SXAMG: a Serial Algebraic Multigrid Solver Library

VERSION 1.0

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Contents

Chapter 1

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 Citation

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/.

Chapter 2

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
```

```
  --disable-FEATURE       do not include FEATURE (same as --enable-FEATURE=no)
  --enable-FEATURE[=ARG]  include FEATURE [ARG=yes]
  --enable-rpath          enable use of rpath (default)
  --disable-rpath         disable use of rpath
  --with-rpath-flag=FLAG  compiler flag for rpath (e.g., "-Wl,-rpath,")
  --disable-assert        turn off assertions
  --enable-big-int        use long int for 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:
  CC          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 `/usr/local/sxamg/`. A different directory can be set by `--prefix=DIR` when configuring, such as `--prefix=/usr/sxamg/`.

Chapter 3

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
typedef double                  SX_FLOAT;
#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

sx_blas_vec_norm2 calculates L2 norm.

```
SX_FLOAT sx_blas_vec_norm2(SX_VEC *x);
```

sx_blas_vec_dot calculates dot product.

```
SX_FLOAT sx_blas_vec_dot(SX_VEC *x, SX_VEC *y);
```

sx_blas_vec_axpyz computes: $z = a * x + y$.

```
void sx_blas_vec_axpyz(const SX_FLOAT a, SX_VEC *x, SX_VEC *y, SX_VEC *z);
```

sx_blas_vec_axpy computes: $y = a * x + y$.

```
void sx_blas_vec_axpy(const SX_FLOAT a, SX_VEC *x, SX_VEC *y);
```

3.4.2 Matrix-Vector

sx_blas_mat_amxpy computes: $y = y + a * A * x$,

```
void sx_blas_mat_amxpy(const SX_FLOAT alpha, SX_MAT *A, SX_VEC *x, SX_VEC *y);
```

sx_blas_mat_mxy computes: $y = A * x$,

```
void sx_blas_mat_mxy(SX_MAT *A, SX_VEC *x, SX_VEC *y);
```

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);
```

Chapter 4

AMG Solver

4.1 Data Structures

SX_SM_TYPE defines smoother types. Nine smoothers are implemented.

```
typedef enum
{
    SX_SM_JACOBI    = 1,  /**< Jacobi smoother */
    SX_SM_GS        = 2,  /**< Gauss-Seidel smoother */
    SX_SM_SGS       = 3,  /**< Symmetric Gauss-Seidel smoother */
    SX_SM_SOR       = 4,  /**< SOR smoother */
    SX_SM_SSOR      = 5,  /**< SSOR smoother */
    SX_SM_GSOR      = 6,  /**< GS + SOR smoother */
    SX_SM_SGSOR     = 7,  /**< SGS + SSOR smoother */
    SX_SM_POLY      = 8,  /**< Polynomial smoother */
    SX_SM_L1DIAG    = 9,  /**< L1 norm diagonal scaling smoother */

} SX_SM_TYPE;
```

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;
```

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

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

```
    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 */
    SX_INT   maxit;              /** maximal number of iterations of AMG */

    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 */
    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);
```

Chapter 5

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);
```

Chapter 6

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.);
    }
}
```

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++) {
```

```
        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.