SMG2S Manual

For SMG2S Release 1.0.1

Version 1.0

Xinzhe Wu

Maison de la Simulation, Gif-sur-Yvette, France

September 14, 2018
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 Introduction .................................................. 5
  1.1 Getting Started ........................................... 5
  1.2 Installation ................................................ 6
  1.3 CMake Options ............................................. 7
  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 Templated 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 Templated 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 Generating 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 Interface 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 Interface .................................. 23
## 6 Verification of Eigenvalues

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1 Prerequisites</td>
<td>24</td>
</tr>
<tr>
<td>6.2 Verification by Shifted Inverse Power Method</td>
<td>24</td>
</tr>
<tr>
<td>6.3 Script for result cleaning</td>
<td>25</td>
</tr>
<tr>
<td>6.4 Plot by Graphic User Interface</td>
<td>26</td>
</tr>
<tr>
<td>6.4.1 Prerequisites for GUI</td>
<td>26</td>
</tr>
<tr>
<td>6.4.2 How to use the GUI</td>
<td>26</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Getting Started

SMG2S (Scalable Matrix Generator with Given Spectrum) [1, 2] is a software which provides for generating 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 in parallel on distributed memory platforms.

Iterative linear algebra methods are essential 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 propose 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.

The functionality proposed inside SMG2S can verify the ability of SMG2S to keep the accuracy of a given spectrum. This function is based on the shift inverse power method. SMG2S also gives a 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**: this part presents the functions implemented in SMG2S to establish parallel vector and matrix over distributed memory platforms.

- **Nilpotent Matrix Object**: this part presents a special nilpotent matrix object for the matrix generation procedure in SMG2S.

- **Generating Matrix with prescribed eigenvalues**: this part gives the way to use SMG2S to generate required test matrices.

- **Interface to Other Languages/Libraries**: this part introduces the interface of SMG2S to other languages and existing scientific computational libraries such as PETSc and Trilinos.

- **Verification of Eigenvalues of Generated Matrix**: this part gives the way to verify the accuracy of eigenvalues of generated matrices comparing
with given spectrum. A graphic user interface is also provided to facilitate the comparison.

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.

In the main directory:

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

The `main.cpp` will generate an executable smg2s.exe to demonstrate a minimum sample:

```
make
```

For testing the software in your platforms:

```
make test
```

The output of the test should be like:

```bash
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 .. Passed 0.66 sec

100% tests passed, 0 tests failed out of 4

Total Test time (real) = 4.29 sec
```
1.3 CMake Options

We use CMake 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 in CMakeLists.txt.

```cmake
option(INSTALL_TO_USE "Install SMG2S include files?" OFF)
```

1.4 Copyright and Licensing of SMG2S

SMG2S is an 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 \http://www.gnu.org/licenses/\.

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

Place cite these papers if you want to reference 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} }
- @inproceedings{wu2018parallel, title={A Parallel Generator of Non-Hermitian Matrices computed from Given Spectra}, author={Wu, Xinzhe and Petiton, Serge and Lu, Yutong}, booktitle={VECPAR 2018: 13th International Meeting on High Performance Computing for Computational Science}, year={2018} }

1.7 Directory Structure

The directory structure of SMG2S is given as follows:

```
SMG2S
   ├── parVector
```
1.8 List of SMG2S Contributors

This is the list of SMG2S contributors:

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xinzhe Wu</td>
<td>main contributor</td>
<td><a href="mailto:xinzhe.wu@ed.univ-lille1.fr">xinzhe.wu@ed.univ-lille1.fr</a></td>
</tr>
<tr>
<td>Serge Petiton</td>
<td>Supervisor</td>
<td><a href="mailto:serge.petiton@univ-lille1.fr">serge.petiton@univ-lille1.fr</a></td>
</tr>
<tr>
<td>Quentin Petit</td>
<td>GUI Implementation (Intern)</td>
<td><a href="mailto:quentin.petit@polyetch-lille.net">quentin.petit@polyetch-lille.net</a></td>
</tr>
</tbody>
</table>
Chapter 2

Templated SMG2S Parallel Matrix and Vector

2.1 Parallel Vector

The distributed vector inside SMG2S is implemented using the C++ programming language and MPI. The parallel vector implementation is composed of two main classes: `parVectorMap` and `parVector`. `parVectorMap` class is a vector index map which controls the partitioning and distribution over the processes, and `parVector` is the parallel vector itself, which contains the actual distributed data and the corresponding functions controlling the data.

