SXAMG: a Serial Algebraic Multigrid Solver Library

VERSION 1.0

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Introduction

1.1 Overview

SXAMG is an AMG (Algebraic Multi-Grid) solver library for sparse linear system, Ax = b. The package is designed for Linux, Unix and Mac systems. It is also possible to compile under Windows if USE_UNIX is set to 0. The code is written by C, and it is serial.

The initial code is from FASP solver, http://fasp.sourceforge.net, which implements a collection of Krylov solvers, AMG solvers and preconditioners.

The purpose of this refactorization is to provide a standalone AMG solver to support other numerical applications and to validate new ideas in the future. The SXAMG can serve as a solver and a preconditioning method. SXAMG rewrites all the data structures, subroutines, and file structures, and it removes many components of the original implementation and third-party package dependency.

1.2 License

The package uses General Public License (GPL) license. If you have any issue, please contact: hui.sc.liu@gmail.com

1.3 Cite

The SXAMG library can be cited as,

```
@misc{sxamg-library,
   author="Hui Liu",
   title="SXAMG: a Serial Algebraic Multigrid Solver Library",
```

```
year="2017",
note={\url{https://github.com/huijwliu/sxamg/}}
}
```

1.4 Website

The official website for SXAMG is https://github.com/huijwliu/sxamg/.

Installation

SXAMG uses autoconf and make to detect system parameters, to build and to install.

2.1 Configuration

The simplest way to configure is to run command:

```
./configure
```

This command will try to find optional packages if applicable and set system parameters.

2.2 Options

The script configure has many options, if user would like to check, run command:

```
./configure --help
```

Output will be like this,

```
'configure' configures this package to adapt to many kinds of systems.

Usage: ./configure [OPTION]... [VAR=VALUE]...

To assign environment variables (e.g., CC, CFLAGS...), specify them as VAR=VALUE. See below for descriptions of some of the useful variables.

....

Optional Features:
--disable-option-checking ignore unrecognized --enable/--with options
```

```
do not include FEATURE (same as --enable-FEATURE=no)
 --disable-FEATURE
 --enable-FEATURE[=ARG] include FEATURE [ARG=yes]
                    enable use of rpath
 --enable-rpath
                         enable use of rpath (default)
 --disable-rpath
 --with-rpath-flag=FLAG compiler flag for rpath (e.g., "-Wl,-rpath,")
                    turn off assertions
 --disable-assert
                     use long int for INT
 --enable-big-int
 --disable-big-int
                       use int for INT (default),
 --with-int=type integer type(long|long long)
 --enable-long-double use long double for FLOAT
 --disable-long-double use double for FLOAT (default)
Some influential environment variables:
             C compiler command
 CFLAGS
             C compiler flags
 LDFLAGS
            linker flags, e.g. -L<lib dir> if you have libraries in a
             nonstandard directory <lib dir>
 LIBS
             libraries to pass to the linker, e.g. -l<library>
 CPPFLAGS
            (Objective) C/C++ preprocessor flags, e.g. -I<include dir> if
             you have headers in a nonstandard directory <include dir>
 CXX
             C++ compiler command
 CXXFLAGS
             C++ compiler flags
 FC
             Fortran compiler command
 FCFLAGS
             Fortran compiler flags
 CPP
             C preprocessor
 CXXCPP
             C++ preprocessor
```

The most important options are,

- --prefix=PATH where to install the library, and default directory is /usr/local/sxamg/;
- --enable-rpath and --disable-rpath, use rpath or not, and it is enabled by default;
- --enable-big-int and --disable-big-int, use big integer or not, and use int by default;
- --with-int=type, type is long or long long. This option is checked when big integer is enabled (--enable-big-int);
- --enable-long-double and --disable-long-double, use long double or not, and double is used by default;

2.3 Compilation

After configuration, Makefile and related scripts will be set correctly. A simple make command can compile the package,

make

2.4 Installation

Run command:

make install

The package will be installed to a directory. The default is <code>/usr/local/sxamg/</code>. A different directory can be set by <code>--prefix=DIR</code> when configuring, such as <code>--prefix=/usr/sxamg/</code>.

Basics

This chapter introduces basic types, matrix and vector management.

