SMG2S Manual

For SMG2S Release 1.0.0

Version 1.0

Xinzhe Wu

August 31, 2018

Copyright ©2018 smg2s.github.io ALL RIGHTS RESERVED. Report may not be copied for commercial redistribution, republication, or dissemination without the explicit permission

Abstract

Iterative linear algebra methods are the important parts of the overall computing time of applications in various fields since decades. Recent research related to social networking, big data, machine learning and artificial intelligence has increased the necessity for non-hermitian solvers associated with much larger sparse matrices and graphs. The analysis of the iterative method behaviors for such problems is complex, and it is necessary to evaluate their convergence to solve extremely large non-Hermitian eigenvalue and linear problems on parallel and/or distributed machines. This convergence depends on the properties of spectra. Then, it is necessary to generate large matrices with known spectra to benchmark the methods. These matrices should be non-Hermitian and non-trivial, with very high dimension. A scalable parallel matrix generator SMG2S that uses the user-defined spectrum to construct large-scale sparse matrices and ensures their eigenvalues as the given ones with high accuracy is implemented based on MPI and C++11. This report gives the manual of SMG2S.

Contents

1	Inti	roduction	5
	1.1	Getting Started	5
	1.2	Installation	5
	1.3	CMake Options	6
	1.4	Copyright and Licensing of SMG2S	7
	1.5	Programming Language in SMG2S	7
	1.6	Referencing SMG2S	7
	1.7	Directory Structure	7
	1.8	List of SMG2S Contributors	8
2	Ten	nplated SMG2S Parallel Matrix and Vector	9
	2.1	Parallel Vector	9
		2.1.1 Vector Map	9
		2.1.2 Creating a Distributed Vector	10
		2.1.3 Parallel Matrix	12
		2.1.4 Creating a Distributed Matrix	13
3	Ten	nplated Nilpotent Matrix Object	14
	3.1	Introduction	14
	3.2	Different Types of Nilpotent Matrix	15
	3.3	Creating a Nilpotent Matrix Object	15
	3.4	Parameter Validation for Nilpotent Matrix	15
4	Ger	nerating Matrix with SMG2S	16
	4.1	SMG2S Class	16
	4.2	Generation Workflow	16
	4.3	Creation of Given Spectrum	17
	4.4	Customize the Low Band of Initial Matrix	18
5	Inte	erface to Other Languages/Libraries	19
	5.1	Interface to C	19
	5.2	Interface to Python	21
	5.3	Interface to PETSc	22
	5.4	Interface to Trilinos/Teptra	22
	5.5	Create Your Inferface	23

6	3 Verification of Eigenvalues			
	6.1	Prerequisites	24	
	6.2	Verification by Shifted Inverse Power Method	24	
	6.3	Script for result cleaning	25	
	6.4	Plot by Graphic User Interface		
		6.4.1 Prerequisites for GUI	26	
		6.4.2 How to use the GUI	26	

Introduction

1.1 Getting Started

SMG2S (Scalable Matrix Generator with Given Spectrum) is a software which provides to generator the non-Hermitian Matrices with User-customized eigenvalues. SMG2S is implemented in parallel based on MPI (Message Passing Interface) and C++11 to support efficiently the generation of test matrices on distributed memory platforms.

Iterative linear algebra methods are important for the applications in various fields. The analysis of the iterative method behaviors is complex, and it is necessary to evaluate their convergence to solve extremely large non-Hermitian eigenvalue and linear problems on parallel and/or distributed machines. This convergence depends on the properties of spectra. Thus, we propse SMG2S to generate large matrices with known spectra to benchmark these methods. The generated matrices are non-Hermitian and non-trivial, with very high dimension. SMG2S can generate the non-Hermitian matrices with user-custormized eigenvalues.

The ability of SMG2S to keep the accuracy of given spectrum can be verified by the functionality proposed inside SMG2S. This function is based the shift inverse power method. SMG2S gives also an graphic user interface to compare the given and final spectral distribution for the verification.

