SXAMG: a Serial Algebraic Multigrid Solver Library

VERSION 1.0

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Chapter 1

Introduction

1.1 Overview

SXAMG is an AMG (Algebraic Multi-Grid) solver library for sparse linear system, Ax = b. The initial code is from FASP project, http://fasp.sourceforge.net, which implements a collection of Krylov solvers, AMG solvers and preconditioners.

The library is serial and written by C. It is designed for Linux, Unix and Mac systems. However, it is also possible to compile under Windows if user generates a file include/config.h manually, where USE_UNIX should be set to 0.

SXAMG rewrites all the data structures, subroutines, and file structures, and it removes many components of the original implementation and third-party package dependency. 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.

1.2 License

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

1.3 Citation

If you use this library for your research, proper citation will be appreciated. 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/huiscliu/sxamg/}}
}
```

1.4 Website

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

Chapter 2

Installation

SXAMG uses autoconf and make to detect system parameters, to set default 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
```

A library, `libsxamg.a`, will be generated under, `lib/`.

2.4 Installation

Run command:

```
make install
```

The package will be installed to a user-defined directory by `--prefix=DIR` during configuring, such as `--prefix=/usr/sxamg/`. The default destination is `/usr/local/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, respectively. 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, such as long int and long double. User can control through configure options.

3.2 Matrix

SX_MAT defines a CSR matrix. The index is from 0 (zero) following C convention. The meanings of the members are the same as usual.

```
typedef struct SX_MAT
{
    SX_INT num_rows;   /* number of rows */
    SX_INT num_cols;   /* number of columns */
    SX_INT num_nnzs;   /* number of non-zeros (entries) */

    SX_INT   *Ap;      /* offset of each row */
    SX_INT   *Aj;      /* column indices */
    SX_FLOAT *Ax;      /* values */

} SX_MAT;
```

3.2.1 Matrix Management

3.2.1.1 Create

sx_mat_struct_create creates the structure of a matrix. The memory is allocated but 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 by user input. This function allocates memory and copies values to the 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 of 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 $m(m \geq 0)$.

```
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: $x[i] = val$.

```
void sx_vec_set_entry(SX_VEC *x, SX_INT i, SX_FLOAT val);
```

3.3.1.4 Get Value

sx_vec_get_entry returns value of $x[i]$.

```
SX_FLOAT sx_vec_get_entry(const SX_VEC *x, SX_INT i);
```

3.3.1.5 Copy

sx_vec_cp copies values from source vector and to destination vector, and the two vectors should have the same length.

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

3.4 BLAS Operations

Some level 1 and level 2 BLAS operations are implemented for internal use.

3.4.1 Vector

sx_blas_vec_norm2 calculates L2 norm.

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

sx_blas_vec_dot calculates dot product.

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

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

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

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

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

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

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

sx_blas_vec_axpby computes: $y = a * x + b * y$.

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

3.4.2 Matrix-Vector

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

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

sx_blas_mat_mxy computes: $y = A * x$.

