Fenics Parallel Computing

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Introduction to Fenics solver

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- Fenics version: 2018.1.0

Introduction to Differential Algebraic Equations (DAEs)

Dof: degree of freedom (nodes on a mesh cell)

Size of a problem: small: < 10k dofs, medium: 30k < dofs, large: others

System of liner equations: Ax = b System of non-liner equations: F(x) = b

All of them are called Differential Algebraic Equations (DAEs)

Choose solver:

LU factorization: LU is simple and robust, but only suitable for small and linear problem *Iterative method:* Newton solver, Krylov solvers

- *Newton* is suitable for small or medium problem with linearity or non-linearity, because it computes Jabcobian matrix F' which is very expensive for large system, and for storing.
- Krylov solvers: GMRES, Conjuate Gradient (CG), BiCG, BiCGS, BiCGSTAB, TFQMR, IDRs, QMR, MINRES, etc
 - originally, Krylov solvers are designed for linear problem.
 - avoid to compute Jacobian matrix F', so that, they are suitable to compute large system
 - GMRES: save a basic of the Krylov subspace at each iteration. May lead to out of memory, the algorithm

will restart using the last approximated solution as the initial guess.

- BiCGSTAB is the 4th upgrade version of CG family, ie CG, BiCG, BiCGS and BiCGSTAB. It's dedicated to avoid storing a new basic vector of the krylov subspace at each iteration likes GMRES. However, it is not stable as GMRES
- Newton-Krylov solvers: Newton-GMRES, Newton-CG, Newton-BiCG etc
 - use the benefits of the Krylov solvers to solve non-linear large system
 - Recommend to use Newton-BiCGSTAB for a huge system likes 1 million dofs

C.T. Kelley – solving nonlinear equations with Newton's Method (1987)

Introduction to Differential Algebraic Equations (DAEs)

Example: Poisson problem

$$\begin{split} -\nabla^2 u(\boldsymbol{x}) &= f(\boldsymbol{x}), \quad \ \boldsymbol{x} \text{ in } \varOmega, \\ u(\boldsymbol{x}) &= u_{\scriptscriptstyle \mathrm{D}}(\boldsymbol{x}), \quad \boldsymbol{x} \text{ on } \partial \varOmega. \end{split}$$

$$\int_{\varOmega} \nabla u \cdot \nabla v \, \mathrm{d}x = \int_{\varOmega} f v \, \mathrm{d}x.$$

Numerical approximate integral Applied boundary conditions

(Thank to Fenics)

Ax = b or

$$F(x)=b$$

DEAs

Strong form

Weak form

Fenics code for weak form

High level call solver:

$$solve(a == L, u, bc)$$

$$solve(F == 0, u, bc)$$

Fenics will run with default setting

Built-in packages can solve DAEs in Fenics

Packages contains algorithms to solve DAEs is called: Linear algebra packages (LAP) To check how many LAP installed in your Fenics version:

```
print(list linear algebra backends())
     Linear algebra backends |
                            Description
                            Template-based linear algebra library
     Eigen
                             Powerful MPI parallel linear algebra library (default)
     PETSc
To know which LAP you are using:
print(parameters['linear algebra backend']) → PETSc
                                                                (by default)
To change your current LAP:
 parameters['linear algebra backend'] = 'Eigen'
 print(parameters['linear_algebra_backend']) → Eigen
Print all solvers:
print(list_linear_solver_methods())
print(list_krylov_solver_methods())
```

Built-in packages can solve DAEs in Fenics

PETSc

| PETSc: all line Solver method | |
|----------------------------------|--|
| bicgstab | Biconjugate gradient stabilized method |
| cg | Conjugate gradient method |
| default | default linear solver |
| gmres | Generalized minimal residual method |
| minres | Minimal residual method |
| mumps | MUMPS (MUltifrontal Massively Parallel Sparse direct Solver) |
| petsc | PETSc built in LU solver |
| richardson | Richardson method |
| superlu | SuperLU |
| tfqmr | Transpose-free quasi-minimal residual method |
| umfpack None | UMFPACK (Unsymmetric MultiFrontal sparse LU factorization) |

| PETSc: all krylov Krylov method | |
|------------------------------------|--|
| Ki y cov ilic cirod | beset ip cion |
| | |
| bicgstab | Biconjugate gradient stabilized method |
| cg | Conjugate gradient method |
| default | default Krylov method |
| gmres | Generalized minimal residual method |
| minres | Minimal residual method |
| richardson | Richardson method |
| tfqmr | Transpose-free quasi-minimal residual method |
| None | |

