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Processor Farming in Homogenization of Coupled Heat and Moisture Transfer

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Abstract

Coupled heat and moisture transport in extremely heterogeneous materials like a masonry still cannot be solved for large strucutres. Multi-scale methods with the macro and meso-scale levels are usually used. The biggest disadvantage of such methods stems from their enormous computational demands. Small coupled problem on the meso-scale level has to be solved for every integration point of the macro-scale problem. The number of the integration points is in thousands or tens of thousands. The multi-scale method can be efficiently implemented in parallel because the particular computations connected with the integration points are totally independent. The strategy denoted the processor farming can be used.

Keywords: coupled heat and moisture transport, Künzel model, parallel computing.

1 Introduction

Coupled heat and moisture transport is becoming very important in civil engineering because its result has a strong influence on mechanical behaviour of materials and structures. In the past, the temperature and relative humidity (or water content) were included into mechanical models as additional material parameters and it was not possible to take into account their time dependence. Contemporary state of the art mechanical models are coupled with the heat and moisture transport which is solved simultaneously with the mechanical analysis.

The coupled heat and moisture transport in extremely heterogeneous material like masonry is hardly solvable even with modern computers. The reason is that there are relatively small mortar layers in comparison with bricks which enforce a very dense finite element mesh. Therefore, only details of structures can be solved.

In order to solve the whole structures, multi-scale techniques are usually used. The

classical first order homogenization in a spatial domain in the framework of the twostep multiscale computational scheme was proposed in [1]. This technique is based on a meso or micro-scale problems and a macro-scale problem. Whether the micro or meso scale level is used depends on the characteristic size of the representative volumes which describe the real complicated geometry. In masonry structures, the representative volume contains several bricks and adjacent mortar layers and therefore the meso-scale level is used. The macro-scale problem describes the problem solved by relatively coarse mesh because homogenized material parameters are obtained from meso-scale level. The multi-scale technique sends the actual values from the macro-scale level problem to the meso-scale problem where the appropriate material parameters are obtained and sent back to the macro-scale problem.

It is evident that the multi-scale method is very demanding because a meso-scale problem has to be solved for each macro-scale finite element. If the number of macroscale finite elements is in thousands only, the solution of meso-scale problems is very demanding even if each meso-scale problem contains only hundreds of degrees of freedom. The multi-scale problems are ideal for parallelization because the mesoscale problems are completely independent and only reasonable amount of data has to be sent between the macro-scale problem and the meso-scale problems.

In this contribution, the coupled heat and moisture transport is described by the Künzel material model which was introduced in 1995 in reference [2]. The Künzel model is based on the temperature and relative humidity which have to satisfy the mass and heat balance equations in the form of partial differential equations.

2 Künzel model of coupled heat and moisture transport

Künzel introduced in 1995 in his thesis material model suitable for the coupled heat and moisture transport in building components. Very brief overview of the model is sketched in this section. Basic form of the mass balance equation is

$$\frac{\partial w}{\partial t} = -\operatorname{div}(\boldsymbol{q}_l + \boldsymbol{q}_v) + S_w , \qquad (1)$$

where w is the water content, q_l is the liquid flux density, q_v is the vapour diffusion flux density and S_w denotes the moisture source or sink. Substitution of several relationships, which can be found in [2] or [3], into the balance equation (1) results in

$$\frac{\partial w}{\partial t} = \operatorname{div}\left(\left(D_{\varphi} + \delta_p p_{vs}\right)\nabla\varphi + \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T}\nabla T\right) + S_w , \qquad (2)$$

where D_{φ} is the liquid conduction coefficient, δ_p is the water vapour permeability and p_{vs} denotes the saturated water vapour pressure which depends on the temperature. The heat balance equation has basically the form

$$\frac{\partial H}{\partial t} = -\operatorname{div} \boldsymbol{q}_T + S_h = -\operatorname{div} \boldsymbol{q}_T - h_v \operatorname{div} \boldsymbol{q}_v , \qquad (3)$$

where H is the enthalpy, q_T is the heat flux density and S_h is the source or sink of the heat which is expressed with the help of the vapour diffusion flux density and the latent heat of phase change, h_v . Similarly to the mass balance equation, after substitution of several relationships the following form is obtained

$$\frac{\partial H}{\partial t} = \operatorname{div}\left(h_v \delta_p p_{vs} \nabla \varphi + \left(\lambda + h_v \delta_p \varphi \frac{\mathrm{d} p_{vs}}{\mathrm{d} T}\right) \nabla T\right) \,. \tag{4}$$