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 integers. Basically, `parVectorMap` handles the definition of global and local indices for the mapping across the processes. Here we give some methods of `parVectorMap < S >`:

```cpp
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();
```
2.1.2 Creating a Distributed Vector

A parallel vector \textit{parVector} across the processes can be created with the help of \textit{parVectorMap}. The entries of \textit{parVector} are distributed over different processes referring to the \textit{parVectorMap}. \textit{parVector} \texttt{< T,S >} is implemented with the C++ template, with \( T \) the data type of entry, and \( S \) the data type of index.

This is the constructor of \textit{parVector}, with \texttt{MPI_Comm ncomm} the working MPI communicator, \texttt{S lbound} and \texttt{S ubound} respectively the lower and upper bound of vector global indices on each proc.

\begin{verbatim}
/* constructor */
parVector(MPI_Comm ncomm, S lbound, S ubound);
\end{verbatim}

Here we give some methods of \textit{parVector}:

\begin{verbatim}
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 integer number for all procs;
T *GetArray(); // Get the array containing the entries on each proc;
void SetValueLocal(S row, T value); // insert value in the local index named row;
\end{verbatim}
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 by SMG2S:

```c++
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);
```
2.1.3 Parallel Matrix

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

This is the constructor of \textit{parMatrixSparse}:

\begin{verbatim}
/* constructor */
parMatrixSparse(parVector<T, S> *Vec, parVector<T, S> *Vec);
\end{verbatim}

Here we given some methods of the \textit{parMatrixSparse} object:

\begin{verbatim}
parVectorMap<S> *GetYMap(); // return the matrix mapping of the columns;
MPI_Comm 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 LocSetValueLocal(S row, S col, T value); // insert value in the local index row;
void LocSetValuesLocal(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 global index named row;
void SetValuesGocal(S nindex, S *rows, T *values); // insert array in the global indices named rows;
void LocSetValue(S row, S col, T value); // Set the entry (row, col) of parMatrix with value;
void LocSetDiagonal(parVector<T, S> *diag); // set the diagonal of matrix to a given vector;
void Loc_MatScale(T scale); // Scaling the matrix;
\end{verbatim}
```cpp
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 a distributed matrix with the mapping of parallel vector:

```cpp
/* 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);
```
Chapter 3

Templated Nilpotent Matrix Object

3.1 Introduction

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

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, referring 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 nilpotent matrix will influence the sparsity pattern of the final generated matrix.

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

3.3 Creating a Nilpotent Matrix Object

```c++
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 should be even;
- NilpType3: validation of parameter length is complex. length should be divisible by p.
Chapter 4

Generating Matrix with SMG2S

4.1 SMG2S Class

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

```cpp
template<typename T, typename S>
parMatrixSparse<T,S> *smg2s(
    S probSize,
    Nilpotency<S> nilp,
    S lbandwidth,
    std::string spectrum,
    MPI_Comm 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 matrix 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

1. Include the head file

```cpp
#include <smg2s/smg2s.h>
```
2. Generate the Nilpotent Matrix Object:

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

3. Create the parallel Sparse Matrix Object Mt:

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

4. Generate a new matrix by SMG2S:

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

Here, the `probsize` parameter represents 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.

