Multiscale Physics

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1 Heat Conduction

Fourier's Law and conservation of energy read

$$q_i = -a_{ij}\frac{\partial u}{\partial x_j}, \quad \frac{\partial q_i}{\partial x_i} = f$$

where $f = f(x)$ is a volumetric heat source. Thus, the governing equation for heat conduction is

$$\frac{\partial}{\partial x_i}(a_{ij}\frac{\partial u}{\partial x_j}) = -f(x)$$

We want to derive an equation for the homogenized conductivity tensor $\bar{a}_{ij}$. We follow the approach of periodic homogenization and think of the space being built up from a slow and fast coordinate x and y respective. Assuming the scales are sufficiently separated to treat these as independent, y is the position within the microstructure and x is the macroscopic variable. Thus, we can write

$$\frac{\partial}{\partial x_i^\eta}(a_{ij}\frac{\partial u^\eta}{\partial x_j^\eta}) = -f(x)$$

$$\frac{\partial}{\partial x_i^\eta} = \frac{\partial}{\partial x_i} + \frac{1}{\eta}\frac{\partial}{\partial y_i}, \quad u^\eta = u_0(x) + u_1(x,y)$$

Plugging this in reads

$$\left(\frac{\partial}{\partial x_i} + \frac{1}{\eta}\frac{\partial}{\partial y_i}\right)a_{ij}\left(\frac{\partial u_0}{\partial x_j} + \eta\frac{\partial u_1}{\partial x_j} + \frac{\partial u_1}{\partial y_j}\right) = -f$$

Grouping by the two lowest powers of η, we obtain two governing equations for the two-scale problem:

$$\frac{\partial}{\partial y_i}\left(a_{ij}\frac{\partial u_1}{\partial y_j}\right) = -\frac{\partial}{\partial y_i}\left(a_{ij}\frac{\partial u_0}{\partial x_j}\right)$$

$$a_{ij}\frac{\partial^2 u_0}{\partial x_i \partial x_j} + a_{ij}\frac{\partial^2 u_1}{\partial x_i \partial x_j} + \frac{\partial}{\partial y_i}\left(a_{ij}\frac{\partial u_1}{\partial x_j}\right) = -f(x)$$

The first equation shows the microscale problem is driven by macroscopic temperature gradients which are constant over the microstructure. The problem is linear, so it suffices to know the microstructural response to unit temperature gradients in each direction. Thus, we can write

$$u_1(x, y) = \chi_m \frac{\partial u_0}{\partial x_m}$$

Plugging this into the second governing equation, we can see that the equation cannot be satisfied pointwise. This is because there are a mixing of scales. Instead we require that the equation is satisfied in an average sense over the microstructure. Call the microstructural domain Ω_y and use $|\Omega_y| = 1$. The macroscopic governing equation is

$$\left(\int_\Omega a_{ij} dy\right) \frac{\partial^2 u_0}{\partial x_i \partial x_j} + \left(\int_\Omega a_{ij} \frac{\partial \chi_m}{\partial y_j} dy\right) \frac{\partial^2 u_0}{\partial x_m \partial x_i} = -f(x)$$

The third term when integrated is zero because it is the divergence of a periodic function (by assumption). Thus, we have

$$\left[\int_\Omega a_{ij} \left(\delta_{mj} + \frac{\partial \chi_m}{\partial y_j}\right) dy\right] \frac{\partial^2 u_0}{\partial x_m \partial x_i} = -f(x)$$

and can now identify the homogenized conductivity tensor as

$$\bar{a}_{im} := \int_\Omega a_{ij} \left(\delta_{mj} + \frac{\partial \chi_m}{\partial y_j}\right) dy$$

2 Linear Elasticity

The Navier equation writes stress equilibrium in terms of displacements. We know how to compute multiscale derivatives required for the strain and the divergence of the stress tensor. We know that the displacement is expanded into a coarse and fine scale contribution. We need a constitutive relation to proceed. For simplicity, assume that the constitutive tensor only depends on the microscale coordinate, otherwise the math becomes extremely cumbersome. Note that it is possible to carry through x dependence of the constitutive tensor. Assuming you have spent enough time with these derivations, doing this gives you exactly what you would expect. The multiscale stress-strain relation is

$$\sigma_{ij}^\eta(x, y) = C_{ijk\ell}(y) \epsilon_{k\ell}^\eta(x, y) \tag{1}$$

Substituting this into stress equilibrium, we can use symmetries of the material tensor to simplify the resulting expression. Note that the body force only depends on the macroscale coordinate:

$$\frac{d}{dx_j^\eta} C_{ijk\ell}(y) \frac{du_k^\eta}{dx_\ell^\eta} = -b_i(x)$$

Substituting the definition of the multiscale derivative and the two-term aymptotic expansion for the displacement, this becomes

$$\left(\frac{\partial}{\partial x_j}+\frac{1}{\eta}\frac{\partial}{\partial y_j}\right)C_{ijk\ell}(y)\left(\frac{\partial}{\partial x_\ell}+\frac{1}{\eta}\frac{\partial}{\partial y_\ell}\right)\Big(u_k^0(x)+\eta u_k^1(x,y)\Big)=-b_i(x)$$

This expression can be expanded, and the terms grouped in powers of η. It is a length calculation to show that, when keeping the two lowest powers of η, the Navier equation is

$$\frac{1}{\eta}\left(\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^0}{\partial x_\ell}\right)+\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^1}{\partial y_\ell}\right)\right)+C_{ijk\ell}\frac{\partial^2 u_k^0}{\partial x_j\partial x_\ell} \\ +C_{ijk\ell}\frac{\partial^2 u_k^1}{\partial x_j\partial y_\ell}+\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^1}{\partial x_\ell}\right)=-b_i \quad (2)$$