Let new notation be introduced in the form

$$\begin{pmatrix} \boldsymbol{q}_{\varphi} \\ \boldsymbol{q}_{T} \end{pmatrix} = \begin{pmatrix} \boldsymbol{D}_{\varphi\varphi} & \boldsymbol{D}_{\varphi T} \\ \boldsymbol{D}_{T\varphi} & \boldsymbol{D}_{TT} \end{pmatrix} \begin{pmatrix} \boldsymbol{g}_{\varphi} \\ \boldsymbol{g}_{T} \end{pmatrix} =$$
(5)

$$= \begin{pmatrix} D_{\varphi} + \delta_{p} p_{vs} & \delta_{p} \varphi \frac{\mathrm{d} p_{vs}}{\mathrm{d} T} \\ h_{v} \delta_{p} p_{vs} & \lambda + h_{v} \delta_{p} \varphi \frac{\mathrm{d} p_{vs}}{\mathrm{d} T} \end{pmatrix} \begin{pmatrix} \nabla \varphi \\ \nabla T \end{pmatrix}.$$
(6)

With the new notation, the balance equations have the form

$$\frac{\mathrm{d}w}{\mathrm{d}\varphi}\frac{\partial\varphi}{\partial t} = \mathrm{div}\left(\boldsymbol{D}_{\varphi\varphi}\nabla\varphi + \boldsymbol{D}_{\varphi T}\nabla T\right) , \qquad (7)$$

$$\frac{\mathrm{d}H}{\mathrm{d}T}\frac{\partial T}{\partial t} = \mathrm{div}\left(\boldsymbol{D}_{T\varphi}\nabla\varphi + \boldsymbol{D}_{TT}\nabla T\right) \,. \tag{8}$$

3 Multi-scale method

On the macro-scale, the coordinates are denoted \boldsymbol{x} , $T(\boldsymbol{x})$ is the temperature and $\varphi(\boldsymbol{x})$ stands for the relative humidity. All variables on the meso-scale are denoted by a bar, i.e. $\bar{\boldsymbol{x}}$, $\bar{T}(\boldsymbol{x})$ and $\bar{\varphi}(\boldsymbol{x})$. The vector of coordinates on the meso-scale has the form

$$\bar{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{\xi} \tag{9}$$

and functions defined on the meso-scale can be written in the form

$$\bar{f}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}) .$$
(10)

A function defined on the meso-scale can be written in the form

$$\bar{f}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = f(\boldsymbol{x}) + (\nabla f(\boldsymbol{x}))^T (\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{f}^*(\bar{\boldsymbol{x}}) , \qquad (11)$$

where $f(\boldsymbol{x})$ is the function defined on the macro-scale, $\nabla f(\boldsymbol{x})$ is the gradient of the function $f(\boldsymbol{x})$ with respect to the macro-scale coordinates and $\bar{f}^*(\bar{\boldsymbol{x}})$ is the function of fluctuations defined on the meso-scale. This formulation corresponds to the first order homogenization where only the function value and the gradient of the macro-scale function is used on the meso-scale.

Volume averaging is defined in the form

$$\langle f(\boldsymbol{x}) \rangle = \frac{1}{|\bar{V}|} \int_{\bar{V}} \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}) \mathrm{d}\bar{V}$$
 (12)

and the surface averaging can be written as

$$\langle f(\boldsymbol{x}) \rangle_{S} = \frac{1}{|\bar{S}|} \int_{\bar{S}} \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}) \mathrm{d}\bar{S} .$$
 (13)

The previous averaged values are valid in a macro-scale point and they are obtained by integration of a function over the representative volume or surface. Volume integral of a function has the form

$$\int_{V} f(\boldsymbol{x}) dV = \int_{V} \langle f(\boldsymbol{x}) \rangle dV = \int_{V} \left(\frac{1}{|\bar{V}|} \int_{\bar{V}} \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}) d\bar{V} \right) dV$$
(14)

and surface integral can be written in the form

$$\int_{S} f(\boldsymbol{x}) dS = \int_{S} \langle f(\boldsymbol{x}) \rangle_{S} dS = \int_{S} \left(\frac{1}{|\bar{S}|} \int_{\bar{S}} \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}) d\bar{S} \right) dS .$$
(15)

Averaging of coordinates leads to the result

$$\langle \bar{\boldsymbol{x}} - \boldsymbol{x} \rangle = 0$$
. (16)

In the multi-scale approach, two gradients are defined. One is defined on the macroscale and second on the meso-scale in the form

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \end{pmatrix} \qquad \bar{\nabla} \bar{f}(\bar{\boldsymbol{x}}) = \begin{pmatrix} \frac{\partial f}{\partial \bar{x}_1} \\ \frac{\partial \bar{f}}{\partial \bar{x}_2} \\ \frac{\partial \bar{f}}{\partial \bar{x}_3} \end{pmatrix} \qquad (17)$$