We will describe the following subset of the SMG2S.

- Parallel Vector and Matrix:
- Nilpotency Matrix Object:
- Generating Matrix with predescribed eigenvalues:
- Interface to Other Languages/Libraries:
- Verification of Eigenvalues of Generated Matrix:

1.2 Installation

To obtain SMG2S, please follow the instructions at the SMG2S download page: https://smg2s.github.io/download.html.

Prerequisites:

- C++ Compiler with c++11 support;
- Cmake (version minimum 3.6);
- (Optional) PETSc and SLPEc are necessary for the verification of the ability to keep the given spectrum.

Int the main directory:

```
cmake . –DCMAKE_INSTALL_PREFIX=${INSTALL_DIRECTORY}
```

The $\mbox{main.cpp}$ will generate an exectutable smg2s.exe to demonstrate a minimum sample :

```
_{\mathrm{make}}
```

The main part of SMG2S is a collection of header files. Install the header files into \${INSTALL_DIRECTORY}

```
make install
```

For testing:

```
make test
```

The output of test should be like:

```
Running tests...
Test project /User/name/SMG2S
Start 1: Test_Size_10000_w_proc1
1/4 Test #1: Test_Size_10000_w_proc1 .. Passed 1.20 sec
Start 2: Test_Size_20000_w_proc2
2/4 Test #2: Test_Size_20000_w_proc2 .. Passed 1.22 sec
Start 3: Test_Size_10000_s_proc1
3/4 Test #3: Test_Size_10000_s_proc1 .. Passed 1.20 sec
Start 4: Test_Size_10000_s_proc2
4/4 Test #4: Test_Size_10000_s_proc2
100% tests passed, 0 tests failed out of 4
Total Test time (real) = 4.29 sec
```

1.3 CMake Options

We uses CMake is to build, test and package SMG2S. If you do not have PETSc and SLEPc in your platform, please make sure the option below is OFF.

```
option(INSTALL_TO_USE "Install_SMG2S_include_files?" OFF)
```

1.4 Copyright and Licensing of SMG2S

SMG2S is a open source software published under the GNU Lesser General Public License v3.0. SMG2S can be redistributed and modified under the terms of this license.

SMG2S is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version. SMG2S is 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 for more details. You should have received a copy of the GNU Lesser General Public License along with SMG2S. If not, see jhttp://www.gnu.org/licenses/j.

1.5 Programming Language in SMG2S

SMG2S is a collection of templated header files written in C++. The wrappers to C and Python codes are provided. The users of PETSc or Trilinos can directly use SMG2S with the interfaces implemented inside.

1.6 Referencing SMG2S

@article{galichergenerate, title={Generate Very Large Sparse Matrices Starting from a Given Spectrum}, author={Galicher, Hervé and Boillod-Cerneux, France and Petiton, Serge and Calvin, Christophe}}

1.7 Directory Structure

SMG2S is a collection of header files, and its directory structure is given as follows:

```
parVector

parVectorMap.h ♦ implementation of distributed vector map

parVector.h ♦ implementation of distributed vector

parMatrix

MatrixCSR.h ♦ implementation of serial CSR Matrix

parMatrixSparse.h ♦ distributed sparse matrix

smg2s

specGen.h ♦ Function to provide given spectrum

smg2s.h ♦ implementation of smg2s generator

utlis

MPI_DataType.h

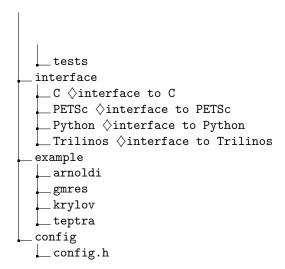
utlis.h

logo.h

verification

powerIverse.cpp ♦ verfication impl based on SLEPc

UI ♦ GUI for comparison based on SLEPc
```



1.8 List of SMG2S Contributors

This is the list of SMG2S contributors:

Xinzhe Wu	main constributor	xinzhe.wu@cea.fr	
Serge Petiton	Supervisor	serge.petiton@univ-lille1.fr	
Quentin Petit	GUI Implementation (Intern)	quentin.petit@polyetch-lille.net	

Templated SMG2S Parallel Matrix and Vector

2.1 Parallel Vector

2.1.1 Vector Map

The distribution of a set of integer labels (or elements) across the processes is here called a parVectorMap. In SMG2S, it is implemented with the help of std:map, which maps the proc number and related intergers. Bascically, parVectorMap handles the definition of global and local indices for the mapping across the processes. Here we give some methods of parVectorMap < S >:

```
S Loc2Glob(S local_index);
//convert local index to global index;

S Glob2Loc(S global_index);
//convert local index to global index;

int GetRank();
//Get proc index;

S GetLowerBound();
//Get lower bound index for each proc;

S GetUpperBound();
//Get upper bound index for each proc;

S GetLocalSize();
//Get index number for each proc;

S GetGlobalSize();
//Get total interger number for all procs.
```

2.1.2 Creating a Distributed Vector

A distributed vector parVector across the processes can be created with the help of parVectorMap. The entries of parVector is distributed over different processes refering to the parVectorMap. parVector < T, S > is implemented with C++ template supported, with T the data type of entry, and S the data type of index.

This is the constructor of parVector, with $MPI_Comm\ ncomm$ the working MPI communicator, Slbound and Subound respectively the lower and upper bound of vector global indices on each proc.

```
/*constructor*/
parVector(MPLComm ncomm, S lbound, S ubound);
```

Here we give some methods of parVector:

```
parVectorMap<S> *GetVecMap();
 //return the related parVectorMap of parVector;
S Loc2Glob(S local_index);
//convert local index to global index;
S Glob2Loc(S global_index);
 //convert local index to global index;
 int GetRank();
 //Get\ proc\ index;
S GetLowerBound();
 //Get lower bound index for each proc;
S GetUpperBound();
 //Get upper bound index for each proc;
S GetLocalSize();
 //Get index number for each proc;
S GetGlobalSize();
 //Get total interger number for all procs;
T *GetArray();
 //Get the array containg the entries on each proc;
void SetValueLocal(S row, T value);
//insert value in the local index named row;
 void SetValuesLocal(S nindex, S *rows, T *values);
 //insert array in the local indices named rows;
 void SetValueGocal(S row, T value);
 //insert value in the gocal index named row;
```

```
void SetValuesGocal(S nindex, S *rows, T *values);
  //insert array in the gocal indices named rows;
  void SetTovalue(T value);
 //Set the entries of parVector all to same given value;
 void VecAdd(parVector *v);
 //Add another vector v with same mapping;
 void VecScale(T scale);
 //Scaling the vector;
 T VecDot(parVector *v);
 //vector dot product operation;
 void ReadExtVec(std::string spectrum);
 //read vector from local file;
 void VecView();
 //display the vector;
 void specGen(std::string spectrum);
//Generate/loal a special vector containing given spectrum
```

Here we give an example to generate a parVector

```
int world_size;
int world_rank;
int span, lower_b, upper_b;
MPI_Comm_size(comm, &world_size);
MPI_Comm_rank(comm, &world_rank);
span = int(ceil(double(probSize)/double(world_size)));
if(world_rank == world_size - 1){
    lower_b = world_rank * span;
    upper_b = probSize - 1 + 1;
}else{
    lower_b = world_rank * span;
    upper_b = (world_rank + 1) * span - 1 + 1;
}
parVector<T,S> *vec = new parVector<T,S>(
comm, lower_b , upper_b );
vec->SetTovalue(T val);
```

2.1.3 Parallel Matrix

The one-dimensional row-major parallel matrix parMatrixSparse in SMG2S is distributed with the same parVectorMap of a given parVector. On each proces, the columns indices and the entries values are stored by a std :: map < T, S > with S data type of indices and T data type of entries.