We obtain two governing equations by claiming that terms of equal powers of η must be equal individually. This results in

$$\eta^{-1}: \quad \frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^1}{\partial y_\ell}\right)=-\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^0}{\partial x_\ell}\right) \quad (3a)$$

$$\eta^{0}: \quad C_{ijk\ell}\frac{\partial^2 u_k^0}{\partial x_j\partial x_\ell}+C_{ijk\ell}\frac{\partial^2 u_k^1}{\partial x_j\partial y_\ell}+\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial u_k^1}{\partial x_\ell}\right)=-b_i \quad (3b)$$

The first equation only involves y derivatives. Because the macroscopic coordinate is assumed to not change with the microscale coordinate (scale separation assumption), the term $\partial u_k^0/\partial x_\ell$ is a constant with respect to y. Because this equation is linear, we can write

$$u_i^1(x,y)=\chi(y)_{imn}\frac{\partial u_m^0}{\partial x_n}(x) \quad (4)$$

The 3-index tensor function χ is interpreted as giving the displacement components of the RVE under the action of applied macroscopic unit strains. Because $u^1(x,y)$ is periodic in y, the process of solving for unit response will enforce periodicity in $\chi_{imn}(y)$. In order to solve for the RVE's response to unit strains, use Eq. 4 with $\partial u_k^0/\partial x_\ell=\delta_{ka}\delta_{\ell b}$ and the first governing equation:

$$\frac{\partial}{\partial y_j}\left(C_{ijk\ell}\frac{\partial \chi_{kab}}{\partial y_\ell}\right)=-\frac{\partial}{\partial y_j}\Big(C_{ijk\ell}\delta_{ka}\delta_{\ell b}\Big) \quad (5)$$

This is the governing equation for $\chi(y)$. A given value of indices a and b, yields an equation for the displacement components. Because the strain tensor is symmetry, not every combination of indices needs to be computed. Note that this equation has the form of stress equilibrium in the RVE for a body force proportional to spatial variations in the constitutive tensor. Turning now to the second of Eqs. 3, we can substitute Eq. 4 in order to remove any $u^1(x, y)$ dependence. Because the RVE unit response function χ only dependence on the microscale coordinate y and the first term in the displacement expansion u^0 only depends on x, we have

$$C_{ijk\ell}\frac{\partial^2 u_k^0}{\partial x_j \partial x_\ell} + C_{ijk\ell}\frac{\partial \chi_{kab}}{\partial y_\ell}\frac{\partial^2 u_a^0}{\partial x_j \partial x_b} + \frac{\partial}{\partial y_j}\left(C_{ijk\ell}\chi_{kab}\frac{\partial^2 u_a^0}{\partial x_b \partial x_\ell}\right) = -b_i \tag{6}$$

Notice how the assumption that $C_{ijk\ell} = C_{ijk\ell}(y)$ is used throughout–if the microstructure varied macroscopically, then the unit response χ would as well. Eq. 6 cannot be satisfied pointwise in x and y. The body force and displacement gradients are purely macroscopic, whereas the constitutive tensor and unit response χ are purely microscopic. The macroscale coordinate x is essentially naive to the small scale variations in the structure's material and mechanics captured by y. Returning to the analogy of zooming into a complex microstructure at each x point, we argue that the microscale interacts with the macroscopic mechanics through an average. Thus, we average the influence of the microstructure and say the averaged multiscale equation is satisfied pointwise in x:

$$\begin{aligned}\left(\frac{1}{|\Omega^y|}\int_{\Omega^y} C_{ijk\ell}\,dy\right)\frac{\partial^2 u_k^0}{\partial x_j \partial x_\ell} + \left(\frac{1}{|\Omega^y|}\int_{\Omega^y} C_{ijk\ell}\frac{\partial \chi_{kab}}{\partial y_\ell}\,dy\right)\frac{\partial^2 u_a^0}{\partial x_j \partial x_b} \\ + \left(\frac{1}{|\Omega^y|}\int_{\Omega^y} \frac{\partial}{\partial y_j}(C_{ijk\ell}\chi_{kab})\,dy\right)\frac{\partial^2 u_a^0}{\partial x_b \partial x_\ell} = -b_i\end{aligned} \tag{7}$$

The third term on the left-hand side of this equation is the divergence of a periodic function (both the material tensor and RVE unit response are periodic). The divergence theorem can be used to show the integral of the divergence of a periodic function is zero. Introducing delta functions to manage indices, we obtain the following expression:

$$\left(\frac{1}{|\Omega^y|}\int_{\Omega^y} C_{ijk\ell}\left(\delta_{ka}\delta_{\ell b} + \frac{\partial \chi_{kab}}{\partial y_\ell}\right)dy\right)\frac{\partial^2 u_a^0}{\partial x_j \partial x_b} = -b_i \tag{8}$$

The integral is a four-index object with no x or y dependence. Eq. 8 is the Navier equation in terms of the macroscopic coordinate x for a constant constitutive tensor. Thus, we recognize the integral in parentheses as the homogenized material tensor:

$$C_{ijab}^H := \frac{1}{|\Omega^y|}\int_{\Omega^y} C_{ijk\ell}\left(\delta_{ka}\delta_{\ell b} + \frac{\partial \chi_{kab}}{\partial y_\ell}\right)dy \tag{9}$$

The homogenized tensor furnishes the effective material properties of a material which exhibits periodic heterogeneities on a small scale. It can be computed once the unit response of the RVE is known.

