Notes on Transformation Elasticity

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1 Inhomogeneous Elasticity Solver

Given an original supercell $\mathbf{x} = \mathbf{s}\mathbf{H}_0$, $\mathbf{s} \in [0, 1)$, we would like to solve the following problem:

$$F^{\mathrm{el}}[\mathbf{H}, \boldsymbol{\epsilon}^0(\mathbf{x})] \;\equiv\; \min_{\mathbf{u}(\mathbf{x})} F^{\mathrm{el}}[\mathbf{u}(\mathbf{x})|\mathbf{H}, \boldsymbol{\epsilon}^0(\mathbf{x})] \tag{1}$$

$$F^{\mathrm{el}}[\mathbf{u}(\mathbf{x})|\mathbf{H}, \boldsymbol{\epsilon}^0(\mathbf{x})] \equiv \frac{1}{2}\int d^3\mathbf{x} c_{ijpq}(\mathbf{x})(\epsilon_{ij}(\mathbf{x}) - \epsilon^0_{ij}(\mathbf{x}))(\epsilon_{pq}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x})) \tag{2}$$

where $\mathbf{u}(\mathbf{x}) \equiv \mathbf{x}' - \mathbf{x}$, the difference between the new position $\mathbf{x}'$ and the old position $\mathbf{x}$, and

$$\epsilon_{ij}(\mathbf{x}) \;\equiv\; \frac{u_{i,j} + u_{j,i}}{2}. \tag{3}$$

$\mathbf{H}$ is the new supercell: $\mathbf{H} = \mathbf{H}_0(\mathbf{I} + \bar{\boldsymbol{\epsilon}})$. Global rotation of $\mathbf{H}$ does not matter anyhow to (2) to first order in the global rotation angle, and is therefore ignored in this leading-order theory. Note that the untransformed material in $\mathbf{H}_0$ does not have to be stress free. The entire role of $\mathbf{H}_0$ in the above is to provide a reference grid.

(2) is motivated by the following idea experiment. One first cuts up the *untransformed supercell* $\mathbf{H}_0$ into many blocks $d^3\mathbf{x}$. Then imagine for instance the temperature is raised, and phase transformation / plasticity may induce some blocks to transform to a new state. Each block, if left alone (stress free), would like to transform to a new strain state $\boldsymbol{\epsilon}^0(\mathbf{x})$. Additional local rotation $\mathbf{R}(\mathbf{x})$ of the block does not matter to the internal Helmholtz free energy of *this* block [1, 2], but needs to be globally optimized since $\mathbf{R}(\mathbf{x})$ must be globally consistent with $\mathbf{u}(\mathbf{x})$.

Because of the periodic boundary condition, there must be

$$\mathbf{u}(\mathbf{x} + \mathbf{h}_0) - \mathbf{u}(\mathbf{x}) \;=\; \mathbf{h}_0\bar{\boldsymbol{\epsilon}} \tag{4}$$

where $\mathbf{h}_0$ is one of the $\mathbf{H}_0$ edge vectors. So

$$\int_0^{\mathbf{h}_0} d\mathbf{x}' \cdot \frac{d\mathbf{u}(\mathbf{x} + \mathbf{x}')}{d\mathbf{x}'} \;=\; \mathbf{h}_0\bar{\boldsymbol{\epsilon}} \;\;\rightarrow\;\; \int d^3\mathbf{x}\frac{d\mathbf{u}}{d\mathbf{x}} = \det|\mathbf{H}_0|\bar{\boldsymbol{\epsilon}}. \tag{5}$$

Note that $\{\epsilon_{ij}(\mathbf{x})\}$, because of (3), need to satisfy three compatibility constraints

$$\epsilon_{ii,jj} + \epsilon_{jj,ii} \; = \; 2\epsilon_{ij,ij}, \quad \forall i \neq j \tag{6}$$

which means the $\{\epsilon_{ij}(\mathbf{x})\}$ fields are not independent fields in the variational functional (the $\{u_i(\mathbf{x})\}$ fields are). On the other hand, there is no compatibility constraint [3] on the stress-free strain fields $\{\epsilon^0_{ij}(\mathbf{x})\}$, which are "given" in the elastic constant minimization problem.

The functional to be minimized in (2) represents a quadratic expansion approximation of the Helmholtz free energy [2] around the *freely transformed* block. As such, there should be a conversion factor $\det|d^3\mathbf{x}'|/\det|d^3\mathbf{x}|$ as well as tensor rotation using $\mathbf{R}(\mathbf{x})$ to convert the isothermal elastic constant of the transformed material to $c_{ijpq}(\mathbf{x})$, which is based on the original volume and observation coordinates. However, this effect is higher order, same as the higher-order terms ignored in (3).

Unlike the more general nonlinear formulation of [3], the merit of the quadratic expansion is that (2) is quadratic in $\mathbf{u}(\mathbf{x})$, whose minimization (in principle at least) entertains a close-formed solution in the form of a matrix inverse, after real-space discretization of $\mathbf{u}(\mathbf{x})$ and representation of ∇^2-like operators. We have the stress equilibrium equation in structurally inhomogeneous and elastically inhomogeneous material:

$$(c_{ijpq}(\mathbf{x})(u_{p,q}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x})))_{,j} \; = \; 0, \quad \forall i = 1..3 \tag{7}$$

1.1 Homogeneous Special Case

If the system is elastically homogeneous [4], $c_{ijpq}(\mathbf{x}) = c^0_{ijpq}$, there is translational symmetry in the problem:

$$c^0_{ijpq}(u_{p,q}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x}))_{,j} \; = \; 0, \quad \forall i = 1..3 \tag{8}$$

and the inverse can be done in the Fourier space on a $\mathbf{k}$-by-$\mathbf{k}$ basis. We first note that $u_p(\mathbf{x})$ can be decomposed into a secularly growing component in $\mathbf{x}$, plus a periodic component:

$$u_p(\mathbf{x}) \; \equiv \; \mathbf{x}\bar{\boldsymbol{\epsilon}} + \tilde{u}_p(\mathbf{x}) \tag{9}$$

Then stress equilibrium requires that in $\mathbf{k}$-space:

$$-\, c^0_{ijpq} k_q k_j \tilde{u}_p(\mathbf{k}) \; = \; i c^0_{ijpq} \epsilon^0_{pq}(\mathbf{k}) k_j \tag{10}$$

where

$$\tilde{u}_p(\mathbf{k}) \equiv \int d^3\mathbf{x}\tilde{u}_p(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}, \quad \tilde{u}_p(\mathbf{x}) = \frac{1}{\det|\mathbf{H}_0|}\sum_{\mathbf{k}}\tilde{u}_p(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{11}$$

and similarly $\epsilon^0_{pq}(\mathbf{k}) \leftrightarrow \epsilon^0_{pq}(\mathbf{x})$. If we define symmetric matrix $\mathbf{C}(\hat{\mathbf{k}})$ [4]

$$C_{ip}(\hat{\mathbf{k}}) \equiv c^0_{ijpq}\hat{k}_q\hat{k}_j, \quad \hat{\mathbf{k}} \equiv \frac{\mathbf{k}}{|\mathbf{k}|}, \tag{12}$$

the inverse matrix is also real and symmetric: $\mathbf{\Omega}(\hat{\mathbf{k}}) \equiv \mathbf{C}^{-1}(\hat{\mathbf{k}})$. Let us also define strain-free stress:

$$\sigma^0_{ij}(\mathbf{x}) \equiv c^0_{ijpq}\epsilon^0_{pq}(\mathbf{x}), \quad \sigma^0_{ij}(\mathbf{k}) \equiv c^0_{ijpq}\epsilon^0_{pq}(\mathbf{k}), \tag{13}$$

then

$$-|\mathbf{k}|^2 C_{ip}(\hat{\mathbf{k}})\tilde{u}_p(\mathbf{k}) = i\sigma^0_{ij}(\mathbf{k})k_j \tag{14}$$

and $\tilde{u}_p(\mathbf{k})$ is obtained explicitly as

$$\tilde{u}_p(\mathbf{k}) = \frac{\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})k_{j'}}{i|\mathbf{k}|^2}. \tag{15}$$

Since $i\sigma^0_{ij}(\mathbf{k})k_j$ represents the divergence of stress, or net force, $-\frac{\Omega_{pi}(\hat{\mathbf{k}})}{|\mathbf{k}|^2}$ is just the infinite-space Green's function relating force to displacement in this translationally invariant system. This Green's function is short-ranged in reciprocal space (in fact $\mathbf{k}$-by-$\mathbf{k}$ local), but long-ranged in real space. Thus it is advantageous to solve homogeneous-material problems in reciprocal space, which is more generally called the spectral method.