3.1 Functions defined in meso-scale problem

The following functions are needed in the meso-scale problem. The temperature

$$\bar{T}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = T(\boldsymbol{x}) + (\nabla T(\boldsymbol{x}))^T (\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{T}^*(\bar{\boldsymbol{x}}) , \qquad (18)$$

the test function for temperature

$$\bar{\chi}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \chi(\boldsymbol{x}) + (\nabla \chi(\boldsymbol{x}))^T (\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{\chi}^*(\bar{\boldsymbol{x}}) , \qquad (19)$$

the relative humidity

$$\bar{\varphi}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \varphi(\boldsymbol{x}) + (\nabla \varphi(\boldsymbol{x}))^T (\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{\varphi}^*(\bar{\boldsymbol{x}}) , \qquad (20)$$

the test function for relative humidity

$$\bar{\psi}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \psi(\boldsymbol{x}) + (\nabla \psi(\boldsymbol{x}))^T (\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{\psi}^*(\bar{\boldsymbol{x}}) .$$
(21)

The gradients of the previously defined functions have the form

$$\overline{\nabla}\overline{T}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla T(\boldsymbol{x}) + \overline{\nabla}\overline{T}^*(\bar{\boldsymbol{x}}) , \qquad (22)$$

$$\bar{\nabla}\bar{\chi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\chi(\boldsymbol{x}) + \bar{\nabla}\bar{\chi}^*(\bar{\boldsymbol{x}}) , \qquad (23)$$

$$\bar{\nabla}\bar{\varphi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\varphi(\boldsymbol{x}) + \bar{\nabla}\bar{\varphi}^*(\bar{\boldsymbol{x}}) , \qquad (24)$$

$$\bar{\nabla}\bar{\psi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\psi(\boldsymbol{x}) + \bar{\nabla}\bar{\psi}^*(\bar{\boldsymbol{x}}) .$$
(25)

3.2 Heat balance equation

The energy balance equation has to be satisfied on the macro-scale as well as on the meso-scale, therefore

$$\frac{\mathrm{d}H}{\mathrm{d}T}\frac{\partial T}{\partial t} = \nabla^T \left(\boldsymbol{D}_{TT} \nabla T + \boldsymbol{D}_{T\varphi} \nabla \varphi \right) , \qquad (26)$$

$$\frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}}\frac{\partial\bar{T}}{\partial t} = \bar{\nabla}^T \left(\bar{\boldsymbol{D}}_{TT}\bar{\nabla}\bar{T} + \bar{\boldsymbol{D}}_{T\varphi}\bar{\nabla}\bar{\varphi} \right) \ . \tag{27}$$

Equation (26) is multiplied by χ , the balance equation (27) is multiplied by the test function $\bar{\chi}$ and then averaged. Finally, both equations are integrated over the volume and they are added up and the following equation is obtained

$$\int_{V} \left\langle \bar{\chi} \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \frac{\partial \bar{T}}{\partial t} \right\rangle \mathrm{d}V - \int_{V} \left\langle \bar{\chi} \,\bar{\nabla}^{T} \left(\bar{\boldsymbol{D}}_{TT} \bar{\nabla}\bar{T} + \bar{\boldsymbol{D}}_{T\varphi} \bar{\nabla}\bar{\varphi} \right) \right\rangle \mathrm{d}V = \\
= \int_{V} \chi \frac{\mathrm{d}H}{\mathrm{d}T} \frac{\partial T}{\partial t} \mathrm{d}V - \int_{V} \chi \,\nabla^{T} \left(\boldsymbol{D}_{TT} \nabla T + \boldsymbol{D}_{T\varphi} \nabla\varphi \right) \mathrm{d}V.$$
(28)

Substitution of the functions (18)–(21) and the gradients (22)–(25) to the heat balance equation (28) results in the form

$$\int_{V} \left\langle (\chi(\boldsymbol{x}) + (\nabla\chi(\boldsymbol{x}))^{T}(\bar{\boldsymbol{x}} - \boldsymbol{x}) + \bar{\chi}^{*}(\bar{\boldsymbol{x}})) \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \frac{\partial\bar{T}}{\partial t} \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\nabla\chi(\boldsymbol{x}) + \bar{\nabla}\bar{\chi}^{*}(\bar{\boldsymbol{x}}))^{T} \bar{\boldsymbol{D}}_{TT} (\nabla T(\boldsymbol{x}) + \bar{\nabla}\bar{T}^{*}(\bar{\boldsymbol{x}})) \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\nabla\chi(\boldsymbol{x}) + \bar{\nabla}\bar{\chi}^{*}(\bar{\boldsymbol{x}}))^{T} \bar{\boldsymbol{D}}_{T\varphi} (\nabla\varphi(\boldsymbol{x}) + \bar{\nabla}\bar{\varphi}^{*}(\bar{\boldsymbol{x}})) \right\rangle \mathrm{d}V - \\
- \int_{S} \left\langle \bar{\chi}\boldsymbol{n}^{T} \bar{\boldsymbol{q}}_{T} \right\rangle \mathrm{d}S - \int_{S} \left\langle \bar{\chi}\boldsymbol{n}^{T} \bar{\boldsymbol{q}}_{\varphi} \right\rangle \mathrm{d}S = \\
= \int_{V} \chi \frac{\mathrm{d}H}{\mathrm{d}T} \frac{\partial T}{\partial t} \mathrm{d}V + \int_{V} (\nabla\chi)^{T} \boldsymbol{D}_{TT} \nabla T \mathrm{d}V + \int_{V} (\nabla\chi)^{T} \boldsymbol{D}_{T\varphi} \nabla\varphi \mathrm{d}V - \\
- \int_{S} \chi \boldsymbol{n}^{T} \boldsymbol{q}_{T} \mathrm{d}S - \int_{S} \chi \boldsymbol{n}^{T} \boldsymbol{q}_{\varphi} \mathrm{d}S .$$
(29)