3 Viscoelasticity

$$\frac{\partial \sigma_{ij}^{\eta}}{\partial x_j} + b_i = 0$$

$$\sigma_{ij}^{\eta} = \int_0^t C_{ijk\ell}(y, t-\tau)\frac{\partial \epsilon_{k\ell}^{\eta}}{\partial \tau} d\tau$$

$$\frac{\partial}{\partial x_j^{\eta}} \int_0^t C_{ijk\ell}(y, t-\tau)\frac{\partial^2 u_k^{\eta}}{\partial x_\ell^{\eta}\partial \tau} d\tau = -b_i$$

For a single-scale linear viscoelastic material with no spatial variation, the governing equation (analogous to Navier equation) is

$$\int_0^t C_{ijk\ell}(t-\tau)\frac{\partial^3 u_k}{\partial x_\ell \partial x_j \partial \tau} d\tau = -b_i$$

We will attempt to recover an equation of this form in order find the effective viscoelastic properties. Turning to the multiscale problem, we plug in the two scale expansion and definition of multiscale derivative

$$\left(\frac{\partial}{\partial x_j} + \frac{1}{\eta}\frac{\partial}{\partial y_j}\right) \int_0^t C_{ijk\ell}(y, t-\tau)\frac{\partial}{\partial \tau}\left[\left(\frac{\partial}{\partial x_j} + \frac{1}{\eta}\frac{\partial}{\partial y_j}\right)\left(u_k^0(x) + \eta u_k^1(x,y)\right)\right] d\tau = -b_i$$

$$= \left(\frac{\partial}{\partial x_j} + \frac{1}{\eta}\frac{\partial}{\partial y_j}\right) \int_0^t C_{ijk\ell}(y, t-\tau)\left[\frac{\partial^2 u_k^0}{\partial x_\ell \partial \tau} + \eta\frac{\partial^2 u_k^1}{\partial x_\ell \partial \tau} + \frac{\partial^2 u_k^1}{\partial y_\ell \partial \tau}\right] d\tau$$

$$= \int_0^t C_{ijk\ell}(t-\tau)\frac{\partial^3 u_k^0}{\partial x_\ell \partial x_j \partial \tau} d\tau + \frac{1}{\eta}\int_0^t \frac{\partial}{\partial y_j}\left(C_{ijk\ell}(t-\tau)\frac{\partial^2 u_k^0}{\partial x_\ell \partial \tau}\right) d\tau + \int_0^t \frac{\partial}{\partial y_j}\left(C_{ijk\ell}(t-\tau)\frac{\partial^2 u_k^1}{\partial x_\ell \partial \tau}\right) d\tau$$
$$+ \int_0^t C_{ijk\ell}(t-\tau)\frac{\partial^3 u_k^1}{\partial x_j \partial y_\ell \partial \tau} d\tau + \frac{1}{\eta}\int_0^t \frac{\partial}{\partial y_j}\left(C_{ijk\ell}(t-\tau)\frac{\partial^2 u_k^1}{\partial y_\ell \partial \tau}\right) d\tau$$

The order η^{-1} equation describes the response of the microscale:

$$\int_0^t \frac{\partial}{\partial y_j}\left(C_{ijk\ell}(t-\tau)\frac{\partial^2 u_k^1}{\partial y_\ell \partial \tau}\right) d\tau = -\int_0^t \frac{\partial}{\partial y_j}\left(C_{ijk\ell}(t-\tau)\frac{\partial^2 u_k^0}{\partial x_\ell \partial \tau}\right) d\tau$$

Assume the time dependence of the applied macroscopic strain is a step function $H(t)$ so that

$$\frac{\partial^2 u_k^0}{\partial x_\ell \partial \tau} = \frac{\partial}{\partial \tau}\left(\frac{\partial u_k^0}{\partial x_\ell} H(\tau)\right) = \delta(\tau)\frac{\partial u_k^0}{\partial x_\ell}$$

This means that the RHS of the microscale governing equation becomes

$$= -\frac{\partial}{\partial y_j} C_{ijk\ell}(t) \frac{\partial u_k^0}{\partial x_\ell}$$

The equations are linear, so we can write

$$u_i^1 = \chi_{imn}(y,t) \frac{\partial u_m^0}{\partial x_n}$$

$\chi_{imn}(y,t)$ records the i-th time-dependent displacement response at point y in the microstructure for a unit applied strain in direction (m,n). This assumes linear viscoelasticity. We can plug this relation into the macroscale governing equation (order η) and integrate over the microscale domain ($|\Omega_y| = 1$). The divergence term will be zero because all functions are periodic.

$$\int_0^t \left(\int_\Omega C_{ijk\ell}(y, t-\tau) d\Omega \right) \frac{\partial^3 u_k^0}{\partial x_\ell \partial x_j \partial \tau} d\tau + \int_0^t \int_\Omega C_{ijk\ell}(y, t-\tau) \frac{\partial}{\partial \tau} \left(\frac{\partial \chi_{kmn}}{\partial y_\ell} \frac{\partial^2 u_m^0}{\partial x_n \partial x_j} \right) d\Omega d\tau$$

But we do not recover the Navier equation because the two terms being differentiated in the second integral are time dependent. Thus, the homogenized constitutive relation is not directly analogous to the single scale viscoelastic solid. Evaluating the time derivative and re-arranging, we get

$$\int_0^t \left(\int_\Omega C_{ijk\ell}(y, t-\tau) d\Omega \right) \frac{\partial^3 u_k^0}{\partial x_\ell \partial x_j \partial \tau} d\tau + \int_0^t \int_\Omega C_{ijk\ell}(y, t-\tau) \frac{\partial^2 \chi_{kmn}}{\partial y_\ell \partial \tau} \frac{\partial^2 u_m^0}{\partial x_n \partial x_j} + C_{ijk\ell}(y, t-\tau) \frac{\partial \chi_{kmn}}{\partial y_\ell} \frac{\partial^3 u_m^0}{\partial x_n \partial x_j \partial \tau} d\Omega d\tau$$

This relation can be interpreted as giving two homogenized tensors:

$$\underline{\nabla} \cdot \left(\int_0^t \underline{\underline{\underline{\underline{C}}}}^1 (t-\tau) : \frac{\partial \underline{\underline{\epsilon}}}{\partial \tau} + \underline{\underline{\underline{\underline{C}}}}^2 (t-\tau) : \underline{\underline{\epsilon}}(\tau) d\tau \right) = -\underline{b}$$

The first homogenized tensor is similar to the usual elastic homogenized tensor (average of microstructure constitutive relation plus flux from unit strains), whereas the second involves time derivatives of the microstructure to the unit strains. Apparently, it also changes the viscoelastic constitutive relation to depend on the strain directly, as opposed to its time derivative. Does this make sense?