3.1 Data Types

SXAMG has two data types, SX_FLOAT and SX_INT, for floating-point number and integer. They are defined as:

```
#if USE_LONG_DOUBLE
typedef long double
                                  SX_FLOAT;
#else
                                  SX_FLOAT;
typedef double
#endif
#if USE_LONG_LONG
typedef signed long long int
                                  SX_INT;
#elif USE_LONG
typedef signed long int
                                  SX_INT;
#else
typedef signed int
                                  SX_INT;
#endif
```

The macros, USE_LONG_DOUBLE, USE_LONG_LONG and USE_LONG, are set by configure to control the real types. User can control through configure options.

3.2 Matrix

SX_MAT defines CSR matrix. The index is from zero. The meanings of the members are clear.

```
typedef struct SX_MAT
```

```
{
    SX_INT num_rows;
    SX_INT num_cols;
    SX_INT num_nnzs;

    SX_INT *Ap;
    SX_INT *Aj;
    SX_FLOAT *Ax;
} SX_MAT;
```

3.2.1 Matrix Management

3.2.1.1 Create

sx_mat_struct_create creates the structure of a matrix, and no value is set:

```
SX_MAT sx_mat_struct_create(const SX_INT nrow, const SX_INT ncol, const SX_INT nnz);
```

sx_mat_create creates a CSR matrix:

```
SX_MAT sx_mat_create(SX_INT nrow, SX_INT ncol, SX_INT *Ap, SX_INT *Aj, SX_FLOAT *Ax);
```

3.2.1.2 Destroy

sx_mat_destroy destroys a matrix and frees its memory:

```
void sx_mat_destroy(SX_MAT *A);
```

3.2.1.3 Transpose

sx_mat_trans gets transpose a matrix:

```
SX_MAT sx_mat_trans(SX_MAT *A);
```

3.2.1.4 Sort

sx_mat_sort sorts column indices in ascending manner.

```
void sx_mat_sort(SX_MAT *A);
```

3.3 Vector

 SX_VEC defines floating-point vector. n is the length of the vector, and d stores the values.

```
typedef struct SX_VEC
{
    SX_INT n;
    SX_FLOAT *d;
} SX_VEC;
```

3.3.1 Vector Management

3.3.1.1 Create

 sx_vec_create creates a vector of length m.

```
SX_VEC sx_vec_create(SX_INT m);
```

3.3.1.2 Destroy

sx_vec_destroy destroys a vector and frees its memory.

```
void sx_vec_destroy(SX_VEC *u);
```

3.3.1.3 Set Value

sx_vec_set_value sets equal value to each component.

```
void sx_vec_set_value(SX_VEC *x, SX_FLOAT val);
```

```
sx_vec_set_entry sets value: x[index] = val,
void sx_vec_set_entry(SX_VEC *x, SX_INT index, SX_FLOAT val);
```

3.3.1.4 Get Value

```
sx_vec_get_entry returns value of x[index],
```

```
SX_FLOAT sx_vec_get_entry(SX_VEC *x, SX_INT index);
```

3.3.1.5 Copy

```
sx_vec_cp copies source vector to destination vector.
```

```
void sx_vec_cp(SX_VEC *src, SX_VEC *des);
```

3.4 BLAS Operations

3.4.1 Vector

```
 \begin{split} & \texttt{sx\_blas\_vec\_norm2} \text{ calculates L2 norm.} \\ & \texttt{SX\_FLOAT sx\_blas\_vec\_norm2}(\texttt{SX\_VEC *x}); \\ & \texttt{sx\_blas\_vec\_dot} \text{ calculates dot product.} \\ & \texttt{SX\_FLOAT sx\_blas\_vec\_dot}(\texttt{SX\_VEC *x}, \ \texttt{SX\_VEC *y}); \\ & \texttt{sx\_blas\_vec\_axpyz} \text{ computes: } z = a * x + y. \\ & \texttt{void sx\_blas\_vec\_axpyz}(\texttt{const SX\_FLOAT a, SX\_VEC *x, SX\_VEC *y, SX\_VEC *z}); \\ & \texttt{sx\_blas\_vec\_axpy} \text{ computes: } y = a * x + y. \\ & \texttt{void sx\_blas\_vec\_axpy}(\texttt{const SX\_FLOAT a, SX\_VEC *x, SX\_VEC *y}); \\ & \texttt{void sx\_blas\_vec\_axpy}(\texttt{const SX\_FLOAT a, SX\_VEC *x, SX\_VEC *y}); \\ \end{aligned}
```

