On coupled field modeling

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1 Introduction

Many real life phenomena and processes are of coupled, often multi-physical nature. In order to reproduce the most important physical effects they have to be described by various fields that interact in space and time and are governed by different laws involving dependent variables. Therefore they require advanced mathematical formulations, numerical methods and computational techniques [1, 3, 5]. The objective of this report is to present general classification of coupled fields problems and details of formulation as well as discretization for a selected example.

2 Classification of coupled field problems

A brief preliminary classification of coupled field problems is presented in this section. The classification was inspired by paper by Hameyer et al. [3].

Considering type of physical effects accounted for one may distinguish the following problems:

1. Exclusively mechanical problems due to independent treatment of
   - displacement and stress
   - displacement, strain and stress.
2. Mechanical processes coupled with other physical effects, that induce strain distortions in solids resulting from e.g.
   - temperature change → thermo-mechanical problems
   - shrinkage or expansion of a composite component (e.g. shrinkage of concrete, reinforcement rust development in concrete) → chemo-mechanical problems.
3. Fluid-structure interaction (porous media, aeroelasticity, offshore structures, ...) → fluid-solid coupling.
4. Acoustic-elastic problems.
5. Bio-heat generation and transfer.
6. Electro-mechanical problems.
7. More than two-field problems, like thermo-hydro-mechanical, welding (CFD, EM, heat, solidification), electro-magneto-fluid.

8. Other.

The above presented classification may be illustrated graphically (Fig. 1). Mechanics is here in the central position since displacements, strains and stresses are of primary interest in civil engineering.

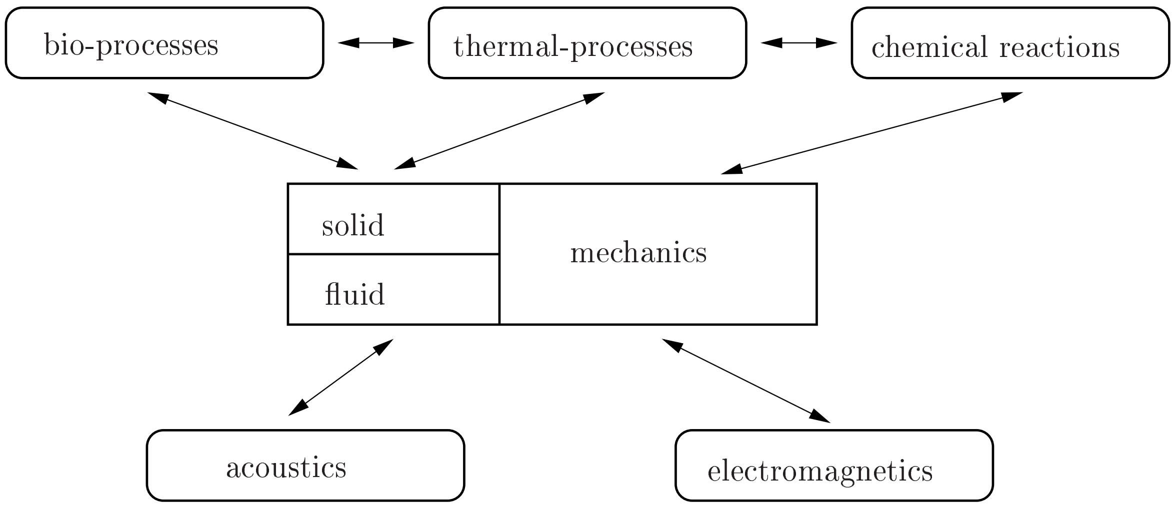

Figure 1: Graphical presentation of systematic for selected coupled problems.

Domain of analysis may lead to:

1. multi-domain (coupling on an interface)
2. one-domain (coupling in the bulk).

Scale, which is accounted for, classifies computation as

1. one scale analysis
2. multiscale analysis.

Despite the forward models also inverse problems, sensitivity analysis, optimization or uncertainty are considered.