4 Nonlinear Heat Conduction

It may be the case that the thermal conductivity depends on the temperature in a heat conduction problem. The simplest form of this dependence would be linear. The governing equation for heat transfer would be

$$\frac{\partial}{\partial x_i}\left(au\frac{\partial u}{\partial x_i}\right)+r=0$$

where r is a volumetric heat source. Now consider a multiscale heat conduction problem of this sort, where the thermal conductivity, which is assumed to isotropic and hence a scalar, varies on the small scale only. We define a new microscale coordinate $y_i = x_i/\eta$ where η is a perturbatively small parameter. Treating these two coordinates as independent and expanding the temperature field with $u^\eta = u^0 + \eta u^1$, as is always done in the method of asymptotic homogenization, we can write this problem as

$$\frac{\partial}{\partial x_i^\eta}\left(a(y)u^\eta\frac{\partial u^\eta}{\partial x_i^\eta}\right)=\left(\frac{\partial}{\partial x_i}+\frac{1}{\eta}\frac{\partial}{\partial y_i}\right)\left(a(y)(u^0+\eta u^1)\left(\frac{\partial}{\partial x_i}+\frac{1}{\eta}\frac{\partial}{\partial y_i}\right)(u^0+\eta u^1)\right)$$

As usual, this is where lots of tedious algebra is required. The need for tedious calculations is exacerbated by the nonlearity. We often assume that the first order term in the temperature expansion u^0 is independent of the microscale coordinate. This can be proven by looking at the expression at lowest order of η:

$$\eta^{-2}:\frac{\partial}{\partial y_i}\left(a(y)u^0\frac{\partial u^0}{\partial y_i}\right)=0$$

The only way that this equation can be zero, which has no volumetric forcing and is not driven by the boundaries, is when u^0 is independent of the microscale coordinate y. The governing equation simplifies to

$$=\left(\frac{\partial}{\partial x_i}+\frac{1}{\eta}\frac{\partial}{\partial y_i}\right)\left(a(y)\left[u^0\frac{\partial u^0}{\partial x_i}+\eta u^1\frac{\partial u^0}{\partial x_i}+\eta u^0\frac{\partial u^1}{\partial x_i}\right.\right.$$
$$\left.\left.+\eta^2u^1\frac{\partial u^1}{\partial x_i}+u^0\frac{\partial u^1}{\partial y_i}+\eta u^1\frac{\partial u^1}{\partial y_i}\right]\right)+r=0$$

We can now pick out terms at the next lowest order of η. This reads

$$\eta^{-1}:\frac{\partial}{\partial y_i}\left(au^0\frac{\partial u^0}{\partial x_i}\right)+\frac{\partial}{\partial y_i}\left(au^0\frac{\partial u^1}{\partial y_i}\right)=0$$

Note that u^0 does not depend on y and can be factored out of this microscale equation. This makes the microscale problem linear, even though the physics are nonlinear. We have the usual "cell" problem from a linear elliptic equation:

$$\eta^{-1}:\frac{\partial}{\partial y_i}\left(a\frac{\partial u^1}{\partial y_i}\right)=-\frac{\partial a}{\partial y_i}\frac{\partial u^0}{\partial x_i}$$

Because the problem is linear, we can write the solution to the cell problem as a linear combination of solutions to unit temperature gradients, weighted by the actual temperature gradient coming in from the macroscale to the cell problem. This reads

$$u^1(x,y) = \chi_i(y)\frac{\partial u^0}{\partial x_i}$$

Lastly, we turn to the third highest order of η, which corresponds to the macroscale equation. Picking out orders of η from the governing equation, this is

$$\frac{\partial}{\partial x_i}\left(au^0\frac{\partial u^0}{\partial x_i}\right) + \frac{\partial}{\partial y_i}\left(au^1\frac{\partial u^0}{\partial x_i}\right) + \frac{\partial}{\partial y_i}\left(au^0\frac{\partial u^1}{\partial x_i}\right) \\ + \frac{\partial}{\partial x_i}\left(au^0\frac{\partial u^1}{\partial y_i}\right) + \frac{\partial}{\partial y_i}\left(au^1\frac{\partial u^1}{\partial y_i}\right) + r = 0$$

We can plug in the expression for the microscale temperature involving the macroscale temperature gradient. This reads

$$a\frac{\partial}{\partial x_i}\left(u^0\frac{\partial u^0}{\partial x_i}\right) + \frac{\partial}{\partial y_i}\left(a\chi_j\frac{\partial u^0}{\partial x_j}\frac{\partial u^0}{\partial x_i}\right) + \frac{\partial}{\partial y_i}\left(au^0\chi_j\frac{\partial^2 u^0}{\partial x_j \partial x_i}\right) \\ + \frac{\partial}{\partial x_i}\left(au^0\frac{\partial \chi_j}{\partial y_i}\frac{\partial u^0}{\partial x_j}\right) + \frac{\partial}{\partial y_i}\left(a\chi_k\frac{\partial u^0}{\partial x_k}\frac{\partial \chi_j}{\partial y_i}\frac{\partial u^0}{\partial x_j}\right) + r = 0$$

