_dcsr_pcg(&A, &b, &x, pc, tol, maxit, stop_type, print_level);
84
85      // Step 5. Clean up memory
86      if (pc_type!=PREC_NULL) fasp_mem_free(pc->data);
87      fasp_dcsr_free(&A);
88      fasp_dvec_free(&b);
89      fasp_dvec_free(&x);
90
91      return FASP_SUCCESS;
92  }
93
94  /*--------------------------------*/
95  /*--        End of File          --*/
96  /*--------------------------------*/
```

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):

```
||   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:             2
Solver type:                    1
Solver precond type:            2
Solver max num of iter:         500
Solver tolerance:               1.00e-06
Solver stopping type:           1
––––––––––––––––––––––––––––––––––––––––––––––––


––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
  Level    Num of rows    Num of nonzeros    Avg. NNZ / row
––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
    0           3969            27281               6.87
    1           1985            28523              14.37
    2            541             7951              14.70
    3            141             1803              12.79
––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
  Grid complexity = 1.672  |  Operator complexity = 2.403
––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
Classical AMG setup costs 0.0042 seconds.
––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
It Num |   ||r||/||b||   |      ||r||     |  Conv. Factor
––––––––––––––––––––––––––––––––––––––––––––––––––––––––––––
     0 |  1.000000e+00   |  7.514358e+00  |     -.--
     1 |  1.156153e-02   |  8.687750e-02  |    0.0116
     2 |  3.127181e-04   |  2.349876e-03  |    0.0270
     3 |  4.813471e-06   |  3.617014e-05  |    0.0154
     4 |  5.312526e-08   |  3.992022e-07  |    0.0110
Number of iterations = 4 with relative residual 5.312526e-08.
```

2.4   How to change parameters in 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:

```
 1  %————————————————————————————————————%
 2  % input parameters                    %
 3  % lines starting with % are comments   %
 4  % must have spaces around the equal sign "="   %
 5  %————————————————————————————————————%
 6
 7  workdir = ../data/    % work directory, no more than 128 characters
 8  print_level = 3        % 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
16                                    % UA unsmoothed aggregation
17  AMG_cycle_type          = V      % V V−cycle | W W−cycle
18                                    % A AMLI−cycle | NA Nonlinear AMLI−cycleA
19  AMG_tol                 = 1e−8   % tolerance for AMG
20  AMG_maxit               = 100    % number of AMG iterations
21  AMG_levels              = 20     % max number of levels
22  AMG_coarse_dof          = 500    % max number of coarse degrees of freedom
23  AMG_coarse_scaling      = OFF    % switch of scaling of the coarse grid correction
24  AMG_amli_degree         = 2      % degree of the polynomial used by AMLI cycle
25  AMG_nl_amli_krylov_type = 6      % Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCG
26
27  %————————————————————————————————————%
28  % parameters for AMG smoothing                %
29  %————————————————————————————————————%
30
31  AMG_smoother            = GS     % GS | JACOBI | SGS
32                                    % SOR | SSOR | GSOR | SGSOR | POLY
33  AMG_ILU_levels          = 0      % number of levels using ILU smoother
34  AMG_Schwarz_levels      = 0      % number of levels using Schwarz smoother
35  AMG_relaxation          = 1.1    % relaxation parameter for SOR smoother
36  AMG_polynomial_degree   = 3      % degree of the polynomial smoother
37  AMG_presmooth_iter      = 2      % number of presmoothing sweeps
38  AMG_postsmooth_iter     = 2      % number of postsmoothing sweeps
39
40  %————————————————————————————————————%
41  % parameters for classical AMG SETUP          %
42  %————————————————————————————————————%
43
44  AMG_coarsening_type     = 1      % 1 Modified RS
45                                    % 3 Compatible Relaxation
46                                    % 4 Aggressive
47  AMG_interpolation_type  = 1      % 1 Direct | 2 Standard | 3 Energy−min
48  AMG_strong_threshold    = 0.6    % Strong threshold
49  AMG_truncation_threshold = 0.4   % Truncation threshold
50  AMG_max_row_sum         = 0.9    % Max row sum
51
52  %————————————————————————————————————%
53  % parameters for aggregation−type AMG SETUP    %
```