In order to illustrate coupled field modeling let us consider the following exemplary problems:
A – incompressible material
B – shrinkage of concrete with thermo-mechanical effects.

The first problem is exclusively mechanical of stationary type and its main difficulty is material incompressibility (Poisson ratio $\nu = 0.5$) resulting generally in impossibility of expressing stresses in terms of displacements. The second problem involves two physical effects – mechanical and chemical, and the coupling results from mechanical deformations induced by chemical reactions.

3 Mathematical model

A variety of physical fields present in the coupled field problems makes the corresponding mathematical models more sophisticated than in the case of classical e.g. mechanical processes. In this section we present the most important mathematical issues of coupled problems.

1. Energy spaces used in formulations are the following:
   - $L_2(\Omega)$ (e.g. displacements, temperature defined by first order equations) – space of square integrable functions, continuity is not required
   - $H^1(\Omega)$ (e.g. displacements, temperature defined by second order equations) – space of functions with square integrable first derivatives, continuity is required
   - $H^1(\mathrm{curl}, \Omega)$ (e.g. electric or magnetic fields) – space of vector valued functions with square integrable curl, continuity of tangential component is required
   - $H^1(\mathrm{div}, \Omega)$ (e.g. stresses) – space of vector (tensor) functions with square integrable divergence, continuity of normal (traction) component is required.
2. Coupling between the fields that are used may be
   - weak (called also one-way or load transfer or loose) – dependent variables can be eliminated (mixed formulations resulting from operator splitting)
   - strong (called also two-way or direct or tight) – dependent variables usually cannot be eliminated.
3. Dependent variables result from
   - either physical problem (e.g. displacement and temperature)
   - or formulation itself (e.g. displacement and stresses, stresses and Lagrange multipliers).

The exemplary problem formulations are shown below.

A – mixed formulation e.g. Hellinger–Reissner principle: *find stress field* $\boldsymbol{\sigma} \in \mathrm{H}^1_{\hat{t}}(\mathrm{div}, \Omega, \mathbb{S})$ *and displacement field* $\boldsymbol{u} \in \mathrm{L}^2(\Omega, \mathbb{V})$*, such that:*

$$\left\{ \begin{array}{ll} \int\limits_{\Omega} \boldsymbol{\tau} : \boldsymbol{C}^{-1} \boldsymbol{\sigma} \, \mathrm{d}\Omega + \int\limits_{\Omega} \mathbf{div}\, \boldsymbol{\tau} \cdot \boldsymbol{u} \, \mathrm{d}\Omega & = \int\limits_{\partial\Omega_u} \boldsymbol{\tau}\, \boldsymbol{n} \cdot \hat{\boldsymbol{u}} \, \mathrm{d}s \\ \int\limits_{\Omega} \boldsymbol{v} \cdot \mathbf{div}\, \boldsymbol{\sigma} \, \mathrm{d}\Omega & = -\int\limits_{\Omega} \boldsymbol{v} \cdot \boldsymbol{b} \, \mathrm{d}\Omega \end{array} \right. \tag{1}$$

$$\forall\, \boldsymbol{\tau} \in \mathrm{H}^1_0(\mathrm{div}, \Omega, \mathbb{S}), \quad \forall\, \boldsymbol{v} \in \mathrm{L}^2(\Omega)$$

where: C denotes elasticity tensor, $\mathrm{H}^1_0(\mathrm{div}, \Omega, \mathbb{S})$ and $\mathrm{H}^1_{\hat{t}}(\mathrm{div}, \Omega, \mathbb{S})$ stand for the spaces of stresses with square integrable divergence and vanishing or equal to $\hat{\boldsymbol{t}}$ tractions on $\partial\Omega_t$, $\mathbb{S}$ is the space of second order symmetric tensors, $\hat{\boldsymbol{u}}$ is displacement known on $\partial\Omega_u$, $\partial\Omega_u \cup \partial\Omega_t = \partial\Omega$, $\partial\Omega_u \cap \partial\Omega_t = \emptyset$.