The strain field that corresponds to the (15) displacement field is

$$\tilde{\epsilon}_{pq}(\mathbf{k}) = \frac{ik_q\tilde{u}_p(\mathbf{k}) + ik_p\tilde{u}_q(\mathbf{k})}{2} = \frac{\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_q + \Omega_{qi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_p}{2}, \tag{16}$$

$$\epsilon_{pq}(\mathbf{x}) = \bar{\epsilon}_{pq} + \tilde{\epsilon}_{pq}(\mathbf{x}), \quad \int d^3\mathbf{x}\tilde{\epsilon}_{pq}(\mathbf{x}) = 0. \tag{17}$$

The rotation field $\mathbf{R}(\mathbf{x}) = \mathbf{I} + \mathbf{W}(\mathbf{x})$ that corresponds to (15) displacement field is

$$W_{pq}(\mathbf{k}) = \frac{\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_q - \Omega_{qi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_p}{2}. \tag{18}$$

The stress field is

$$\sigma_{ij}(\mathbf{x}) = \quad c^0_{ijpq}\bar{\epsilon}_{pq} + c^0_{ijpq}\tilde{\epsilon}_{pq}(\mathbf{x}) - \sigma^0_{ij}(\mathbf{x}) \tag{19}$$

$$\begin{aligned}
\sigma_{ij}(\mathbf{k}) = & \quad \det|\mathbf{H}_0| c^0_{ijpq}\bar{\epsilon}_{pq}\delta_{\mathbf{k}} + c^0_{ijpq}\tilde{\epsilon}_{pq}(\mathbf{k}) - \sigma^0_{ij}(\mathbf{k}) \qquad (20)\\
= & \quad \det|\mathbf{H}_0| c^0_{ijpq}\bar{\epsilon}_{pq}\delta_{\mathbf{k}} + \frac{c^0_{ijpq}\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_q + c^0_{ijpq}\Omega_{qi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_p}{2} - \sigma^0_{ij}(\mathbf{k})
\end{aligned}$$

We see that the $\sigma_{ij}(\mathbf{k})$ solution above satisfy stress equilibrium:

$$\begin{aligned}
\sigma_{ij}(\mathbf{k})k_j = & \quad |\mathbf{k}|\frac{c^0_{ijpq}\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_q\hat{k}_j + c^0_{ijpq}\Omega_{qi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_p\hat{k}_j}{2} - |\mathbf{k}|\sigma^0_{ij}(\mathbf{k})\hat{k}_j\\
= & \quad |\mathbf{k}|\frac{C_{ip}(\hat{\mathbf{k}})\Omega_{pi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'} + C_{iq}(\hat{\mathbf{k}})\Omega_{qi'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}}{2} - |\mathbf{k}|\sigma^0_{ij}(\mathbf{k})\hat{k}_j\\
= & \quad |\mathbf{k}|\frac{\delta_{ii'}\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'} + \delta_{ii'}\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}}{2} - |\mathbf{k}|\sigma^0_{ij}(\mathbf{k})\hat{k}_j\\
= & \quad 0. \qquad (21)
\end{aligned}$$

(2) is then relaxed to be:

$$\begin{aligned}
F^{\mathrm{el}}[\mathbf{H}, \boldsymbol{\epsilon}^0(\mathbf{x})] = & \quad \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\epsilon^0_{pq}(\mathbf{x}) - \int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\epsilon_{pq}(\mathbf{x}) + \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\epsilon_{ij}(\mathbf{x})\epsilon_{pq}(\mathbf{x})\\
= & \quad \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\epsilon^0_{pq}(\mathbf{x}) - \int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\bar{\epsilon}_{pq} + \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\bar{\epsilon}_{ij}\bar{\epsilon}_{pq}\\
- & \quad \int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\tilde{\epsilon}_{pq}(\mathbf{x}) + \int \frac{d^3\mathbf{x}}{2} c^0_{p'q'pq}\tilde{\epsilon}_{p'q'}(\mathbf{x})\tilde{\epsilon}_{pq}(\mathbf{x})\\
= & \quad \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\epsilon^0_{pq}(\mathbf{x}) - \bar{\epsilon}_{pq}\int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x}) + \frac{\det|\mathbf{H}_0|}{2} c^0_{ijpq}\bar{\epsilon}_{ij}\bar{\epsilon}_{pq}\\
- & \quad \frac{1}{\det|\mathbf{H}_0|}\sum_{\mathbf{k}} \sigma^0_{pq}(\mathbf{k})\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j\hat{k}_q\\
+ & \quad \frac{1}{2\det|\mathbf{H}_0|}\sum_{\mathbf{k}} c^0_{p'q'pq}\Omega_{p'i'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_{q'}\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j\hat{k}_q \qquad (22)
\end{aligned}$$

where we have used the property: $\sigma_{pq}(-\mathbf{k}) = \sigma^*_{pq}(\mathbf{k})$ for real $\sigma_{pq}(\mathbf{x})$ field.

But

$$
\begin{aligned}
c^0_{p'q'pq}\Omega_{p'i'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\hat{k}_{q'}\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j\hat{k}_q = \quad & C_{p'p}(\hat{\mathbf{k}})\Omega_{p'i'}(\hat{\mathbf{k}})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j \\
= \quad & \delta_{i'p}\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j \\
= \quad & \sigma^0_{pj'}(\mathbf{k})\hat{k}_{j'}\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j \\
= \quad & \hat{k}_{j'}\sigma^0_{j'p}(\mathbf{k})\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j. \qquad (23)
\end{aligned}
$$

So the final relaxed elastic energy [4] is

$$
\begin{aligned}
F^{\mathrm{el}}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})] = \quad & \int \frac{d^3\mathbf{x}}{2} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x})\epsilon^0_{pq}(\mathbf{x}) - \bar{\epsilon}_{pq}\int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{ij}(\mathbf{x}) + \frac{\det|\mathbf{H}_0|}{2} c^0_{ijpq}\bar{\epsilon}_{ij}\bar{\epsilon}_{pq} \\
- \quad & \frac{1}{2\det|\mathbf{H}_0|}\sum_{\mathbf{k}} \hat{k}_q\sigma^0_{qp}(\mathbf{k})\Omega_{pi}(\hat{\mathbf{k}})\sigma^{0*}_{ij}(\mathbf{k})\hat{k}_j, \qquad (24)
\end{aligned}
$$

the last term being the non-affine relaxation energy.

The supercell stress $\bar{\boldsymbol{\sigma}}$ is

$$
\begin{aligned}
\bar{\sigma}_{ij} \equiv \quad & \frac{1}{\det|\mathbf{H}_0|}\left.\frac{\partial F^{\mathrm{el}}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})]}{\partial \bar{\epsilon}_{ij}}\right|_{\boldsymbol{\epsilon}^0(\mathbf{x})} \\
= \quad & c^0_{ijpq}\bar{\epsilon}_{pq} - \frac{1}{\det|\mathbf{H}_0|}\int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{pq}(\mathbf{x}) \\
= \quad & \frac{1}{\det|\mathbf{H}_0|}\int d^3\mathbf{x} c^0_{ijpq}\epsilon_{pq}(\mathbf{x}) - \frac{1}{\det|\mathbf{H}_0|}\int d^3\mathbf{x} c^0_{ijpq}\epsilon^0_{pq}(\mathbf{x}) \\
= \quad & \frac{1}{\det|\mathbf{H}_0|}\int d^3\mathbf{x}\sigma_{ij}(\mathbf{x}), \qquad (25)
\end{aligned}
$$

which is physically intuitive.