```
54  %————————————————————————————————%
55
56  AMG_strong_coupled       = 0.08    % Strong coupled threshold
57  AMG_max_aggregation      = 20      % Max size of aggregations
58  AMG_tentative_smooth     = 0.67    % Smoothing factor for tentative prolongation
59  AMG_smooth_filter        = OFF     % Switch for filtered matrix for smoothing
```

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 (§3.7).

- Line 56–59 gives the parameters for the setup phase of the aggregation-base AMG methods (§3.7).

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

```
AMG_type                 = SA
```

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

```
===================================
||   FASP: 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
b: n = 3969


        Parameters in AMG_param
———————————————————————————————————————————
AMG print level:              3
AMG max num of iter:          100
AMG type:                     2
AMG tolerance:                1.00e−08
```

```
AMG max levels:                    20
AMG cycle type:                    1
AMG coarse solver type:            0
AMG scaling of coarse correction:  0
AMG smoother type:                 2
AMG smoother order:                1
AMG num of presmoothing:           2
AMG num of postsmoothing:          2
Aggregation type:                  1
Aggregation number of pairs:       2
Aggregation quality bound:         8.00
_____


Calling SA AMG ...
_____

   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 seconds.
_____

It Num |    ||r||/||b||    |       ||r||      |  Conv. Factor
_____

      0 |   1.000000e+00    |   7.514358e+00   |    -.--
      1 |   4.345463e-02    |   3.265336e-01   |    0.0435
      2 |   8.041967e-03    |   6.043022e-02   |    0.1851
      3 |   3.808810e-03    |   2.862076e-02   |    0.4736
      4 |   1.838990e-03    |   1.381883e-02   |    0.4828
      5 |   8.675952e-04    |   6.519421e-03   |    0.4718
      6 |   4.089274e-04    |   3.072827e-03   |    0.4713
      7 |   1.939823e-04    |   1.457653e-03   |    0.4744
      8 |   9.276723e-05    |   6.970862e-04   |    0.4782
      9 |   4.471799e-05    |   3.360270e-04   |    0.4820
     10 |   2.171249e-05    |   1.631554e-04   |    0.4855
     11 |   1.060934e-05    |   7.972239e-05   |    0.4886
     12 |   5.212246e-06    |   3.916668e-05   |    0.4913
     13 |   2.572464e-06    |   1.933042e-05   |    0.4935
     14 |   1.274466e-06    |   9.576797e-06   |    0.4954
     15 |   6.333891e-07    |   4.759512e-06   |    0.4970
     16 |   3.155926e-07    |   2.371476e-06   |    0.4983
     17 |   1.575755e-07    |   1.184079e-06   |    0.4993
     18 |   7.881043e-08    |   5.922098e-07   |    0.5001
     19 |   3.947044e-08    |   2.965950e-07   |    0.5008
     20 |   1.978978e-08    |   1.487075e-07   |    0.5014
     21 |   9.931176e-09    |   7.462641e-08   |    0.5018
Number of iterations = 21 with relative residual 9.931176e-09.
AMG solve costs 0.0053 seconds.
AMG totally costs 0.0083 seconds.
```

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

```
=============================================
||   FASP: AMG example −− C version    ||
=============================================

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

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

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

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

Chapter 3

Data structures and basic usage

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

3.1   Vectors and sparse matrices

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

Vectors

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

```
330
331  /**
332   * \struct dvector
333   * \brief Vector with n entries of REAL type
334   */
335  typedef struct dvector{
336
337      //! number of rows
338      INT row;
339
340      //! 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*

$$\begin{pmatrix} 1 & 1.5 & 0 & 0 & 12 \\ 0 & 1 & 6 & 7 & 1 \\ 3 & 0 & 6 & 0 & 0 \\ 1 & 0 & 2 & 0 & 5 \end{pmatrix}$$

(i) COO format

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

```
192
193   /**
194    * \struct dCOOmat
195    * \brief Sparse matrix of REAL type in COO (or IJ) format
196    *
197    * Coordinate Format (I,J,A)
198    *
199    * \note The starting index of A is 0.
200    * \note Change I to rowind, J to colind. To avoid with complex.h confliction on I.
201    */
202   typedef struct dCOOmat{
203
204       //! row number of matrix A, m
205       INT row;
206
207       //! column of matrix A, n
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
135    * \brief Sparse matrix of REAL type in CSR format
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
146        //! column of matrix A, n
147        INT col;
148
149        //! number of nonzero entries
150        INT nnz;
151
152        //! integer array of row pointers, the size is m+1
153        INT *IA;
154
155        //! integer array of column indexes, the size is nnz
156        INT *JA;
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

$$IA = \left\| \, 0 \, \right\| \, 3 \, \left\| \, 7 \, \right\| \, 9 \, \left\| \, 12 \, \right\|$$