If the function $\chi(x)$ is factored in (29), the balance equation on the macro-scale is obtained

$$\int_{V} \left(\left\langle (\chi(\boldsymbol{x}) + (\nabla\chi(\boldsymbol{x}))^{T}(\bar{\boldsymbol{x}} - \boldsymbol{x})) \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \frac{\partial\bar{T}}{\partial t} \right\rangle - \chi \frac{\mathrm{d}H}{\mathrm{d}T} \frac{\partial T}{\partial t} \right) \mathrm{d}V + \\
+ \int_{V} (\nabla\chi(\boldsymbol{x}))^{T} \left(-\boldsymbol{D}_{TT} \nabla T + \left\langle \bar{\boldsymbol{D}}_{TT} (\nabla T(\boldsymbol{x}) + \bar{\nabla}\bar{T}^{*}(\bar{\boldsymbol{x}})) \right\rangle \right) \mathrm{d}V + \\
+ \int_{V} (\nabla\chi(\boldsymbol{x}))^{T} \left(-\boldsymbol{D}_{T\varphi} \nabla\varphi + \left\langle \bar{\boldsymbol{D}}_{T\varphi} (\nabla\varphi(\boldsymbol{x}) + \bar{\nabla}\bar{\varphi}^{*}(\bar{\boldsymbol{x}})) \right\rangle \right) \mathrm{d}V = 0. \quad (30)$$

If the function $\bar{\chi}(\boldsymbol{x})$ is factored in (29), the balance equation on the meso-scale is obtained

$$\int_{V} \left\langle \bar{\chi}^{*}(\bar{\boldsymbol{x}}) \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \frac{\partial\bar{T}}{\partial t} \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\bar{\nabla}\bar{\chi}^{*}(\bar{\boldsymbol{x}}))^{T} \bar{\boldsymbol{D}}_{TT} (\nabla T(\boldsymbol{x}) + \bar{\nabla}\bar{T}^{*}(\bar{\boldsymbol{x}})) \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\bar{\nabla}\bar{\chi}^{*}(\bar{\boldsymbol{x}}))^{T} \bar{\boldsymbol{D}}_{T\varphi} (\nabla\varphi(\boldsymbol{x}) + \bar{\nabla}\bar{\varphi}^{*}(\bar{\boldsymbol{x}})) \right\rangle \mathrm{d}V - \\
- \int_{S} \left\langle \bar{\chi}^{*} \boldsymbol{n}^{T} \boldsymbol{q}_{T} \right\rangle \mathrm{d}S - \int_{S} \left\langle \bar{\chi}^{*} \boldsymbol{n}^{T} \boldsymbol{q}_{\varphi} \right\rangle \mathrm{d}S = 0.$$
(31)

The balance equations on both levels are discretized by the finite element method in the classical sense. The number of degrees of freedom on the macro-scale is denoted N while the number of degrees of freedom on the meso-scale is denoted n. After discretization, the gradients (22)–(25) have the form

$$\bar{\nabla}\bar{T}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla T(\boldsymbol{x}) + \bar{\nabla}\bar{T}^*(\bar{\boldsymbol{x}}) = \boldsymbol{B}_T \boldsymbol{u}_T + \bar{\boldsymbol{B}}_T \bar{\boldsymbol{u}}_T^* , \qquad (32)$$

$$\bar{\nabla}\bar{\chi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\chi(\boldsymbol{x}) + \bar{\nabla}\bar{\chi}^*(\bar{\boldsymbol{x}}) = \boldsymbol{B}_T \boldsymbol{v}_T + \bar{\boldsymbol{B}}_T \bar{\boldsymbol{v}}_T^* , \qquad (33)$$

$$\bar{\nabla}\bar{\varphi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\varphi(\boldsymbol{x}) + \bar{\nabla}\bar{\varphi}^*(\bar{\boldsymbol{x}}) = \boldsymbol{B}_{\varphi}\boldsymbol{u}_{\varphi} + \bar{\boldsymbol{B}}_{\varphi}\bar{\boldsymbol{u}}_{\varphi}^*, \qquad (34)$$

$$\bar{\nabla}\bar{\psi}(\boldsymbol{x},\bar{\boldsymbol{x}}) = \nabla\psi(\boldsymbol{x}) + \bar{\nabla}\bar{\psi}^*(\bar{\boldsymbol{x}}) = \boldsymbol{B}_{\varphi}\boldsymbol{v}_{\varphi} + \bar{\boldsymbol{B}}_{\varphi}\bar{\boldsymbol{v}}_{\varphi}^*, \qquad (35)$$