1.2 General Solver

Wang, Jin and Khachaturyan (WJK) proposed an iterative solver to (7) based on an operator splitting technique. The idea is one wants to avoid direct handling of $\mathbf{u}(\mathbf{x})$, and real-space representations of ∇^2-like operators, as in the usual finite-difference scheme. The finite-difference or finite-element schemes are philosophically similar to atomistic simulations. It is known that solving elasticity problems in real space often have slow convergence. In the WJK treatment, the section 1.1 solver is used as a "pre-conditioner". If the system is close to an elastically homogeneous state, the inhomogeneity can be regarded as a perturbation and convergence should be fast.

The key idea in [4] is the introduction of a reference homogeneous system c°_{ijpq}, which has the same displacement field $\mathbf{u}(\mathbf{x})$, strain field $\boldsymbol{\epsilon}(\mathbf{x})$ and stress field $\boldsymbol{\sigma}(\mathbf{x})$ as the real inhomogeneous system. This can always be done by tuning the virtual stress-free strain field $\epsilon^\circ_{pq}(\mathbf{x})$:

$$c_{ijpq}(\mathbf{x})(u_{p,q}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x})) \;=\; c^\circ_{ijpq}(u_{p,q}(\mathbf{x}) - \epsilon^\circ_{pq}(\mathbf{x})) \tag{26}$$

where there are as many equations (stress components) as unknowns (stress-free strain components, which do not need to satisfy compatibility [3]), and have unique solution for positive definite c°_{ijpq}. So there is one-to-one mapping between a given inhomogeneous system to a virtual homogeneous system, and vice versa, similar to the mapping from interacting-electrons system to fictitious non-interacting-electrons system in density functional theory (DFT) [5]. In hindsight, the success of the Kohn-Sham treatment of DFT and associated planewave solvers (in contrast to older Thomas-Fermi treatment, which forced to be completely local) largely originated from the splitting of the kinetic energy ∇^2 operator which has nonlocal effects, such as boundary sensitivity, from the total energy, Eq. (2) in [5]. The remainder part, defined as exchange-correlation energy, is more local. The WJK treatment which takes advantage of planewave solver for virtual homogeneous system is philosophically quite similar to the Kohn-Sham treatment.

Suppose *we know* what $\boldsymbol{\epsilon}^\circ(\mathbf{x})$ should be used, it is easy to obtain $\mathbf{u}(\mathbf{x})$, $\boldsymbol{\epsilon}(\mathbf{x})$ and $\boldsymbol{\sigma}(\mathbf{x})$ based on section 1.1 nonlocal planewave solver:

$$\boldsymbol{\epsilon}^\circ(\mathbf{x}) \;\rightarrow\; \mathbf{u}(\mathbf{x}), \boldsymbol{\epsilon}(\mathbf{x}), \boldsymbol{\sigma}(\mathbf{x}). \tag{27}$$

This set of $\boldsymbol{\epsilon}(\mathbf{x}), \boldsymbol{\sigma}(\mathbf{x})$ is supposed to be identical as that of the inhomogeneous system. But, is is true? We can plug into (26) *locally* and check:

$$c^\circ_{ijpq}\epsilon^\circ_{pq}(\mathbf{x}) \;=\; c_{ijpq}(\mathbf{x})\epsilon^0_{pq}(\mathbf{x}) + (c^\circ_{ijpq} - c_{ijpq}(\mathbf{x}))\epsilon_{pq}(\mathbf{x}). \tag{28}$$

The above should be satisfied exactly if we have an exact guess for $\boldsymbol{\epsilon}^\circ(\mathbf{x})$. But if our guess of $\boldsymbol{\epsilon}^\circ(\mathbf{x})$ contains some error, the LHS will not be exactly the same as the RHS. But then we can invert the RHS to update the guess $\epsilon^\circ_{pq}(\mathbf{x})$, and repeat the process until convergence is reached.

When convergence is reached, we have from (2)

$$
\begin{aligned}
F^{\mathrm{el}}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})] = & \quad \frac{1}{2} \int d^3\mathbf{x} \sigma_{pq}(\mathbf{x})(\epsilon_{pq}(\mathbf{x}) - \epsilon^{\circ}_{pq}(\mathbf{x}) + \epsilon^{\circ}_{pq}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x})) \\
= & \quad F^{\mathrm{el}\circ}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^{\circ}(\mathbf{x})] + \int \frac{d^3\mathbf{x}}{2} \sigma_{pq}(\mathbf{x})(\epsilon^{\circ}_{pq}(\mathbf{x}) - \epsilon^0_{pq}(\mathbf{x})).
\end{aligned}
\tag{29}
$$

So the mapping of energy needs a correction.

The supercell stress $\bar{\boldsymbol{\sigma}}$ is

$$
\begin{aligned}
\bar{\sigma}_{ij} \equiv & \quad \frac{1}{\det|\mathbf{H}_0|} \left. \frac{\partial F^{\mathrm{el}}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})]}{\partial \bar{\epsilon}_{ij}} \right|_{\boldsymbol{\epsilon}^0(\mathbf{x})} \\
= & \quad \frac{1}{\det|\mathbf{H}_0|} \left. \frac{\partial F^{\mathrm{el}\circ}[\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})]}{\partial \bar{\epsilon}_{ij}} \right|_{\boldsymbol{\epsilon}^0(\mathbf{x})}.
\end{aligned}
\tag{30}
$$

The reason is that in (29), the value of F^{el} obviously depends parametrically on $\boldsymbol{\epsilon}^{\circ}(\mathbf{x})$, and with change in $\bar{\boldsymbol{\epsilon}}$ there will be associated $\delta\boldsymbol{\epsilon}^{\circ}(\mathbf{x})$. However,

$$
\frac{\delta F^{\mathrm{el}}[\boldsymbol{\epsilon}^{\circ}(\mathbf{x})|\bar{\boldsymbol{\epsilon}}, \boldsymbol{\epsilon}^0(\mathbf{x})]}{\delta \boldsymbol{\epsilon}^{\circ}(\mathbf{x})} = 0 \tag{31}
$$

so (25) can still be used, which is physically intuitive.

1.3 3D Isotropic Media

A 3D isotropic medium has

$$
c_{ijpq} = \lambda \delta_{ij} \delta_{pq} + \mu(\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp}). \tag{32}
$$

The relationship between the Lamé parameters λ, μ and E, ν are:

$$
\lambda = \frac{2\nu\mu}{1-2\nu} = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}, \tag{33}
$$

and the relationship between stress and strain is:

$$
\sigma^0_{ij}(\mathbf{k}) = (\lambda \epsilon^0_{pp}(\mathbf{k}))\delta_{ij} + 2\mu\epsilon^0_{ij}(\mathbf{k}), \quad \sigma^0_{ij}(\mathbf{x}) = (\lambda \epsilon^0_{pp}(\mathbf{x}))\delta_{ij} + 2\mu\epsilon^0_{ij}(\mathbf{x}). \tag{34}
$$

Then (12) becomes:

$$C_{ip}(\hat{\mathbf{k}}) = c_{ijpq}\hat{k}_j\hat{k}_q = \lambda\hat{k}_i\hat{k}_p + \mu\delta_{ip} + \mu\hat{k}_p\hat{k}_i = \mu\delta_{ip} + (\lambda+\mu)\hat{k}_i\hat{k}_p \tag{35}$$

or

$$\mathbf{C}(\hat{\mathbf{k}}) \;=\; \mu\mathbf{I} + (\lambda+\mu)\hat{\mathbf{K}} \tag{36}$$

with $K_{ip} \equiv \hat{k}_i\hat{k}_p$. The $\hat{\mathbf{K}}$ matrix is real and symmetric. It is also idempotent: $\hat{\mathbf{K}}^n = \hat{\mathbf{K}}$.

