

9 April 2021

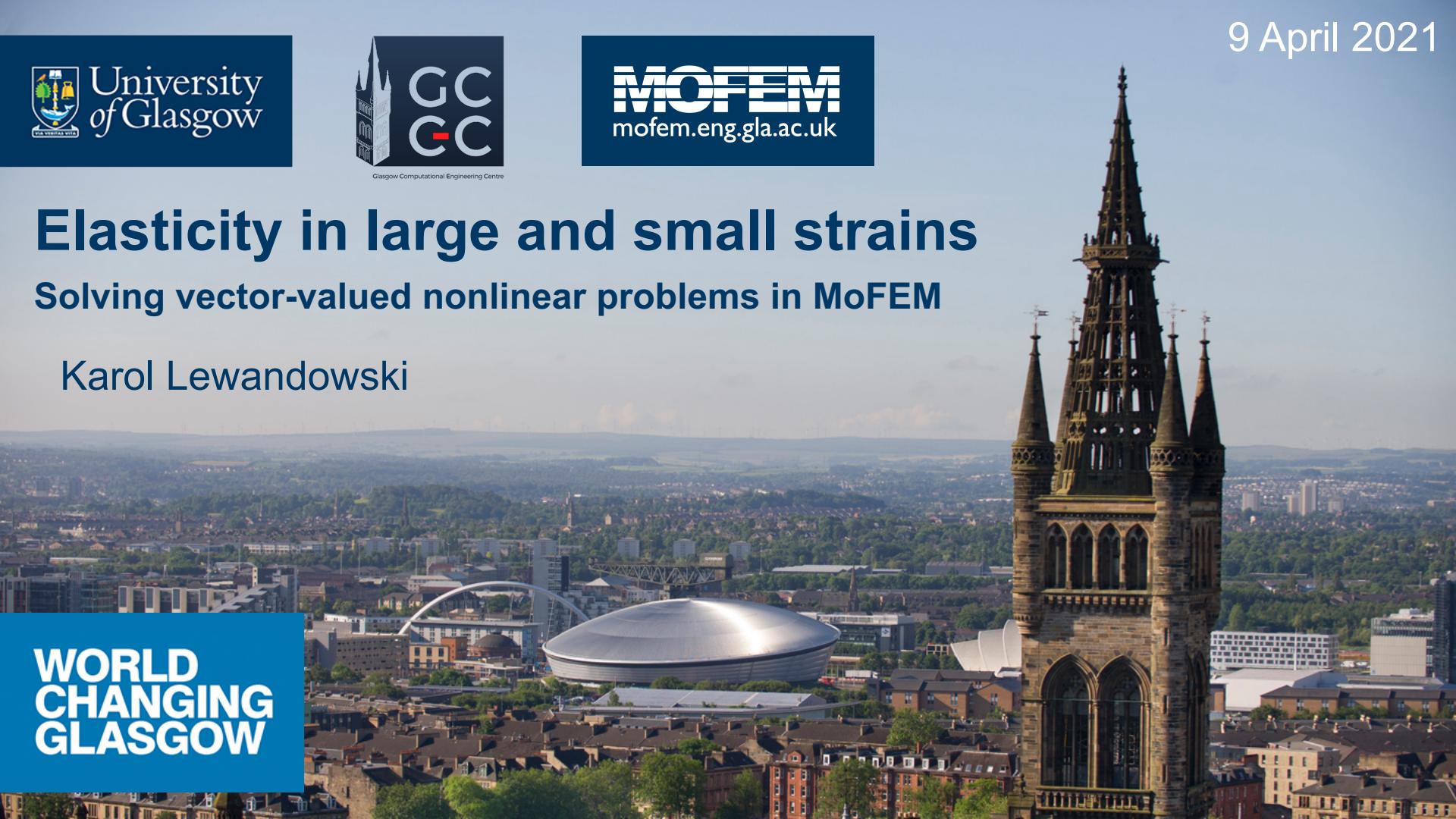


Elasticity in large and small strains

Solving vector-valued nonlinear problems in MoFEM

Karol Lewandowski

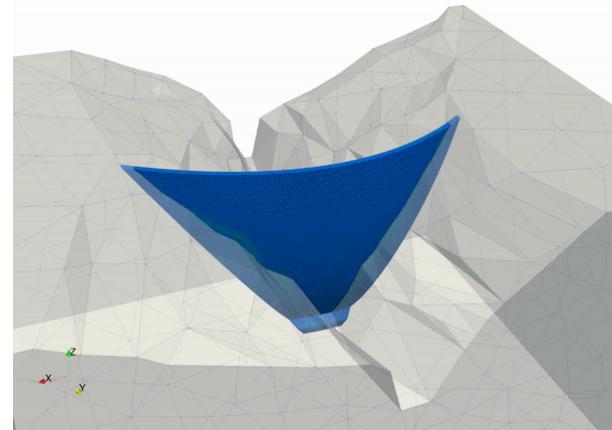
**WORLD
CHANGING
GLASGOW**



Elasticity problem

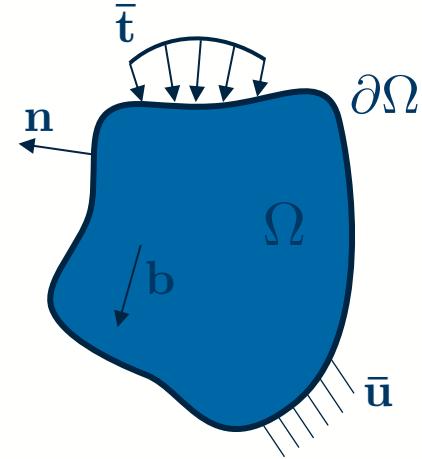
Outline

- Governing equations
- Implementation
- Result
- Large strains example
- Implementing and solving nonlinear problems
- Summary



VEC-0 <http://mofem.eng.gla.ac.uk/mofem/html/tutorials.html>

Governing equations



- Physical example: Deformation of an elastic body with arbitrary load

- Balance of momentum

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}(\mathbf{x})) + \mathbf{b} = 0 & \text{in } \Omega \\ \mathbf{u}(\mathbf{x}) = \bar{\mathbf{u}} & \text{on } \partial\Omega^u \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} & \text{on } \partial\Omega^t \end{cases}$$

- Constitutive equation

$$\boldsymbol{\sigma} = \mathbb{D} : \frac{1}{2} (\nabla \mathbf{u}^T + \nabla \mathbf{u})$$

- Weak form – find $\mathbf{u} \in \mathbf{H}^1(\Omega)$