3.4.2 Matrix-Vector

```
 \begin{split} & \texttt{sx\_blas\_mat\_amxpy} \text{ computes: } y = y + a * A * x, \\ & \texttt{void sx\_blas\_mat\_amxpy}(\texttt{const SX\_FLOAT alpha, SX\_MAT *A, SX\_VEC *x, SX\_VEC *y)}; \\ & \texttt{sx\_blas\_mat\_mxy} \text{ computes: } y = A * x, \\ & \texttt{void sx\_blas\_mat\_mxy}(\texttt{SX\_MAT *A, SX\_VEC *x, SX\_VEC *y)}; \end{split}
```

3.4.3 Matrix-Matrix

```
sx_blas_mat_rap returns the matrix-matrix product: R*A*P, SX_MAT sx_blas_mat_rap(SX_MAT *R, SX_MAT *A, SX_MAT *P);
```

AMG Solver

4.1 Data Structures

SX_SM_TYPE defines smoother types. Nine smoothers are implemented.

SX_COARSEN_TYPE defines coarsening types, including classical RS coarsening and classical RS coarsening with positive off-diagonals.

```
typedef enum
{
    SX_COARSE_RS = 1, /**< Classical */
    SX_COARSE_RSP = 2, /**< Classical, with positive offdiags */
} SX_COARSEN_TYPE;</pre>
```

SX_INTERP_TYPE defines interpolation types, including direct interpolation and standard interpolation.

```
typedef enum
{
    SX_INTERP_DIR = 1, /**< Direct interpolation */</pre>
```

```
SX_INTERP_STD = 2, /**< Standard interpolation */
} SX_INTERP_TYPE;
```

SX_AMG_PARS defines AMG parameters. The meaning of each member is explained as comment. For example, cycle_itr determines the cycle type: 1 for V-cycle, 2 for W-cycle..

```
typedef struct SX_AMG_PARS
     SX_INT verb;
     SX_INT cycle_itr; /** type of AMG cycle, 1 is for V, 2 for W */
SX_FLOAT tol; /** stopping tolerance for AMG solver */
SX_FLOAT ctol; /** stopping tolerance for coarsest solver */
                                 /** maximal number of iterations of AMG */
     SX_INT maxit;
     SX_COARSEN_TYPE cs_type; /** coarsening type */
     SX_INT max_levels;
                                         /** max number of levels of AMG */
     SX_INT coarse_dof;
                                         /** max number of coarsest level DOF */
     SX_SM_TYPE smoother; /** smoother type */
     SX_FLOAT relax; /** relax parseter for SOR smoother */
SX_INT cf_order; /** False (0): nature order, True (1): C/F order */
SX_INT pre_iter; /** number of presmoothers */
SX_INT post_iter; /** number of postsmoothers */
SY_INT poly deg: /** degree of the polynomial smoother */
     SX_INT poly_deg;
                                         /** degree of the polynomial smoother */
     SX_INTERP_TYPE interp_type; /** interpolation type */
     SX_FLOAT strong_threshold; /** strong connection threshold for coarsening */
     SX_FLOAT max_row_sum; /** maximal row sum parseter */
     SX_FLOAT trunc_threshold; /** truncation threshold */
} SX_AMG_PARS;
```

SX_RTN is for return values.

```
typedef struct SX_RTN
{
    SX_FLOAT ares;    /* absolute residual */
    SX_FLOAT rres;    /* relative residual */
    SX_INT nits;    /* number of iterations */
} SX_RTN;
```

4.2 Management

4.2.1 Initialize Parameters

sx_amg_pars_init sets default parameters.

```
void sx_amg_pars_init(SX_AMG_PARS *pars);
```

4.2.2 Setup

sx_amg_setup setups the hierarchical struture of AMG solver,

```
SX_AMG * sx_amg_setup(SX_MAT *A, SX_AMG_PARS *pars);
```

4.2.3 Solve

sx_solver_amg_solve solves the linear system using AMG method,

```
SX_RTN sx_solver_amg_solve(SX_AMG *mg, SX_VEC *x, SX_VEC *b);
```

sx_solver_amg solves the linear system using AMG method. This function is a high level interface, and user can call it only to solve a linear system, which will setup the AMG solver, solve and destroy the AMG solver.

```
SX_RTN sx_solver_amg(SX_MAT *A, SX_VEC *x, SX_VEC *b, SX_AMG_PARS *pars);
```