The inversion of $\mathbf{C}(\hat{\mathbf{k}})$ can be done by matrix series expansion:

$$\boldsymbol{\Omega}(\hat{\mathbf{k}}) \;=\; \frac{1}{\mu}\sum_{n=0}^{\infty}(-\frac{\lambda+\mu}{\mu})^n\hat{\mathbf{K}}^n = \frac{1}{\mu}(\mathbf{I} - \frac{\lambda+\mu}{\mu}\frac{\hat{\mathbf{K}}}{1+\frac{\lambda+\mu}{\mu}}) = \frac{1}{\mu}(\mathbf{I} - \frac{\lambda+\mu}{\lambda+2\mu}\hat{\mathbf{K}}). \tag{37}$$

Define dimensionless quantity

$$\alpha \;\equiv\; \frac{\lambda+\mu}{\lambda+2\mu} = \frac{1}{2(1-\nu)}, \tag{38}$$

we then have $\boldsymbol{\Omega}(\hat{\mathbf{k}}) = (\mathbf{I} - \alpha\hat{\mathbf{K}})/\mu$.

So (15) would become

$$\tilde{u}_p(\mathbf{k}) \;=\; \frac{(\delta_{pi'} - \alpha\hat{k}_p\hat{k}_{i'})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}}{\mu i|\mathbf{k}|} = \frac{\sigma^0_{pj'}(\mathbf{k})\hat{k}_{j'} - \alpha\hat{k}_p\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{i'}\hat{k}_{j'}}{\mu i|\mathbf{k}|}. \tag{39}$$

Define vector and scalar

$$\mathbf{f}(\mathbf{k}) \;\equiv\; \boldsymbol{\sigma}^0(\mathbf{k})\cdot\hat{\mathbf{k}}, \quad g(\mathbf{k}) \;\equiv\; \hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}), \tag{40}$$

which can be pre-computed, we then have

$$\tilde{\mathbf{u}}(\mathbf{k}) \;=\; \frac{\mathbf{f}(\mathbf{k}) - \alpha g(\mathbf{k})\hat{\mathbf{k}}}{\mu i|\mathbf{k}|}. \tag{41}$$

The periodic part of the strain field is then

$$\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) \;=\; \frac{i\tilde{\mathbf{u}}(\mathbf{k})\mathbf{k} + i\mathbf{k}\tilde{\mathbf{u}}(\mathbf{k})}{2} \;=\; \frac{\mathbf{f}(\mathbf{k})\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) - 2\alpha g(\mathbf{k})\hat{\mathbf{K}}}{2\mu}, \tag{42}$$

with $\mathrm{tr}(\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}) = \mathrm{tr}(\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})) = \hat{\mathbf{k}} \cdot \mathbf{f}(\mathbf{k}) = g(\mathbf{k})$, $\mathrm{tr}(\tilde{\boldsymbol{\epsilon}}(\mathbf{k})) = (1-\alpha)g(\mathbf{k})/\mu$, and

$$\boldsymbol{\epsilon}(\mathbf{x}) \;=\; \bar{\boldsymbol{\epsilon}} + \tilde{\boldsymbol{\epsilon}}(\mathbf{x}), \qquad \int d^3\mathbf{x}\tilde{\boldsymbol{\epsilon}}(\mathbf{x}) = 0. \tag{43}$$

The rotation field $\mathbf{R}(\mathbf{x}) = \mathbf{I} + \mathbf{W}(\mathbf{x})$ field is

$$\mathbf{W}(\mathbf{k}) \;=\; \frac{\mathbf{f}(\mathbf{k})\hat{\mathbf{k}} - \hat{\mathbf{k}}\mathbf{f}(\mathbf{k})}{2\mu}. \tag{44}$$

The $c^0_{ijpq}\tilde{\epsilon}_{pq}(\mathbf{k})$ stress component in (20) is simplified to be

$$\begin{aligned}\lambda\mathrm{tr}(\tilde{\boldsymbol{\epsilon}}(\mathbf{k}))\mathbf{I} + 2\mu\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) = &\quad \frac{\lambda(1-\alpha)g(\mathbf{k})}{\mu}\mathbf{I} + \mathbf{f}(\mathbf{k})\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) - 2\alpha g(\mathbf{k})\hat{\mathbf{K}} \\ = &\quad \beta g(\mathbf{k})\mathbf{I} + \mathbf{f}(\mathbf{k})\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) - 2\alpha g(\mathbf{k})\hat{\mathbf{K}}\end{aligned} \tag{45}$$

where

$$\beta \;\equiv\; \frac{\lambda(1-\alpha)}{\mu} = \frac{\nu}{1-\nu} \tag{46}$$

so

$$\boldsymbol{\sigma}(\mathbf{k}) = \quad \det|\mathbf{H}_0| c^0_{ijpq}\bar{\epsilon}_{pq}\delta_{\mathbf{k}} + \mathbf{f}(\mathbf{k})\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) + \frac{\nu\mathbf{I} - \hat{\mathbf{K}}}{1-\nu}g(\mathbf{k}) - \sigma^0_{ij}(\mathbf{k}). \tag{47}$$

In the real-space inversion of (28):

$$c^{\circ}_{ijpq}\epsilon^{\circ}_{pq}(\mathbf{x}) \;=\; \tau_{ij}(\mathbf{x}), \qquad \lambda\mathrm{tr}(\boldsymbol{\epsilon}^{\circ})\mathbf{I} + 2\mu\boldsymbol{\epsilon}^{\circ} \;=\; \boldsymbol{\tau}, \tag{48}$$

we note that

$$3\lambda\mathrm{tr}(\boldsymbol{\epsilon}^{\circ}) + 2\mu\mathrm{tr}(\boldsymbol{\epsilon}^{\circ}) \;=\; \mathrm{tr}(\boldsymbol{\tau}), \qquad \mathrm{tr}(\boldsymbol{\epsilon}^{\circ}) \;=\; \frac{\mathrm{tr}(\boldsymbol{\tau})}{3\lambda + 2\mu}, \tag{49}$$

so

$$\boldsymbol{\epsilon}^{\circ} \;=\; \frac{\boldsymbol{\tau}}{2\mu} - \frac{\lambda}{2\mu}\frac{\mathrm{tr}(\boldsymbol{\tau})}{3\lambda + 2\mu}\mathbf{I}. \tag{50}$$

1.3.1 Sanity Check 1

To perform a sanity check, consider:

$$\nu^{\circ} = 0, \;\; \lambda^{\circ} = 0, \;\; \alpha^{\circ} = \frac{1}{2}, \;\; \beta^{\circ} = 0 \tag{51}$$

In this case

$$\boldsymbol{\sigma}^\circ(\mathbf{x}) \;=\; 2\mu\tilde{\boldsymbol{\epsilon}}^\circ(\mathbf{x}). \tag{52}$$

One requires:

$$\nabla\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{x}) \;=\; \nabla\cdot\boldsymbol{\sigma}^\circ(\mathbf{x}) \tag{53}$$

or

$$i\mathbf{k}\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{k}) \;=\; i\mathbf{k}\cdot\boldsymbol{\sigma}^\circ(\mathbf{k}) = i|\mathbf{k}|(\hat{\mathbf{k}}\cdot\boldsymbol{\sigma}^\circ(\mathbf{k})) \equiv i|\mathbf{k}|\mathbf{f}(\mathbf{k}) \tag{54}$$