$$\int_{\Omega} \nabla \delta \mathbf{u} : \boldsymbol{\sigma}(\mathbf{u}) d\Omega = - \int_{\Omega} \delta \mathbf{u} \cdot \mathbf{b} d\Omega + \int_{\partial\Omega^t} \delta \mathbf{u} \cdot \bar{\mathbf{t}} dS \quad \forall \delta \mathbf{u} \in \mathbf{H}_0^1(\Omega)$$

Discretisation

- Approximation

$$\mathbf{u} \approx \mathbf{u}^h = \sum_{j=0}^{N-1} \phi_j \bar{\mathbf{u}}_j \quad \delta \mathbf{u} \approx \delta \mathbf{u}^h = \sum_{j=0}^{N-1} \phi_j \delta \bar{\mathbf{u}}_j$$

- Substitute to the weak form

- Global system

$$\mathbf{KU} = \mathbf{F}$$

where

$$\mathbf{K}_{ij}^e = \int_{\Omega^e} \nabla \phi_i \mathbb{D} \nabla \phi_j \, d\Omega \approx \sum_q \nabla \phi_i (\mathbf{x}_q) \mathbb{D} \nabla \phi_j (\mathbf{x}_q) w_q$$

$$\mathbf{F}_i^e = \int_{\partial \Omega^e} \phi_i \mathbf{t} \, dS + \int_{\Omega^e} \phi_i \mathbf{b} \, d\Omega \approx \sum_q \phi_i (\mathbf{x}_q) \mathbf{t} (\mathbf{x}_q) w_q + \sum_q \phi_i (\mathbf{x}_q) \mathbf{b} (\mathbf{x}_q) w_q$$

Implementation: Setup

```
constexpr int SPACE_DIM = 2; //< Space dimension of problem, mesh
```

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem(); // Call to MoFEMFunctionBegin
    MoFEMFunctionReturn(0);
}
```