where $\boldsymbol{u}_T, \boldsymbol{v}_T, \boldsymbol{u}_{\varphi}, \boldsymbol{v}_{\varphi} \in R^N$ are the vector of nodal temperatures, the vector of nodal values of the test function $\bar{\chi}$, the vector of nodal relative humidities and the vector of nodal values of the test function $\bar{\psi}$, respectively. The matrices $\boldsymbol{B}_T, \boldsymbol{B}_{\varphi} \in R^{3 \times N}$ are the matrices of gradients of basis functions. The same basis functions are used for a quantity and its test function. All previously mentioned vectors and matrices are defined on the macro-scale. Similar vectors and matrices $\bar{\boldsymbol{u}}_T^*, \bar{\boldsymbol{v}}_T^*, \bar{\boldsymbol{u}}_{\varphi}^*, \bar{\boldsymbol{v}}_{\varphi}^* \in R^n$, $\bar{\boldsymbol{B}}_T, \bar{\boldsymbol{B}}_{\varphi} \in R^{3 \times n}$ are defined also on the meso-scale.

Substitution of the finite element approximation to the balance equation on the macro-scale leads to the form

$$\int_{V} \boldsymbol{v}_{T}^{T} \boldsymbol{B}_{T}^{T} \left(-\boldsymbol{D}_{TT} \nabla T(\boldsymbol{x}) + \left\langle \bar{\boldsymbol{D}}_{TT} (\nabla T(\boldsymbol{x}) + \bar{\boldsymbol{B}}_{T} \bar{\boldsymbol{u}}_{T}^{*}) \right\rangle \right) \mathrm{d}V + \\ + \int_{V} \boldsymbol{v}_{T}^{T} \boldsymbol{B}_{T}^{T} \left(-\boldsymbol{D}_{T\varphi} \nabla \varphi(\boldsymbol{x}) + \left\langle \bar{\boldsymbol{D}}_{T\varphi} (\nabla \varphi(\boldsymbol{x}) + \bar{\boldsymbol{B}}_{\varphi} \bar{\boldsymbol{u}}_{\varphi}^{*}) \right\rangle \right) \mathrm{d}V = 0.$$
(36)

If new matrices are defined in the form

$$\boldsymbol{L}_{TT} = \left\langle \bar{\boldsymbol{D}}_{TT} \bar{\boldsymbol{B}}_T \right\rangle \in R^{3 \times n} \qquad \boldsymbol{L}_{T\varphi} = \left\langle \bar{\boldsymbol{D}}_{T\varphi} \bar{\boldsymbol{B}}_{\varphi} \right\rangle \in R^{3 \times n} , \qquad (37)$$

the discrete version of the heat balance equation on the macro-scale is

$$-\boldsymbol{D}_{TT}\nabla T - \boldsymbol{D}_{T\varphi}\nabla\varphi + \langle \bar{\boldsymbol{D}}_{TT} \rangle \nabla T + \langle \bar{\boldsymbol{D}}_{T\varphi} \rangle \nabla\varphi + \boldsymbol{L}_{TT}\bar{\boldsymbol{u}}_{T}^{*} + \boldsymbol{L}_{T\varphi}\bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0}.$$
(38)

Substitution of the finite element approximation to the balance equation on the mesoscale leads to the form

$$\int_{V} \left\langle \bar{\chi}^{*}(\bar{\boldsymbol{x}}) \right\rangle \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \frac{\partial\bar{T}}{\partial t} \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\bar{\boldsymbol{v}}_{T}^{*})^{T} \bar{\boldsymbol{B}}_{T}^{T} \bar{\boldsymbol{D}}_{TT} (\nabla T(\boldsymbol{x}) + \bar{\boldsymbol{B}}_{T} \bar{\boldsymbol{u}}_{T}^{*}) \right\rangle \mathrm{d}V + \\
+ \int_{V} \left\langle (\bar{\boldsymbol{v}}_{T}^{*})^{T} \bar{\boldsymbol{B}}_{T}^{T} \bar{\boldsymbol{D}}_{T\varphi} (\nabla \varphi(\boldsymbol{x}) + \bar{\boldsymbol{B}}_{\varphi} \bar{\boldsymbol{u}}_{\varphi}^{*}) \right\rangle \mathrm{d}V - \\
- \int_{S} \left\langle \bar{\chi}^{*} \boldsymbol{n}^{T} \boldsymbol{q}_{T} \right\rangle \mathrm{d}S - \int_{S} \left\langle \bar{\chi}^{*} \boldsymbol{n}^{T} \boldsymbol{q}_{\varphi} \right\rangle \mathrm{d}S = 0.$$
(39)