This equation cannot be satisfied pointwise because the volumetric heat source only varies on the macroscale whereas the temperature necessarily varies on both scales. We average over the microstructure domain, which has a volume of 1 by definition. Note that the third term in the above equation is the divergence of the product of periodic functions, thus its integral is zero. This can be verified by use of the divergence theorem. This equation becomes:

$$\frac{\partial}{\partial x_i}\left(u^0\frac{\partial u^0}{\partial x_i}\right)\left(\int a d\Omega\right) + \frac{\partial u^0}{\partial x_j}\frac{\partial u^0}{\partial x_i}\left(\int \frac{\partial}{\partial y_i}(a\chi_j) d\Omega\right) \\ + \frac{\partial}{\partial x_i}\left(u^0\frac{\partial u^0}{\partial x_j}\right)\left(\int a\frac{\partial \chi_j}{\partial y_i} d\Omega\right) + \frac{\partial u^0}{\partial x_k}\frac{\partial u^0}{\partial x_j}\left(\int \frac{\partial}{\partial y_i}\left(a\chi_k\frac{\partial \chi_j}{\partial y_i}\right) d\Omega\right) + r = 0$$

The microscale equation is linear, so we do not end up with a coupling between scales. However, we end up with a complex nonlinear problem at the macroscale. Perhaps this equation can be simplified further. With all the indices floating around, what we can see is that the conductivity is now a matrix. It makes sense that microstructural variations could introduce anisotropy into the heat conduction problem. It also seems that we will not recover an "effective conductivity" matrix. If such a thing existed, we would be able to write

$$\frac{\partial}{\partial x_i}\left(C_{ij}u^0\frac{\partial u^0}{\partial x_j}\right)$$

where $\underline{\underline{C}}$ is an expression involving integrals over the microstructure. It does not appear possible to rearrange this equation to have this form. This can be seen by noting that there are terms multiplying the product of gradients that never multiply the product of the temperature and the Laplacian of temperature. The two would need to have the same factors in order to recover a form of this sort. Thus, the homogenization procedure has shown that the physics of the macroscale are governed by some new physics. The problem will have the general form of

$$u^0 C^1_{ij} \frac{\partial^2 u^0}{\partial x_i \partial x_j} + C^2_{ij} \frac{\partial u^0}{\partial x_i} \frac{\partial u^0}{\partial x_j} + r = 0$$

5 1D Finite Strain Elasticity

A 1D St. Venant Kirchoff model of elasticity is

$$\frac{\partial}{\partial x^\eta} E(y) \left(\frac{\partial u^\eta}{\partial x^\eta} + \frac{1}{2} \left(\frac{\partial u^\eta}{\partial x^\eta} \right)^2 \right) = b(x)$$

The η superscripts denote multiscale quantities. The problem is geometrically non-linear, but the material behavior is linear. This is examlpe is taken as a first pass at non-linear homogenization. We expand the displacement field and derivatives in the usual way, and carry through the laborious expansions and simplifications.

$$u^\eta(x,y) = u^0(x) + \eta u^1(x,y), \quad \frac{\partial}{\partial x^\eta} = \frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y}$$

$$= \left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right) E(y) \left(\left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right)(u^0 + \eta u^1) + \frac{1}{2} \left[\left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right)(u^0 + \eta u^1) \right]^2 \right)$$

$$= \left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right) E(y) \left(u^0_x + \eta u^1_x + u^1_y + \frac{1}{2} \left[u^0_x + \eta u^1_x + u^1_y \right]^2 \right)$$

$$= \left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right) E(y) \left(u^0_x + \eta u^1_x + u^1_y + \frac{1}{2} \Big[(u^0_x)^2 + \eta^2 (u^1_x)^2 + (u^1_y)^2 + 2\eta (u^1_y u^1_x + u^0_x u^1_x + u^1_y u^0_x) \Big] \right)$$

Look at each term individually!

$$\left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y} \right) \left(E(y) u^0_x \right) = E u^0_{xx} + \eta^{-1} \frac{\partial}{\partial y}(E u^0_x)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(E(y)\eta u_x^1\Big)=\eta E u_{xx}^1+\frac{\partial}{\partial y}(Eu_x^1)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(E(y)u_y^1\Big)=E u_{xy}^1+\eta^{-1}\frac{\partial}{\partial y}(Eu_y^1)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(\frac{1}{2}E(y)(u_x^0)^2\Big)=E u_x^0 u_{xx}^0+\eta^{-1}\frac{\partial}{\partial y}\left(\frac{E}{2}(u_x^0)^2\right)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(\frac{1}{2}E(y)\eta^2(u_x^1)^2\Big)=\eta^2 E u_x^1 u_{xx}^1+\eta\frac{\partial}{\partial y}\left(\frac{E}{2}(u_x^1)^2\right)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(\frac{1}{2}E(y)(u_y^1)^2\Big)=E u_y^1 u_{xy}^1+\eta^{-1}\frac{\partial}{\partial y}\left(\frac{E}{2}(u_y^1)^2\right)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(E(y)\eta u_y^1 u_x^1\Big)=\eta\frac{\partial}{\partial x}(Eu_y^1u_x^1)+\frac{\partial}{\partial y}(Eu_y^1u_x^1)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(E(y)\eta u_x^0 u_x^1\Big)=\eta\frac{\partial}{\partial x}(Eu_x^0u_x^1)+\frac{\partial}{\partial y}(Eu_x^0u_x^1)$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Big(E(y)\eta u_y^1 u_x^0\Big)=\eta\frac{\partial}{\partial x}(Eu_y^1u_x^0)+\frac{\partial}{\partial y}(Eu_y^1u_x^0)$$

Now group terms corresponding to the two lowest order power of η and ignore the rest:

$$\eta^{-1}:\quad \frac{\partial}{\partial y}(Eu_x^0)+\frac{\partial}{\partial y}(Eu_y^1)+\frac{\partial}{\partial y}\left(\frac{E}{2}(u_x^0)^2\right)+\frac{\partial}{\partial y}\left(\frac{E}{2}(u_y^1)^2\right)=0$$

$$\frac{\partial}{\partial y}\Big[E(y)\Big(u_y^1+\frac{1}{2}(u_y^1)^2\Big)\Big]=-\frac{\partial}{\partial y}\Big[E(y)\Big(u_x^0+\frac{1}{2}(u_x^0)^2\Big)\Big]$$