Eigen

```
Eigen: all linear solvers
                 Description
                 Biconjugate gradient stabilized method
bicgstab
                 Conjugate gradient method
cg
cholesky
                 Simplicial LDLT
cholmod
                  'CHOLMOD' sparse Cholesky factorisation
                 default linear solver
default
                 Generalised minimal residual (GMRES)
amres
minres
sparselu
                 Supernodal LU factorization for general matrices
                 UMFPACK (Unsymmetric MultiFrontal sparse LU factorization)
umfpack
lone
```

```
Eigen: all krylov solvers
Krylov method | Description
bicgstab | Biconjugate gradient stabilized method
cg | Conjugate gradient method
default | default Eigen Krylov method
gmres | Generalised minimal residual (GMRES)
minres | Minimal residual
None
```

Preconditioners

Preconditioner is matrix C that multiplied to linear DAEs to speed up the convergence rate $C^{-1}A_X = C^{-1}b$

```
print(list_krylov_solver_preconditioners())
```

PETSc

```
PETSc: all krylov preconditioners
Preconditioner
                    Description
                    Algebraic multigrid
                    default preconditioner
default
                    Hypre algebraic multigrid (BoomerAMG)
hypre amg
                    Hypre parallel incomplete LU factorization
hypre euclid
                    Hypre parallel sparse approximate inverse
hypre parasails
                    Incomplete Cholesky factorization
icc
ilu
                    Incomplete LU factorization
iacobi
                    Jacobi iteration
                    No preconditioner
none
                    PETSc algebraic multigrid
petsc amq
                    Successive over-relaxation
sor
None
```

Eigen

```
Eigen: all krylov solvers

Krylov method | Description

bicgstab | Biconjugate gradient stabilized method
cg | Conjugate gradient method
default | default Eigen Krylov method
gmres | Generalised minimal residual (GMRES)
minres | Minimal residual
None
```

Introduction to solver 'parameters'

All parameters regarding the solver, likes absolute tolerance, relative tolerance and maximum of iteration, are set in a built-in **dictionary** in Fenics called parameters.

To print on terminal the parameters

info(parameters, True)

To save parameters into file

File('parameters.xml') << parameters</pre>

To read parameters from file

File('parameters.xml') >> parameters

Introduction to solver 'parameters'

To print on terminal the parameters | info(parameters, True)

Set of parameters: 'dolfin' (father of all), 'form_compiler', 'krylov_solver', 'lu_solver'

Example:

'linear_algera_backend' is a parameter of set 'dolfin'

To call a set of parameters:

```
info(parameters['form_compiler'], True)
info(parameters['lu_solver'], True)
info(parameters['krylov_solver'], True)
```

To change the default setting of a parameter:

```
parameters[set_name][name] = 123 or 'abc'
```

| dolfin | type | | | | | range | change |
|----------------------------------|-----------|------------|-----------|--------------------|---------------|------------------|--------|
| allow extrapolation | bool | | | | | Not set | |
| dof ordering library | string | SC0TCH | | | | | |
| ghost mode | string | | | | | | |
| graph coloring library | string | Boost | | | | | |
| inear algebra backend | string | PETSc | | | | [Eigen,PETSc] | |
| nesh partitioner | string | SC0TCH- | | | [None, Page 1 | arMETIS,SCOTCH) | |
| artitioning approach | string | PARTITION | | [PA | RTITION, REFI | NE, REPARTITION] | |
| rint mpi thread support level | | | | | | Not set | |
| efinement algorithm | string | plaza | [plaza,pl | aza_with | _parent_face | ts,regular_cut] | |
| elative line width | double | 0.025000 | | | | Not set | |
| eorder_cells_gps | bool | | | | | Not set | |
| eorder dofs serial | | | | | | Not set | |
| eorder_vertices_gps | bool | | | | | Not set | |
| td_out_all_processes | bool | | | | | Not set | |
| imer_prefix | string | | | | | Not set | |
| se_petsc_signal_handler | bool | | | | | Not set | |
| arn_on_xml_file_size | | 100 | | | | Not set | |
| Parameter set "form_compiler" co | ntaining: | | | arameter access | | | |
| compiter | Lyp | | I aliye | | criange | | |
| add tabulate tensor timing | boo | | Not set | | | | |
| cache dir | strin | g | Not set | | | | |
| convert exceptions to warnings | boo | | Not set | | | | |
| cpp optimize | | | Not set | | | | |
| cpp optimize flags | strin | g -02 | Not set | | | | |
| epsilon | | e 0.000000 | Not set | | | | |
| | | | Not set | | | | |
| external_include_dirs | strin | | Not set | | | | |
| external includes | strin | | Not set | | | | |
| external libraries | | | Not set | | | | |
| external_library_dirs | strin | | Not set | | | | |
| form_postfix | | | Not set | | | | |
| format | İstrin | | Not set | | | | |

