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Hybrid finite elements for nonlinear thermal and hygral problems

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ABSTRACT

The performance of a hybrid finite element formulation developed for the solution of nonlinear transient problems is assessed. The formulation, already applied to the solution of heat transfer and moisture transport problems, develops from the uncoupling of the approximation of the state variables and the mapping of the geometry. The formulation qualifies as hybrid because the state variable and its gradient are approximated independently. Orthogonal bases are used to enhance numerical stability under high-order approximations. The resulting solving system is highly sparse and well-suited to adaptive refinement and parallel processing. Besides the benchmarks used in the assessment of conform elements, the rates and patterns of convergence of the hybrid element are defined and its sensitivity to shape distortion is analysed. Also illustrated is the simulation of singular heat flow fields in cracked plates and the hygro-thermo-chemical modelling of cement hydration in concrete structures.

1. Introduction

Nonlinear transient problems are usually solved using the conventional (conform) formulation of the finite element method (FEM) ever since the applications of Zienkiewicz and Cheung [1], as well as of Bathe and Khoshgoftaar [2] to heat transfer. Although literature is rich in using alternative hybrid formulations of FEM in a wide range of application fields, their use in the solution of heat transfer problems has been very limited since the work of Fraeijs de Veubeke and Hogge [3] on steady-state applications. Besides its extension to transient analyses using the Trefftz variant [4], reports on the application of hybrid formulations to thermal problems remain limited in scope, restricted to thermo-elastic fracture, inverse heat conduction and convection-diffusion problems [5–7].

The modelling flexibility offered by hybrid formulations is substantially increased when the approximations of geometry and state variables are uncoupled. They can be implemented using unstructured, coarse meshes of high-degree elements, to yield sparse solving systems well-suited to adaptive refinement and parallel processing. Examples are the use of hybrid elements for simulating cement hydration in early age concrete structures and in fire protection of structural elements strengthened with CFRP laminates [8–10].

Those reports focus on assessing the use of conform and hybrid variants of FEM in the solution of nonlinear and coupled transient problems. The focus of the present paper is distinct: it aims to characterize the performance of the hybrid element in terms of rates and patterns of convergence, under both p- and h-refinement, and its sensitivity to gross mesh distortion. A benchmark test set in [2] is also assessed to illustrate an axisymmetric application. These tests are complemented with the modelling of temperature fields in cracked plates, to illustrate the extension of the finite element approximation basis to model singular heat flows. Numerical testing closes with the simulation of cement hydration in a concrete block to show that the formulation written here for heat transfer problems can be readily extended, in this particular case to hygro-thermo-chemical analyses.

Besides defining the mathematical model, the paper addresses the procedures used to approximate the geometry and the state variables, to characterize the approximation bases and to discuss the properties of the resulting solving system. Comments on numerical implementation are limited to essential aspects, as the detailed information presented in [8,10] remains valid for the present extension to singular flux fields. For simplicity, the mathematical model, the finite element formulation and all testing problems are presented for heat transfer problems, with the exception of the closing application, which is used to comment the extension to moisture transport problems.

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2. Mathematical model

The domain conditions that govern the thermal field, $T(\boldsymbol{x},t)$, in the domain V^e of a finite element with boundary Γ^e, assigned to space and time systems of reference $\boldsymbol{x}$ and t, respectively, can be summarized as follows:

$$\boldsymbol{\nabla}^T\boldsymbol{\sigma} + c\dot{T} = \dot{Q} \quad in\ V^e \tag{1}$$

$$\boldsymbol{\varepsilon} = \boldsymbol{\nabla}T \quad in\ V^e \tag{2}$$

$$\boldsymbol{\sigma} = -\boldsymbol{k}\boldsymbol{\varepsilon} \quad in\ V^e \tag{3}$$

In the thermal equilibrium Eq. (1), $\boldsymbol{\nabla}^T\boldsymbol{\sigma}$ is the divergence of the heat flow, c is the volumetric specific heat and $\dot{Q}$ represents the heat source. Eq. (2) defines the temperature gradient, $\boldsymbol{\varepsilon}$, and Eq. (3) represents the constitutive relation, as $\boldsymbol{k}$ is the local conductivity matrix. Conditions (1)–(3) are often combined to obtain the state equation:

$$\boldsymbol{\nabla}^T\boldsymbol{k}\boldsymbol{\nabla}T + \dot{Q} = c\dot{T} \quad in\ V^e \tag{4}$$