B – thermomechanics with shrinkage: *find* $\boldsymbol{u} \in \mathrm{H}^1_0(\Omega) + \boldsymbol{h}$ *and* $\Theta \in \mathrm{H}^1_0 + T$, *such that:*

$$\begin{cases} \int\limits_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{C}\, \boldsymbol{\varepsilon}(\boldsymbol{u})\, \mathrm{d}\Omega - \int\limits_\Omega \mathrm{tr}(\boldsymbol{\varepsilon}(\boldsymbol{v}))\, c\, \Theta\, \mathrm{d}\Omega &= \int\limits_{\partial\Omega_t} \boldsymbol{v}\boldsymbol{q}\, \mathrm{d}s + \int\limits_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{C}\, \boldsymbol{\varepsilon}_{c,as}\, \mathrm{d}\Omega \\ \int\limits_\Omega \boldsymbol{\psi}\, k\, \nabla\Theta\, \mathrm{d}\Omega &= \int\limits_{\partial\Omega_s} \boldsymbol{\psi}\boldsymbol{S}\, \mathrm{d}s \end{cases} \tag{2}$$

$$\forall\, \boldsymbol{v} \in H^1_0(\Omega), \qquad \forall\, \boldsymbol{\psi} \in H^1_0(\Omega)$$

where: k is thermal conductivity, c denotes thermal expansion coefficient, $\boldsymbol{S}$ is a heat source, $\boldsymbol{\varepsilon}_{c,as}$ is the example of concrete shrinkage [4], i.e.

$$\boldsymbol{\varepsilon}_{c,as} = \varepsilon_{c,as} \cdot \boldsymbol{I} \tag{3}$$

$\varepsilon_{c,as} = \varepsilon_{c,aso}(f_{cm}) \cdot \beta_{as}(t)$, $\boldsymbol{I}$ is the identity matrix

$$\varepsilon_{c,aso}(f_{cm}) = -\alpha_{as} - \left(\frac{\frac{f_{cm}}{f_{cmo}}}{6 + \frac{f_{cm}}{f_{cmo}}} \right)^{2.5} \cdot 10^{-6} \tag{4}$$

$$\beta_{as}(t) = 1 - \exp\left[-0.2 \left(\frac{t}{t_1} \right)^{0.5} \right] \tag{5}$$

where: f_{cm} is the average strength of concrete after 28 days, α_{as} is a coefficient depending on the type of cement used.

4 Approximation

Appropriate mathematical formulation (existence of solution) does not, in general, guarantee convergence and therefore possibility of obtaining reliable numerical results. Therefore, additionally the following conditions have to be satisfied

1. Approximability - the best approximation error approaches zero when number of DOF approaches infinity (complete polynomials satisfy this condition)

2. Stability verified by the *inf-sup condition* or the *de Rham diagram commutativity* or interior approximation for elliptic problems

Further numerical issues that should be carefully considered to obtain efficient numerical techniques for coupled field problems include:

1. Algorithm

    - directly coupled (one system of equations)

- staggered (separate systems of equations)

2. Methods (exclusively FEM or FEM+BEM, e.g. for infinite domains)

3. Compatible meshes either in the bulk or over the interface

4. Domain decomposition

Mixed formulation used in the example problem A requires a careful selection of approximation functions. First, the symmetry of stresses cannot be enforced a-priori but in a weak sense [2, 6]. Therefore formulation (1) must be transformed to the following form: *find* $\boldsymbol{\sigma} \in \mathrm{H}^1_{\hat{t}}(\mathrm{div}, \Omega, \mathbb{M})$, $\boldsymbol{u} \in \mathrm{L}^2(\Omega, \mathbb{V})$ *and tensor valued Lagrange multiplier* $\boldsymbol{p} \in \mathrm{L}^2(\Omega, \mathbb{K})$ *such that:*