```plaintext
%%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.

```plaintext
%%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 `specGen` 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. Additionally, 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 LocSetValue implemented in parMatrixSparse. LocSetValue uses the global indices of matrix to set values.
Chapter 5

Interface to Other Languages/Libraries

Until now, 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 parMatrixSparseRealDoubleInt *m;
   m = newParMatrixSparseRealDoubleInt();
   ```

5. Generate by SMG2S:

   ```
   smg2sRealDoubleInt(m, 10, n, 3,"\" ,MPI\_COMM\_WORLD);
   ```

6. Release Nilpotency Object and parMatrixSparse Object:

   ```
   ReleaseNilpotencyInt(&n);
   ReleaseParMatrixSparseRealDoubleInt(&m);
   ```
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 Nilpotent Matrix object is implemented for both `int` and `longint` as below:

```c
struct NilpotencyInt;
struct NilpotencyLongInt;
```

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

- `ComplexDoubleLongInt`;
- `ComplexDoubleInt`;
- `ComplexSingleLongInt`;
- `ComplexSingleInt`;
- `RealDoubleLongInt`;
- `RealDoubleInt`;
- `RealSingleLongInt`;
- `RealSingleInt`.

```c
// long int case
struct parMatrixSparseSUFFIX;
/* parVectorMap C wrappers */
struct parVectorMapLongInt *newparVectorMapLongInt(void);
/* complex double long ints */
struct parMatrixSparseComplexSUFFIX *newPar\MatrixSparseSUFFIX(void);
void ReleaseParMatrixSparseSUFFIX(struct \parMatrixSparseSUFFIX **ppInstance);
void LOC_MatViewSUFFIX(struct parMatrix\SparseSUFFIX *m);
void GetLocalSizeSUFFIX(struct parMatrix\SparseSUFFIX *m, int64_t *rs, int64_t *cs);
void Loc_CSRGetRowsArraySizesSUFFIX(struct parMatrix\SparseComplexDoubleLongInt *m);
void Loc_CSRGetRowsArraysSUFFIX(struct parMatrix\SparseSparseSUFFIX *m, int64_t *size, int64_t *size2);
void smg2sSUFFIX(struct parMatrixSparseSUFFIX *m, int64_t probSize, struct NilpotencyLongInt *nilp, int64_t lbandwidth, char *spectrum, MPIComm 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

# build in local
cc . / 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 utilization, make sure that mpi4py is installed.

This is a little example of usage:

```
from mpi4py import MPI
import smg2s
import sys

size = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()
name = MPI.Get_processor_name()

sys.stdout.write("Hello, World! I am process %d of %d on %s.
")
% (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.COMM_WORLD)

5.3 Interface to PETSc

SMG2S provides the interface to scientific computational softwares PETSc/SLEPc.

The way of Usage:
Include the header file:

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

Create parMatrixSparse type matrix:

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

Restore this matrix into CSR format:

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

Create PETSc MAT type:

```c
MatCreate(PETSC_COMM_WORLD,&A);
```

Convert to PETSc MAT format:

Create PETSc MAT type:

```c
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

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

Create parMatrixSparse type matrix:

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

Create Trilinos/Teptra MAT type:

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

Convert to Trilinos MAT format:

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

Here is a full example of Trilinos.
5.5 Create Your Interface

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

```cpp
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*/
for (T i = 0; i < lsize; i++){
    for (it = dynloc[i].begin(); it != dynloc[i].end(); ++it){
        col = it->first;
        val = it->second;
    }
}
```
Chapter 6

Verification of Eigenvalues

SMG2S provides the functionality to verify the ability 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 [SLEPc 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 below:

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

LENGTH=$(awk -v N="2\{print $1\}" vector.txt)

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

Here we list the meaning of the critical 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:

```bash
#!/bin/bash

grep "@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 -l tmp4.txt | awk '{print $1}'`
awk 'BEGIN{print "$NB" " "$NB" " "$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 arguments 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 included 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:

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

Install modules to Python 3.X:

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

6.4.2 How to use the GUI

To use the GUI:

```bash
python main.py
```

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

The first step is to select the files which will be displayed. When you have selected a file, the button changes to 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:

It will be generated with automatic lens scaling, but you can generate it with your own scales as Fig. 6.4.2:
Figure 6.1: Home Screen Capture

Figure 6.2: Home Screen Capture After Selection
Figure 6.3: Home Screen Plot Capture

Figure 6.4: Home Screen Plot Capture with Lens Scaling
Bibliography