The mathematical model is completed with the following set of boundary and initial conditions:

$$\boldsymbol{n}^T\boldsymbol{\sigma} = -\boldsymbol{n}^T\boldsymbol{k}\boldsymbol{\nabla}T = q_N \quad on\ \Gamma^e_N \tag{5}$$

$$T = T_D \quad on\ \Gamma^e_D \tag{6}$$

$$T = T_0\ at\ t = t_0 \quad in\ V^e \tag{7}$$

Eqs. (5) and (6) assume that the element boundary, with a unit outward normal $\boldsymbol{n}$, is uncoupled into complementary Neumann and Dirichlet parts,

$$\Gamma^e = \Gamma^e_N \cup \Gamma^e_D \tag{8}$$

which are decomposed as follows, under the notation defined below:

$$\Gamma^e_N = \Gamma^e_q \cup \Gamma^e_{cr} \cup \Gamma^e_{cd} \tag{9}$$

$$\Gamma^e_D = \Gamma^e_T \cup \Gamma^e_i \tag{10}$$

The Neumann condition (5) is used to model prescribed heat flux fields, $\overline{q}$, convection-radiation and conductance conditions:

$$q_N = \overline{q} \quad on\ \Gamma^e_q \tag{11}$$

$$q_N = h_{cr}(T - T_a) \quad on\ \Gamma^e_{cr} \tag{12}$$

$$q_N = h_{cd}(T - T_k) \quad on\ \Gamma^e_{cd} \tag{13}$$

In the equations above, T_a is the ambient temperature and T_k the surface temperature of a connecting element. The radiation condition is set letting $h_{cr} = h_r(T + T_k)(T^2 + T_a^2)$ in Eq. (12), with h_r representing the radiation coefficient.

The Dirichlet Eq. (6) is used to model prescribed temperature fields, $\overline{T}$, and inter-element thermal continuity:

$$T_D = \overline{T} \quad on\ \Gamma^e_T \tag{14}$$

$$T_D = T_k \quad on\ \Gamma^e_i \tag{15}$$

The prescribed temperature and heat flux fields and the ambient temperature are defined as functions of time and space. The specific heat and the conductivity coefficients, as well as the convection, radiation and conductance coefficients, are defined in a similar way and may vary with temperature.

3. Discretization in space and time

The hybrid formulation presented below is implemented on coarse meshes of high-degree elements. Most elements are regular in shape, as the domain decomposition is mainly constrained by the medium geometry and by inhomogeneity of its properties.

Although no conceptual constraints limit the topology of hybrid elements, *e.g.* [11], domain decomposition has been implemented using parametric descriptions,

$$\boldsymbol{x} = \boldsymbol{N}(\boldsymbol{\xi})\boldsymbol{c} \quad in\ V \tag{16}$$

where vector $\boldsymbol{c}$ defines the coordinates of the element control nodes, $\boldsymbol{N}$ is the shape function matrix and $\boldsymbol{\xi}$ represents the parametric co-ordinate system. It is noted that mapping (16) is independent of the approximation of the state variables of the problem, as shown in Section 4.

Following the usual practice in the solution of the first-order problems, time integration of temperature T is based on trapezoidal rules with a fixed time increment, δt,

$$T = T_0 + \gamma_0\delta t\dot{T}_0 + \gamma\delta t\dot{T} \tag{17}$$

where γ and γ_0 are integration constants ($\gamma = \gamma_0 = \frac{1}{2}$ in the tests presented below).

4. Finite element approximations

Either the temperature or the heat flow fields can be selected for primary approximation in a hybrid formulation of thermal problems. The first option, also used in the derivation of conform elements, is designed to locally enforce the thermal gradient and the conductivity conditions (2) and (3), while the second is designed to satisfy Eq. (3) and the thermal equilibrium condition (1).

These are the approaches followed in the early contribution of Fraeijs de Veubeke and Hogge [3], with the aim of bounding the error of FEM solutions of steady-state heat conduction problems. The first option is chosen here because in most thermal applications the main concern of the analyst is to directly control the quality of the temperature approximation. It is written assuming separation of variables in time and space,

$$T(\boldsymbol{x},t) = \boldsymbol{\Theta}(\boldsymbol{\xi})\boldsymbol{T}(t) \quad in\ V^e \tag{18}$$

where vector $\boldsymbol{T}$ defines the amplitudes of the temperature modes listed in row-vector $\boldsymbol{\Theta}$. The temperature approximation basis is defined as the product of (naturally hierarchical, orthogonal) Legendre polynomials,

$$\boldsymbol{\Theta} = \{\cdots \quad L_i(\xi)L_j(\eta)L_k(\zeta) \quad \cdots\} \tag{19}$$

expressed in the natural element co-ordinate system. The dimension of this basis is,

$$N_D = \prod_{j=1}^{D} \begin{cases} \frac{1}{D!}(d+j) & if\ d_\xi = d_\eta = d_\zeta = d \\ (d_j + 1) & if\ independently\ set \end{cases} \tag{20}$$

for two-dimensional ($D = 2$) and three-dimensional ($D = 3$), depending on whether the same or different degrees of approximation are implemented in each direction.

The same basis is used to approximate the temperature rate and, as for conform elements, the thermal gradient and the heat flow rate fields are determined enforcing conditions (2) and (3) for the assumed temperature approximation:

$$\dot{T} = \boldsymbol{\Theta}\dot{\boldsymbol{T}} \quad in\ V^e \tag{21}$$

$$\boldsymbol{\varepsilon} = (\boldsymbol{\nabla}\boldsymbol{\Theta})\boldsymbol{T} \quad in\ V^e \tag{22}$$