This is the constructor of parMatrixSparse:

```
/*constructor*/
parMatrixSparse(parVector<T,S> *Vec, parVector<T,S> *Vec);
```

Here we given some methods of the parMatrixSparse object:

```
parVectorMap<S> *GetYMap();
//return the matrix mapping of the columns;
MPLComm GetComm();
//Get current working MPI communicator;
std :: map < S, T > *GetDynMatLoc();
//Get the map storing cols and entries on each proc;
void LOC_MatView();
//display the parallel matrix
void Loc_SetValueLocal( S row, S col, T value);
//insert value in the local index row;
void Loc_SetValuesLocal(S nindex, S *rows, S *cols, \
T *values);
//insert array in the local index rows;
void SetValueGocal(S row, T value);
//insert value in the gocal index named row;
void SetValuesGocal(S nindex, S *rows, T *values);
//insert array in the gocal indices named rows;
void Loc_SetValue(S row, S col, T value);
//Set the entriy (row, col) of parMatrix with value;
void Loc_SetDiagonal(parVector<T,S> *diag);
//set the diagonal of matrix to a given vector;
void Loc_MatScale(T scale);
//Scaling the matrix;
void Loc_MatAXPY(parMatrixSparse<T,S> *X, T scale);
//AXPY operation;
void Loc_MatAYPX(parMatrixSparse<T,S> *X, T scale);
```

```
//AYPX operation;
void Loc_ZeroEntries();
//Zeros all entries and keep the previous matrix pattern;
void MA(Nilpotency <S> nilp, parMatrixSparse <T,S> *prod);
//matrix multiple a special nilpotent matrix;
void AM(Nilpotency <S> nilp, parMatrixSparse <T,S> *prod);
//special nilpotent matrix multiple another matrix;
```

2.1.4 Creating a Distributed Matrix

The is an example of creating distributed matrix with the mapping of distributed vector.

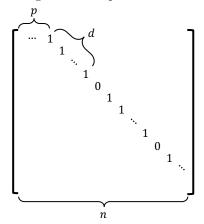
```
/*lower_b and upper_b of each proc is given*/
parVector<T,S> *vec = new parVector<T,S>(
comm,lower_b, upper_b);
parMatrixSparse<T,S> *A=new parMatrixSparse<T,S>(vec,vec);
```

Templated Nilpotent Matrix Object

3.1 Introduction

The nilpotent matrix is very important for the generation of test matrices with given spectrum. Il can be defined by several parameters, the explicit implementation is not necessary.

Figure 3.1: Nilpotent Matrix



The three parameters defined a nilpotent matrix is listed as:

- **dIagPostion**: the distance of the off-diagonal to the diagonal, referring to p in Fig. 3.1;
- **length**: the continuous one on the off-diagonal of nilpotent matrix, refering to d in Fig. 3.1;
- **probSize**: the number of row/column of nilpotent matrix, referring to n in Fig. 3.1.

3.2 Different Types of Nilpotent Matrix

The different nilptent matrix will influence the sparsity pattern of final generated matrix.

```
NilpType1: diagPostion = 2
NilpType2: diagPostion = 3
NilpType3: diagPostion > 3
```

3.3 Creating a Nilpotent Matrix Object

```
Nilpotency < int > nilp;
nilp.NilpType1(length, probSize);
//
nilp.NilpType2(length, probSize);
//
nilp.NilpType3(diagPostion, length, probSize);
```

3.4 Parameter Validation for Nilpotent Matrix

- NilpType1: parameter length can be any integer value > 0;
- NilpType2: parameter length sould be even;
- • NilpType3: validation of parameter length is complex. length should be divisible by p.