$$\begin{cases} \int\limits_\Omega \boldsymbol{\tau} : \boldsymbol{C}^{-1}\boldsymbol{\sigma}\,\mathrm{d}\Omega + \int\limits_\Omega \mathbf{div}\,\boldsymbol{\tau}\cdot\boldsymbol{u}\,\mathrm{d}\Omega + \int\limits_\Omega \boldsymbol{\tau}\cdot\boldsymbol{p}\,\mathrm{d}\Omega = \int\limits_{\partial\Omega_u} \boldsymbol{\tau}\boldsymbol{n}\cdot\hat{\boldsymbol{u}}\,\mathrm{d}s \\ \int\limits_\Omega \boldsymbol{v}\cdot\mathbf{div}\,\boldsymbol{\sigma}\,\mathrm{d}\Omega = -\int\limits_\Omega \boldsymbol{v}\cdot\boldsymbol{b}\,\mathrm{d}\Omega \\ \int\limits_\Omega \boldsymbol{q}\cdot\boldsymbol{\sigma}\,\mathrm{d}\Omega = 0 \end{cases} \tag{6}$$

$$\forall\, \boldsymbol{\tau} \in \mathrm{H}^1_0(\mathrm{div}, \Omega, \mathbb{M}), \quad \forall\, \boldsymbol{v} \in \mathrm{L}^2(\Omega, \mathbb{V}), \quad \forall\, \boldsymbol{q} \in \mathrm{L}^2(\Omega, \mathbb{K})$$

where $\mathbb{M}$ is the space of second order (now, not necessary symmetric) tensors, $\mathbb{K}$ is the space of skew-symmetric tensors. The matrix representation looks as follows:

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} & \boldsymbol{C} \\ \boldsymbol{B}^T & \mathbf{0} & \mathbf{0} \\ \boldsymbol{C}^T & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\sigma} \\ \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{c} \\ \boldsymbol{d} \\ \mathbf{0} \end{bmatrix} \tag{7}$$

Formulation (6) was used for 2D problems with discretization described below. 9 node quadrilateral elements, shown schematically in Fig.2, were used. The nodes are ordered in the following way:

- vertex nodes: a_1, a_2, a_3, a_4 (used only for geometry)

- edge nodes: a_5, a_6, a_7, a_8

- middle node: a_9.

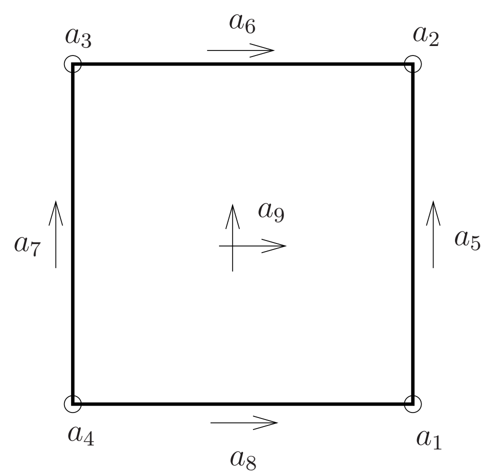

Figure 2: Master finite element $\hat{\mathrm{K}}$.

All shape functions are defined as products of the following two sets of 1D functions that contain integrated Legendre polynomials

$$\begin{array}{rclcrcl} \hat{\psi}_1(t) & = & 1 & \quad\text{or}\quad & \hat{\varphi}_1(t) & = & 1-t \\ \hat{\psi}_2(t) & = & t-\frac{1}{2} & & \hat{\varphi}_2(t) & = & t \end{array} \tag{8}$$

supplemented with the following higher order shape functions

$$\begin{array}{rcl} \hat{\psi}_3(t) = \hat{\varphi}_3(t) & = & t(t-1) \\ \hat{\psi}_4(t) = \hat{\varphi}_4(t) & = & t(t-1)(t-2) \\ \dots & & \end{array} \tag{9}$$

where $t \in [0,1]$.