But

$$i\mathbf{k}\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{k}) = i|\mathbf{k}|2\mu\hat{\mathbf{k}}\cdot\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) = i|\mathbf{k}|\mu\hat{\mathbf{k}}\cdot(i\mathbf{k}\tilde{\mathbf{u}}(\mathbf{k}) + i\tilde{\mathbf{u}}(\mathbf{k})\mathbf{k}), \tag{55}$$

so

$$\tilde{\mathbf{u}}(\mathbf{k}) + (\hat{\mathbf{k}}\cdot\tilde{\mathbf{u}}(\mathbf{k}))\hat{\mathbf{k}} \;=\; \frac{\mathbf{f}(\mathbf{k})}{i|\mathbf{k}|\mu} \tag{56}$$

$$2\hat{\mathbf{k}}\cdot\tilde{\mathbf{u}}(\mathbf{k}) \;=\; \frac{\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k})}{i|\mathbf{k}|\mu} \tag{57}$$

$$\tilde{\mathbf{u}}(\mathbf{k}) \;=\; \frac{\mathbf{f}(\mathbf{k})}{i|\mathbf{k}|\mu} - \frac{(\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}}}{2i|\mathbf{k}|\mu} \tag{58}$$

$$\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) \;=\; \frac{1}{2}\left(\frac{\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})}{\mu} - \frac{\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}}}{2\mu} + \frac{\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}}{\mu} - \frac{\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}}}{2\mu}\right) \;=\; \frac{\hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) + \mathbf{f}(\mathbf{k})\hat{\mathbf{k}} - (\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}}\hat{\mathbf{k}}}{2\mu} \tag{59}$$

so

$$\tilde{\boldsymbol{\sigma}}(\mathbf{k}) \;=\; \hat{\mathbf{k}}\mathbf{f}(\mathbf{k}) + \mathbf{f}(\mathbf{k})\hat{\mathbf{k}} - (\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}}\hat{\mathbf{k}} \tag{60}$$

It's clear that

$$\hat{\mathbf{k}}\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{k}) \;=\; \mathbf{f}(\mathbf{k}) + (\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))\hat{\mathbf{k}} - (\hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}))(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}})\hat{\mathbf{k}} \;=\; \mathbf{f}(\mathbf{k}) \tag{61}$$

which satisfies the stress equilibrium condition.

1.3.2 Sanity Check 2: Green's function

Imagine a point force $\mathbf{F}$ at $\mathbf{x}=0$, compensated by a uniform $-\mathbf{F}$ (jellium) spread over the entire supercell. When one performs Fourier transform on this external force field $\mathbf{F}\delta(\mathbf{x}) - \mathbf{F}/\det|\mathbf{H}_0|$, all finite-$\mathbf{k}$ Fourier component are $\mathbf{F}$, while the $\mathbf{k}=0$ component is 0. We can identify $-i|\mathbf{k}|\mathbf{f}(\mathbf{k})$ in (54) with $\mathbf{F}$, in which case

$$\mathbf{f}(\mathbf{k}) \;=\; \frac{i\mathbf{F}}{|\mathbf{k}|}, \quad g(\mathbf{k}) = \hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}) = \frac{i\hat{\mathbf{k}}\cdot\mathbf{F}}{|\mathbf{k}|}. \tag{62}$$

The displacement, according to (41), should be

$$\tilde{\mathbf{u}}(\mathbf{k}) \;=\; \frac{\mathbf{F}-\alpha(\hat{\mathbf{k}}\cdot\mathbf{F})\hat{\mathbf{k}}}{\mu|\mathbf{k}|^2}. \tag{63}$$

Consider a problem

$$\nabla^2\phi_{\mathrm{G}}(\mathbf{x}) \;=\; \frac{4\pi}{\det|\mathbf{H}_0|} - 4\pi\delta(\mathbf{x}), \tag{64}$$

from electrostatics point-charge solution we know that near $\mathbf{x}=0$, $\phi_{\mathrm{G}}(\mathbf{x})$ should behave as $\frac{1}{|\mathbf{x}|}$. On the other hand, if we do Fourier transform in the supercell, we will have

$$-|\mathbf{k}|^2\phi_{\mathrm{G}}(\mathbf{k}) \;=\; -4\pi, \quad \forall\mathbf{k}\neq 0. \tag{65}$$

Thus $4\pi|\mathbf{k}|^{-2}$ is the Fourier transform of $\phi_{\mathrm{G}}(\mathbf{x})\approx\frac{1}{|\mathbf{x}|}$. Furthermore, suppose

$$\nabla^2\psi_{\mathrm{G}}(\mathbf{x}) \;\equiv\; 2\phi_{\mathrm{G}}(\mathbf{x}) \tag{66}$$

from real space we see that $\psi_{\mathrm{G}}(\mathbf{x})\approx|\mathbf{x}|$ would work well near $\mathbf{x}=0$. Thus,

$$\psi_{\mathrm{G}}(\mathbf{k}) \;=\; -\frac{2\phi_{\mathrm{G}}(\mathbf{k})}{|\mathbf{k}|^2} = -\frac{8\pi}{|\mathbf{k}|^4}, \tag{67}$$

and so the real-space correspondent to $-\frac{k_ik_j}{|\mathbf{k}|^4}$ would be $\partial_i\partial_j(-\psi_{\mathrm{G}}(\mathbf{x})/8\pi) = -\partial_i\partial_j\frac{|\mathbf{x}|}{8\pi}$. Thus, the real-space displacement near the origin (or anywhere, with $\mathbf{H}_0\to\infty$) is

$$\mathbf{u}_{\mathrm{G}}(\mathbf{x}) \;=\; \frac{\mathbf{F}\phi_{\mathrm{G}}(\mathbf{x})/4\pi - \alpha\nabla(\mathbf{F}\cdot\nabla\psi_{\mathrm{G}}(\mathbf{x}))/8\pi}{\mu} \;\approx\; \frac{\mathbf{F}}{4\pi\mu|\mathbf{x}|} - \frac{\alpha}{8\pi\mu}\nabla(\mathbf{F}\cdot\nabla|\mathbf{x}|) \tag{68}$$

which agrees with Eqn (2.5) of [6].

1.3.3 Sanity Check 3: Cylindrical Inclusion

Imagine a cylindrical inclusion of radius R which would like to undergo spontaneous transformation strain ϵ^0_{12}, with equal modulus before and after the transformation. According to

Eqn (2.8) of [6]:

$$u_i = \frac{\epsilon^0_{12}}{4\pi(1-\nu)}\psi_{,i12} - \frac{\epsilon^0_{12}}{2\pi}\phi_{,1}\delta_{i2} - \frac{\epsilon^0_{12}}{2\pi}\phi_{,2}\delta_{i1} \tag{69}$$

$$\phi(\mathbf{x}) = \int_{\text{cylinder}} \frac{d^3\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|} = \int_R^r \frac{-4\pi\cdot\pi R^2}{2\pi r}dr = -2\pi R^2 \ln r \tag{70}$$

Also from Eqn (2.9) of [6],

$$\nabla^2\psi(\mathbf{x}) = 2\phi(\mathbf{x}) \quad \rightarrow \quad r^{-1}\partial_r(r\partial_r\psi(r)) = -4\pi R^2 \ln r \tag{71}$$

so $\psi(r) = \pi R^2(r^2 - r^2\ln r)$.

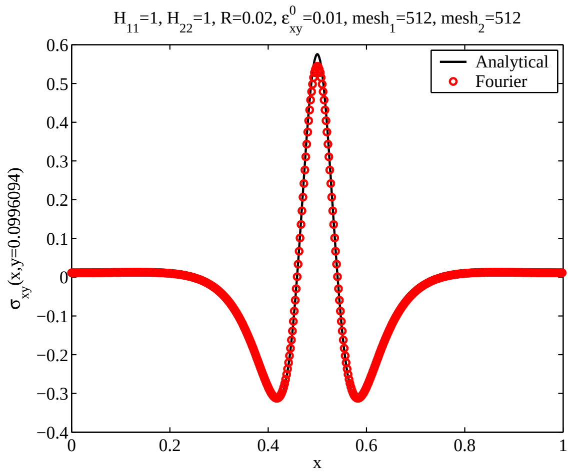


Figure 1:

Using Mathematica[7] to do the differentiations, we obtain:

$$\sigma_{xy}(x,y) = \frac{\mu\epsilon^0_{12}R^2(x^4-6x^2y^2+y^4)}{(x^2+y^2)^3(1-\nu)}, \quad x^2+y^2 > R^2 \tag{72}$$

The comparison with numerical solution is shown in Fig. 1.