Generating Matrix with SMG2S

4.1 SMG2S Class

The header file ./smg2s/smg2s.h implement the matrix generation method. It is defined as:

```
template<typename T, typename S>
parMatrixSparse<T,S> *smg2s(
S probSize,
Nilpotency<S> nilp,
S lbandwidth,
std::string spectrum,
MPLComm comm
)
```

Inside the definition, typename T is to define the size of matrix, and typename S is to define the scalar types of entries of matrix. We give the meaning of the input parameter as below:

- S ProbSize: the size of matrix to generate;
- Nilpotency<S> nilp: the nilpotent matirx object for generation;
- S lbandwidth: the bandwidth of lower-diagonal band of initial matrix;
- std::string spectrum: the file path of spectra file;
- MPI_Comm comm: the working MPI communicator.

4.2 Generation Workflow

Include the head file:

```
\#include < smg2s/smg2s.h>
```

Generate the Nilpotent Matrix Object:

```
Nilpotency<int> nilp;
nilp.NilpType1(length, probSize);
```

Create the parallel Sparse Matrix Object Mt:

```
parMatrixSparse<std::complex<double>,int> *Mt;
```

Generate a new matrix by SMG2S:

```
MPLComm comm; //working MPI Communicator
Mt = smg2s<std::complex<double>,int>(probSize, nilp,
lbandwidth, spectrum, comm);
```

Here, the **probsize** parameter represent the matrix size, **nilp** is the nilpotency matrix object that we have declared previously, **lbandwidth** is the bandwidth of lower-diagonal band. **spectrum** is the file path of spectra file, if **spectrum** is set as " ", SMG2S will use the mechanism inside to generate the spectral distribution. **comm** is the basic object used by MPI to determine which processes are involved in a communication.

The given spectra file is in **pseudo-Matrix Market Vector format**. For the complex eigenvalues, the given spectrum is stored in three columns, the first column is the coordinates, the second column is the real part of complex values, and the third column is the imaginary part of complex values.

```
%%MatrixMarket matrix coordinate complex general
3 3 3
1 10 6.5154
2 10.6288 3.4790
3 10.7621 5.0540
```

For the eigenvalues values, the given spectrum is stored in two columns, the first column is the coordinates, the second column is related values.

```
%%MatrixMarket matrix coordinate complex general 3 3 1 10 2 10.6288 3 10.7621
```

4.3 Creation of Given Spectrum

In the directory ./verification/tests, we give an example to generate the file of given spectrum, which can be reused by the users to create their own values. This is a small C++ file named as vecgen.cpp.

If the users want to generate the eigenvalues in time without loading from local file, they can customize their eigenvalues generation by the function spec-Gen in the file ./verification/tests/specGen.h, and set the parameter spectrum of smg2s to be "".

```
template<typename T, typename S>
void parVector<T,S>::specGen(std::string spectrum)
```

In this function, the eigenvalues are stored by the distributed vector text-colorblueparVector. And the filling of values on this parVector can be done by the method SetValueGlobal implemented in parVector, which takes the global indices to set values.

4.4 Customize the Low Band of Initial Matrix

We know that the low band bandwidth of initial matrix can be set by the parameter lbandwidth of smg2s. Additionaly, the distribution of entries of initial matrix can also be customized by the function matInit provided by the file ./verification/tests/specGen.h. En default, these entries are filled in random. The different mechanism to fill them will influence the sparsity of final generated sparse matrix.

```
template<typename T, typename S>
void matInit(
parMatrixSparse<T,S> *Am,
parMatrixSparse<T,S> *matAop,
S probSize,
S lbandwidth
)
```

In this function, distributed matrix Am and matAop should be filled with the same way. And these entries of matrix can be filled by the method Loc_SetValue implemented in parMatrixSparse. Loc_SetValue uses the global indices of matrix to set values.

Interface to Other Languages/Libraries

SMG2S provides interfaces to C, Python, PETSc and Trilinos.

5.1 Interface to C

SMG2S install command will generate a shared library libsmg2s.so (libsmg2s2c.dylib on OS X platform) into \${INSTALL_DIRECTORY}/lib. It can be used to profit the C wrapper of SMG2S.