This is the governing equation for the microscale displacement driven by the macroscale displacement gradients. This equation is non-linear, so we cannot conclude that the solution depends linearly on the macroscopic strains. This means that microscale and macroscale equations will be coupled. Anticipating a finite element problem, the weak form of this equation is

$$\int\Big[E(y)\Big(u_y^1+\frac{1}{2}(u_y^1)^2\Big)\Big]w_y dy=-\int\Big[E(y)\Big(u_x^0+\frac{1}{2}(u_x^0)^2\Big)\Big]w_y dy$$

Turning to the next order of η, we can write down the macroscale governing equation:

$$\eta^0: \quad Eu^0_{xx} + \frac{\partial}{\partial y}(Eu^1_x) + Eu^1_{xy} + Eu^0_x u^0_{xx} + Eu^1_y u^1_{xy}$$
$$+ \frac{\partial}{\partial y}(Eu^1_y u^1_x) + \frac{\partial}{\partial y}(Eu^0_x u^1_x) + \frac{\partial}{\partial y}(Eu^1_y u^0_x) = b(x)$$

As in the linear case, this equation cannot be satisfied pointwise. The body force depends only on the macroscale coordinate, so if it were to be satisfied pointwise there could be no microscale fluctuations. Thus we require that it is satisfied in an average sense, so we integrate over the microscale coordinate. Note that the microscale displacement and the modulus are periodic over the microstructure. The macroscale displacement is constant over the microstructure. Thus the terms with microscale derivatives vanish when averaged. The macroscale governing equation is

$$\left(\int E(y)dy\right)(1 + u^0_x)u^0_{xx} + \int E(y)(1 + u^1_y)u^1_{xy}dy = b(x)$$

From the microscale governing equation, we know that $u^1 = u^1\big(y, u^0_x\big)$, ie there is no explicit x dependence, but that the microscale displacement does implicitly depend on the macroscale through the macroscale displacement gradient. Thus, we have that

$$\frac{\partial^2 u^1}{\partial x \partial y} = \frac{\partial^2 u^1}{\partial y \partial u^0_x} u^0_{xx}$$

The macroscale governing equation becomes

$$\left(\int E(y)dy\right)(1 + u^0_x)u^0_{xx} + \left(\int E(y)(1 + u^1_y)\frac{\partial^2 u^1}{\partial y \partial u^0_x}dy\right)u^0_{xx} = b(x)$$

Perhaps it is simpler to write this as this way, which somewhat resembles the Navier equation and a homogenized tensor:

$$\left[\left(\int E(y)dy\right)(1 + u^0_x) + \left(\int E(y)(1 + u^1_y)\frac{\partial^2 u^1}{\partial y \partial u^0_x}dy\right)\right]u^0_{xx} = b(x)$$

The above is not the right way to go about the problem. Instead, we should write recognize that derivatives can be factored out and plan to integrate these by parts when weakening the problem. First, recognize that we can write

$$\bar{E}\frac{\partial}{\partial x}\left(u^0_x + \frac{1}{2}(u^0_x)^2\right) + \frac{\partial}{\partial x}\left(\int E(y)\left(u^1_y + \frac{1}{2}(u^1_y)^2\right)dy\right) = b(x)$$

Now we weaken the problem and integrate by parts (ignore sign on the body force for now). We will assume zero boundaries on the macroscale domain.

$$\int_{\Omega^x} \bar{E}\frac{\partial}{\partial x}\left(u_x^0 + \frac{1}{2}(u_x^0)^2\right)w_x dx + \int_{\Omega^x}\left(\int_{\Omega^y} E(y)\left(u_y^1 + \frac{1}{2}(u_y^1)^2\right)dy\right)w_x dx = \int_{\Omega^x} b(x) w dx$$

$$\int_{\Omega^y}\left[E(y)\left(u_y^1 + \frac{1}{2}(u_y^1)^2\right)\right]w_y dy = -\int_{\Omega^y}\left[E(y)\left(u_x^0 + \frac{1}{2}(u_x^0)^2\right)\right]w_y dy$$

These are the governing equations for the so-called "FE2" scheme of nonlinear multiscale problems. No homogenized material properties can be computed, rather boundary value problems on the microstructure need to be solved at every Newton iteration.

6 1D Isotropic Phase Field Model

In the strong form, the governing equations for the 1D phase field model are

$$\frac{\partial}{\partial x}\left(E(\phi - 1)^2\frac{\partial u}{\partial x}\right) + b = 0$$

$$(\phi - 1)E\left(\frac{\partial u}{\partial x}\right)^2 + \frac{G}{\ell}\phi - \frac{\partial}{\partial x}\left(G\ell\frac{\partial \phi}{\partial x}\right) = 0$$

We will try to use a multiscale expansion to arrive at multiscale phase field equations. Define y as the microscale variable and x as the macroscale variable. The superscript η indicates a multiscale quantity. Start with the stress equilibrium equation:

$$\frac{\partial}{\partial x^\eta}\left(E(y)(\phi^\eta - 1)^2\frac{\partial u^\eta}{\partial x^\eta}\right) + b = 0$$

The modulus only varies on the microscale. Use the following multiscale relations:

$$\frac{\partial}{\partial x^\eta} = \frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y}, \quad u^\eta = u^0(x) + \eta u^1(x,y), \quad \phi^\eta = \phi^0(x) + \eta\phi^1(x,y)$$