```
///! [Set up problem]
MoFEMErrorCode Example::setupProblem() {
    MoFEMFunctionBegin;
    Simple *simple = mField.getInterface<Simple>();
    // Add field
    CHKERR simple->addDomainField("U", H1, AINSWORTH_LEGENDRE_BASE, SPACE_DIM);
    CHKERR simple->addBoundaryField("U", H1, AINSWORTH_LEGENDRE_BASE, SPACE_DIM);
    int order = 2;
    CHKERR PetscOptionsGetInt(PETSC_NULL, "", "-order", &order, PETSC_NULL);
    CHKERR simple->setFieldOrder("U", order);
    CHKERR simple->setUp();
    MoFEMFunctionReturn(0);
}
```

Implementation: Elasticity tensor

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();----->
    CHKERR boundaryCondition();
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
constexpr auto t_kd = FTensor::Kronecker_Delta_symmetric<int>();
constexpr double A =
    (SPACE_DIM == 2) ? 2 * shear_modulus_G /
                       (bulk_modulus_K + (4. / 3.) * shear_modulus_G) : 1;
auto t_D = getFTensor4DdgFromMat<SPACE_DIM, SPACE_DIM, 0>(*matDPtr);

t_D(i, j, k, l) = 2 * shear_modulus_G * ((t_kd(i, k) ^ t_kd(j, l)) / 4.) +
                  A * (bulk_modulus_K - (2. / 3.) * shear_modulus_G) *
                      t_kd(i, j) * t_kd(k, l);
```

$$\mathbb{D}_{ijkl} = G [\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] + A(K - \frac{2}{3}G) [\delta_{ij}\delta_{kl}]$$

where for 3D or plane strain:

$$A = 1$$

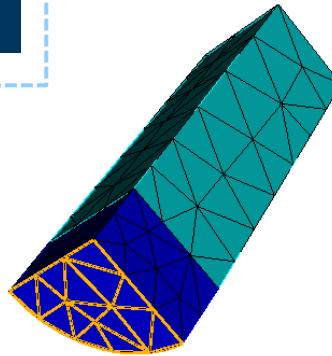
plane stress:

$$A = \frac{2G}{K + \frac{4}{3}G}$$

Implementation: Dirichlet BC

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition(); // Call to boundaryCondition()
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
CHKERR remove_ents(fix_disp("FIX_X"), 0, 0);
CHKERR remove_ents(fix_disp("FIX_Y"), 1, 1);
CHKERR remove_ents(fix_disp("FIX_Z"), 2, 2);
CHKERR remove_ents(fix_disp("FIX_ALL"), 0, 3);
```



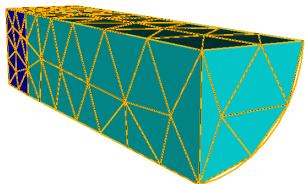
Implementation: Neumann BC

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition(); //<----->
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
auto set_body_force = [&]() {
    FTensor::Index<'i', SPACE_DIM> i;
    MoFEMFunctionBegin;
    auto t_force = getFTensor1FromMat<SPACE_DIM, 0>(*bodyForceMatPtr);
    t_force(i) = 0;
    t_force(1) = -1;
    MoFEMFunctionReturn(0);
};

pipeline_mng->getOpDomainRhsPipeline().push_back(new OpBodyForce(
    "U", bodyForceMatPtr, [](double, double, double) { return 1.; }));

```



$$\mathbf{F}_i^e = \int_{\Omega^e} \phi_i \mathbf{b} \, dV$$

Implementation: Assembly

Pushing UDOs into pipelines

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem(); //<----- Pipeline insertion point
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
using OpK = FormsIntegrators<DomainEleOp>::Assembly<PETSC>::BiLinearForm<
GAUSS>::OpGradSymTensorGrad<1, SPACE_DIM, SPACE_DIM, 0>;
```