The way to use: 1. Add this shared library to LD_LIBRARY_PATH:

```
export LD_LIBRARY_PATH=${INSTALL DIRECTORY}/lib
```

2. Include the header file:

```
#include <interface/C/c_wrapper.h>
```

3. create Nilpotency object:

```
struct NilpotencyInt *n;
n = newNilpotencyInt();
NilpType1(n, 2, 10);
```

4. After that, you need to create the parallel Sparse Matrix Object Mt like this :

```
struct parMatrixSparseDoubleInt *m;
m = newParMatrixSparseDoubleInt();
```

5. Generate by SMG2S:

```
smg2s(m, 10, n, 3 ," ¬", MPLCOMMLWORLD);
```

6. Release Nilpotency Object and parMatrixSparse Object :

```
smg2s (m, 10, n, 3 ," _",MPLCOMM_WORLD);
```

SMG2S provides the C interface to different data types. For the data type of matrix size, it can be either *int* or *longint*; for the data type of matrix entries, it can be either *complex* or *real* with *single* or double precision.

The Nilpotency Matrix object is implemented for both int and longint as below:

```
      struct
      NilpotencyInt;

      struct
      NilpotencyLongInt;
```

The interface of C for parMatrixSparse Object and smg2s function can be defined as below, ____ can be replaced by the selected data type, as one of :

- ComplexDoubleLongInt;
- ComplexDoubleInt;
- ComplexSingleLongInt;
- ComplexSingleInt;

- RealDoubleLongInt;
- RealDoubleInt;
- RealSingleLongInt;
- \bullet Real Signle Int.

```
//double + complex + int64
struct parMatrixSparse____;
/*parVectorMap C wrapper*/
struct parVectorMapInt *newparVectorMapInt(void);
struct parVectorMapLongInt *newparVectorMapLongInt(void);
/*complex double long int*/
struct parMatrixSparseComplex____ *newPar\
MatrixSparse____(void);
void ReleaseParMatrixSparse____(struct \)
parMatrixSparse____ **ppInstance);
void LOC_MatView____(struct parMatrix\
void GetLocalSize.....(struct parMatrix\
Sparse____ *m, __int64_t *rs, __int64_t *cs);
void Loc_ConvertToCSR____(struct parMatrix\
SparseComplexDoubleLongInt *m);
void Loc_CSRGetRowsArraySizes____(struct parMatri\
xSparse_____ *m, __int64_t *size,__int64_t *size2);
void Loc_CSRGetRowsArrays____(struct par\
void smg2s-----(struct parMatrixSparse-----
*m, __int64_t probSize, struct NilpotencyLongInt \
*nilp, __int64_t lbandwidth, char *spectrum, MPL-Comm comm);
```

5.2 Interface to Python

SMG2S uses SWIG to generate the wrapper of SMG2S to Python. Generate the shared library and install the python module of smg2s.

```
#install online from pypi
CC=mpicxx pip install smg2s

#bulid in local
cd ./interface/python;
CC=mpicxx python setup.py build_ext —inplace
#or
CC=mpicxx python setup.py build
#or
CC=mpicxx python setup.py install

#run
mpirun —np 2 python generate.py
```

Before the utilisation, make sure that **mpi4py** is installed.

This is a little example of usge:

```
from mpi4py import MPI
import smg2s
import sys
size = MPI.COMMLWORLD. Get_size()
rank = MPI.COMMLWORLD.Get_rank()
name = MPI. Get_processor_name()
sys.stdout.write(
"Hello, _World! _I _am_ process _%d_ of _%d_on _%s.\n"
% (rank, size, name))
if rank = 0:
    print ('INFO_]>_Starting_...')
    print("INFO_]>_The_MPI_World_Size_is_%d" %size)
#bandwidth for the lower band of initial matrix
lbandwidth = 3
#create the nilpotent matrix
nilp = smg2s. NilpotencyInt()
#setup the nilpotent matrix:
nilp.NilpType1(2,10)
Mt = smg2s.parMatrixSparseDoubleInt()
#Generate Mt by SMG2S
#vector.txt is the file that stores the given
```

```
spectral distribution in local filesystem.
Mt=smg2s.smg2sDoubleInt(10,nilp,lbandwidth,
"vector.txt", MPI.COMMWORLD)
```