- JA is of size $IA(5) - 1 = 12$

$$JA = \left\| \, 0 \, \right| \, 1 \, \left| \, 4 \, \right\| \, 1 \, \left| \, 3 \, \right| \, 2 \, \left| \, 4 \, \right\| \, 0 \, \left| \, 2 \, \right\| \, 2 \, \left| \, 4 \, \right| \, 0 \, \left\| \right.$$

- val is of the same size as JA and

$$val = \left\| \, 1. \, \right| \, 1.5 \, \left| \, 12. \, \right\| \, 1. \, \left| \, 7. \, \right| \, 6. \, \left| \, 1. \, \right\| \, 3. \, \left| \, 6. \, \right\| \, 2. \, \left| \, 5. \, \right| \, 1. \, \left\| \right.$$

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:

$$IA = \left\| \; 0 \; \right\| \; 2 \; \left\| \; 5 \; \right\| \; 7 \; \right\|,$$

$$JA = \left\| \; 0 \; \right| \; 2 \; \left\| \; 1 \; \right| \; 2 \; \left| \; 3 \; \right\| \; 1 \; \left| \; 3 \; \right\| \; 0 \; \left| \; 1 \; \right| \; 2 \; \right\|,$$

and

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

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    */
258   typedef struct dCSRLmat{
259
260       //! number of rows
261       INT row;
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
270        INT dif;
271
272        //! nz_diff[i]: the i-th different value in 'nzrow'
273        INT *nz_diff;
274
275        //! row index of the matrix (length-grouped): rows with same nnz are together
276        INT *index;
277
278        //! j in {start[i],...,start[i+1]-1} means nz_diff[i] nnz in index[j]-row
279        INT *start;
280
281        //! column indices of all the nonzeros
282        INT *ja;
283
284        //! values of all the nonzero entries
285        REAL *val;
```

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

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:

$$IA = \left\| \; 0 \; \right\| \; 8 \; \left\| \; 16 \; \right\|,$$

$$JA = \left\| \; 0 \; \right| \; 1 \; \left\| \; 0 \; \right| \; 1 \; \right\|,$$

and

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

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
80    * \brief Block REAL CSR matrix format
81    *
82    * \note The starting index of A is 0.
83    */
84   typedef struct block_dCSRmat {
85
86       //! row number of blocks in A, m
87       INT brow;
88
89       //! column number of blocks A, n
90       INT bcol;
91
92       //! blocks of dCSRmat, point to blocks[brow][bcol]
93       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 ,
837                           dCSRmat *A ,
838                           dvector *b );
839
840  void fasp_dcsrvec2_read ( const char *filemat ,
841                           const char *filerhs ,
842                           dCSRmat *A ,
843                           dvector *b  );
844
845  void fasp_dcsr_read ( const char *filename ,
846                        dCSRmat *A );
847
848  void fasp_dcoo_read ( const char *filename ,
849                        dCSRmat *A );
850
851  void fasp_dcoo1_read ( const char *filename ,
852                         dCOOmat *A );
853
854  void fasp_dcoo_shift_read ( const char *filename ,
855                              dCSRmat *A );
856
857  void fasp_dmtx_read ( const char *filename ,
858                        dCSRmat *A );
859
860  void fasp_dmtxsym_read ( const char *filename ,
861                           dCSRmat *A );
862
863  void fasp_dstr_read ( const char *filename ,
864                        dSTRmat *A );
865
866  void fasp_dbsr_read ( const char *filename ,
867                        dBSRmat *A );
868
869  void fasp_dvecind_read ( const char *filename ,
870                           dvector *b );
871
872  void fasp_dvec_read ( const char *filename ,
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
885  void fasp_dcsrvec2_write ( const char *filemat ,
886                            const char *filerhs ,
887                            dCSRmat *A ,
```