```
if (SPACE_DIM == 2) {
    pipeline_mng->getOpDomainLhsPipeline().push_back(
        new OpCalculateInvJacForFace(invJac));
    pipeline_mng->getOpDomainLhsPipeline().push_back(
        new OpSetInvJacH1ForFace(invJac));
}
pipeline_mng->getOpDomainLhsPipeline().push_back(new OpK("U", "U", matDPtr));
```

$$\mathbf{K}_{ij}^e = \int_{\Omega^e} \nabla \phi_i \mathbb{D} \nabla \phi_j \, d\Omega$$

Implementation: Solve

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
///! [Solve]
MoFEMErrorCode Example::solveSystem() {
    MoFEMFunctionBegin;
    auto *simple = mField.getInterface<Simple>();
    auto *pipeline_mng = mField.getInterface<PipelineManager>();
    auto solver = pipeline_mng->createKSP();
    CHKERR KSPSetFromOptions(solver);
    CHKERR KSPSetUp(solver);

    auto dm = simple->getDM();
    auto D = smartCreateDMVector(dm);
    auto F = smartVectorDuplicate(D);

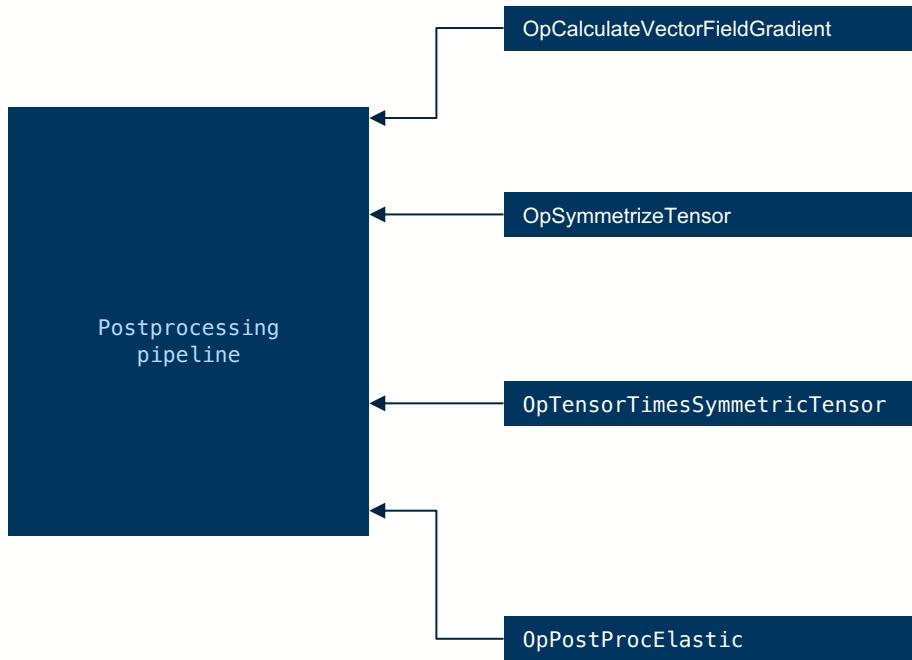
    CHKERR KSPSolve(solver, F, D);
    CHKERR VecGhostUpdateBegin(D, INSERT_VALUES, SCATTER_FORWARD);
    CHKERR VecGhostUpdateEnd(D, INSERT_VALUES, SCATTER_FORWARD);
    CHKERR DMoFEMMeshToLocalVector(dm, D, INSERT_VALUES,
                                   SCATTER_REVERSE);
    MoFEMFunctionReturn(0);
}
```

Implementation: Postprocessing

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
pipeline_mng->getDomainLhsFE().reset();
auto post_proc_fe = boost::make_shared<PostProcEle>(mField);
post_proc_fe->generateReferenceElementMesh();
post_proc_fe->getOpPtrVector().push_back(
    new OpCalculateVectorFieldGradient<SPACE_DIM, SPACE_DIM>("U",
                                                               matGradPtr));
post_proc_fe->getOpPtrVector().push_back(
    new OpSymmetrizeTensor<SPACE_DIM>("U", matGradPtr, matStrainPtr));
post_proc_fe->getOpPtrVector().push_back(
    new OpTensorTimesSymmetricTensor<SPACE_DIM, SPACE_DIM>(
        "U", matStrainPtr, matStressPtr, matDPtr));
post_proc_fe->getOpPtrVector().push_back(new OpPostProcElastic<SPACE_DIM>(
    "U", post_proc_fe->postProcMesh, post_proc_fe->mapGaussPts, matStrainPtr,
    matStressPtr));
post_proc_fe->addFieldValuesPostProc("U");
pipeline_mng->getDomainRhsFE() = post_proc_fe;
CHKERR pipeline_mng->loopFiniteElements();
CHKERR post_proc_fe->writeFile("out_elastic.h5m");
```

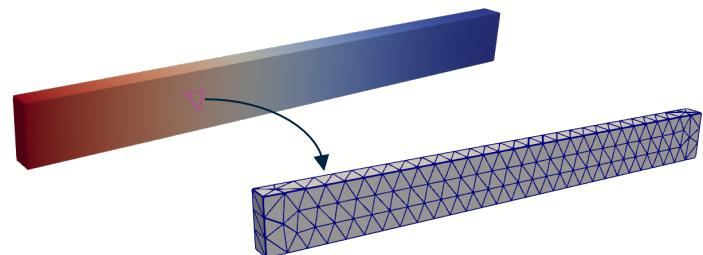
Implementation: Postprocessing



$$\nabla \mathbf{u}^h = \sum_{m=0}^{N-1} \nabla \phi_m \bar{\mathbf{u}}_m$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u}^T + \nabla \mathbf{u})$$

$$\boldsymbol{\sigma} = \mathbb{D} : \boldsymbol{\varepsilon}$$



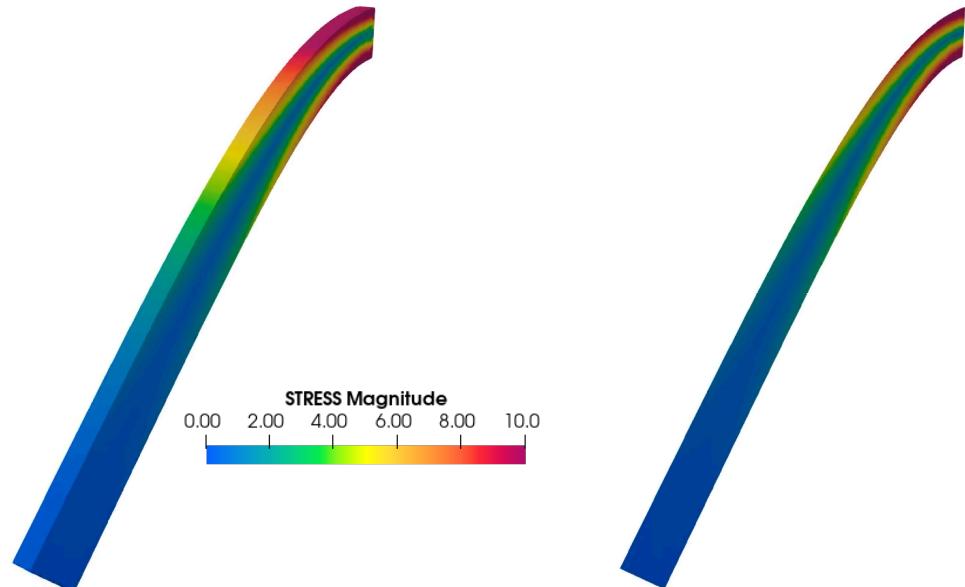
Results: 2D and 3D