generate dummy tabulate tensor

no-evaluate basis derivatives

relative tolerance

<Parameter set "krylov solver" containing 8 parameter(s) and parameter set(s)>

<Parameter set "lu solver" containing 3 parameter(s) and parameter set(s)>

Introduction to solver 'parameters'

Example: change some parameters in Krylov solver

```
prm = parameters['krylov_solver'] # for short form
prm['absolute_tolerance'] = 1E-10
prm['relative_tolerance'] = 1E-6
prm['maximum_iterations'] = 1000
```

If you change these parameters at the beginning of your code, they will **globally** applied hereafter

| <pre><parameter "krylov_solver"="" 8="" and="" containing="" parameter="" parameter(s)="" set="" set(s)=""></parameter></pre> | | | | | | | |
|---|--|---|---|---|-----------------------|-----------------------|--|
| krylov_solver | | type | value | range | access | change | |
| absolute_tolerance divergence_limit error_on_nonconvergence maximum_iterations monitor_convergence nonzero_initial_guess relative_tolerance report | | double double bool int bool double | <unset> /unset></unset></unset></unset></unset></unset></unset></unset></unset></unset></unset></unset></unset> | Not set Not set Not set Not set Not set | 0 0 0 0 0 | 0 0 0 0 0 | |

| <pre><parameter "krylov_solver"="" 8="" and="" containing="" parameter="" parameter(s)="" set="" set(s)=""></parameter></pre> | | | | | | | | |
|---|------------------|-----------------|--------------------|--------|--------|--|--|--|
| krylov_solver | type | value | range | access | change | | | |
| absolute_tolerance | double | | Not set | | | | | |
| <pre>divergence_limit error_on_nonconvergence</pre> | double bool | <unset></unset> | Not set Not set | 0 0 | 0 0 | | | |
| <pre>maximum_iterations monitor_convergence</pre> | int bool | | Not set Not set | | 0 0 | | | |
| nonzero_initial_guess relative_tolerance | bool double | | Not set Not set | | | | | |
| report | bool | <unset></unset> | Not set | | | | | |

Before After

Introduction to Newton algorithm

ALGORITHM 5.3.1.
$$newton(x, F, \tau)$$

- 1. $r_0 = ||F(x)||$
- 2. Do while $||F(x)|| > \tau_r r_0 + \tau_a$
 - (a) Compute F'(x)

 - (c) Solve LUs = -F(x)
 - (d) x = x + s
 - (e) Evaluate F(x).

$$F(x)=0$$
,

$$F(x)=0,$$

$$F'(x_{n}) \approx \frac{F(x_{n+1}) - F(x_{n})}{x_{n+1} - x_{n}}, \quad x_{n+1} = x_{n} + F'(x_{n})^{-1} (F(x_{n+1}) - F(x_{n})),$$

$$\|F(x)\| \gg \|F(x_{n})\| \Rightarrow 0 \quad \text{So that } x_{n} = x_{n} - F'(x_{n})^{-1} F(x_{n})$$

(a) Compute
$$F'(x)$$

(b) Factor $F'(x) = LU$.
(c) Solve $LUs = -F(x) = S_n$ $||F(x_n)|| \gg ||F(x_{n+1})|| \to 0$ So that $x_{n+1} = x_n - F'(x_n)^{-1} F(x_n)$ or $x_{n+1} - x_n = -F'(x_n)^{-1} F(x_n)$