Plugging this into the equation for stress equilibrium, we get

$$\left(\frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y}\right)\left[E(y)\left((\phi^0)^2 + \eta^2(\phi^1)^2 + 1 + 2\eta\phi^0\phi^1 - 2\phi^0 - 2\eta\phi^1\right)\left(u_x^0 + \eta u_x^1 + u_y^1\right)\right] + b = 0$$

$$\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\Bigg[E(y)\Bigg(u_x^0(\phi^0)^2+\eta^2u_x^0(\phi^1)^2+u_x^0+2\eta u_x^0\phi^0\phi^1-2u_x^0\phi^0-2\eta u_x^0\phi^1$$
$$+\eta u_x^1(\phi^0)^2+\eta^3u_x^1(\phi^1)^2+\eta u_x^1+2\eta^2u_x^1\phi^0\phi^1-2\eta u_x^1\phi^0-2\eta^2u_x^1\phi^1$$
$$+u_y^1(\phi^0)^2+\eta^2u_y^1(\phi^1)^2+u_y^1+2\eta u_y^1\phi^0\phi^1-2u_y^1\phi^0-2\eta u_y^1\phi^1\Bigg)\Bigg]+b=0$$

Now group terms by orders of η:

$$\eta^{-1}:\quad \frac{\partial}{\partial y}\left(E(y)u_x^0(\phi^0)^2\right)+\frac{\partial}{\partial y}\left(E(y)u_x^0\right)-2\frac{\partial}{\partial y}\left(E(y)u_x^0\phi^0\right)$$
$$+\frac{\partial}{\partial y}\left(E(y)u_y^1(\phi^0)^2\right)+\frac{\partial}{\partial y}\left(E(y)u_y^1\right)-2\frac{\partial}{\partial y}\left(E(y)u_y^1\phi_0\right)$$

This can be written more compactly as

$$\frac{\partial}{\partial y}\left(E(y)(\phi^0-1)^2u_y^1\right)=-\frac{\partial}{\partial y}\left(E(y)(\phi^0-1)^2u_x^0\right)$$

This is the microscale stress equation. The microscale displacement is linear in the macroscopic strain but depends on the macroscopic damage. We can write

$$u^1(x,y)=\chi(\phi^0,y)\frac{\partial u^0}{\partial x}$$

where χ is the solution to the microscale stress problem at a given macroscopic damage level and for an applied unit strain. Note that the damage variable ϕ^0 is constant over the microstructure. Now turn the next order of η:

$$\eta^0:\quad \frac{\partial}{\partial x}\left(E(y)u_x^0(\phi^0)^2\right)+\frac{\partial}{\partial x}\left(E(y)u_x^0\right)+2\frac{\partial}{\partial y}\left(E(y)u_x^0\phi^0\phi^1\right)-2\frac{\partial}{\partial x}\left(E(y)u_x^0\phi^0\right)$$
$$-2\frac{\partial}{\partial y}\left(E(y)u_x^0\phi^1\right)+\frac{\partial}{\partial y}\left(E(y)u_x^1(\phi^0)^2\right)+\frac{\partial}{\partial y}\left(E(y)u_x^1\right)-2\frac{\partial}{\partial y}\left(E(y)u_x^1\phi^0\right)$$
$$+\frac{\partial}{\partial x}\left(E(y)u_y^1(\phi^0)^2\right)+\frac{\partial}{\partial x}\left(E(y)u_y^1\right)+2\frac{\partial}{\partial y}\left(E(y)u_y^1\phi^0\phi^1\right)-2\frac{\partial}{\partial x}\left(E(y)u_y^1\phi^0\right)-2\frac{\partial}{\partial y}\left(E(y)u_y^1\phi^1\right)$$

This can be written more compactly as

$$\frac{\partial}{\partial x}\left(E(y)(\phi^0-1)^2u_x^0\right)+\frac{\partial}{\partial y}\left(E(y)(\phi^0-1)^2u_x^1\right)+\frac{\partial}{\partial x}\left(E(y)(\phi_1^0)^2u_y^1\right)$$
$$+2\frac{\partial}{\partial y}\left(E(y)u_x^0\phi^1(\phi^0-1)\right)+2\frac{\partial}{\partial y}\left(E(y)u_y^1\phi^1(\phi^0-1)\right)$$

The macroscale equation cannot be satisfied pointwise, so we average over the microstructure. All terms involving y derivatives of periodic functions will vanish in the averaging operation. The functions $E(y)$, u^1,ϕ^1 and their products are periodic, but not their derivatives. The second and fourth terms drop out when averaged. The governing equation becomes

$$(\phi^0-1)^2\left(\int Edy\right)u_{xx}^0+\frac{\partial}{\partial x}\left((\phi^0-1)^2\int Eu_y^1dy\right)+2(\phi^0-1)\int\frac{\partial}{\partial y}(Eu_y^1\phi^1)dy+b=0$$

Now we can use the definition of the microscale displacement in terms of the macroscopic strain to write

$$(\phi^0-1)^2\left(\int Edy\right)u_{xx}^0+(\phi^0-1)^2u_{xx}^0\int E\frac{\partial\chi(\phi^0)}{\partial y}dy+2(\phi^0-1)u_x^0\int\frac{\partial}{\partial y}\left(E\frac{\partial\chi(\phi^0)}{\partial y}\phi^1\right)dy+b=0$$

For now, there are no further simplification that can be made. This is the governing equation for the macroscopic stress equilibrium with damage. Now we turn to the governing equation for the multiscale evolution of the phase field. We assume that like the moduluIs, the energy release rate varies over the microstructure.

$$(\phi^\eta-1)E(y)\left(\frac{\partial u^\eta}{\partial x^\eta}\right)^2+\frac{G(y)}{\ell}\phi^\eta-\frac{\partial}{\partial x^\eta}\left(G(y)\ell\frac{\partial\phi^\eta}{\partial x^\eta}\right)=0$$

$$=(\phi^0+\eta\phi^1-1)E(u_x^0+\eta u_x^1+u_y^1)^2+\frac{G}{\ell}(\phi^0+\eta\phi^1)-\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\left(G\ell\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)(\phi^0+\eta\phi^1)\right)$$

$$=E(y)(\phi^0+\eta\phi^1-1)\left((u_x^0)^2+\eta^2(u_x^1)^2+(u_y^1)^2+2u_x^0u_y^1+2\eta u_x^1u_x^0+2\eta u_x^1u_y^1\right)+\frac{G}{\ell}(\phi^0+\eta\phi^1)$$
$$-\left(\frac{\partial}{\partial x}+\frac{1}{\eta}\frac{\partial}{\partial y}\right)\left(G\ell(\phi_x^0+\eta\phi_x^1+\phi_y^1)\right)$$