```
void sx_blas_mat_mxy(const SX_MAT *A, const 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(const SX_MAT *R, const SX_MAT *A, const SX_MAT *P);
```

Chapter 4

AMG Solver

If A is a positive-definite square matrix, the AMG methods [5, 4, 1, 2, 3, 6] have proved to be efficient methods and they are also scalable [7].

AMG methods have hierarchical structures, which is shown in Figure 4.1. A coarse grid is constructed when entering a coarser level. To calculate a coarser matrix, a restriction operator R_l and an interpolation (prolongation) operator P_l need to be determined. In general, the restriction operator R_l is the transpose of the interpolation (prolongation) operator P_l:

$$R_l = P_l^T.$$

The matrix on the coarser grid is calculated as

$$A_{l+1} = R_l A_l P_l. \tag{4.1}$$

We know that a high frequency error is easier to converge on a fine grid than a low frequency error, and for the AMG methods, the restriction operator, R_l, projects the error from a finer grid onto a coarser grid and converts a low frequency error to a high frequency error. The interpolation operator transfers a solution on a coarser grid to that on a finer grid. Its setup phase for the AMG methods on each level l $(0 \leq l < L)$ is formulated in Algorithm 1, where a coarser grid, an interpolation operator, a restriction operator, a coarser matrix and post- and pre-smoothers are constructed. By repeating the algorithm, an L-level system can be built. The solution of the AMG methods is recursive and is formulated in Algorithm 2, which shows one iteration of AMG.

The Cleary-Luby-Jones-Plassman (CLJP) coarsening algorithm was proposed by Cleary [9] based on the algorithms developed by Luby [11] and Jones and Plassman [10]. The standard RS coarsening algorithm has also been parallelized [8]. Falgout et al. developed a parallel coarsening algorithm, the Falgout coarsening algorithm, which has been implemented in HYPRE [8]. Yang et al. proposed HMIS and PMIS coarsening algorithms for a coarse grid selection [12]. Various parallel smoothers and interpolation operators have also been studied by Yang et al [8, 12].

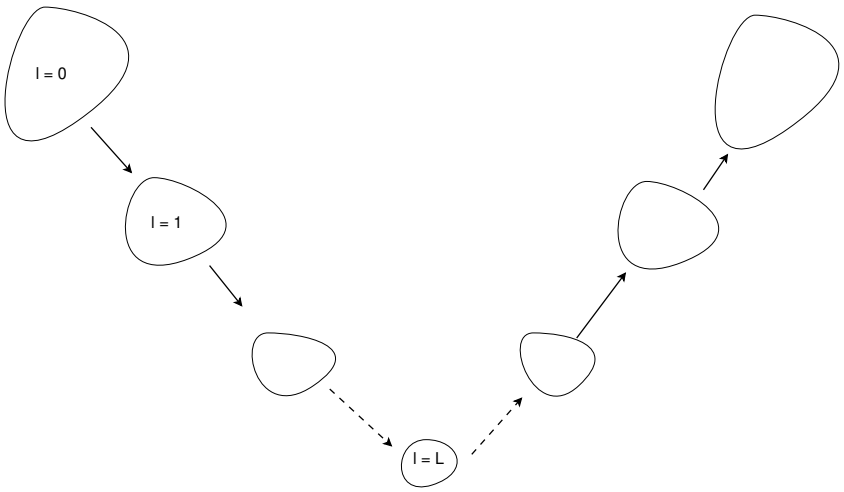

Figure 4.1: Structure of AMG solver.

Algorithm 1 AMG setup Algorithm

1: Calculate strength matrix S.
2: Choose coarsening nodes set ω_{l+1} according to strength matrix S, such that $\omega_{l+1} \subset \omega_l$.
3: Calculate prolongation operator P_l.
4: Derive restriction operator $R_l = P_l^T$.
5: Calculate coarse matrix A_{l+1}: $A_{l+1} = R_l \times A_l \times P_l$.
6: Setup pre-smoother S_l and post-smoother T_l.

Algorithm 2 AMG V-cycle Solution Algorithm: amg_solve(l)

Require: b_l, x_l, A_l, R_l, P_l, S_l, T_l, $0 \leq l < L$

$b_0 = b$
if $(l < L)$ **then**
  $x_l = S_l(x_l, A_l, b_l)$
  $r = b_l - A_l x_l$
  $b_{r+1} = R_l r$
  amg_solve$(l + 1)$
  $x_l = x_l + P_l x_{l+1}$
  $x_l = T_l(x_l, A_l, b_l)$
else
  $x_l = A_l^{-1} b_l$
end if
x $= x_0$

4.1 Data Structures

SX_SM_TYPE defines smoother types. The following 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, W if greater than 1 */
    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 using given parameters.

```
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. The AMG object has to be set up before using, the x has initial value and b is the right-hand side.

```
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 to solve a linear system, which will setup the AMG object, solve and destroy the AMG object. If pars is NULL, then default parameters will be applied.

```
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 outputs will be stored to log file too.

```
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 Solver

This example shows how to use SXAMG as a solver. Five steps are required to call:

1. sx_amg_pars_init initializes default AMG parameters, and user can check their value from source code;
2. Re-define parameters. This step is optional.
3. Input matrix, initial guess and right-hand side should be constructed.
4. sx_solver_amg setups, solves and destroys the AMG system, and the solution is stored by x.
5. Free memories.

```
{
    SX_AMG_PARS pars;
    SX_MAT A;
    SX_VEC b, x;
    int verb = 2;
    SX_RTN rtn;

    /* step 1: default pars */
    sx_amg_pars_init(&pars);

    /* step 2: redefine parameters */
    pars.maxit = 1000;
    pars.verb = 2;

    /* step 3: set A, b, initial x */
    ....
```

```
    /* step 4: solve the system */
    rtn = sx_solver_amg(&A, &x, &b, &pars);

    /* step 5: free memory */
    sx_mat_destroy(&A);
    sx_vec_destroy(&b);
    sx_vec_destroy(&x);
}
```

6.2 Lower Level Interface

Sometimes user needs to store the AMG object and re-uses it, such as preconditioner. This example exposes more details of the AMG solver, where seven steps are required:

1. initialize default parameters;
2. re-define parameters if default parameters do not meet requirement;
3. setup input matrix `A`, which is a standard CSR matrix;
4. setup AMG object;
5. setup initial guess and right-hand side;
6. solve the linear system using given `x` and `b`;
7. free memories;

Here user can call step 1) to 4) once in the beginning stage, call 5) and 6) as many as required, and call step 7) in the end stage of the program.

```
{
    SX_AMG_PARS pars;
    SX_MAT A;
    SX_VEC b, x;
    int verb = 2;
    SX_AMG *mg;
    SX_RTN rtn;

    /* step 1: initialize pars */
    sx_amg_pars_init(&pars);

    /* step 2: re-define parameters */
    pars.maxit = 1000;
    pars.verb = 2;

    /* step 3: input A */
    ....
```

```
    /* Step 4: setup AMG setup object */
    mg = sx_amg_setup(&A, &pars);

    /* Step 5: setup 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);

    /* step 6: solve */
    rtn = sx_solver_amg_solve(mg, &x, &b);

    /* step 7: free memories */
    sx_mat_destroy(&A);
    sx_vec_destroy(&b);
    sx_vec_destroy(&x);
    sx_amg_data_destroy(&mg);
}
```

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