and

 $k \leq k_{max}$

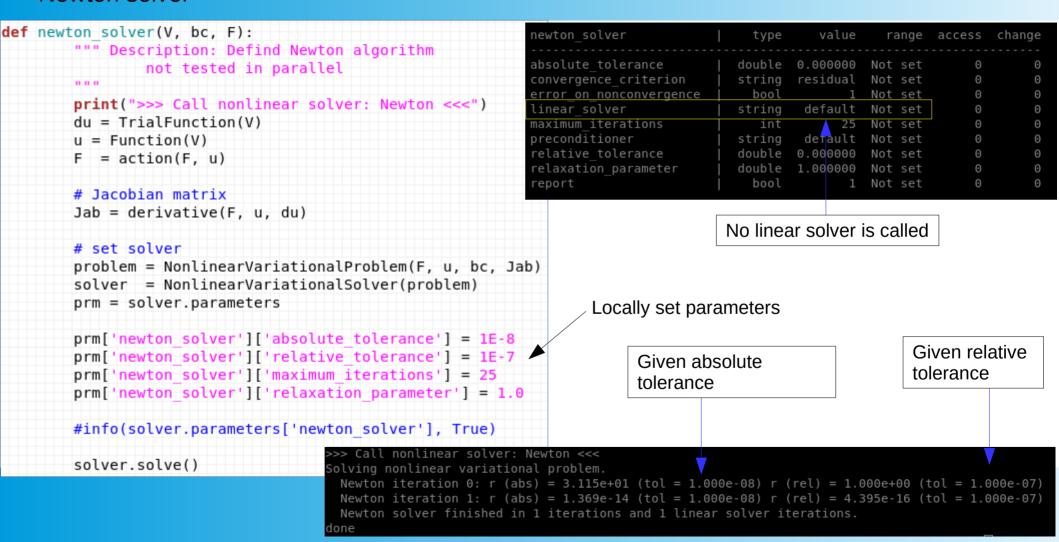
Newton method:
$$\begin{aligned} s_n &:= x_{n+1} - x_n \\ F'(x_n) s_n &= -F(x_n) \\ x_{n+1} &= x_n + s_n \end{aligned}$$

$$||F(x)|| \le \tau_r ||F(x_0)|| + \tau_\alpha$$
 τ_r Relative error tolerance

 τ_r Relative error tolerance

 τ_{α} Absolute error tolerance

Newton solver



Introduction to GMRES algorithm

ALGORITHM 3.4.2. $gmresa(x, b, A, \epsilon, kmax, \rho)$

1.
$$r = b - Ax$$
, $v_1 = r/||r||_2$, $\rho = ||r||_2$, $\beta = \rho$, $k = 0$

- 2. While $\rho > \epsilon ||b||_2$ and k < kmax do
 - (a) k = k + 1
 - (b) for j = 1, ..., k $h_{jk} = (Av_k)^T v_j$
 - (c) $v_{k+1} = Av_k \sum_{j=1}^k h_{jk} v_j$ arnoldi
 - (d) $h_{k+1,k} = ||v_{k+1}||_2$
 - (e) $v_{k+1} = v_{k+1} / ||v_{k+1}||_2$
 - (f) $e_1 = (1, 0, ..., 0)^T \in R^{k+1}$ Minimize $\|\beta e_1 - H_k y^k\|_{R^{k+1}}$ over R^k to obtain y^k .
 - (g) $\rho = \|\beta e_1 H_k y^k\|_{R^{k+1}}$.
- $3. \ x_k = x_0 + V_k y^k.$

Solve linear problem

$$Ax = b$$

Iteratively

GMRES solver

```
def gmres solver(V, bc, a, L):
        """ Description: linear solver GMRES
                can not run in parallel
        print(">>> Call linear solver: GMRES <<<")</pre>
        u = Function(V)
        # define problem and solver
        problem = LinearVariationalProblem(a, L, u, bc)
        solver = LinearVariationalSolver(problem)
        # choose algorithms GMRES with ILU preconditioner
        solver.parameters['linear solver'] = "gmres"
        solver.parameters['preconditioner'] = "ilu"
        #solver.parameters['print rhs'] = True
        # set local parameters
        prm = solver.parameters['krylov solver'] # short form
        prm['absolute tolerance'] = 1E-7
        prm['relative tolerance'] = 1E-4
        prm['maximum iterations'] = 1000
        prm['monitor convergence'] = True
        prm['report'] = True
        info(solver.parameters, True)
        solver.solve()
                               Print convergence message
        return u
```

```
>> Call linear solver: GMRES <<<
<Parameter set "linear variational solver" containing 7 parameter(s) and parameter set(s).</p>
 linear variational solver |
 linear solver
                                      amres Not set
                                        ilu Not set
                                             Not set
 print matrix
                                bool
                                bool
                                             Not set
 svmmetric
                                          0 Not set
 <Parameter set "krylov solver" containing 8 parameter(s) and parameter set(s)>
   krylov solver
   absolute tolerance
                              double 0.000000 Not set
   divergence limit
                              double
   error on nonconvergence
                                      <unset> Not set
   nonzero initial guess
   relative tolerance
                                             1 Not set
 <Parameter set "lu solver" containing 3 parameter(s) and parameter set(s)>
   lu solver | type value range access change
                          1 Not set
   svmmetric
                          0 Not set
                          0 Not set
```

