Mathematical and numerical multiscale modelling

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Abstract

We discuss the role of thermodynamic consistency in multiphysics and multiscale models, and how it can be preserved among scales. The quest for consistency and adoption of thermodynamic non equilibrium models has led to remarkable results in the field of fluid-solid interaction problems such as an improved model for drying shrinkage in concrete or the possibility to model non-isothermal leaching of calcium in concrete. The problem of thermodynamical consistency in case of asymptotic homogenization is also mentioned.

Keywords: multiphysics, multiscale models, thermodynamical consistency.

1. Introduction

Multiscale methods are nowadays very popular in the community dealing with computational methods in applied sciences and engineering. At the extreme, these methods allow to bridge the scales from quantum mechanics to the continuum at macroscopic level [20]. In such instances the scale bridging method is mainly of numerical nature [23]. In multi physics problems however it is often advantageous to use multiscale procedures already at mathematical level when formulating the model. In this case seldom more than two or three scales are involved. This is particularly the case of multi-physics problems with overlapping domains where diffusion, advection, adsorption, phase change, deformation, chemical reactions and other phenomena take place. In such a case a mathematical multi-scale approach is useful to obtain the proper form of the interaction and exchange terms among the fields. Purely macroscopic approaches often yield to confusion and to wrong forms of the interaction terms. Using appropriate approaches such as the hybrid mixture theory [11] which in fact is an averaging method, or the thermodynamically constrained averaging theory TCAT [12] allows assuring that the second law of thermodynamics is satisfied. In the hybrid mixture theory the system thermodynamics is postulated directly at the average scale (i.e. the macro scale) and thus does not account for some of the sub scale deviations in thermodynamic properties, and the thermodynamic statements do not necessarily downscale to the microscale. On the other hand, the thermodynamically constrained averaging theory TCAT involves averaging established microscale thermodynamic principles to the macroscale. In doing so, it inherently assures consistency between microscale and macroscale forms.

Thermodynamic consistency of the mathematical model improves the performance of the ensuing numerical model. This is due to the fact that unwanted and uncontrolled dissipation is eliminated. The fact that thermodynamically consistent models behave better than others is known from CFD where numerical dissipation is introduced for this purpose. Numerical dissipation enters stability estimates which, physically speaking, can be understood as energy estimates. But, if well designed, the same dissipation enters in entropy estimates and helps to guarantee that entropy is never decreasing. For a compressible flow setting, see T.R.J. Hughes et al. [15,16]. A more mathematically oriented exposition of the concept is due to Johnson and Szepessy [18] and Szepessy [22], where the relationship between dissipation and entropy inequalities is shown for hyperbolic equations. More recently, the connection between entropy conditions and numerical dissipation is being exploited by Guermond [14].

In the computational fluid-solid interaction community (FSI, interaction in the domain) the thermodynamical consistency is investigated by Coussy [6,7], Baggio et al. [1], Schrefler [21], Hutter et al. [17], de Boer et al. [8], Borja [2]. We shall show how such consistency can be obtained in FSI. With an appropriate multiscale procedure such as TCAT remarkable result can be achieved which cannot be obtained with a macroscopic continuum theory of thermodynamics [2].

Another case of interest is the asymptotic theory of homogenization which is often used in solid mechanics problems [3,4,5,24]. The expansion is usually truncated after a few terms. What matters here in conserving the thermodynamical consistency is the size of the unit cell. As long as it is infinitesimally small it is generally accepted that the O(1) theory is as good as anything else. The problem is finite size of the cell which usually appears in numerical exploitation of the method. Here the question is still open as it is in the case of numerical multiscale procedures like those mentioned at the beginning of this paper.

We shall show some examples for mathematical and numerical multiscale methods belonging to stress measures in partially saturated media and their effects on drying shrinkage modelling in concrete, to calcium leaching in concrete and to three scale homogenization with application to nuclear fusion technology.
2. Numerical examples

2.1. Drying shrinkage of concrete

As first case we consider drying shrinkage of young concrete where a proper choice of the stress tensor allows avoiding the need for an experimentally obtained shrinkage coefficient (valid only for each particular case) linking relative humidity with shrinkage strain. However, the functional dependence of the Helmholtz free energy must be sufficiently rich to properly represent the physical reality. The stress form obtained by Coussy [7]

\[ d\sigma = d\sigma + \alpha dp^s; \]
\[ dp^s = dp^s - S_w dp^w \]

(1)

with a Helmholtz free energy for the solid phase depending only on \( S_w \) the water degree of saturation, \( \theta \) the absolute temperature and \( E_s \) the Lagrangian strain tensor is not sufficient to simulate the strain behaviour at low values of relative humidity. On the other hand the generalized Skempton stress tensor containing the disjoining pressure,

\[ \sigma^s = \sigma^s + \alpha dp^f \]
\[ p^f = p^s - \chi^w \rho^s \]
\[ \rho^f = \rho^s - \chi^w f^s \]

(2)

where the Helmholtz free energy depends also on the specific interface areas [13] allows following the experimentally observed strain behaviour down to very low values of the relative humidity [10], Figure 1.

