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Hybrid parallel approach to homogenization of transport processes in masonry

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ABSTRACT

Numerical simulations of transport processes, e.g., heat and moisture transport, in heterogeneous masonry structures performed on single processor computers are very time consuming. The classical description by the finite element method leads to enormous numbers of degrees of freedom. It is caused by the fact that there are relatively thin layers of mortar in contrary to large bricks or stones. The mortar and stones have very different material parameters and the finite element mesh has to be able to describe the temperature and moisture fields in the thin layers of mortar and in their vicinity. An application of a multi-scale approach in connection with parallel computing can be successfully exploited. The whole structure is described by a reasonably coarse finite element mesh, called the macro-scale problem, and the material parameters are obtained from the lower-level problems, called the meso-scale problem, by a homogenization procedure. In this procedure, the macro-problem is assigned to the master processor and the meso-scale problems belong to the slave processors. This proposed approach is called hybrid parallel method.

1. Introduction

Restoration and reconstruction of historical masonry structures need complex analyses combining both experimental work and numerical simulations. By way of example, the last reconstruction of Charles bridge in Prague can be mentioned together with the information system [1] integrating detailed geometrical description of the bridge including changes resulting from previous reconstructions, historical and contemporary materials forming the bridge as well as novel materials and technologies used to improve its durability and serviceable life. A thermo-hygro-mechanical simulation of the response of masonry structures to climatic loadings can be shown as a suitable example of such complex numerical analysis.

Numerical modelling of coupled heat and moisture transport in masonry structures by the finite element method leads to huge number of degrees of freedom. It is caused mainly by an effort to create suitable finite element mesh in mortar between stones and in its vicinity in order to capture correct temperature and moisture distribution. Such problems with too many degrees of freedom are hardly solvable on single processor computers. Several possible solutions of the given difficulties are presented in references, e.g., parallelization of the problem is proposed in [2]. Further, when non-linear dynamic analyses are performed [3], the utilization of homogenization into a nested finite element approach is prohibitive. An alternative is also using rigid elements and homogenized interfaces presented in [4], where the problem is decoupled into meso and macro-scale.

This paper presents hybrid parallel method which is an application of a multi-scale approach in connection with parallelization. In the hybrid method, each macro-scopic integration point or each finite element is connected with a certain meso-scopic problem represented by an appropriate periodic unit cell. The solution of a meso-scale problem then provides effective parameters needed on the macro-scale. Such an analysis is suitable for parallel computing because the meso-scale problems can be distributed among many processors and the amount of transferred data is small. In this regard, the master-slave strategy can be efficiently exploited. An application of the hybrid parallel method is illustrated by a numerical analysis of coupled heat and moisture transfer in Charles bridge in Prague.

Two-scale approach with a macro-scale problem dealing with the structure and a meso-scale problem describing the type of masonry has been previously introduced in [5]. This formulation corresponds to the first order homogenization, where only the function value and the gradient of the macro-level function is used on the meso-level. Governing equations of the coupled heat and moisture transport are derived in the framework of coupled two-scale analysis of finite element type [6]. It is presumed that the

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homogenized macro-scale fields are found from the solution of a certain sub-scale (meso-scale) problem performed on a representative volume element (RVE) which is represented by a periodic unit cell (PUC). Regular and irregular meso-structures have been approached either directly in the framework of stochastic finite elements [7] or indirectly by introducing the concept of statistically equivalent periodic unit cell (SEPUC) [8]. Such a unit cell is then constructed to match the real meso-structure, at least in a statistical sense, as close as possible.

The presented hybrid parallel computing method based on multi-scale analysis differs from classical parallel computing methods which come out from the domain decomposition. The macro-problem is assigned to the master processor while the solution at the meso-level is carried out on slave processors, see, e.g., [9,10]. At each time step the current temperature and moisture together with the increments of their gradients at a given macro-scopic integration point are passed to the slave processor (imposed onto the associated periodic cell), which, upon completing the small scale analysis, sends the homogenized data (effective conductivities, averaged storage terms and fluxes) back to the master processor. It means that the conductivity and capacity matrix of an element of the macro-scale problem are assembled as a result of the homogenization on meso-scale. The meso-scale problems are solved n times, where n denotes the number of all integration points or elements. In case of too large meso-scale problems, the meso-scale problems are solved only once for aggregates of elements with averaged values of temperature and moisture fields and their gradients. The hybrid method has been implemented into a parallel version of SIFEL code [11] with the distributed memory scheme and the MPI communication library. The code uses the master and slaves concept, where the master processor manages communication among all processors and it also controls the computation.

This paper consists of six sections. After the first Introduction, the basic approach based on Künzel and Kiessl's coupled heat and moisture transfer model is summarized in Section 2. The first order homogenization procedure is described in Section 3. Then the basic principles of the hybrid method are explained in Section 4 and results of a numerical simulation of heat and moisture transfer in Charles bridge in Prague are illustrated in Section 5. Finally, the benefits of the hybrid method are discussed in Conclusions.

2. Description of coupled heat and moisture transfer and numerical solution

The presented hybrid parallel approach is based on the Künzel and Kiessl model [12]. This phenomenological model introduces two unknowns, relative humidity φ (-) and temperature T (K) in a material point. The practical usage of the main advantages of this model can be seen, e.g., in [13,14], where building structures are simulated under common climatic conditions with help of material properties measured experimentally.