1.3.4 Sanity Check 4: Cylindrical Void

Imagine a cylindrical hole of radius R under a far field stress $\sigma^\infty_{ij} = 0$ except $\sigma^\infty_{22} > 0$. This is a plane-strain condition, where $\sigma_{33}(x,y)$ is tuned to make $\epsilon_{33}(x,y) = 0$. We have non-zero

$\epsilon_{11}(x,y)$, $\epsilon_{22}(x,y)$, $\epsilon_{12}(x,y)$ that must satisfy the compatibility constraint:

$$\epsilon_{11,22} + \epsilon_{22,11} \;=\; 2\epsilon_{12,12}. \tag{73}$$

There are two stress equilibrium equations:

$$\sigma_{11,1} + \sigma_{12,2} \;=\; 0, \quad \sigma_{21,1} + \sigma_{22,2} \;=\; 0 \tag{74}$$

the finite $\sigma_{33}(x,y)$ is canceled for finite-thickness samples near the hole exit by 3D indentation like local stress field. Define Airy stress function:

$$\varphi_{,22} \equiv \sigma_{11}, \;\; \varphi_{,12} \equiv -\sigma_{12}, \;\; \varphi_{,11} \equiv \sigma_{22} \tag{75}$$

Stress equilibrium is satisfied. We also have $\sigma_{33} = \lambda(\epsilon_{11} + \epsilon_{22})$, $\sigma_{22} = \lambda(\epsilon_{11} + \epsilon_{22}) + 2\mu\epsilon_{22}$, $\sigma_{11} = \lambda(\epsilon_{11} + \epsilon_{22}) + 2\mu\epsilon_{11}$, so $\mathrm{tr}(\boldsymbol{\sigma}) = (3\lambda + 2\mu)(\epsilon_{11} + \epsilon_{22})$, and based on (50):

$$\boldsymbol{\epsilon} \;=\; \frac{\boldsymbol{\sigma}}{2\mu} - \frac{\lambda}{2\mu}\frac{\mathrm{tr}(\boldsymbol{\sigma})}{3\lambda + 2\mu}\mathbf{I}. \tag{76}$$

Plugging above back into (73), we get

$$\nabla^4\varphi \;=\; (\partial_{11} + \partial_{22})(\partial_{11} + \partial_{22})\varphi \;=\; (r^{-1}\partial_r(r\partial_r) + r^{-2}\partial_\theta^2)^2\varphi \;=\; 0. \tag{77}$$

Converting to cylindrical coordinate, we also have

$$\sigma_{rr} = r^{-1}\partial_r\varphi + r^{-2}\partial_\theta^2\varphi, \quad \sigma_{\theta\theta} = \partial_r^2\varphi, \quad \sigma_{r\theta} = -\partial_r(r^{-1}\partial_\theta\varphi) \tag{78}$$

Since $\sigma_{22}^\infty = \sigma_{22}(x, y \to \infty) = \varphi_{,11}(x, y \to \infty)$, we see that $\varphi(x,y)$ must contain $\sigma_{22}^\infty x^2/2 = \sigma_{22}^\infty r^2\cos^2(\theta)/2 = \sigma_{22}^\infty r^2(\cos(2\theta) + 1)/4$ as the leading-order term. Presume $\varphi = r^m g(\theta)$, a $\cos(n\theta)$ angular term excites in (77):

$$0 \;=\; (r^{-1}\partial_r(r\partial_r) - n^2r^{-2})^2 f(r) \;=\; r^{m-4}((m-2)^2 - n^2)(m^2 - n^2), \tag{79}$$

which means $m = \pm n, 2 \pm n$. For $n = 0$, the solution can be r^2, $r^2\ln r$, 1, $\ln r$. So we know the general solution should look like

$$\varphi \;=\; \frac{\sigma_{22}^\infty}{4}\left[(r^2 + ar^{-2} + b + 0r^4)\cos(2\theta) + (c\ln r + r^2)\cos(0\theta)\right] \tag{80}$$

$0r^4$ because we know it does not satisfy the far-field asymptote. Thus,

$$\begin{aligned}
\sigma_{rr} = &\quad r^{-1}\partial_r\varphi + r^{-2}\partial_\theta^2\varphi \\
= &\quad \frac{\sigma_{22}^\infty}{4}\left[\cos(2\theta)(r^{-1}(2r - 2ar^{-3}) - 4r^{-2}(r^2 + ar^{-2} + b)) + r^{-1}(2r + cr^{-1})\right] \\
= &\quad \frac{\sigma_{22}^\infty}{4}\left[\cos(2\theta)(-2 - 6ar^{-4} - 4br^{-2}) + 2 + cr^{-2}\right]
\end{aligned} \tag{81}$$

$$\begin{aligned}
\sigma_{r\theta} = &\quad -\partial_r(r^{-1}\partial_\theta\varphi) \\
= &\quad \frac{\sigma_{22}^\infty}{4}\left[2\sin(2\theta)(\partial_r(r + ar^{-3} + br^{-1}))\right] \\
= &\quad \frac{\sigma_{22}^\infty}{4}\left[2\sin(2\theta)(1 - 3ar^{-4} - br^{-2}\right]
\end{aligned} \tag{82}$$

To satisfy the traction-free boundary condition: $0 = \sigma_{rr}(r = R, \theta)$, $0 = \sigma_{r\theta}(r = R, \theta)$, we should have: $c = -2R^2$, $1 + 3aR^{-4} + 2bR^{-2} = 0$. Also,

$$1 - 3aR^{-4} - bR^{-2} \;=\; 0 \tag{83}$$

then $b = -2R^2$, $a = R^4$. So

$$\varphi \;=\; \frac{\sigma_{22}^\infty}{4}\left[\cos(2\theta)(r^2 + R^4r^{-2} - 2R^2) + r^2 - 2R^2\ln r\right] \tag{84}$$

$$\sigma_{\theta\theta} \;=\; \frac{\sigma_{22}^\infty}{2}\left[\cos(2\theta)(1 + 3R^4r^{-4}) + 1 + R^2r^{-2}\right]. \tag{85}$$

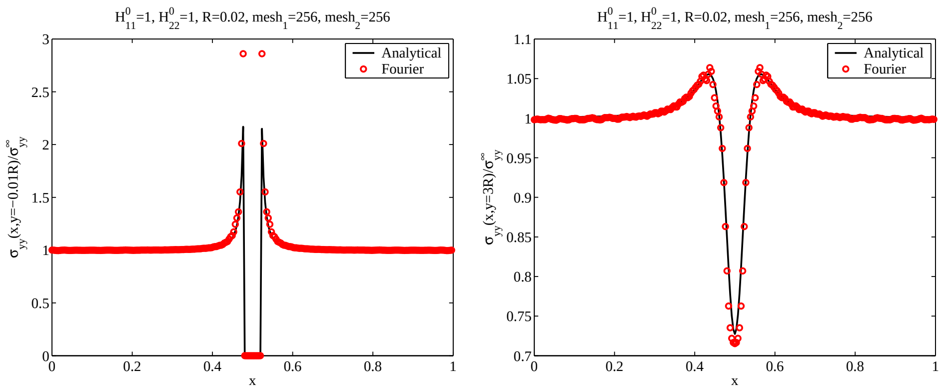
$$\sigma_{rr} = \frac{\sigma_{22}^\infty}{2}\left[\cos(2\theta)(-1 - 3R^4r^{-4} + 4R^2r^{-2}) + 1 - R^2r^{-2}\right]. \tag{86}$$

$$\sigma_{r\theta} = \frac{\sigma_{22}^\infty}{2}\left[\sin(2\theta)(1 - 3R^4r^{-4} + 2R^2r^{-2})\right]. \tag{87}$$

And

$$\sigma_{yy}(x, y) = \sigma_{22}^\infty\frac{2(x^2 + y^2)^4 + 3R^4(x^4 - 6x^2y^2 + y^4) + R^2(x^6 + 13x^4y^2 + 7x^2y^4 - 5y^6)}{2(x^2 + y^2)^4} \tag{88}$$

The above solution is independent of ν and plane strain vs plane stress condition. The only difference between those lies in the displacement field, not in the stress field.