```
constexpr int SPACE_DIM = 3; //< Space dimension of problem, mesh
```

Execute program:

```
./elastic -file_name beam_3D.cub -order 2
```

- Cantilever beam
- Uniform body force
- *mbconvert* tool
- *Paraview*
WarpByVector filter



Nonlinear problem

Small strain theory cannot deal with large rotations!

Introduce Hencky measures [1]:

- Logarithmic strain

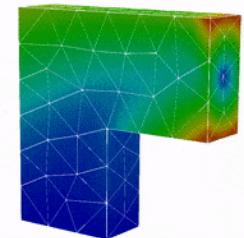
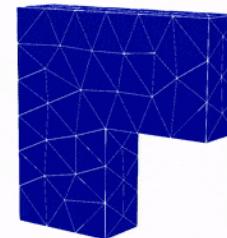
$$\mathbf{E} := \frac{1}{2} \ln(\mathbf{F}^T \mathbf{F})$$

- Work conjugate stress:

$$\mathbf{T} = \mathbb{D} : \mathbf{E}$$

- Geometric postprocessor:

$$\mathbf{P} = \mathbf{F} \mathbf{T} : 2\partial_C \mathbf{E}$$



Nonlinear problem

The solution to a nonlinear problem will be obtained in increments:

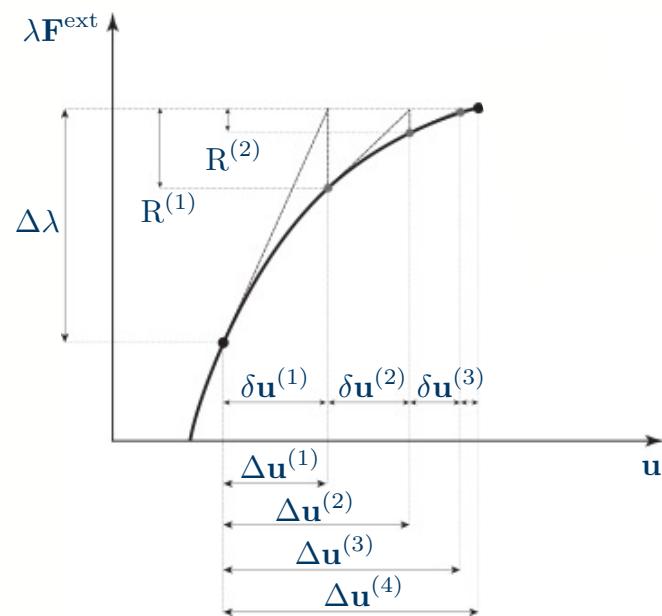
$$\bar{\mathbf{u}}_{n+1} = \bar{\mathbf{u}}_n + \Delta\bar{\mathbf{u}}$$

System of previous linear equations is restated as:

$$\mathbf{F}^{\text{int}}(\bar{\mathbf{u}}) - \mathbf{F}^{\text{ext}} = \mathbf{0}$$

$$\mathbf{F}^{\text{int}}(\bar{\mathbf{u}}_0 + \delta\bar{\mathbf{u}}) = \mathbf{F}^{\text{int}}(\bar{\mathbf{u}}_0) + \left[\frac{\partial \mathbf{F}(\bar{\mathbf{u}})}{\partial \bar{\mathbf{u}}} \right] \cdot \delta\bar{\mathbf{u}}$$

$$[K_T]_{\bar{\mathbf{u}}_0} \delta\bar{\mathbf{u}} = \Delta\lambda \mathbf{F}^{\text{ext}} - \mathbf{F}^{\text{int}}(\bar{\mathbf{u}})$$



Implementation: Assemble

Operators push both to RHS and LHS

Pushing UDOs into pipelines

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem(); //<----- Pipeline insertion point
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
auto add_domain_base_ops = [&](auto &pipeline) {
    MoFEMFunctionBegin;

    pipeline.push_back(new OpCalculateVectorFieldGradient<SPACE_DIM,
                       SPACE_DIM>("U", matGradPtr));

    pipeline.push_back(
        new OpCalculateEigenVals<SPACE_DIM>("U",
                                              commonHenkyDataPtr));
    pipeline.push_back(
        new OpCalculateLogC<SPACE_DIM>("U", commonHenkyDataPtr));
    pipeline.push_back(
        new OpCalculateLogC_dC<SPACE_DIM>("U", commonHenkyDataPtr));
    pipeline.push_back(
        new OpCalculateHenckyStress<SPACE_DIM>("U",
                                                 commonHenkyDataPtr));
    pipeline.push_back(
        new OpCalculatePiolaStress<SPACE_DIM>("U",
                                                commonHenkyDataPtr));

    MoFEMFunctionReturn(0);
};
```