The model supposes the moisture transport mechanisms relevant to numerical analysis in the field of building physics are just water vapour diffusion and liquid transport. Vapour diffusion is most important for large pores, whereas liquid transport takes place on pore surfaces and in small capillaries. Vapour diffusion in porous media is described in the model by the Fick's diffusion and effusion in the form

$$J_v = -\delta_p \nabla p = -\frac{\delta}{\mu}\nabla p, \tag{1}$$

where δ_p [kg m s^{-1} Pa^{-1}] is the vapour permeability of the porous material, p denotes vapour pressure [Pa], μ is the vapour diffusion resistance number and δ [kg m s^{-1} Pa^{-1}] is the vapour diffusion coefficient in air.

The liquid transport mechanism includes liquid flow in the absorbed layer (surface diffusion) and in the water filled capillaries (capillary transport). The driving potential in both cases is capillary pressure (suction stress) or relative humidity φ. The flux of liquid water is described in the form

$$J_w = -D_\varphi \nabla \varphi, \tag{2}$$

where the liquid conductivity $D_\varphi = D_w \frac{\mathrm{d}w}{\mathrm{d}\varphi}$ [kg m s^{-1}] is the product of the liquid diffusivity D_w [m^2 s^{-1}] and the derivative of water retention function. w [kg m^{-3}] is the water content of the material.

The heat flux is proportional to the thermal conductivity of the moist porous material and the temperature gradient (Fourier's law)

$$q = -\lambda \nabla T, \tag{3}$$

where λ [W m^{-1} K^{-1}] is the thermal conductivity of the moist material.

The heat and moisture balance equations are closely coupled because the moisture content depends on the total enthalpy and thermal conductivity while the temperature depends on the moisture flow. The resulting set of differential equations for the description of simultaneous heat and moisture transfer, expressed in terms of temperature, T, and relative humidity, φ, have the form of partial differential equations defined on a domain Ω

$$\frac{\partial w}{\partial \varphi}\frac{\partial \varphi}{\partial t} = \nabla^{\mathrm{T}}\left(D_\varphi \nabla \varphi + \delta_p \nabla(\varphi p_{\mathrm{sat}})\right), \tag{4}$$

$$\left(\rho C + \frac{\partial H_w}{\partial T}\right)\frac{\partial T}{\partial t} = \nabla^{\mathrm{T}}\left(\lambda\ \nabla T\right) + h_v \nabla^{\mathrm{T}}\left(\delta_p \nabla(\varphi p_{\mathrm{sat}})\right), \tag{5}$$

where H_w [J m^{-3}] is the enthalpy of the material moisture, h_v [J kg^{-1}] is the evaporation enthalpy of the water, p_{sat} [Pa] is the water vapour saturation pressure, ρ [kg m^{-3}] is the material density, C [J kg^{-1} K^{-1}] is the specific heat capacity and t [s] denotes time. Boundary of the domain Ω is split into parts Γ_T, Γ_φ, Γ_{qpT}, $\Gamma_{Jp\varphi}$, Γ_{qcT} and $\Gamma_{Jc\varphi}$ which are disjoint and their union is the whole boundary Γ.

The system of Eqs. (4) and (5) is accompanied with three types of boundary conditions:

- Dirichlet boundary conditions

$$T(\boldsymbol{x}, t) = \overline{T}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_T \tag{6}$$

$$\varphi(\boldsymbol{x}, t) = \overline{\varphi}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_\varphi \tag{7}$$

- Neumann boundary conditions

$$-\lambda \frac{\mathrm{d}T}{\mathrm{d}\boldsymbol{n}} = \boldsymbol{q}(\boldsymbol{x}, t) = \bar{\boldsymbol{q}}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_{qpT}, \tag{8}$$

$$-D_\varphi \frac{\mathrm{d}\varphi}{\mathrm{d}\boldsymbol{n}} = \boldsymbol{J}(\boldsymbol{x}, t) = \bar{\boldsymbol{J}}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_{Jp\varphi}, \tag{9}$$

- Cauchy boundary conditions

$$\boldsymbol{q}(\boldsymbol{x}, t) = \alpha(T(\boldsymbol{x}, t) - T_\infty(\boldsymbol{x}, t)), \qquad \boldsymbol{x} \in \Gamma_{qcT}, \tag{10}$$

$$\boldsymbol{J}(\boldsymbol{x}, t) = \beta(p(\boldsymbol{x}, t) - p_\infty(\boldsymbol{x}, t)), \qquad \boldsymbol{x} \in \Gamma_{Jc\varphi}, \tag{11}$$

where $\overline{T}(\boldsymbol{x}, t)$ is the prescribed temperature, $\overline{\varphi}(\boldsymbol{x}, t)$ is the prescribed relative humidity, $\bar{\boldsymbol{q}}(\boldsymbol{x}, t)$ is the prescribed heat flux, $\bar{\boldsymbol{J}}(\boldsymbol{x}, t)$ is the prescribed moisture flux, α [W m^{-2} K^{-1}] and β [kg s^{-1} Pa^{-1}] are the heat and mass transfer coefficient, T_∞ is the ambient temperature and p_∞ is the ambient water vapour pressure.

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