![Figure 1: Drying process of a concrete sample: comparison between experimental values and numerical results obtained according to the theories [7] and [10].](image)

2.2. Leaching of concrete

The second example deals with calcium leaching of concrete which is particularly important for containment structures for nuclear waste disposal. Equilibrium based models show convergence problems because of the sudden appearance of large source terms which must attain equilibrium instantaneously. Models which consider thermodynamic imbalance of the calcium in solid and liquid phases, allowing for the description of process kinetics behave numerically much better [9]. The correct evolution of the chemical process is captured through the introduction, for each chemical component, of the relaxation time which would be zero in equilibrium type models but not in reality and in process kinetics based models. As additional bonus of such a kind of approach, it allows for introducing non isothermal leaching by means of the thermal diffusion of ionic species and the temperature dependence of the chemical reaction through an Arrhenius-like relationship.

![Figure 2: Calcium content in the solid skeleton after 7500 days at two different temperatures [9].](image)

![Figure 3: Calcium concentration in the liquid solution after 7500 days at two different temperatures [9].](image)
As example we show the case of non isothermal leaching of a cubic specimen (side=4 cm) in direct contact with deionised water at two different temperatures: 25°C and 60°C. Fig 2 and 3 show the calcium content in the solid skeleton and in the saline solution after 7500 days. For further information about material properties and boundary conditions used in the numerical simulation, see [9].

2.3. Asymptotic homogenization for ITER strands

The third case deals with the thermo-mechanical analysis of a superconducting strand used to wind the coils of the thermo-nuclear experimental reactor (ITER), which is now under construction. In the strand (Fig. 4) a three-level hierarchy can be identified [3,4,19]: the single filament (micro-scale, on the right), groups of filaments (meso-scale, in the centre) and the superconducting strand (macro-scale, on the left). In this example we compute the effective characteristics and the strain field due to the cool down of the strand from its reaction temperature (923K) to the coil working condition (4K). We assume that the strand components are in equilibrium at 923K without eigenstresses or eigenstrains, which are relaxed since the strand remains for several hours at high temperature. We have to deal with non-linear, temperature-dependent material characteristics.

Asymptotic theory of homogenisation is adopted for the non linear situation and the three scales are bridged by applying it in concurrent manner. From a mathematical point of view, the theory of homogenisation is a limit theory which uses the asymptotic expansion and the assumption of periodicity to substitute the differential equations with rapidly oscillating coefficients, with differential equations whose coefficients are constant or slowly varying in such a way that the solutions are close to the initial equations. The first important assumption for asymptotic analysis is that it must be possible to distinguish two length scales associated with the macroscopic and microscopic phenomena. The second basic assumption is that the periodicity of the material characteristics imposes an analogous periodical perturbation on quantities describing the mechanical behaviour of the body. The method consists in modelling the real microstructure of only a sub-volume of the domain, which is assumed to repeat itself: the repetitive unit cell (RUC) (Fig. 5).

Asymptotic expansion of displacements, temperature, stress fields in the RUC are carried out and the solution of the governing field equations can be obtained numerically (finite difference, finite element or boundary element methods). Appropriate boundary conditions ensure that the deformation of an RUC remains consistent with the deformation of its neighbours. In this way the effective coefficients are obtained from the unit cell analysis. If applied iteratively, asymptotic theory of homogenization may also be used for non-linear situations. Furthermore, it can obviously be used to bridge several scales. The particular nature of the thermo-elastic-plastic process has allowed the use of a tangent stiffness procedure, which avoids costly equilibrium iterations of a Newton-Raphson procedure at macroscopic level. In the adopted procedure the updating of the cell is compulsory to avoid to drift away from equilibrium path. The results are remarkably accurate as shown in Fig. 6, where the computed and measured residual strains after the cool down process are compared.

3. Concluding remarks

It is not straightforward to maintain thermodynamic consistency in multiphysics and multiscale models. Its importance is now generally admitted in computational mechanics and is exploited in CFD since a long time ago. In fluid structure interaction problems with interaction in the domain it is pursued mainly when writing the mathematical multiscale model. This quest for thermodynamic consistency has led to improved models for simulating drying shrinkage through adoption of a more appropriate stress tensor which includes disjoining pressure. Adoption of thermodynamic non equilibrium approach has then permitted to simulate non-isothermal leaching in concrete and has led to models which show less convergence difficulties. Finally the preservation of thermodynamic consistency in case of asymptotic expansion, another popular multiscale method, appears to be still an open problem, worth to be investigated.
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References


