

Use of PETSc and SLEPc in the SplineFEM library

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1 Installation of PETSc

The latest version of PETSc can be downloaded from the webpage <http://www.mcs.anl.gov/petsc/petsc-as/>. When writing this note the tarball has the name `petsc-3.1-p5.tar.gz`. Save the file to the directory where you want to install PETSc. Then unpack the tarball by writing

```
> tar xvfz petsc-3.1-p5.tar.gz
```

This should produce a directory named `petsc-3.1-p5`. Before the library can be compiled the environment variable `PETSC_DIR` must be set to the path of the PETSc home directory. For instance, if the library was unpacked at `$HOME/libs/PETSc`, the variable can be set by writing

```
> export PETSC_DIR=$HOME/libs/PETSc/petsc-3.1-p5
```

in the terminal window. Alternatively, the path can be set in the `.bashrc` file under the home directory to define the variable when a new terminal window is opened on the machine.

Now the PETSc library can be compiled from `$PETSC_DIR` by first calling the configuration script to generate the Makefile. In my installation I have used the following configuration options

```
> ./config/configure.py --with-cc=gcc --with-fc=gfortran
--download-f-blas-lapack --download-mpich --with-clanguage=c++
--download-ml --download-superlu --download-superlu_dist
--download-parmetis --with-shared=0
```

If you already have a version of some of the library on your machine the `download` command can be replaced by the `with` command specifying the path of the installed library. See the PETSc homepage for more information on options for the configuration script. To run in parallel MPI must be installed on the machine. Moreover, the use of the distributed SuperLU solver requires that ParMetis is installed. Trilinos/ML is not supported by the linear solver interface of the SplineFEM library, but will be included at a later stage to give access to algebraic multigrid preconditioners.

After the configuration script has been runned, the code can be compiled and tested by

```
> make all test
```

2 Installation of SLEPc

SLEPc is a library which is built on top of PETSc for computing eigenvalues and eigenvalues. It can be downloaded from the webpage <http://www.grycap.upv.es/slepc/>. At the time of writing the tarball is named `slepc-3.1-p4.tgz`. Unpack the library by calling

```
> tar xvfz slepc-3.1-p4.tgz
```

To compile the library PETSc must be installed and the environment variables `PETSC_DIR` and `SLEPC_DIR` must be set. For example, if SLEPc is installed at the directory `$HOME/libs/SLEPc/slepc-3.1-p4` write

```
> export SLEPC_DIR=$HOME/libs/SLEPc/slepc-3.1-p4
```

From the `$SLEPC_DIR` directory the library can be compiled by calling

```
> ./configure
> make
```

3 Compilation of SplineFEM with PETSc/SLEPc

To compile the SplineFEM library and application code with PETSc and SLEPc the Makefiles in the `SplineFEM/src` and `SplineFEM/src/Apps` directories must be modified. Uncomment the line

```
#include ${SLEPC_DIR}/conf/slepc_common_variables
```

to include the necessary variables from PETSc/SLEPc. Then uncomment one of the `PETSCOPT` lines depending on whether you want to run the code sequential or in parallel. Then compile the SplineFEM library and application code as usual.

4 Input files when running with PETSc

The input files must be modified slightly to run with PETSc. The linear solver parameters are defined in the `LINEARSOLVER` block which has the following parameters and default values

```
LINEARSOLVER 8
type      = gmres      # Krylov solver
pc        = ilu        # Preconditioner
package   = petsc     # Software package used for linear solver
levels    = 0         # Number of levels for ilu
atol      = 1.0e-6    # Absolute tolerance for residual
rtol      = 1.0e-6    # Relative tolerance for residual
dtol      = 1.0e-6    # Divergence tolerance
maxits    = 1000      # Maximal number of iterations
```

If some parameters are not specified in the input file, the default value is used. Note that not all solvers and preconditioners are available both for serial and parallel computations. For instance, the `ilu` preconditioner is not available in parallel. See the PETSc documentation for legal choices. To use the distributed SuperLU solver the following input is given

```
LINEARSOLVER 3
type      = preonly
pc        = lu
package   = superlu_dist
```

In parallel computations the patches must be specified by the `PATCHFILE` command and a global numbering of the unknowns must be specified by the `NODEFILE` command. A special numbering scheme is required by PETSc, and can be generated from the patchfile using the `gpm.getGNO` program with the option `-petsc`. Parallelization using PETSc is only available for multi-patch cases and the user must specify the distribution of patches to each process in the `PARTITIONING` block at the beginning of the input file. For instance, the input

```
PARTITIONING 2
# proc first last
  0   1   2
  1   3   3
```

specifies a case with 3 patches which is run on 2 processes. Process 0 is assigned patches 1 and 2, while process 1 gets patch 3. Consecutive patch numbers must be assigned to the processes because of the special numbering scheme used by PETSc.

5 Running application code using PETSc

To run application code compiled in serial mode, it is sufficient to give the option `-petsc` to the executable. For example, running `line13D` with input file `CanTS-p1.inp` using PETSc

```
> ./line13D -petsc CanTS-p1.inp
```

To run in parallel MPI must be called with the correct number of processes. If the input file has at least two patches, the program can be run in parallel by

```
> mpiexec -np 2 ./line13D -petsc CanTS-p1.inp
```

For parallel simulations the output will be written to individual files for each process. For instance, the case given above will produce the output files `CanTS-p1_p0000.vtf` and `CanTS-p1_p0001.vtf`. The `glue` program can then be used to merge the different VTF-files in a pre-processing step. The command

```
> ./glue -FileBaseIn CanTS-p1 -NoFileIn 2 -format ASCII
```

will generate a file named `CanTS-p1.vtf` containing the results for all patches.