5.3 Interface to PETSc

SMG2S provides the interface to scientific computational softwares PETSc/SLEPc. The way of Usage:

Include header file: Include the header file:

```
#include <interface/PETSc/petsc_interface.h>
```

Create parMatrixSparse type matrix :

```
parMatrixSparse<std::complex<double>,int> *Mt;
```

Restore this matrix into CSR format:

```
Mt->Loc_ConvertToCSR();
```

Create PETSc MAT type :

```
{\tt MatCreate} (PETSC_COMM_WORLD,&A);
```

Convert to PETSc MAT format :

Create PETSc MAT type:

```
A = ConvertToPETSCMat(Mt);
```

Here are the example of Arnoldi, GMRES, and another Krylov method.

5.4 Interface to Trilinos/Teptra

SMG2S is able to convert its distributed to the CSR one-dimensional distributed matrix defined by Teptra in Trilinos.

The way of usage:

Include header file

```
#include <interface/Trilinos/trilinos_interface.hpp>
```

Create parMatrixSparse type matrix:

```
parMatrixSparse<std::complex<double>,int> *Mt;
```

Create Trilinos/Teptra MAT type:

```
parMatrixSparse<std::complex<double>,int> *Mt;
```

Convert to Trilinos MAT format :

```
K = ConvertToTrilinosMat(Mt);
```

Here is a full example of Trilinos.

5.5 Create Your Inferface

On each process, the submatrix is stored by the std::map<T,S> provided by C++, which can be get the function GetDynMatLoc implemented in the sparse matrix implementation. The column index and related entry value can be gotten by the C++ iterator.

```
parMatrixSparse<S, T > *M
T col;
S val;
/*On each process*/
parVectorMap<T> *pmap = M->GetYMap();
/* Get row number on each proc*/
T lsize = pmap->GetLocalSize();
std := map < T, S * dynloc;
std::map < T, S>::iterator it;
dynloc = M->GetDynMatLoc();
/* Get col indices and values*/
\mathbf{for}(\mathbf{T} \ \mathbf{i} = 0; \ \mathbf{i} < \mathbf{lsize}; \ \mathbf{i} + +)
 for (it = dynloc[i].begin(); it != dynloc[i].end(); ++it){
          col = it \rightarrow first;
          val = it -> second;
 }
```

Verification of Eigenvalues

SMG2S provides the functionality to verify the abilibity to keep given spectrum. In the directory of ./verification/. The implementation of the functionality is powerInverse.cpp.

6.1 Prerequisites

The verification method is implemented based on the shifted inverse method proposed by PETSc/SLEPc. Before the starting of verification, it is necessary to have the two on the platforms.

If not, the download and installation of PETSc can be found: [PETSc Download] and [SLPEc Installation]. The download and installation of PETSc can be found: [SLEPc Download] and [SLEPc Installation].

6.2 Verification by Shifted Inverse Power Method

1. compile the file powerInverse.cpp by the command

```
make
```

This will generate an executable powerInverse.exe.

2. Suppose the given eigenvalues are stored in the file vector.txt by the pseudo-Matrix Matrix Vector format, run the verification script as blow:

```
#!/bin/bash
EXEC=./powerInverse.exe
N=100
L=10
TEST_TOL=0.00001
DEGREE=4

LENGTH=$(awk 'NR==2{print $1}' vector.txt)
echo "Test_Eigenvalues_number_=_" ${LENGTH}

for ((i=3;i<=${LENGTH}+2;i++))
do
```

```
real=$(awk 'NR=='$i'{print $2}' vector.txt)
imag=$(awk 'NR=='$i'{print $3}' vector.txt)
srun -n 1 ${EXEC} -n ${N} -1 ${L} -eps_monitor_conv \
-eps_power_shift_type constant -st_type sinvert \
-exact_value ${real}+${imag}i -test_tol ${TEST_TOL} \
-degree ${DEGREE}
done
```

Here we list the meaning of the important parameters in the script above:

- N: the size of matrix to generate, which should be equal to the number of given eigenvalues;
- L: the bandwidth of low part diagonal of matrix to generate;
- TEST_TOL: the tolerance to check if the accuracy of one eigenvalue can be accepted or not;
- DEGREE: the continuous one for the nilpotency matrix.