Preconditioner 'ilu' can not run in parallel, use 'hypre euclid' instead

```
Solving linear variational problem.

Solving linear system of size 549 x 549 (PETSc Krylov solver).

done
```

```
Solving linear variational problem.
Solving linear system of size 549 x 549 (PETSc Krylov solver).
0 KSP preconditioned resid norm 1.087833032130e+01 true resid norm 8.944633496442e+00 ||r(i)||/||b|| 1.000000000000e+00
1 KSP preconditioned resid norm 3.177442391705e+00 true resid norm 3.237513682686e+00 ||r(i)||/||b|| 3.619504012069e-01
2 KSP preconditioned resid norm 1.646247475198e+00 true resid norm 1.709854243620e+00 ||r(i)||/||b|| 1.911597880786e-01
```

3 KSP preconditioned resid norm 1.133144175467e+00 true resid norm 1.042557609266e+00 ||r(i)||/||b|| 1.165567722457e-01

Introduction to Newton-GMRES algorithm

ALGORITHM 6.2.1. fdgmres
$$(s, x, F, h, \eta, kmax, \rho)$$
1. $s = 0, r = -F(x), v_1 = r/\|r\|_2, \rho = \|r\|_2, \beta = \rho, k = 0$
2. While $\rho > \eta \|F(x)\|_2$ and $k < kmax$ do

(a) $k = k + 1$

(b) $v_{k+1} = D_h F(x : v_k)$ Inexact termination condition for $j = 1, \dots k$

i. $h_{jk} = v_{k+1}^T v_j$

ii. $v_{k+1} = v_{k+1} - h_{jk} v_j$

(c) $h_{k+1,k} = \|v_{k+1}\|_2$

(d) $v_{k+1} = v_{k+1} / \|v_{k+1}\|_2$

ALGORITHM 6.3.1.
$$nsolgm(x, F, \tau, \eta)$$

- 1. $r_c = r_0 = ||F(x)||_2 / \sqrt{N}$ Termination condition
- 2. Do while $||F(x)||_2/\sqrt{N} > \tau_r r_0 + \tau_a$
 - (a) Select η .
 - (b) $fdgmres(s, x, F, \eta) = S$ (c) x = x + s
 - (d) Evaluate F(x)
 - (e) $r_{+} = ||F(x)||_{2} / \sqrt{N}, \sigma = r_{+} / r_{c}, r_{c} = r_{+}$
 - (f) If $||F(x)||_2 \le \tau_r r_0 + \tau_a$ exit.

GMRES is originally designed for solving linear problem

$$Ax = b$$

Newton algorithm uses GMRES to find S_n

$$F'(x)s=F(x)$$

Forward difference GMRES algorithm

(e) $e_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^{k+1}$

(f) $\rho = \|\beta e_1 - H_k y^k\|_{R^{k+1}}$.

3. $s = V_k y^k$. output

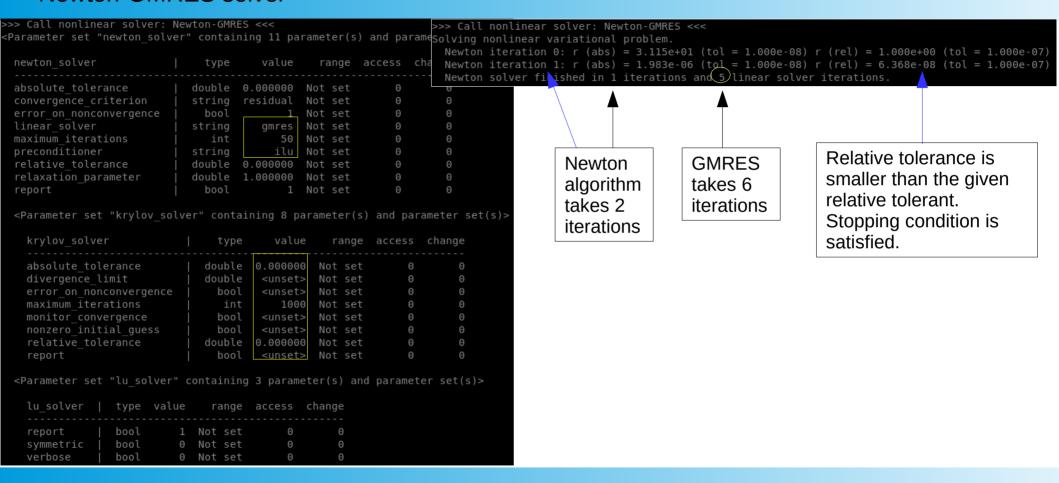
C.T. Kelley – solving nonlinear equations with Newton's Method (1987)

Minimize $\|\beta e_1 - H_k y^k\|_{R^{k+1}}$ to obtain $y^k \in \mathbb{R}^k$.

