Solvers for solid mechanics - Recent progress

Mika Malinen, D.Sc. (Tech.)

Aalto University Department of Mathematics and Systems Analysis and CSC – IT Center for Science (on leave)

April 15, 2021



The most notable "recent" developments (introduced in Elmer release 8.4., Dec 2018, or later)

- User-defined materials (UMAT) interface for nonlinear elasticity solver, together with documentation
- A nonlinear version of shell solver
- Support for solving strongly coupled FSI problems in frequency domain

Ongoing work

• A tight coupling of 3D elasticity and 2D shell equations

 $\ensuremath{\mathsf{red}}\xspace$ = the special subjects of this presentation

伺 と く ヨ と く ヨ と

I Overview of solvers for solid mechanics

Volumetric discretizations of 2-D/3-D solids

- Linear elasticity (the module StressSolve)
 - Basic material laws, with possible anisotropy
 - Modal and stability analysis
 - Harmonic analysis (complex-valued fields)
 - Mesh adaptivity
- Nonlinear elasticity (ElasticSolve)
 - Finite deformations
 - Neo-Hookean and St Venant-Kirchhoff materials in-built
 - Note: A St Venant-Kirchhoff material intended for large displacements and small extensional strains
 - A special formulation for an incompressible material
 - Anisotropy for a St Venant-Kirchhoff material
 - User-defined materials (UMAT) interface to handle more general classes of solids (beyond elasticity)

伺 と く ヨ と く ヨ と

Models obtained via dimensional reduction

- 1-D beams (BeamSolver3D)
 - Shear-deformable (Timoshenko's theory) and allows torsional stiffness
 - A beam can be embedded freely in the 3-dimensional space
 - A linearly elastic material
 - A recent addition (May, 2019)
- 2-D Reissner-Mindlin model for linearly elastic plates (SMITC)
- 2-D shell equations (ShellSolver)

- 2-D shell equations (ShellSolver)
 - finite deformations (a linear model as a special case)
 - a St Venant-Kirchhoff material only
 - an extensible director assumed
 - in some aspects a research version (non-standard developments)
 - to replace the (undocumented) facet shell solver (FacetShellSolver)

Nonlinear shell analysis: A cantilever benchmark

• A cantilever is subject to a shear force at an end



米部 とくほと くほと

3

Nonlinear shell analysis: A cantilever benchmark



Nonlinear shell analysis: A pinched cylinder benchmark

• A straight cylindrical shell is subject to a pinching force and has rigid end diaphragms allowing axial slip



- 4 回 ト - 4 回 ト

Nonlinear shell analysis: A pinched cylinder benchmark



Nonlinear shell analysis: An open hemisphere benchmark

• An open hemispherical shell is subject to inward and outward pinching forces



< 回 > < 回 > < 回 >

Nonlinear shell analysis: An open hemisphere benchmark



Additional utilities

- Pointwise springs and masses (SpringAssembly)
 - an additional assembly procedure to add springs and masses
 - allows the assembly although the mesh files do not specify point elements
 - a recent addition (Apr, 2020)

To sum up:

- Basic models available, limitations on available material models and postprocessing
- Higher-order discretizations may not be an option
- Pure solid mechanics has not really been on focus

伺 と く ヨ と く ヨ と

A typical question

"I need to apply a special nonlinear material model. Does Elmer support such a simulation?"

A typical answer

"In principle yes, but you need to program the material law ..."

A local enhancement suffices:

- Only a special subroutine has to be written
- The code of the solver need not be touched

Some historical comments:

- Our UMAT development was initiated in a project
- The project goal was to enable interfacing with material models written for ABAQUS
- The interface was published later under open source
- A thesis (M.Sc.) also utilized the UMAT interface: http://URN.fi/URN:NBN:fi:tty-201810032372

In practice

- UMAT is a Fortran subroutine with a fixed calling convention
- ABAQUS gives its own documentation

Different software work differently:

- Some adaptation on the Elmer side was needed
- For example, Elmer expresses the equilibrium equations in terms of the first Piola-Kirchhoff stress, while UMAT describes the material response in terms of the Cauchy stress
- Use modern Fortran when working with Elmer