6.3 Script for result cleaning

The result file generated during the verification can be cleaned into the pseudo-Matrix Market Vector by the script below:

```
#!/bin/bash

grep "@>_The_eigenvalue" $1 > tmp.txt
awk '{print $5 "_" $7 }' tmp.txt > tmp2.txt
awk '{print substr($0, 1, length($0)-1)}' tmp2.txt \
> tmp3.txt

awk '{print NR "_" $0}' tmp3.txt > tmp4.txt
NB='wc -1 tmp4.txt | awk '{print $1}''
awk 'BEGIN{print '$NB' "_" '$NB' "_" '$NB'}{print}' \
tmp4.txt > tmp5.txt

awk 'BEGIN{print "%%MatrixMarket_matrix_coordinate_\
_real_general"}{print}' tmp5.txt > $2

rm tmp.txt tmp2.txt tmp3.txt tmp4.txt tmp5.txt
```

Execution of this script:

```
./ traitement.sh results.txt results_clean.txt
```

In this command, The 1st and 2nd arugments for the execution are separately the initial results file and the final cleaned and formatted file.

6.4 Plot by Graphic User Interface

6.4.1 Prerequisites for GUI

You need to have Python2.X or Python3.X to run it. Moreover, UI uses some libraries to support a dynamic and intuitive graphical user interface, you can see the list of libraries. Normally, some of them are include in Python distribution. You can find below the list of necessary libraries of the UI.

- Modules which are bundled in the Python installation : Tkinter, re, sys, decimal ;
- Modules which need to be installed in addition to Python : NumPy & SciPy, Matplotlib, Pillow(PIL)

Install modules to Python 2.X:

```
apt-get install python-tk python-imaging-tk
pip -m install Pillow
python -mpip install -U pip
python -mpip install -U matplotlib
pip install -U numpy scipy
```

Install modules to Python 3.X:

```
sudo apt-get install python3-tk python-imaging-tk
pip -m install Pillow
python -mpip install -U pip
python -mpip install -U matplotlib
pip install -U numpy scipy
```

6.4.2 How to use the GUI

To use the GUI:

```
python main.py
```

When you launch the program, a new windows opens like Fig. 6.4.2:

The first step is to select the files which be display. When you have selected a file, the button change in green color as Fig. 6.4.2 (Attention, the files imported should be in the pseudo-Matrix Market vector format that we have talked):

After that, you can click on "Display" to build and open the graphic on the right side of the window. Click on "New window" to open your graphic on a new window. It's possible to open as many windows as you want like Fig. 6.4.2:

Your will be generate with automatic lens scaling, but your can generate it with your own scales as Fig. 6.4.2:

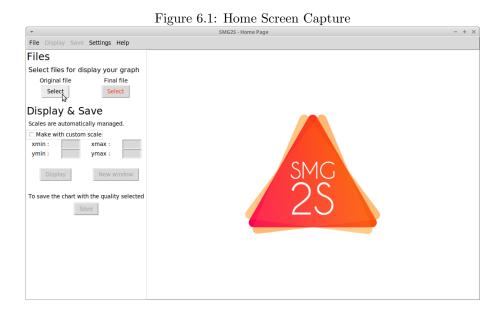


Figure 6.2: Home Screen Capture After Selection SMG2S - Home Page File Display Save Settings Help Files Select files for display your graph Original file Final file Select Select Display & Save Scales are automatically managed. Make with custom scale xmin: xmax : Display New window To save the chart with the quality selected Save