Newton-GMRES solver

```
def newton gmres solver(V, bc, F):
        print(">>> Call nonlinear solver: Newton-GMRES <<<")</pre>
        du = TrialFunction(V)
       u = Function(V)
        F = action(F. u)
       # Jacobian matrix
        Jab = derivative(F, u, du)
       # set problem and solver
        problem = NonlinearVariationalProblem(F, u, bc, Jab)
        solver = NonlinearVariationalSolver(problem)
        prm = solver.parameters
       # set Newton solver
        prm['newton solver']['absolute tolerance'] = 1E-8
        prm['newton solver']['relative tolerance'] = 1E-7
        prm['newton solver']['maximum iterations'] = 50
        prm['newton solver']['relaxation parameter'] = 1.0
        prm['newton solver']['linear solver'] = 'qmres'
        prm['newton solver']['preconditioner'] = 'ilu'
       #info(prm['newton solver'], True)
       # set GMRES solver
        prm['newton solver']['krylov solver']['absolute tolerance'] = 1E-9
        prm['newton solver']['krylov solver']['relative tolerance'] = 1E-7
        prm['newton solver']['krylov solver']['maximum iterations'] = 1000
       #info(prm['newton solver'], True)
        solver.solve()
```

Newton-GMRES solver



Good lecturers and references

http://users.ices.utexas.edu/~noemi/teaching.html

https://fenicsproject.org/pub/course/lectures/2017-nordic-phdcourse/

http://www.math.pitt.edu/~sussmanm/

FEniCS tutorial (Python):http://fenicsproject.org/documentation/tutorial/

Examples:http://fenicsproject.org/_static/tutorial/fenics_tutorial_examples.tar.gz

FEniCS presentations: http://fenicsproject.org/pub/presentations/

FEniCS course:http://fenicsproject.org/pub/course/lectures/

Documented DOLFIN demos (Python):note: the demos are already installed on your

system, see fo ex:/Applications/FeniCS.app/Contents/Resources/share/dolfin/demohttp://

fenicsproject.org/documentation/dolfin/1.1.0/python/demo/index.html

Basic classes and functions in DOLFIN (Python):

http://fenicsproject.org/documentation/dolfin/1.1.0/python/quick_reference.html

All classes and functions in DOLFIN (Python):

http://fenicsproject.org/documentation/dolfin/1.1.0/python/genindex.html

Questions on forum

Use subprocess: object oriented programming https://fenicsproject.org/qa/10701/on-using-mpi/

Marked mesh with GMSH tag does not work in parallel: https://fenicsproject.org/qa/5337/importing-marked-mesh-for-parallel-use/?show=5344#a5344

https://fenicsproject.org/qa/5864/get-access-to-entire-vector-in-parallel/

https://fenicsproject.org/qa/4227/going-parallel-distributed/

https://fenicsproject.org/qa/13142/assemble-system-parallel-and-store-complete-sparse-matrix/

https://fenicsproject.org/qa/3025/solving-a-problem-in-parallel-with-mpi-&-petsc/

Parallel tutorial

https://fenicsproject.org/qa/3154/improve-performance-for-solving-coupled-system-in-parallel/https://fenicsproject.org/qa/3324/using-petsc-direct-solver-in-parallel/https://fenicsproject.org/qa/12217/parallel-solver-calls/

https://fenicsproject.org/qa/8459/what-is-the-simplest-way-to-use-mpi/

http://www.math.pitt.edu/~sussmanm/3040Summer14/fenicsI.pdf

https://media.readthedocs.org/pdf/fenics-handson/latest/fenics-handson.pdf

https://fenicsproject.org/qa/10068/solving-linear-system-in-parallel/

http://andy.terrel.us/papers and talks/FEniCS08Tutorial.pdf

https://www.mcs.anl.gov/petsc/documentation/tutorials/ACTS2006/ACTS2006.pdf

https://cse.buffalo.edu/~knepley/presentations/TutorialFEniCS2008.pdf