(a) (b)

Figure 2:

1.4 2D Isotropic Media

A 2D isotropic medium has

$$c_{ijpq} \;=\; \lambda\delta_{ij}\delta_{pq} + \mu(\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp}). \tag{89}$$

The relationship between the Lamé parameters λ, μ and E, ν are:

$$\lambda = \frac{E\nu}{1-\nu^2} = \frac{2\nu\mu}{1-\nu}, \quad \mu = \frac{E}{2(1+\nu)}, \tag{90}$$

and the relationship between stress and strain is:

$$\sigma^0_{ij}(\mathbf{k}) = (\lambda\epsilon^0_{pp}(\mathbf{k}))\delta_{ij} + 2\mu\epsilon^0_{ij}(\mathbf{k}), \quad \sigma^0_{ij}(\mathbf{x}) = (\lambda\epsilon^0_{pp}(\mathbf{x}))\delta_{ij} + 2\mu\epsilon^0_{ij}(\mathbf{x}). \tag{91}$$

Then (12) becomes:

$$C_{ip}(\hat{\mathbf{k}}) = c_{ijpq}\hat{k}_j\hat{k}_q = \lambda\hat{k}_i\hat{k}_p + \mu\delta_{ip} + \mu\hat{k}_p\hat{k}_i = \mu\delta_{ip} + (\lambda+\mu)\hat{k}_i\hat{k}_p \tag{92}$$

or

$$\mathbf{C}(\hat{\mathbf{k}}) \;=\; \mu\mathbf{I} + (\lambda+\mu)\hat{\mathbf{K}} \tag{93}$$

with $K_{ip} \equiv \hat{k}_i\hat{k}_p$. The $\hat{\mathbf{K}}$ matrix is real and symmetric. It is also idempotent: $\hat{\mathbf{K}}^n = \hat{\mathbf{K}}$.

The inversion of $\mathbf{C}(\hat{\mathbf{k}})$ can be done by matrix series expansion:

$$\mathbf{\Omega}(\hat{\mathbf{k}}) \;=\; \frac{1}{\mu}\sum_{n=0}^{\infty}(-\frac{\lambda+\mu}{\mu})^n\hat{\mathbf{K}}^n = \frac{1}{\mu}(\mathbf{I}-\frac{\lambda+\mu}{\mu}\frac{\hat{\mathbf{K}}}{1+\frac{\lambda+\mu}{\mu}}) = \frac{1}{\mu}(\mathbf{I}-\frac{\lambda+\mu}{\lambda+2\mu}\hat{\mathbf{K}}). \tag{94}$$

Define dimensionless quantity

$$\alpha \;\equiv\; \frac{\lambda+\mu}{\lambda+2\mu} = \frac{1+\nu}{2}, \tag{95}$$

we then have $\mathbf{\Omega}(\hat{\mathbf{k}}) = (\mathbf{I}-\alpha\hat{\mathbf{K}})/\mu$.

So (15) would become

$$\tilde{u}_p(\mathbf{k}) \;=\; \frac{(\delta_{pi'}-\alpha\hat{k}_p\hat{k}_{i'})\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{j'}}{\mu i|\mathbf{k}|} = \frac{\sigma^0_{pj'}(\mathbf{k})\hat{k}_{j'}-\alpha\hat{k}_p\sigma^0_{i'j'}(\mathbf{k})\hat{k}_{i'}\hat{k}_{j'}}{\mu i|\mathbf{k}|}. \tag{96}$$

Define vector and scalar

$$\mathbf{f}(\mathbf{k}) \;\equiv\; \boldsymbol{\sigma}^0(\mathbf{k})\cdot\hat{\mathbf{k}}, \quad g(\mathbf{k}) \;\equiv\; \hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}), \tag{97}$$

which can be pre-computed, we then have

$$\tilde{\mathbf{u}}(\mathbf{k}) \;=\; \frac{\mathbf{f}(\mathbf{k})-\alpha g(\mathbf{k})\hat{\mathbf{k}}}{\mu i|\mathbf{k}|}. \tag{98}$$

The periodic part of the strain field is then

$$\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) \;=\; \frac{i\tilde{\mathbf{u}}(\mathbf{k})\mathbf{k}+i\mathbf{k}\tilde{\mathbf{u}}(\mathbf{k})}{2} \;=\; \frac{\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}+\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})-2\alpha g(\mathbf{k})\hat{\mathbf{K}}}{2\mu}, \tag{99}$$

with $\mathrm{tr}(\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}) = \mathrm{tr}(\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})) = \hat{\mathbf{k}}\cdot\mathbf{f}(\mathbf{k}) = g(\mathbf{k})$, $\mathrm{tr}(\tilde{\boldsymbol{\epsilon}}(\mathbf{k})) = (1-\alpha)g(\mathbf{k})/\mu$, and

$$\boldsymbol{\epsilon}(\mathbf{x}) \;=\; \bar{\boldsymbol{\epsilon}}+\tilde{\boldsymbol{\epsilon}}(\mathbf{x}), \qquad \int d^3\mathbf{x}\tilde{\boldsymbol{\epsilon}}(\mathbf{x}) = 0. \tag{100}$$

The rotation field $\mathbf{R}(\mathbf{x}) = \mathbf{I}+\mathbf{W}(\mathbf{x})$ field is

$$\mathbf{W}(\mathbf{k}) \;=\; \frac{\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}-\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})}{2\mu}. \tag{101}$$

The $c^0_{ijpq}\tilde{\epsilon}_{pq}(\mathbf{k})$ stress component in (20) is simplified to be

$$\begin{aligned}\lambda\mathrm{tr}(\tilde{\boldsymbol{\epsilon}}(\mathbf{k}))\mathbf{I}+2\mu\tilde{\boldsymbol{\epsilon}}(\mathbf{k}) &= \frac{\lambda(1-\alpha)g(\mathbf{k})}{\mu}\mathbf{I}+\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}+\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})-2\alpha g(\mathbf{k})\hat{\mathbf{K}} \\ &= \beta g(\mathbf{k})\mathbf{I}+\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}+\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})-2\alpha g(\mathbf{k})\hat{\mathbf{K}} \end{aligned}\tag{102}$$

where

$$\beta \equiv \frac{\lambda(1-\alpha)}{\mu} = \nu \tag{103}$$

so

$$\boldsymbol{\sigma}(\mathbf{k}) = \det|\mathbf{H}_0| c^0_{ijpq}\bar{\epsilon}_{pq}\delta_{\mathbf{k}}+\mathbf{f}(\mathbf{k})\hat{\mathbf{k}}+\hat{\mathbf{k}}\mathbf{f}(\mathbf{k})+(\nu\mathbf{I}-(1+\nu)\hat{\mathbf{K}})g(\mathbf{k})-\sigma^0_{ij}(\mathbf{k}). \tag{104}$$