Implementation: Assemble

```

F(i, j) = t_grad(i, j) + t_kd(i, j);
C(i, j) = F(k, i) ^ F(k, j);

// rare case when two eigen values are equal
auto nb_uniq = get_uniq_nb(eig);
if (DIM == 3 && nb_uniq == 2)
    sort_eigen_vals(eig, eigen_vec);

auto logC = EigenMatrix::getMat(eig, eigen_vec, f);

T(i, j) = t_D(i, j, k, l) * logC(k, l);

auto dlogC_dC = EigenMatrix::getDiffMat(eig, eigen_vec, f, d_f, nb_uniq);
dlogC_dC(i, j, k, l) *= 2;

S(k, l) = T(i, j) * dlogC_dC(i, j, k, l);
P(i, l) = F(i, k) * S(k, l);

FTensor::Tensor4<double, DIM, DIM, DIM, DIM> dC_dF;
dC_dF(i, j, k, l) = (t_kd(i, l) * F(k, j)) + (t_kd(j, l) * F(k, i));

auto TL = EigenMatrix::getDiffDiffMat(eig, eigen_vec, f, d_f, dd_f, T,
                                      nb_uniq);
TL(i, j, k, l) *= 4;

FTensor::Ddg<double, DIM, DIM> P_D_P_plus_TL;
P_D_P_plus_TL(i, j, k, l) =
    TL(i, j, k, l) +
    (dlogC_dC(i, j, o, p) * t_D(o, p, m, n)) * dlogC_dC(m, n, k, l);
P_D_P_plus_TL(i, j, k, l) *= 0.5;
dP_dF(i, j, m, n) = t_kd(i, m) * (t_kd(k, n) * S(k, j));
dP_dF(i, j, m, n) +=
    F(i, k) * (P_D_P_plus_TL(k, j, o, p) * dC_dF(o, p, m, n));

```

Strain measures:

$$\mathbf{F} = \nabla \mathbf{u} + \mathbf{I} \quad \mathbf{C} = \mathbf{F}^T \mathbf{F}$$

Compute tensor function using MoFEM function:

$$\mathbf{E} = \frac{1}{2} \ln \mathbf{C} \quad \mathbf{T} = \mathbb{D} : \mathbf{E}$$

and derivatives:

$$\mathbf{S} = \mathbf{T} : \mathbb{P}_L \quad \mathbb{P}_L := 2\partial_C \mathbf{E}$$

$$\mathbb{L}_L = 4\partial_{CC} \mathbf{E}$$

Tangent operator for LHS:

$$\mathbb{C}_L^{ep} = \mathbb{P}_L : \mathbb{D} : \mathbb{P}_L + \mathbf{T} : \mathbb{L}_L$$

$$\mathbb{C}_N^{ep} = \mathbb{I}\mathbf{S} + \mathbf{F}\mathbb{C}_L^{ep} : \partial_C \mathbf{F}$$