If new matrices are defined in the form

$$\bar{\boldsymbol{K}}_{TT} = \left\langle \bar{\boldsymbol{B}}_{T}^{T} \bar{\boldsymbol{D}}_{TT} \bar{\boldsymbol{B}}_{T} \right\rangle \in R^{n \times n} , \qquad (40)$$

$$\bar{\boldsymbol{K}}_{T\varphi} = \left\langle \bar{\boldsymbol{B}}_{T}^{T} \bar{\boldsymbol{D}}_{T\varphi} \bar{\boldsymbol{B}}_{\varphi} \right\rangle \in R^{n \times n} , \qquad (41)$$

$$\bar{\boldsymbol{C}}_{TT} = \left\langle \bar{\boldsymbol{N}}_{T}^{T} \frac{\mathrm{d}\bar{H}}{\mathrm{d}\bar{T}} \bar{\boldsymbol{N}}_{T} \right\rangle \in R^{n \times n}, \qquad (42)$$

the discrete version of the heat balance equation on the meso-scale is

$$\bar{\boldsymbol{C}}_{TT}\frac{\mathrm{d}\bar{\boldsymbol{u}}_{T}^{*}}{\mathrm{d}t} + \boldsymbol{L}_{TT}^{T}\nabla T(\boldsymbol{x}) + \boldsymbol{L}_{T\varphi}^{T}\nabla\varphi(\boldsymbol{x}) + \bar{\boldsymbol{K}}_{TT}\bar{\boldsymbol{u}}_{T}^{*} + \bar{\boldsymbol{K}}_{T\varphi}\bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0}.$$
(43)

3.3 Mass balance equation

Discretized version of the mass balance equations on the macro and meso-scales can be obtained in similar way to the equations for heat transport. The whole derivation is not included and only the resulting equations are summarized. The mass balance equation on the macro-scale has the form

$$-\boldsymbol{D}_{\varphi T}\nabla T - \boldsymbol{D}_{\varphi \varphi}\nabla \varphi + \langle \bar{\boldsymbol{D}}_{\varphi T} \rangle \nabla T + \langle \bar{\boldsymbol{D}}_{\varphi \varphi} \rangle \nabla \varphi + \boldsymbol{L}_{\varphi T} \bar{\boldsymbol{u}}_{T}^{*} + \boldsymbol{L}_{\varphi \varphi} \bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0} , \qquad (44)$$

while the mass balance equation on the meso-scale has the form

$$\bar{\boldsymbol{C}}_{\varphi\varphi}\frac{\mathrm{d}\bar{\boldsymbol{u}}_{\varphi}^{*}}{\mathrm{d}t} + \boldsymbol{L}_{\varphi T}^{T}\nabla T(\boldsymbol{x}) + \boldsymbol{L}_{\varphi\varphi}^{T}\nabla\varphi(\boldsymbol{x}) + \bar{\boldsymbol{K}}_{\varphi T}\bar{\boldsymbol{u}}_{T}^{*} + \bar{\boldsymbol{K}}_{\varphi\varphi}\bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0}.$$
(45)

3.4 Solution of multi-scale problem

The multi-scale problem is described by two balance equations on the macro-scale and two equations on the meso-scale. On the meso-scale, the balance equations have the form

$$\bar{\boldsymbol{C}}_{TT} \frac{\mathrm{d}\bar{\boldsymbol{u}}_{T}^{*}}{\mathrm{d}t} + \boldsymbol{L}_{TT}^{T} \nabla T(\boldsymbol{x}) + \boldsymbol{L}_{T\varphi}^{T} \nabla \varphi(\boldsymbol{x}) + \bar{\boldsymbol{K}}_{TT} \bar{\boldsymbol{u}}_{T}^{*} + \bar{\boldsymbol{K}}_{T\varphi} \bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0} \quad (46)$$

$$\bar{\boldsymbol{C}}_{\varphi\varphi}\frac{\mathrm{d}\bar{\boldsymbol{u}}_{\varphi}^{*}}{\mathrm{d}t} + \boldsymbol{L}_{\varphi T}^{T}\nabla T(\boldsymbol{x}) + \boldsymbol{L}_{\varphi\varphi}^{T}\nabla\varphi(\boldsymbol{x}) + \bar{\boldsymbol{K}}_{\varphi T}\bar{\boldsymbol{u}}_{T}^{*} + \bar{\boldsymbol{K}}_{\varphi\varphi}\bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0} \quad (47)$$

On the macro-scale, the balance equations have the form

$$-\boldsymbol{D}_{TT}\nabla T - \boldsymbol{D}_{T\varphi}\nabla\varphi + \langle \bar{\boldsymbol{D}}_{TT} \rangle \nabla T + \langle \bar{\boldsymbol{D}}_{T\varphi} \rangle \nabla\varphi + \boldsymbol{L}_{TT}\bar{\boldsymbol{u}}_{T}^{*} + \boldsymbol{L}_{T\varphi}\bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0} \quad (48)$$

$$-\boldsymbol{D}_{\varphi T}\nabla T - \boldsymbol{D}_{\varphi \varphi}\nabla \varphi + \langle \bar{\boldsymbol{D}}_{\varphi T} \rangle \nabla T + \langle \bar{\boldsymbol{D}}_{\varphi \varphi} \rangle \nabla \varphi + \boldsymbol{L}_{\varphi T} \bar{\boldsymbol{u}}_{T}^{*} + \boldsymbol{L}_{\varphi \varphi} \bar{\boldsymbol{u}}_{\varphi}^{*} = \boldsymbol{0} \quad (49)$$