伺 と く ヨ と く ヨ と

Limitations:

- Not all arguments of the UMAT subroutine are supported
- The implementation shouldn't rely on utility subroutines that are available only within Abaqus
- At the moment just stationary cases, but no technical hindrance to enable transient cases
- An adaptive load incrementation is not supported within Elmer
- That is, some simulation controls doesn't have a meaning within Elmer

伺い イヨン イヨン

How to start

- UMAT subroutine can be compiled independently of the solver of Elmer
- elmerf90 command coming with the installed Elmer can be used for compilation
- A ready template for writing UMAT is a part of the Elmer source code:

../fem/src/modules/UMATLib.F90

- It also contains some examples of basic material models
- See also example cases given as tests

.../fem/tests/UMAT_*

向下 イヨト イヨト

• The file containing UMAT implementation can be named freely, so one may compile for example

elmerf90 MyUMATLib.F90 -o MyUMATLib

- Several material models can also be contained in a single file
- Use the keyword UMAT Subroutine in a material section to specify the file and to pick the subroutine desired

```
Material X
UMAT Subroutine = "MyUMATLib" "my_umat"
...
```

You may also want to specify a path, for example

```
UMAT Subroutine = "./MyUMATLib" "my_umat"
```

▲□ ▶ ▲ □ ▶ ▲ □ ▶ □ ■ ● ● ● ●

Special keywords:

- Number of Material Constants
- Material Constants: Ordering and consistent use are at the responsibility of the user
- Number of State Variables
- Output State Variables: set True in order to obtain stresses (UmatStress), energy variables (UmatEnergy), and additional state variables (UmatState) as fields associated with integration points
- Initialize State Variables: an optional extra call to obtain the state variables in the initial state
- Name

伺 と く ヨ と く ヨ と

Some remarks:

- Calculate Stresses and Calculate Strains create stresses and strains as nodal fields
- Calculate Strains produces the standard material strain
- However, UMAT can define the Cauchy stress to be a function of any strain measure which may be computed in terms of the deformation gradient (switches now to an inexact Newton method)
- With UMAT the in-built convergence criterion is always "residual"
- An incompressible material is not yet supported (via a mixed formulation with an additional pressure variable)

向下 イヨト イヨト

II User-defined material models

The best place to find details is the template UMATLib.F90 and its comment lines

• Specifies a constitutive law

$$\boldsymbol{\sigma}_m(\mathbf{p},t) = \bar{\boldsymbol{\sigma}}(\hat{\boldsymbol{E}}(\boldsymbol{F})(\mathbf{p},t),\mathbf{q}(\mathbf{p},t)).$$

- Here $\hat{E}(F)$ is the strain field, F is the deformation gradient, and is $q = (q_1, \ldots, q_N)$ a N-tuple of state variables
- The stress response function is a composition

$$F \mapsto \bar{\sigma}(\cdot, \mathbf{q}) \circ \hat{E}(F),$$

so we can differentiate as

$$oldsymbol{U}\mapsto Dar{oldsymbol{\sigma}}(\hat{oldsymbol{E}}(oldsymbol{F}),\mathbf{q})[D\hat{oldsymbol{E}}(oldsymbol{F})[oldsymbol{U}]]$$

- ullet The user must specify the derivative $D \bar{oldsymbol{\sigma}}(\hat{m{E}}(m{F}),\mathbf{q})$
- If not possible in a closed form, an approximation may suffice

For some additional details see also Elmer Models Manual

э

(E) < E)</p>

In principle two ways to couple different models:

- a loose numerical coupling (the default strategy in Elmer)
- a tight numerical coupling: all unknowns updated/solved simultaneously

An implementation of a tight numerical coupling may not be an easy task:

- However, it may be the only practical way to handle a very strong physical coupling
- Gradual developments to enable tight coupling procedures

An example here: the coupling of a 2-D shell and a 3-D solid

・ 戸 ・ ・ ヨ ・ ・ ヨ ・

A graphical abstract: the coupling of solids and shells



-

Essential ingredients for enabling a tight coupling:

• An ability to construct a monolithic matrix from constituent blocks, for example to create:

$$\left[\begin{array}{cc} K & D \\ H & A \end{array}\right] \left[\begin{array}{c} U \\ V \end{array}\right] = \left[\begin{array}{c} F \\ G \end{array}\right]$$

where $K \mbox{ and } A$ are the stiffness matrices of 3D solid and shell parts

- Special keyword constructs/procedures so that existing solvers can be utilized to assemble the diagonal blocks
- Special assembly subroutines for creating coupling blocks (here D and H)

▲圖 → ▲ 国 → ▲ 国 →

Remarks:

- After a monolithic system has been created, its solution can be sought by applying a Krylov method
- $\bullet\,$ The block matrix construct within Elmer is generic \Rightarrow should work similarly in different cases
- On the other hand, D and H don't exist as matrices when using a loose coupling \Rightarrow specific code needed
- Block preconditioning to combine the strengths of loose and tight numerical coupling

▲圖 ▶ ▲ 国 ▶ ▲ 国 ▶ …

For details on writing a sif file for a tightly coupled model see Chapter 14 of ElmerSolver Manual, *"Block-matrix construct to build tightly coupled solvers"*

- Two solver sections needed as usual
- The first solver section to assemble the (1,1)-block and to control the solution of the fully coupled system
- The second solver section is subsidiary, integrating the (2,2)-block
- The keyword Structure-Structure Coupling activates the integration of interaction blocks

□ > 《注 > 《注 >

Special keywords:

- Linear System Block Mode: a main switch to create the linear system by using block construct
- Block Solvers(2): pointers to solvers which define constituent blocks
- Pre Solvers(1): activates the execution of a subsidiary solver in the assembly
- Block Monolithic: to create the coupled system as a single object
- Shell Solver Index: to inform that the coupling with the shell solver is wanted

伺 と く ヨ と く ヨ と

- Static and eigenanalysis problems have been considered in verification
- The results have been compared with the results of alternate models of the same problem (for example a pure shell model or solid model)
- Seems to work
- Resources: See test cases .../fem/tests/Shell_with_Solid_* in the code repository

A cylindrical shell problem with bending-dominated asymptotic behaviour, see .../tests/Shell_with_Solid_Eigenanalysis/Readme.txt

Shell and Solid	Shell
EigenSolve: 1: 4.441527E+04	EigenSolve: 1: 4.291169E+04
EigenSolve: 2: 1.302856E+06	EigenSolve: 2: 1.255816E+06
EigenSolve: 3: 4.885759E+06	EigenSolve: 3: 4.836657E+06
EigenSolve: 4: 7.316037E+06	EigenSolve: 4: 7.036570E+06
EigenSolve: 5: 1.032933E+07	EigenSolve: 5: 1.039543E+07
EigenSolve: 6: 1.169052E+07	EigenSolve: 6: 1.118662E+07
EigenSolve: 7: 2.382371E+07	EigenSolve: 7: 2.296068E+07
EigenSolve: 8: 2.429051E+07	EigenSolve: 8: 2.428822E+07
EigenSolve: 9: 2.473271E+07	EigenSolve: 9: 2.503445E+07
EigenSolve: 10: 2.594538E+07	EigenSolve: 10: 2.591956E+07

伺 とう ほうどう ほうどう

3

III Coupling procedures: Verification

The sixth mode as given by the coupled model and the pure shell model (the 2-norm of the displacement vector)



III Coupling procedures: Future work

- Some geometric constraints on the mesh
- Enabling parallelism
- Non-smooth shell mid-surfaces can in general be troublesome and then switching to a drilling rotation formulation seems to have a relative merit
- The construction of coupling blocks is not yet fully general for the drilling rotation formulation



- In future divergence-conforming (and curl-conforming) basis functions could be utilized to create non-standard formulations
- Thanks for your attention!
- Questions or comments?

・ 同 ト ・ ヨ ト ・ ヨ ト

3