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

```
941  void fasp_vector_write (const char *filerhs,
942                                void *b,
943                                INT  flag);
944
945  void fasp_hb_read (const char *input_file,
946                     dCSRmat *A,
947                     dvector *b);
```

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 BLAS

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

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

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

3.5   Iterative methods

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

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

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

```
463       // ILU setup for whole matrix
464       ILU_data LU;
465       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;
469
470        // set preconditioner
471        precond pc;
472        pc.data = &LU;
473        pc.fct  = fasp_precond_ilu;
474
475        // call iterative solver
476        status = fasp_solver_dcsr_itsolver(A,b,x,&pc,itparam);
```

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 §2.4. 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 now left with no choice but introducing "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 */
```

Possible "itsolver_type" includes:

```
/**
 * \brief Definition of solver types for iterative methods
 */
#define SOLVER_DEFAULT          0  /**< Use default solver in FASP */
//-------------------------------------------------------------------------------
```

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

3.6   Geometric multigrid

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 $x_i = ih$, $y_j = jh$ $(i, j = 0, 1, \ldots, n)$. 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:

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

The sample code for this solver can be found in "`test/main/testgmg.c`" and a piece of the source code is listed as follows:

```
254            case 2: // 2 dimension
255
256                u = (REAL *)malloc((nx+1)*(ny+1)*sizeof(REAL));
257                fasp_array_set((nx+1)*(ny+1), u, 0.0);
258
259                b = (REAL *)malloc((nx+1)*(ny+1)*sizeof(REAL));
260                for (i = 0; i <= nx; i++) {
261                    for (j = 0; j <= ny; j++) {
262                        b[j*(nx+1)+i] = h*h*f2d(i, j, nx, ny);
263                    }
264                }
265
266                switch (method) {
267
268                    case 1: // V-cycle
269                        fasp_poisson_gmg_2D(u, b, nx, ny, maxlevel, rtol, prtlvl);
270                        break;
271
272                    case 2: // FMG
273                        fasp_poisson_fgmg_2D(u, b, nx, ny, maxlevel, rtol, prtlvl);
274                        break;
275
276                    case 3: // PCG
277                        fasp_poisson_pcg_gmg_2D(u, b, nx, ny, maxlevel, rtol, prtlvl);
278                        break;
279
280                }
281
282            break;
```

3.7 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).

```c
42      const SHORT    max_levels  = param->max_levels;
43      const SHORT    prtlvl      = param->print_level;
44      const SHORT    amg_type    = param->AMG_type;
45      const SHORT    cycle_type  = param->cycle_type;
46      const INT      nnz = A->nnz, m = A->row, n = A->col;
47
48      // local variables
49      SHORT          status;
50      AMG_data *     mgl = fasp_amg_data_create(max_levels);
51      REAL           AMG_start, AMG_end;
52
53  #if DEBUG_MODE > 0
54      printf("### DEBUG: %s ...... [Start]\n", __FUNCTION__);
55  #endif
56
57      if ( prtlvl > PRINT_NONE ) fasp_gettime(&AMG_start);
58
59      // check matrix data
60      if ( m != n ) {
61          printf("### ERROR: A is not a square matrix!\n");
62          fasp_chkerr(ERROR_MAT_SIZE, __FUNCTION__);
63      }
64
65      if ( nnz <= 0 ) {
66          printf("### ERROR: A has no nonzero entries!\n");
67          fasp_chkerr(ERROR_MAT_SIZE, __FUNCTION__);
68      }
69
70      // Step 0: initialize mgl[0] with A, b and x
71      mgl[0].A = fasp_dcsr_create(m, n, nnz);
72      fasp_dcsr_cp(A, &mgl[0].A);
73
74      mgl[0].b = fasp_dvec_create(n);
75      fasp_dvec_cp(b, &mgl[0].b);
76
77      mgl[0].x = fasp_dvec_create(n);
78      fasp_dvec_cp(x, &mgl[0].x);
79
80      // Step 1: AMG setup phase
81      switch (amg_type) {
82
83          case SA_AMG: // Smoothed Aggregation AMG setup
```