4.2.4 Destroy

```
sx_amg_data_destroy destroys the AMG object,
```

```
void sx_amg_data_destroy(SX_AMG **mg);
```

Utilities

5.1 Print

```
sx_set_log sets log file. If log file is set, all screen prints will be stored to log file,
void sx_set_log(FILE *io);

sx_printf prints info to screen, if log file is set, it prints to log file and screen,
int sx_printf(const char *fmt, ...);
```

5.2 Memory

```
sx_mem_malloc allocates memory,
void * sx_mem_malloc(size_t size);

sx_mem_calloc allocates and initializes memory,
void * sx_mem_calloc(size_t size, SX_INT type);

sx_mem_realloc reallocates memory,
void * sx_mem_realloc(void *oldmem, size_t tsize);

sx_mem_free frees memory,
void sx_mem_free(void *mem);
```

5.3 Performance

```
sx_gettime returns current time stamp, if t is not NULL, result will be written to t,
SX_FLOAT sx_gettime(SX_FLOAT *t);
```

How to Use

6.1 Vector: Set Value

```
SX_VEC v;
SX_INT n, i;

v = sx_vec_create(n);

/* way 1: v[i] = 1. */
sx_vec_set_value(v, 1.);

/* way 2: v[i] = 1 */
for (i = 0; i < n; i++) {
    sx_vec_set_entry(&v, i, 1);
}

/* way 3: v[i] = i / 3. */
for (i = 0; i < n; i++) {
    sx_vec_set_entry(&v, i, i / 3.);
}</pre>
```

6.2 Vector: Get Value

```
{
    SX_VEC v;
    SX_INT n, i;
    SX_FLOAT val;

n = sx_vec_get_size(&v);
    for (i = 0; i < n; i++) {</pre>
```

```
val = sx_vec_get_entry(&v, i);
}
```

6.3 Create a Matrix

```
{
    SX_MAT A;
    SX_INT *Ap, *Aj;
    SX_FLOAT *Ax;

    /* input Ap, Aj, Ax */
    /* gen A */
    A = sx_mat_create(nrow, ncol, Ap, Aj, Ax);
}
```

6.4 Solver

This example shows how to use SXAMG as a solver.

```
SX_AMG_PARS pars;
SX_MAT A;
SX_VEC b, x;
int verb = 2;
SX_RTN rtn;
/* default pars */
sx_amg_pars_init(&pars);
/* redefine parameters */
pars.maxit = 1000;
pars.verb = 2;
/* set A, b, initial x */
. . . .
/* solve the system */
rtn = sx_solver_amg(&A, &x, &b, &pars);
/* free memory */
sx_mat_destroy(&A);
sx_vec_destroy(&b);
sx_vec_destroy(&x);
```

We can see that only two functions are called: 1) **sx_amg_pars_init** initializes default AMG parameters; 2) **sx_solver_amg** setups, solves and destroys the AMG system, and the solution is stored by **x**.

The user needs to provide, matrix, right-hand side and initial guess.

6.5 Lower Level Interface

This example exposes more details of the AMG solver: 1) setup; 2) solve; 3) destroy.

```
SX_AMG_PARS pars;
    SX_MAT A;
    SX_VEC b, x;
    int verb = 2;
    SX_AMG *mg;
    SX_RTN rtn;
    /* pars */
    sx_amg_pars_init(&pars);
    pars.maxit = 1000;
    pars.verb = 2;
    /* input A */
    // Step 1: AMG setup phase
    mg = sx_amg_setup(&A, &pars);
    // Step 2: AMG solve phase
    /* rhs and initial guess */
    x = sx_vec_create(A.num_rows);
    sx_vec_set_value(&x, 1.0);
    b = sx_vec_create(A.num_rows);
    sx_vec_set_value(&b, 1.0);
    /* solve */
    rtn = sx_solver_amg_solve(mg, &x, &b);
    sx_mat_destroy(&A);
    sx_vec_destroy(&b);
    sx_vec_destroy(&x);
    sx_amg_data_destroy(&mg);
}
```

The user can modify this example to use SXAMG as a preconditioner, where the AMG system is assembled once and other solvers can call solving phase in each iteration.