Scalar shape functions $\hat{g}_1, \dots, \hat{g}_9$ related to nodes $a_1, \dots, a_9$ (see Fig.2) are constructed in the following way

$$\begin{array}{rcl} \hat{g}_1(\xi,\eta) & = & \hat{\varphi}_2(\xi)\,\hat{\varphi}_1(\eta) \\ \hat{g}_2(\xi,\eta) & = & \hat{\varphi}_2(\xi)\,\hat{\varphi}_2(\eta) \\ \hat{g}_3(\xi,\eta) & = & \hat{\varphi}_1(\xi)\,\hat{\varphi}_2(\eta) \\ \hat{g}_4(\xi,\eta) & = & \hat{\varphi}_1(\xi)\,\hat{\varphi}_1(\eta) \\ \hat{g}_5(\xi,\eta) & = & \hat{\varphi}_2(\xi)\,\hat{\varphi}_3(\eta) \\ \hat{g}_6(\xi,\eta) & = & \hat{\varphi}_3(\xi)\,\hat{\varphi}_2(\eta) \\ \hat{g}_7(\xi,\eta) & = & \hat{\varphi}_1(\xi)\,\hat{\varphi}_3(\eta) \\ \hat{g}_8(\xi,\eta) & = & \hat{\varphi}_3(\xi)\,\hat{\varphi}_1(\eta) \\ \hat{g}_9(\xi,\eta) & = & \hat{\varphi}_3(\xi)\,\hat{\varphi}_3(\eta) \end{array} \tag{10}$$

Additionally, bilinear shape functions that are used for approximation of stresses, are defined in the following way:

$$
\begin{array}{rcl}
\hat{e}_1(\xi,\eta) & = & \hat{\varphi}_2(\xi)\,\hat{\psi}_1(\eta) \\
\hat{e}_2(\xi,\eta) & = & \hat{\varphi}_2(\xi)\,\hat{\psi}_2(\eta) \\
\hat{e}_3(\xi,\eta) & = & \hat{\psi}_1(\xi)\,\hat{\varphi}_2(\eta) \\
\hat{e}_4(\xi,\eta) & = & \hat{\psi}_2(\xi)\,\hat{\varphi}_2(\eta) \\
\ldots & &
\end{array}
\qquad (11)
$$

One of the shape functions used for stress approximation, is shown in Fig. 3. Such an approximation enables enforcement of only tractions continuity. There is no assumption about stress tensor continuity.

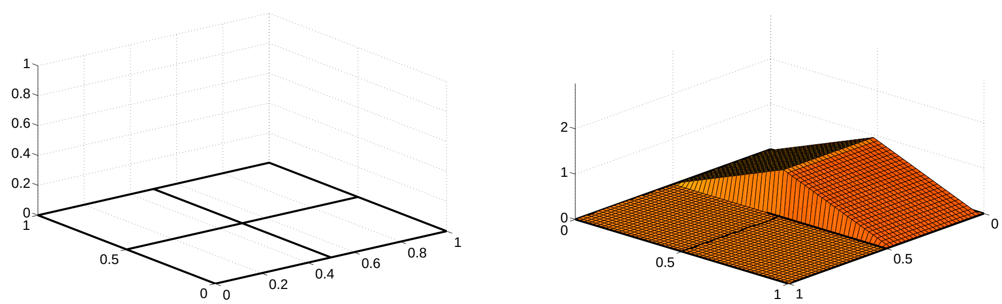

Figure 3: FE discretization with 4 elements. A basis shape function for stress approximation.

Let us consider a plane stress state problem presented in Fig. 4. The model was fixed on the left side and loaded by constant loading on the top. Material data are as follows: Young modulus $E = 200\ GPa$, Poisson ration $\nu = 0.5$. Both mixed and displacement formulations were used to compare results (Fig. 5). One may observe faster convergence for the mixed approach.