```
84              if ( prtlvl > PRINT_NONE ) printf("\nCalling SA AMG ...\n");
85              status = fasp_amg_setup_sa(mgl, param); break;
86
87          case UA_AMG: // Unsmoothed Aggregation AMG setup
88              if ( prtlvl > PRINT_NONE ) printf("\nCalling UA AMG ...\n");
89              status = fasp_amg_setup_ua(mgl, param); break;
90
91          default: // Classical AMG setup
92              if ( prtlvl > PRINT_NONE ) printf("\nCalling classical AMG ...\n");
93              status = fasp_amg_setup_rs(mgl, param);
94
95      }
96
97      // Step 2: AMG solve phase
98      if ( status == FASP_SUCCESS ) { // call a multilevel cycle
99
100         switch (cycle_type) {
101
102             case AMLI_CYCLE: // AMLI-cycle
103                 fasp_amg_solve_amli(mgl, param); break;
104
105             case NL_AMLI_CYCLE: // Nonlinear AMLI-cycle
106                 fasp_amg_solve_nl_amli(mgl, param); break;
107
108             default: // V,W-cycles (determined by param)
109                 fasp_amg_solve(mgl, param); break;
110
111         }
112
113         fasp_dvec_cp(&mgl[0].x, x);
114
115     }
116
117     else { // call a backup solver
118
119         if ( prtlvl > PRINT_MIN ) {
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, prtlvl);
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 §2.4.

- 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  %————————————————————————————%
56  % parameters for multilevel iteration          %
57  %————————————————————————————%
58
59  AMG_type                 = C       % C classic AMG
60                                     % SA smoothed aggregation
61                                     % UA unsmoothed aggregation
62  AMG_cycle_type           = V       % V V−cycle | W W−cycle
63                                     % A AMLI−cycle | NA Nonlinear AMLI−cycleA
64  AMG_tol                  = 1e−6    % tolerance for AMG
65  AMG_maxit                = 1       % number of AMG iterations
66  AMG_levels               = 20      % max number of levels
67  AMG_coarse_dof           = 500     % max number of coarse degrees of freedom
68  AMG_coarse_solver        = 0       % coarsest solver: 0 iterative |
69                                     % 31 SuperLU | 32 UMFPack | 33 MUMPS
70  AMG_coarse_scaling       = OFF     % switch of scaling of the coarse grid correction
71  AMG_amli_degree          = 2       % degree of the polynomial used by AMLI cycle
72  AMG_nl_amli_krylov_type  = 6       % Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCG
73
74  %————————————————————————————%
75  % parameters for AMG smoothing                  %
76  %————————————————————————————%
77
78  AMG_smoother             = GS      % GS | JACOBI | SGS SOR | SSOR |
79                                     % GSOR | SGSOR | POLY | L1DIAG | CG
80  AMG_smooth_order         = CF      % NO: natural order | CF: CF order
81  AMG_ILU_levels           = 0       % number of levels using ILU smoother
82  AMG_Schwarz_levels       = 0       % number of levels using Schwarz smoother
83  AMG_relaxation           = 1.0     % relaxation parameter for SOR smoother
84  AMG_polynomial_degree    = 3       % degree of the polynomial smoother
85  AMG_presmooth_iter       = 1       % number of presmoothing sweeps
86  AMG_postsmooth_iter      = 1       % number of postsmoothing sweeps
87
88  %————————————————————————————%
89  % parameters for classical AMG SETUP            %
90  %————————————————————————————%
91
92  AMG_coarsening_type      = 1       % 1 Modified RS
93                                     % 3 Compatible Relaxation
94                                     % 4 Aggressive
```

```
 95   AMG_interpolation_type   = 1        % 1 Direct | 2 Standard | 3 Energy-min
 96   AMG_strong_threshold     = 0.3      % Strong threshold
 97   AMG_truncation_threshold = 0.1      % Truncation threshold
 98   AMG_max_row_sum          = 0.9      % Max row sum
 99
100   %————————————————————————————————————————%
101   % parameters for aggregation-type AMG SETUP     %
102   %————————————————————————————————————————%
103
104   AMG_aggregation_type     = 2        % 1 Matching | 2 VMB
105   AMG_pair_number          = 2        % Number of pairs in matching
106   AMG_strong_coupled       = 0.08     % Strong coupled threshold
107   AMG_max_aggregation      = 20       % Max size of aggregations
108   AMG_tentative_smooth     = 0.67     % Smoothing factor for tentative prolongation
109   AMG_smooth_filter        = OFF      % Switch for filtered matrix for smoothing
110   AMG_quality_bound        = 8.0      % quality of aggregation: 8.0 sysmm | 10.0 unsymm
```

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

Chapter 4

More advanced features

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

4.1   An OpenMP example

OpenMP[1] (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" and set "openmp" to be "yes".