In the real-space inversion of (28):

$$c^\circ_{ijpq}\epsilon^\circ_{pq}(\mathbf{x}) = \tau_{ij}(\mathbf{x}), \quad \lambda\mathrm{tr}(\boldsymbol{\epsilon}^\circ)\mathbf{I}+2\mu\boldsymbol{\epsilon}^\circ = \boldsymbol{\tau}, \tag{105}$$

we note that

$$2\lambda\mathrm{tr}(\boldsymbol{\epsilon}^\circ)+2\mu\mathrm{tr}(\boldsymbol{\epsilon}^\circ) = \mathrm{tr}(\boldsymbol{\tau}), \quad \mathrm{tr}(\boldsymbol{\epsilon}^\circ) = \frac{\mathrm{tr}(\boldsymbol{\tau})}{2\lambda+2\mu}, \tag{106}$$

so

$$\boldsymbol{\epsilon}^\circ = \frac{\boldsymbol{\tau}}{2\mu}-\frac{\lambda}{2\mu}\frac{\mathrm{tr}(\boldsymbol{\tau})}{2\lambda+2\mu}\mathbf{I}. \tag{107}$$

2 Isotropically Random Strain Matrix

2.1 2D

Consider stress-free transformation strain $\boldsymbol{\epsilon}^0$ of volume elements in an isotropically random material like bulk glass:

$$\boldsymbol{\epsilon}^0 = \begin{pmatrix} \epsilon^0_{11} & \epsilon^0_{12} \\ \epsilon^0_{12} & \epsilon^0_{22} \end{pmatrix} \equiv \boldsymbol{\epsilon}^0_{\mathbf{I}}+\boldsymbol{\eta} \equiv \frac{\mathrm{Tr}\boldsymbol{\epsilon}^0}{2}\mathbf{I}+\begin{pmatrix} \eta_1 & \eta_3 \\ \eta_3 & -\eta_1 \end{pmatrix} \tag{108}$$

where we have decomposed $\boldsymbol{\epsilon}^0$ into a hydrostatic part $\boldsymbol{\epsilon}^0_{\mathbf{I}}$ and a deviatoric part $\boldsymbol{\eta}$. Assuming the hydrostatic part is decoupled from the deviatoric part, one wonders how to sample η_1,

η_3, so the *distribution* of $\boldsymbol{\eta}$ is indistinguishable from that viewed in a rotated frame

$$\tilde{\boldsymbol{\eta}} = \mathbf{R}^T \boldsymbol{\eta} \mathbf{R}, \quad \tilde{\eta}_{ij} = \eta_{i'j'} R_{i'i} R_{j'j} \tag{109}$$

where the rotation matrix is

$$\mathbf{R} \; = \; \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{110}$$

$\mathbf{R}\mathbf{R}^T = \mathbf{I}$, connecting $d\mathbf{x} = \mathbf{R} d\tilde{\mathbf{x}}$, and $(dl)^2 = d\mathbf{x}^T(\mathbf{I} + 2\boldsymbol{\eta})d\mathbf{x} = d\tilde{\mathbf{x}}^T(\mathbf{I} + 2\tilde{\boldsymbol{\eta}})d\tilde{\mathbf{x}}$.

We have

$$\tilde{\eta}_1 \; = \; \begin{bmatrix} \cos\theta & \sin\theta \end{bmatrix} \begin{pmatrix} \eta_1 & \eta_3 \\ \eta_3 & -\eta_1 \end{pmatrix} \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} = \eta_1 \cos 2\theta + \eta_3 \sin 2\theta. \tag{111}$$

$$\tilde{\eta}_3 \; = \; \begin{bmatrix} \cos\theta & \sin\theta \end{bmatrix} \begin{pmatrix} \eta_1 & \eta_3 \\ \eta_3 & -\eta_1 \end{pmatrix} \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix} = -\eta_1 \sin 2\theta + \eta_3 \cos 2\theta. \tag{112}$$

The above is basically Mohr's circle.

Because

$$\begin{bmatrix} \tilde{\eta}_1 \\ \tilde{\eta}_3 \end{bmatrix} \; = \; \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{pmatrix} \begin{bmatrix} \eta_1 \\ \eta_3 \end{bmatrix}, \quad \mathbf{W} \; = \; \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{pmatrix} \tag{113}$$

is a rotational matrix, we get the feeling that η_1 and η_3 are "equivalent" like x- and y-axis. Therefore, the proposal is to sample η_1 and η_3 as independent Gaussians.

The J_2 invariant is

$$J_2 \; \equiv \; -\det(\boldsymbol{\eta}) = \eta_1^2 + \eta_3^2 \tag{114}$$

confirming the view that η_1 and η_3 are "equivalent" dimensions in strain space.

2.2 3D

Consider

$$\boldsymbol{\eta} \; = \; \begin{pmatrix} \eta_1 & \eta_6 & \eta_5 \\ \eta_6 & \eta_2 & \eta_4 \\ \eta_5 & \eta_4 & -\eta_1 - \eta_2 \end{pmatrix} \tag{115}$$

This is more complicated because clearly η_1 and η_2 cannot be drawn independently, because if drawn independently, the first and second diagonals will be uncorrelated, but the first with third diagonals will be negatively correlated, making the third dimension "special".

Because $\boldsymbol{\eta}$ is a symmetric real matrix, which can always be diagonalized into

$$\boldsymbol{\eta} \;=\; \hat{\mathbf{R}}^T \begin{pmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{pmatrix} \hat{\mathbf{R}} \tag{116}$$

i.e. principal-axes representation, we come up with the following algorithm:

1. Draw h_1, h_2, h_3 as three independent Gaussian random variables with equal variance σ^2:
$$dP(h_i, h_i + dh_i) \;=\; \frac{dh_i}{\sqrt{2\pi\sigma^2}} \exp(-\frac{h_i^2}{2\sigma^2}) \tag{117}$$
This creates a spherically symmetric cloud.

2. Compute $\bar{h} = (h_1 + h_2 + h_3)/3$

3. Compute $k_1 = h_1 - \bar{h}$, $k_2 = h_2 - \bar{h}$, $k_3 = h_3 - \bar{h}$. The $[k_1, k_2, k_3]$ cloud falls onto the (111) plane that passes through the origin, which is the requirement, but otherwise has no preference among 1-2-3 permutations.

4. Create a "spherically isotropic" random rotation matrix $\hat{\mathbf{R}}$ (see below).

5. Plug into (116), do the matrix multiplications, to get $\boldsymbol{\eta}$.

To obtain "spherically isotropic" random rotation matrix $\hat{\mathbf{R}}$, one must first know how to draw "spherically isotropic" vector $\mathbf{v}$. This can be done by looking at the 4π solid angle in 3D:

$$4\pi \;=\; -\int_{\theta=0}^{\pi} d\cos\theta \int_{\phi=0}^{2\pi} d\phi. \tag{118}$$

The algorithm is

1. Draw a uniformly random number α from -1 to 1.

2. Obtain $\theta = \cos^{-1}(\alpha) \in (0, \pi)$

3. Draw a uniformly random number $\phi \in (0, 2\pi)$

4. Compute $\mathbf{v} = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]$.

With normalized "spherically isotropic" vector generator, "spherically isotropic" random rotation matrix can be easily generated by:

1. Draw two independent "spherically isotropic" vectors $\mathbf{v}_1$, $\mathbf{v}_2$,
2. Obtain $\mathbf{u}_2 = \mathbf{v}_2 - (\mathbf{v}_2 \cdot \mathbf{v}_1)\mathbf{v}_1$
3. Obtain normalized $\hat{\mathbf{u}}_2 = \mathbf{u}_2/|\mathbf{u}_2|$
4. Obtain cross product $\mathbf{v}_3 = \mathbf{v}_1 \times \hat{\mathbf{u}}_2$
5. $\hat{\mathbf{R}} = [\mathbf{v}_1, \hat{\mathbf{u}}_2, \mathbf{v}_3]$.

Matlab code of the above generator is at http://mt.seas.upenn.edu/Stuff/e/Matlab/RandomStrain3D/. One can verify, via histograms, that any component of $\boldsymbol{\eta}$ and $\tilde{\boldsymbol{\eta}} = \mathbf{R}^T\boldsymbol{\eta}\mathbf{R}$ indeed have the same distribution. For example, η_5 would have the same histogram as $\tilde{\eta}_5$.

References

(**http://mt.seas.upenn.edu/Stuff/e/Notes/Paper/**)

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