Implementation: Assemble

Pushing UDOs into pipelines

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem(); // Dashed box
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
auto add_domain_ops_lhs = [&](auto &pipeline) {
    MoFEMFunctionBegin;

    pipeline.push_back(
        new OpHenckyTangent<SPACE_DIM>("U", commonHenckyDataPtr));
    pipeline.push_back(new OpK("U", "U", commonHenckyDataPtr->getMatTangent()));

    MoFEMFunctionReturn(0);
};
```

$$\mathbf{K}_{ij}^e = \int_{\Omega^e} \nabla \phi_i \mathbb{C}_N^{ep} \nabla \phi_j \, d\Omega$$

```
auto add_domain_ops_rhs = [&](auto &pipeline) {
    MoFEMFunctionBegin;
    // Calculate internal force
    pipeline.push_back(new OpInternalForce(
        "U", commonHenckyDataPtr->getMatFirstPiolaStress()));

    MoFEMFunctionReturn(0);
};
```

$$\mathbf{F}_i^e = \int_{\Omega^e} \nabla \phi_i \cdot \mathbf{P} \, d\Omega$$

Implementation: Solve

```
///! [Run problem]
MoFEMErrorCode Example::runProblem() {
    MoFEMFunctionBegin;
    CHKERR readMesh();
    CHKERR setupProblem();
    CHKERR createCommonData();
    CHKERR boundaryCondition();
    CHKERR assembleSystem();
    CHKERR solveSystem();
    CHKERR outputResults();
    CHKERR checkResults();
    MoFEMFunctionReturn(0);
}
```

```
auto dm = simple->getDM();
auto ts = pipeline_mng->createTS();

// Add monitor to time solver
auto monitor_ptr = boost::make_shared<Monitor>(dm, post_proc_fe);
CHKERR DMMoFEMTSSetMonitor(dm, ts, simple->getDomainFName(), null_fe,
                           null_fe, monitor_ptr);

auto D = smartCreateDMVector(simple->getDM());

CHKERR TSSetSolution(ts, D);
CHKERR TSSetFromOptions(ts);

CHKERR TSSolve(ts, NULL);
```

This snippet will be the similar for all nonlinear problems

$$[K_T]_{\bar{\mathbf{u}}_0} \delta \bar{\mathbf{u}} = \Delta \lambda \mathbf{F}^{\text{ext}} - \mathbf{F}^{\text{int}}(\bar{\mathbf{u}})$$



Results: Nonlinear 3D problem

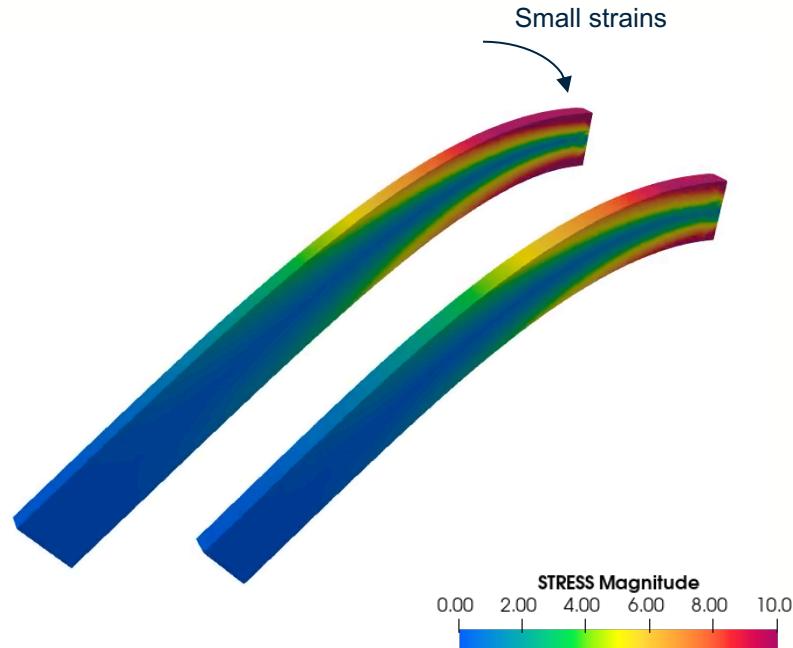
```
constexpr int SPACE_DIM = 3; //< Space dimension of problem, mesh
```

Execute program:

```
./nonlinear_elastic -file_name beam_3D.cub -order 2 -ts_dt 0.05
```

Program output for each load step $\Delta\lambda$:

```
[0] <inform> [petsc] 0 SNES Function norm 1.639129230990e-04  
[0] <inform> [petsc] 1 SNES Function norm 1.459143968364e-02  
[0] <inform> [petsc] 2 SNES Function norm 1.716350367415e-05  
[0] <inform> [petsc] 3 SNES Function norm 9.827788747448e-07  
[0] <inform> [petsc] 4 SNES Function norm 1.108872284616e-12  
[0] <inform> [petsc] 10 TS dt 0.05 time 0.5
```



Verify consistency of tangent matrix

Test Jacobian matrix using finite difference method:

```
./nonlinear_elastic -file_name beam_2D.cub -order 2 -ts_dt 0.05
-snes_test_jacobian
```

Absolute and relative error:

```
[0] <inform> [petsc] ----- Testing Jacobian -----
[0] <inform> [petsc] ||J - Jfd||_F / ||J||_F = 5.22467e-07, ||J - Jfd||_F
= 0.00128756
```

Plotting all entries for implemented matrix:

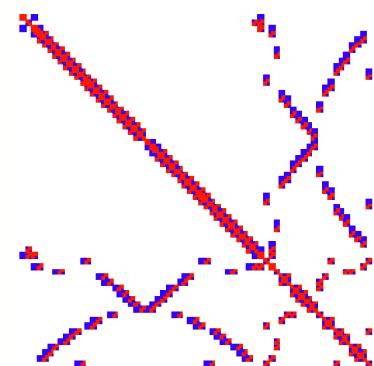
```
-snes_test_jacobian -snes_test_jacobian_display
```

```
[0] <inform> [petsc] Hand-coded minus finite-difference Jacobian with tolerance 1e-05 -----
[0] <inform> [petsc] Mat Object: 1 MPI processes
[0] <inform> [petsc] type: mpiaij
[0] <inform> [petsc] row 0: (0, 7.66377e-05) (1, 4.4597e-05) (4, 5.94409e-05)
[0] <inform> [petsc] row 1: (0, 4.66387e-05) (1, 6.35757e-05) (89, 4.46589e-05)
[0] <inform> [petsc] row 2: (2, 7.66377e-05) (3, 4.45971e-05) (86, 5.94409e-05)
[0] <inform> [petsc] row 3: (2, -4.66387e-05) (3, -6.35735e-05) (89, -4.46588e-05)
```

$$\mathbf{K}_{ij}^e \approx \frac{\mathbf{F}_i^e(\bar{\mathbf{u}} + h\mathbf{e}_j) - \mathbf{F}_i^e(\bar{\mathbf{u}})}{h}$$

Visualising tangent matrix errors:

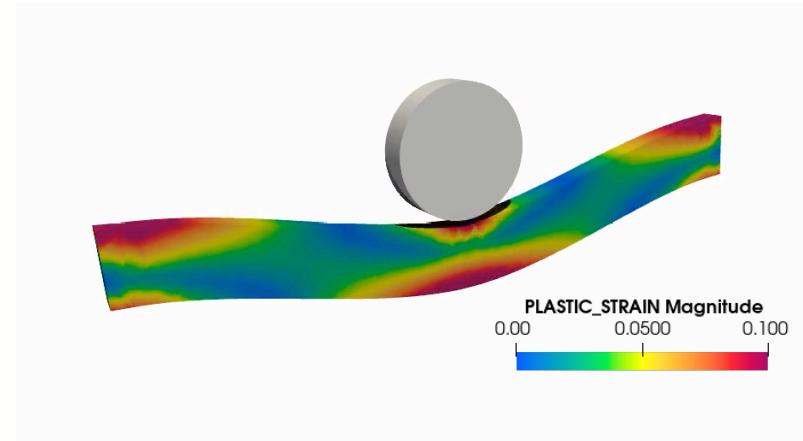
```
-snes_compare_explicit_draw -draw_save
```



Summary

- Implementation of a vector valued problem
- Using operators from MoFEM library
- Solving nonlinear elasticity
- Tools for debugging tangent matrix

- Modular structure can be easily extended with:
 - Contact
 - *Plasticity*
 - ...



Source code:

VEC-0 and VEC-2: <http://mofem.eng.gla.ac.uk/mofem/html/tutorials.html>



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Thank you for your attention!

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