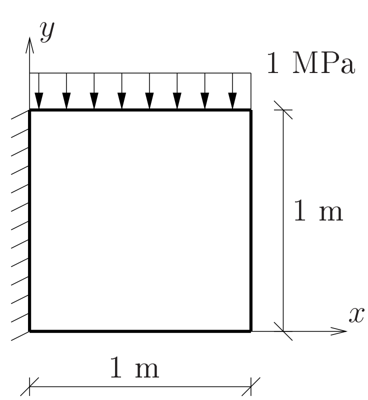

Figure 4: Plane stress state problem. Boundary conditions.

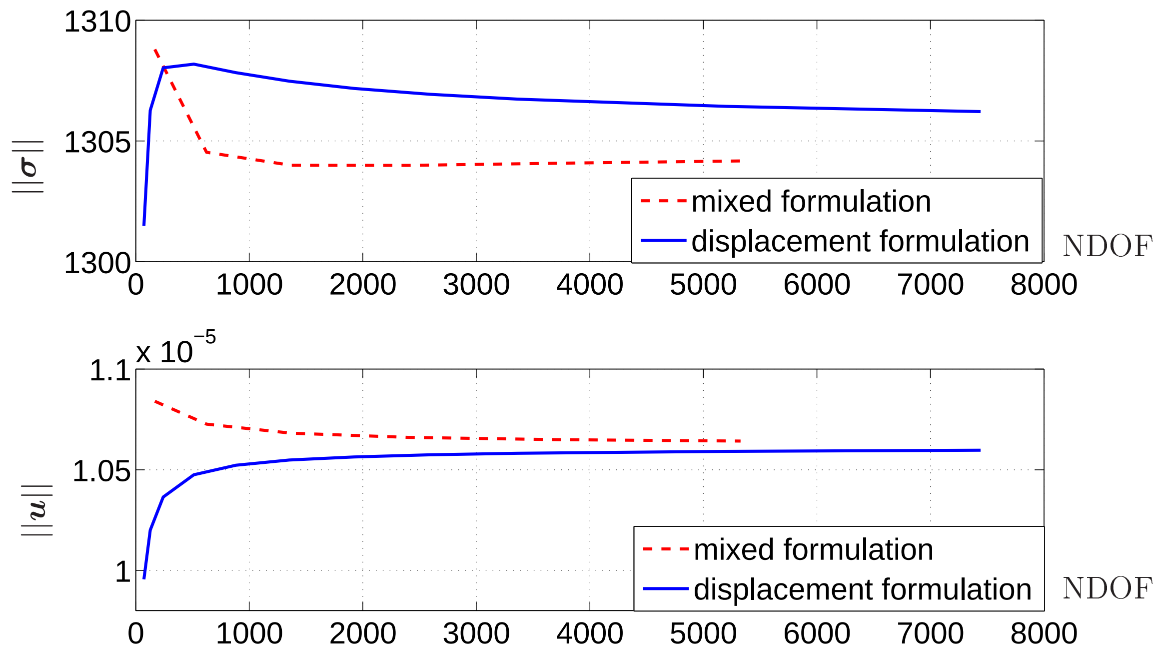

Figure 5: Plate. Convergence of solution norms.

5 Software

The details of approximation described in the previous section influence algorithms used in the computer codes designated for analysis of coupled field problems. Their most important aspects include:

1. Type of coupling
   - Multi-disciplinary - one code generates data for another
   - Multi-physics - all data in one code, weakly or strongly coupled problems
2. Data base (boundary conditions, subdomains) should account for the type of coupling
3. Parallel computing may be particularly profitable in this type of modeling

Nowadays practically all commercial codes claim multi-physics capabilities.

6 Conclusion

The classification of coupled field problems in this report is definitely not complete since we focused only on phenomena and processes related to mechanics. However, even in so restricted coupled problems one may find a wide variety of practical, real-life applications. They always require thorough mathematical, numerical and computer considerations in order to obtain reliable modeling results.

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