We can group terms by powers of η to obtain two governing equations:

$$\eta^{-1}: \quad \frac{\partial}{\partial y}\left(G(y)\ell\phi_y^1\right) = -\frac{\partial}{\partial y}\left(G(y)\ell\phi_x^0\right)$$

The microscale equation for damage has a particularly simple from. The microscale damage is linear in the macroscale damage gradient. Thus, we can write

$$\phi^1(x, y) = \Pi(y)\frac{\partial\phi^0}{\partial x}$$

where Π is the damage response of the microstructure to a damage gradient of unit magnitude. Turning to the next order of η, we have

$$\eta^0: \quad E(\phi^0-1)\left((u_x^0)^2+(u_y^1)^2+2u_x^0u_y^1\right)+\frac{G}{\ell}\phi^0-\frac{\partial}{\partial x}\left(G\ell\phi_x^0\right)-\frac{\partial}{\partial x}\left(G\ell\phi_y^1\right)-\frac{\partial}{\partial y}\left(G\ell\phi_x^1\right)$$

This equation cannot be obeyed pointwise, thus we average over the microstructure.

$$(\phi^0-1)\left((u_x^0)^2\int Edy+\int E(u_y^1)^2dy+2u_x^0\int Eu_y^1dy\right)+\frac{\phi^]}{\ell}\int Gdy$$
$$-\ell\phi_{xx}^0\int Gdy-\ell\int G\phi_{xy}^1dy-\ell\int\frac{\partial}{\partial y}(G\phi_x^1)dy$$

Using the relationship between the macroscopic damage gradient and the microscale damage, this can be written as

$$(\phi^0-1)(u_x^0)^2\left(\int Edy+\int E\left(\frac{\partial\chi}{\partial y}\right)^2dy+2\int E\frac{\partial\chi}{\partial y}dy\right)+\frac{\phi^0}{\ell}\int Gdy$$
$$-\ell\phi_{xx}^0\int Gdy-\ell\int G\phi_{xy}^1dy-\ell\int\frac{\partial}{\partial y}(G\phi_x^1)dy$$

$$(\phi^0-1)(u_x^0)^2\left(\int Edy+\int E\left(\frac{\partial\chi}{\partial y}\right)^2dy+2\int E\frac{\partial\chi}{\partial y}dy\right)+\frac{\phi^0}{\ell}\int Gdy$$
$$-\ell\phi_{xx}^0\int Gdy-\ell\phi_{xx}^0\int G\frac{\partial\Pi}{\partial y}dy-\ell\phi_{xx}^0\int\frac{\partial}{\partial y}(G\Pi)dy$$

$$(\phi^0-1)(u_x^0)^2\left(\int Edy+\int E\left(\frac{\partial\chi}{\partial y}\right)^2dy+2\int E\frac{\partial\chi}{\partial y}dy\right)+\frac{\phi^0}{\ell}\int Gdy$$
$$-\ell\phi_{xx}^0\left(\int Gdy-\int G\frac{\partial\Pi}{\partial y}dy-\int\frac{\partial}{\partial y}(G\Pi)dy\right)=0$$

We can now summarize the governing equations for the problem. There are two microscale problems and two macroscale problems. The microscale problem for the elastic displacement is

$$\frac{\partial}{\partial y}\left(E(y)u_y^1\right) = -\frac{\partial}{\partial y}\left(E(y)u_x^0\right)$$

For whatever reason, there is no influence of the microscale damage on the microscale displacement equation. This equation is linear and is solved for unit strains to obtain $\chi(y)$. The microscale damage equation is

$$\frac{\partial}{\partial y}\left(G(y)\phi_y^1\right) = -\frac{\partial}{\partial y}\left(G(y)\phi_x^0\right)$$

This equation is solved for unit damage gradients to obtain $\Pi(y)$. The macroscale equation of elasticity is

$$(\phi^0-1)^2 u_{xx}^0\left(\int E\left(1+\frac{\partial\chi}{\partial y}\right)dy\right)+2(\phi^0-1)u_x^0\phi_x^0\int\frac{\partial}{\partial y}\left(E\frac{\partial\chi}{\partial y}\Pi\right)dy+b=0$$

The typical expression for the homogenized tensor is reproduced in the first term, but there is an additive correction which involves the microscale damage response and introduces a new coupling term of the damage and displacement gradients. The macroscale equation for the damage evolution is

$$(\phi^0-1)(u_x^0)^2\left(\int E\left(1+2\frac{\partial\chi}{\partial y}+\left(\frac{\partial\chi}{\partial y}\right)^2\right)dy\right)+\frac{\phi^0}{\ell}\int Gdy \\ -\ell\phi_{xx}^0\left(\int G\left(1+\frac{\partial\Pi}{\partial y}\right)dy\right)=0$$

We ignore the last term in the previous version of this equation because the microscale damage response and energy release rate are both periodic so the average of the derivative of their product is zero. The macroscale phase field equation has the same form as the single scale equation, but with different constitutive parameters. The macroscale displacement equation does not have the same form as the single scale case. Introducing notation for the homogenized constitutive parameters, these equations can be written as

$$(\phi^0-1)^2\bar{E}\frac{\partial^2 u^0}{\partial x^2}+2(\phi^0-1)J\frac{\partial u^0}{\partial x}\frac{\partial\phi^0}{\partial x}+b=0$$

$$(\phi^0-1)\bar{\bar{E}}\left(\frac{\partial u^0}{\partial x}\right)^2+\frac{\bar{G}}{\ell}\phi^0-\bar{\bar{G}}\ell\frac{\partial^2\phi^0}{\partial x^2}=0$$