Both balance equations on the meso-scale can be written in the matrix-vector form

$$\begin{pmatrix} \boldsymbol{K}_{TT} & \boldsymbol{K}_{T\varphi} \\ \boldsymbol{K}_{\varphi T} & \boldsymbol{K}_{\varphi \varphi} \end{pmatrix} \begin{pmatrix} \bar{\boldsymbol{u}}_{T}^{*} \\ \bar{\boldsymbol{u}}_{\varphi}^{*} \end{pmatrix} = -\begin{pmatrix} \boldsymbol{L}_{TT}^{T} & \boldsymbol{L}_{T\varphi}^{T} \\ \boldsymbol{L}_{\varphi T}^{T} & \boldsymbol{L}_{\varphi \varphi}^{T} \end{pmatrix} \begin{pmatrix} \nabla T(\boldsymbol{x}) \\ \nabla \varphi(\boldsymbol{x}) \end{pmatrix}, \quad (50)$$

where the right hand side is assembled from the gradients of the macro-scale variables. The solution of system (50) can be formally written in the form

$$\begin{pmatrix} \bar{\boldsymbol{u}}_{T}^{*} \\ \bar{\boldsymbol{u}}_{\varphi}^{*} \end{pmatrix} = -\begin{pmatrix} \boldsymbol{K}_{TT} & \boldsymbol{K}_{T\varphi} \\ \boldsymbol{K}_{\varphi T} & \boldsymbol{K}_{\varphi \varphi} \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{L}_{TT}^{T} & \boldsymbol{L}_{T\varphi}^{T} \\ \boldsymbol{L}_{\varphi T}^{T} & \boldsymbol{L}_{\varphi \varphi}^{T} \end{pmatrix} \begin{pmatrix} \nabla T(\boldsymbol{x}) \\ \nabla \varphi(\boldsymbol{x}) \end{pmatrix} .$$
(51)

Substitution of the solution (51) to the balance equations valid on the macro-scale (48) and (49) leads to the expression

$$-\begin{pmatrix} \boldsymbol{D}_{TT} & \boldsymbol{D}_{T\varphi} \\ \boldsymbol{D}_{\varphi T} & \boldsymbol{D}_{\varphi \varphi} \end{pmatrix}\begin{pmatrix} \nabla T \\ \nabla \varphi \end{pmatrix} + \begin{pmatrix} \langle \bar{\boldsymbol{D}}_{TT} \rangle & \langle \bar{\boldsymbol{D}}_{T\varphi} \rangle \\ \langle \bar{\boldsymbol{D}}_{\varphi T} \rangle & \langle \bar{\boldsymbol{D}}_{\varphi \varphi} \rangle \end{pmatrix}\begin{pmatrix} \nabla T \\ \nabla \varphi \end{pmatrix} +$$
(52)

$$+ \begin{pmatrix} \boldsymbol{L}_{TT} & \boldsymbol{L}_{T\varphi} \\ \boldsymbol{L}_{\varphi T} & \boldsymbol{L}_{\varphi \varphi} \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_{T}^{*} \\ \boldsymbol{u}_{\varphi}^{*} \end{pmatrix} = \boldsymbol{0}$$
(53)

which can be rearranged to the relationship for the conductivity matrix in the form

$$\begin{pmatrix} \mathbf{D}_{TT} & \mathbf{D}_{T\varphi} \\ \mathbf{D}_{\varphi T} & \mathbf{D}_{\varphi \varphi} \end{pmatrix} = \begin{pmatrix} \langle \bar{\mathbf{D}}_{TT} \rangle & \langle \bar{\mathbf{D}}_{T\varphi} \rangle \\ \langle \bar{\mathbf{D}}_{\varphi T} \rangle & \langle \bar{\mathbf{D}}_{\varphi \varphi} \rangle \end{pmatrix} -$$

$$- \begin{pmatrix} \mathbf{L}_{TT} & \mathbf{L}_{T\varphi} \\ \mathbf{L}_{\varphi T} & \mathbf{L}_{\varphi \varphi} \end{pmatrix} \begin{pmatrix} \mathbf{K}_{TT} & \mathbf{K}_{T\varphi} \\ \mathbf{K}_{\varphi T} & \mathbf{K}_{\varphi \varphi} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{L}_{TT}^{T} & \mathbf{L}_{T\varphi}^{T} \\ \mathbf{L}_{\varphi T}^{T} & \mathbf{L}_{\varphi \varphi}^{T} \end{pmatrix} .$$
(54)

The conductivity matrix (54) is used on the macro-scale and it is obtained by homogenization from the meso-scale.