```
37   #
38   # You may use multithread version after you enable OpenMP support. To
```

---

[1]Official website: http://openmp.org/

```
39  # setup the environment, you need
40  #  >> export OMP_NUM_THREADS=4 (for bash)
41  #  >> setenv OMP_NUM_THREADS 4 (for tcsh)
42  # If you want to compile with OpenMP support, uncomment the next line:
43  #
44  # openmp=yes
45  #
```

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:

```
1  /*! \file fasp_const.h
2   *  \brief Definition of all kinds of messages, including error messages,
3   *         solver types, etc.
4   *
5   *  \note  This is internal use only. Do NOT change.
6   *
7   *---------------------------------------------------------------------------------
8   *  Created  by Chensong Zhang on 03/20/2010.
9   *  Modified by Chensong Zhang on 12/06/2011.
10  *  Modified by Chensong Zhang on 12/25/2011.
11  *  Modified by Chensong Zhang on 04/22/2012.
12  *  Modified by Ludmil Zikatanov on 02/15/2013: CG -> SMOOTHER_CG.
13  *  Modified by Chensong Zhang on 02/16/2013: GS -> SMOOTHER_GS, etc.
14  *  Modified by Chensong Zhang on 04/09/2013: Add safe Krylov methods.
15  *  Modified by Chensong Zhang on 09/22/2013: Clean up Doxygen.
16  *  Modified by Chensong Zhang on 09/17/2013: Filename changed from message.h.
17  *---------------------------------------------------------------------------------
18  *
19  */
20
21  #ifndef __FASP_MESSAGES__          /*-- allow multiple inclusions --*/
22  #define __FASP_MESSAGES__
23
24  /**
25   * \brief Definition of return status and error messages
26   */
27  #define FASP_SUCCESS            0  /**< return from function successfully */
28  //---------------------------------------------------------------------------------
```

