An equation-free multiscale method applied to discrete networks

BEEX[1] L.A.A., KERFRIDEN[2] P.

[1] University of Luxembourg, Institute of Computational Engineering, Luxembourg (lars.beex@uni.lu)
[2] Cardiff University, Architectural, Civil & Environmental Engineering, Wales, UK (kerfridenp@cardiff.ac.uk)

Nested multiscale approaches, e.g. the FE^2 framework, come with a number of drawbacks. One of those is the formulation of macro-to-micro and micro-to-macro relations (to which we refer as 'scaling relations'). This involves extracting the correct information of the descriptions at the different length scales and sending this information from one scale to another. It also involves applying appropriate boundary conditions (BCs) at the small-scale models. This is not trivial if the macroscale field is more enhanced than piece-wise linear (see e.g. [1]).

Another disadvantage is that the length scale of the unit cell must be several orders of magnitude smaller than the interpolation elements at the macroscale. This is a disadvantage because the user needs to ensure that scale separation is present. It furthermore leads to large computational efforts if domains in which the small-scale model is used are coupled to domains in which computational homogenization is employed. A side note is that error measures can be utilized to overcome this issue [2].

In this presentation, an equation-free multiscale approach is discussed. The approach is applied to discrete models of discrete mesostructures. The discrete small-scale model is directly incorporated in the macroscale model in the proposed scheme, such that no scaling relations are required (hence, the term 'equation-free'). Separation of scales is also not required.

The price to pay to avoid upscaling relations and scale separation is that each node of the macroscale discretization has as a substantial number of degrees of freedom.

The equation-free multiscale approach is the result of a numerical generalization of the quasicontinuum (QC) method. The QC method was originally proposed for discrete conservative models with a regular charactre (i.e. atomistics, in which each atom is connected to other atoms in the same way) [3]. Recently, several generalizations are proposed to incorporate dissipative phenomena such as (elasto)plasticity, damage and frictional fibre sliding [4-6].

The dissipative QC frameworks could so far however also not deal irregularity at the small scale. The new QC framework presented here is able to deal with irregularity (within a periodic representative volume element). This makes approach considerably more applicable to discrete network models.

In this presentation, the numerical generalization of the QC approach is presented. We will start with an explanation of the QC method for regular structures. In the discussion we will consider the two reduction steps of the QC method (see Fig. 1).

The presented examples focus on discrete planar models with damage, useful to represent discrete mesostructures. The examples use higher order interpolations at the macroscale, showing the relative ease to apply the approach for any order of macroscale interpolation.

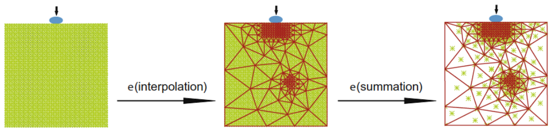

Figure 1. The two reduction steps of the QC method: interpolation and summation (also called sampling, which can be interpreted as reduced integration). Both steps come with an error and the crux is how to apply both steps such that the combined error is sufficiently small.

[1] Kouznetsova V., Geers M.G.D., Brekelmans, W.A.M.. Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenisation scheme. *IJNME*, Vol. **54**, pp. 1235-1260, 2002.
[2] Akbari Rahimadabi A., Kerfriden P., Bordas S.P.A., Scale selection in nonlinear fracture mechanics of heterogeneous materials. *Phil. Mag.*, Vol. **95**(28-30), pp. 3328-3347, 2015.
[2] Tadmor E.B., Phillips R., Ortiz M., Mixed atomistics and continuum models of deformation in solids. Langmuir, Vol. **12**(19), pp. 4529-4534, 1996.
[4] Beex L.A.A., Peerlings R.H.J., Geers M.G.D, A multiscale quasicontinuum method for dissipative lattice models and discrete networks. *JMPS*, Vol. **64**, pp. 154-169, 2014.
[5] Beex L.A.A., Peerlings R.H.J., Geers M.G.D, A multiscale quasicontinuum method for lattice models with bond failure and fiber sliding. *CMAME*, Vol. **269**, pp. 108-122, 2014.
[6] Rokoš O., Beex L.A.A., Zeman J., Peerlings R.H.J., A variational formulation of dissipative quasicontinuum methods. *IJSS*, In press.