Figure 1: Three-dimensional model of the Charles bridges in Prague.

4 Numerical examples

The multi-scale method described in the previous section is demonstrated on the example of analysis of historical masonry bridge. The bridge analyzed is the Charles brigde in Prague, Czech Republic. Three-dimensional model of the bridge is in Figure 1 where the different colours indicate different type of materials. With respect to extremely large demands of the multi-scale method on computer power, only twodimensional problems was solved. Cross section of the bridge was modelled and the mesh together with meso-scale problems are depicted in Figure 2. The boundary conditions were obtained from measured data. The time dependency of the temperature and relative humidity is depicted in Figure 3. Evolution of the temperature and relative humidity in the macro-scale problem is in Figure 4. Figure 5 shows the fluctuations of the temperature and relative humidity in the meso-scale problems in selected points of the bridge. Behaviour of the variables in time is also included.

4.1 Parallel computation

As already discussed in the previous section, the present FE^2 based multi-scale analysis assumes each macroscopic integration point be connected with a certain mesoscopic problem represented by an appropriate periodic unit cell. The solution of a meso-scale problem then provides instantaneous effective data needed on the macroscale. Such an analysis is particularly suitable for a parallel computing because the amount of transferred data is small. In this regard, the master-slave strategy can be efficiently exploited [4]. To that end, the macro-problem is assigned to the master



Figure 2: Cross-section of the brigde and two meso-scale meshes.



Exterior boundary conditions

Figure 3: Boundary conditions (relative humidity and temperature).

Evolution of temperature and moisture



Figure 4: Distribution of the temperature and relative humidity in the cross section.



Figure 5: Distribution of the temperature and relative humidity on the meso-scale meshes.

processor while the solution at the meso-scale is carried out on slave processors. At each time step the current temperature and moisture together with the increments of their gradients at a given macroscopic 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.

If the meso-scale problems are large enough, the ideal solution is to assign one meso-problem to one slave processor. Clearly, even for very small macro-problems with a few thousands of finite elements, the hardware requirements would be in such a case excessive. On the other hand, if the meso-problems are relatively small, i.e. they contain small number of finite elements, the corresponding analysis might be even shorter than the data transfer between the processors. Then, the computational time associated with the data transfer between the master processor and many slave processors may grow excessively. It is worth mentioning that this time consists of two contributions. The first one represents the latency time (the processors make connection) which is independent of the amount of transferred data whilst the second contribution clearly depends on the amount of data being transferred. For small meso-problems it is therefore reasonable to assign several of them to a single slave processor. The master processor then sends a larger package of data from many macroscopic integration points at the same time to each slave processor so that the latency time does not play a crucial role. This approach was adopted hereinafter.

The number of elements in the two meso-problems amounts to 265 (160 nodes) for SEPUC 1 and to 414 (239 nodes) for SEPUC 2, respectively. Similarly to the macro-problem, the meso-problems have to account for the material heterogeneity. Clearly, the ideal speedup and load balancing are obtained when the decomposition of the macro-problem reflects the meso-problem meshes. However, this is considerably more difficult when compared to the classical mesh decomposition.

The finite element mesh used at the macro-level is evident from Fig. 2 featuring 7,081 nodes and 13,794 triangular elements with a single integration point thus amounting to the solution of 13,794 meso-problems at each macroscopic time step. This figure also shows decomposition of the macro-problem into 12 slave processors. The numbers of elements in individual sub-domains being equal to the number of meso-problems handled by the assigned slave processor are listed in Table 1. It should be noted that the assumed decomposition of the macro-problem is not ideal. In comparison with domain decomposition methods, the macro-problem has to be split with respect to the heterogeneity of the material resulting in the variation of number of elements in individual sub-domains between 1046 and 1748.

The actual analysis was performed on a cluster built at our department. Each node of the cluster is a single processor personal computer Dell Optiplex GX620 equipped with 3.54 GB of RAM. The processors are Intel Pentium with the frequency 3.4 GHz. The cluster is based on Debian linux 5.0 and 32-bit architecture. Each time step took 2.08 minute.

Processor No.	1	2	3	4	5	6
	7	8	9	10	11	12
No. of	1218	1748	1046	1052	1214	1210
meso-problems	1052	1054	1046	1052	1054	1048

Table 1: Decomposition of the macro-problem into sub-domains.

5 Conclusion

A multi-scale analysis of simultaneous heat and moisture transport in masonry structures was implemented in the framework of FE^2 computational strategy. Special attention was accorded to the implementation of the method in the parallel format employing the master-slave approach. Although not qualitatively fully acceptable, the two-dimensional example of Charles Bridge raised a number of questions to the solution efficiency particularly with reference to a proper subdivision of the analyzed macro-domain and local finite element mesh of individual meso-scale SEPUCs. The present findings will be utilized in a fully three-dimensional analysis being the subject of our current research effort.

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