```
29  #define ERROR_OPEN_FILE         -10   /**< fail to open a file */
30  #define ERROR_WRONG_FILE        -11   /**< input contains wrong format */
31  #define ERROR_INPUT_PAR         -13   /**< wrong input argument */
32  #define ERROR_REGRESS           -14   /**< regression test fail */
33  #define ERROR_MAT_SIZE          -15   /**< wrong problem size */
34  #define ERROR_NUM_BLOCKS        -18   /**< wrong number of blocks */
35  #define ERROR_MISC              -19   /**< other error */
36  //——————————————————————————————————————————————————————————————————————
37  #define ERROR_ALLOC_MEM         -20   /**< fail to allocate memory */
38  #define ERROR_DATA_STRUCTURE    -21   /**< problem with data structures */
39  #define ERROR_DATA_ZERODIAG     -22   /**< matrix has zero diagonal entries */
40  #define ERROR_DUMMY_VAR         -23   /**< unexpected input data */
41  //——————————————————————————————————————————————————————————————————————
42  #define ERROR_AMG_INTERP_TYPE   -30   /**< unknown interpolation type */
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  //——————————————————————————————————————————————————————————————————————
47  #define ERROR_SOLVER_TYPE       -40   /**< unknown solver type */
48  #define ERROR_SOLVER_PRECTYPE   -41   /**< unknown precond type */
49  #define ERROR_SOLVER_STAG       -42   /**< solver stagnates */
50  #define ERROR_SOLVER_SOLSTAG    -43   /**< solver's solution is too small */
51  #define ERROR_SOLVER_TOLSMALL   -44   /**< solver's tolerance is too small */
52  #define ERROR_SOLVER_ILUSETUP   -45   /**< ILU setup error */
53  #define ERROR_SOLVER_MISC       -46   /**< misc solver error during run time */
54  #define ERROR_SOLVER_MAXIT      -48   /**< maximal iteration number exceeded */
55  #define ERROR_SOLVER_EXIT       -49   /**< solver does not quit successfully */
56  //——————————————————————————————————————————————————————————————————————
57  #define ERROR_QUAD_TYPE         -60   /**< unknown quadrature type */
58  #define ERROR_QUAD_DIM          -61   /**< unsupported quadrature dim */
59  //——————————————————————————————————————————————————————————————————————
60  #define ERROR_LIC_TYPE          -80   /**< wrong license type */
61  //——————————————————————————————————————————————————————————————————————
62  #define ERROR_UNKNOWN           -99   /**< an unknown error type */
63
64  /**
65   * \brief Definition of logic type
66   */
67  #define TRUE                    1   /**< logic TRUE */
68  #define FALSE                   0   /**< logic FALSE */
69
70  /**
71   * \brief Definition of switch
72   */
73  #define ON                      1   /**< turn on certain parameter */
74  #define OFF                     0   /**< turn off certain parameter */
75
76  /**
77   * \brief Print level for all subroutines —— not including DEBUG output
78   */
79  #define PRINT_NONE              0   /**< silent: no printout at all */
80  #define PRINT_MIN               1   /**< quiet:  print error, important warnings */
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  /**
87   * \brief Definition of matrix format
88   **/
89  #define MAT_FREE                0   /**< matrix-free format: only mxv action */
90  #define MAT_CSR                 1   /**< compressed sparse row */
91  #define MAT_BSR                 2   /**< block-wise compressed sparse row */
92  #define MAT_STR                 3   /**< structured sparse matrix */
93  #define MAT_bCSR                4   /**< block matrix of CSR */
94  #define MAT_bBSR                5   /**< block matrix of BSR for bordered systems */
95  #define MAT_CSRL                6   /**< modified CSR to reduce cache missing */
96  #define MAT_SymCSR              7   /**< symmetric CSR format */
97
98  /**
99   * \brief Definition of solver types for iterative methods
100  */
101 #define SOLVER_DEFAULT          0   /**< Use default solver in FASP */
102 //——————————————————————————————————————————————————————————
103 #define SOLVER_CG               1   /**< Conjugate Gradient */
104 #define SOLVER_BiCGstab         2   /**< Bi-Conjugate Gradient Stabilized */
105 #define SOLVER_MinRes           3   /**< Minimal Residual */
106 #define SOLVER_GMRES            4   /**< Generalized Minimal Residual */
107 #define SOLVER_VGMRES           5   /**< Variable Restarting GMRES */
108 #define SOLVER_VFGMRES          6   /**< Variable Restarting Flexible GMRES */
109 #define SOLVER_GCG              7   /**< Generalized Conjugate Gradient */
110 #define SOLVER_GCR              8   /**< Generalized Conjugate Residual */
111 //——————————————————————————————————————————————————————————
112 #define SOLVER_SCG              11  /**< Conjugate Gradient with safety net */
113 #define SOLVER_SBiCGstab        12  /**< BiCGstab with safety net */
114 #define SOLVER_SMinRes          13  /**< MinRes with safety net */
115 #define SOLVER_SGMRES           14  /**< GMRes with safety net */
116 #define SOLVER_SVGMRES          15  /**< Variable-restart GMRES with safety net */
117 #define SOLVER_SVFGMRES         16  /**< Variable-restart FGMRES with safety net */
118 #define SOLVER_SGCG             17  /**< GCG with safety net */
119 //——————————————————————————————————————————————————————————
120 #define SOLVER_AMG              21  /**< AMG as an iterative solver */
121 #define SOLVER_FMG              22  /**< Full AMG as an solver */
122 //——————————————————————————————————————————————————————————
123 #define SOLVER_SUPERLU          31  /**< SuperLU Direct Solver */
124 #define SOLVER_UMFPACK          32  /**< UMFPack Direct Solver */
125 #define SOLVER_MUMPS            33  /**< MUMPS   Direct Solver */
126
127 /**
128  * \brief Definition of iterative solver stopping criteria types
129  */
130 #define STOP_REL_RES            1   /**< relative residual ||r||/||b|| */
131 #define STOP_REL_PRECRES        2   /**< relative B-residual ||r||_B/||b||_B */
132 #define STOP_MOD_REL_RES        3   /**< modified relative residual ||r||/||x|| */
133
134 /**
```

```
135    * \brief Definition of preconditioner type for iterative methods
136    */
137   #define PREC_NULL              0   /**< with no precond */
138   #define PREC_DIAG              1   /**< with diagonal precond */
139   #define PREC_AMG               2   /**< with AMG precond */
140   #define PREC_FMG               3   /**< with full AMG precond */
141   #define PREC_ILU               4   /**< with ILU precond */
142   #define PREC_SCHWARZ           5   /**< with Schwarz preconditioner */
143
144   /**
145    * \brief Type of ILU methods
146    */
147   #define ILUk                   1   /**< ILUk */
148   #define ILUt                   2   /**< ILUt */
149   #define ILUtp                  3   /**< ILUtp */
150
151   /**
152    * \brief Type of Schwarz smoother
153    */
154   #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 */
162   #define SA_AMG                 2   /**< smoothed aggregation AMG */
163   #define UA_AMG                 3   /**< unsmoothed aggregation AMG */
164
165   /**
166    * \brief Definition of aggregation types
167    */
168   #define PAIRWISE               1   /**< pairwise aggregation */
169   #define VMB                    2   /**< VMB aggregation */
170
171   /**
172    * \brief Definition of cycle types
173    */
174   #define V_CYCLE                1   /**< V-cycle */
175   #define W_CYCLE                2   /**< W-cycle */
176   #define AMLI_CYCLE             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 */
183   #define SMOOTHER_GS            2   /**< Gauss-Seidel smoother */
184   #define SMOOTHER_SGS           3   /**< Symmetric Gauss-Seidel smoother */
185   #define SMOOTHER_CG            4   /**< CG as a smoother */
186   #define SMOOTHER_SOR           5   /**< SOR smoother */
187   #define SMOOTHER_SSOR          6   /**< SSOR smoother */
```

```
188  #define SMOOTHER_GSOR            7   /**< GS + SOR smoother */
189  #define SMOOTHER_SGSOR           8   /**< SGS + SSOR smoother */
190  #define SMOOTHER_POLY            9   /**< Polynomial smoother */
191  #define SMOOTHER_L1DIAG         10   /**< L1 norm diagonal scaling smoother */
192
193  /**
194   * \brief Definition of coarsening types
195   */
196  #define COARSE_RS                1   /**< Classical */
197  #define COARSE_RSP               2   /**< Classical, with positive offdiags */
198  #define COARSE_CR                3   /**< Compatible relaxation */
199  #define COARSE_AC                4   /**< Aggressive coarsening */
200  #define COARSE_MIS               5   /**< Aggressive coarsening based on MIS */
201
202  /**
203   * \brief Definition of interpolation types
204   */
205  #define INTERP_DIR               1   /**< Direct interpolation */
206  #define INTERP_STD               2   /**< Standard interpolation */
207  #define INTERP_ENG               3   /**< energy minimization interpolation */
208
209  /**
210   * \brief Type of vertices (DOFs) for coarsening
211   */
212  #define GOPT                    -5   /**< Cannot fit in aggregates */
213  #define UNPT                    -1   /**< Undetermined points */
214  #define FGPT                     0   /**< Fine grid points  */
215  #define CGPT                     1   /**< Coarse grid points */
216  #define ISPT                     2   /**< Isolated points */
217
218  /**
219   * \brief Definition of smoothing order
220   */
221  #define NO_ORDER                 0   /**< Natural order smoothing */
222  #define CF_ORDER                 1   /**< C/F order smoothing */
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 */
229  #define FPFIRST                 -1   /**< F-points first order */
230  #define ASCEND                  12   /**< Ascending order */
231  #define DESCEND                 21   /**< Descending order */
232
233  /**
234   * \brief Some global constants
235   */
236  #define BIGREAL              1e+20   /**< A large real number */
237  #define SMALLREAL            1e-20   /**< A small real number */
238  #define SMALLREAL2           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 */
243  #define MAX_CRATE            20.0   /**< Maximal coarsening ratio */
244  #define MAX_RESTART            20   /**< Maximal restarting number */
245  #define MAX_STAG               20   /**< Maximal number of stagnation times */
246  #define STAG_RATIO           1e-4   /**< Stagnation tolerance = tol*STAGRATIO */
247  #define OPENMP_HOLDS         2000   /**< Smallest size for OpenMP version */
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 and such version is compiled with optimization and no warnings are displayed during the build. How to build the FASP library with debugging enabled is described below.

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

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

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

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

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