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MILTON

Extending the Theory of Composites to Other Areas of Science

> Edited By Graeme W. Milton



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Its available ! http://www.math.utah.edu/~milton/



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Extending the Theory of Composites to Other Areas of Science

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In Chapter 1 we review many of the linear equations of physics, and write them in a canonical form appropriate to the theory of composites. We show how conservation laws, which have played a key role throughout the history of science, can be generalized to equalities which we call "boundary field equalities and inequalities". Chapter 2 reviews the abstract theory of composites, both for the effective tensor and for the associated "Y -tensor". Chapter 3 shows that the problem of finding the Dirichlet-to-Neumann map which governs the response of inhomogeneous bodies, for acoustics, elastodynamics, ***** Read more



Rewriting some of the linear equations of Physics.

Constitutive Law:

$$\begin{pmatrix} \boldsymbol{\epsilon}(\mathbf{x}) \\ \mathbf{d}(\mathbf{x}) \\ \mathbf{b}(\mathbf{x}) \end{pmatrix} = \underbrace{\begin{pmatrix} \boldsymbol{\mathcal{S}}(\mathbf{x}) & \boldsymbol{\mathcal{D}}(\mathbf{x}) & \boldsymbol{\mathcal{Q}}(\mathbf{x}) \\ \boldsymbol{\mathcal{D}}^T(\mathbf{x}) & \boldsymbol{\varepsilon}(\mathbf{x}) & \boldsymbol{\beta}(\mathbf{x}) \\ \boldsymbol{\mathcal{Q}}^T(\mathbf{x}) & \boldsymbol{\beta}^T(\mathbf{x}) & \boldsymbol{\mu}(\mathbf{x}) \end{pmatrix}}_{\boldsymbol{\boldsymbol{\mu}}(\mathbf{x}) \boldsymbol{\boldsymbol{\lambda}}} \begin{pmatrix} \boldsymbol{\sigma}(\mathbf{x}) \\ \mathbf{e}(\mathbf{x}) \\ \mathbf{h}(\mathbf{x}) \end{pmatrix},$$

Differential Constraints:

$$\begin{aligned} \epsilon &= [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]/2, \quad \nabla \cdot \boldsymbol{\sigma} = 0; \\ \nabla \cdot \mathbf{d} &= 0, \quad \mathbf{e} = -\nabla V; \\ \nabla \cdot \mathbf{b} &= 0, \quad \mathbf{h} = -\nabla \psi. \end{aligned}$$

Key Identity:
$$\begin{pmatrix} \mathbf{d}(\mathbf{x}) \\ \mathbf{b}(\mathbf{x}) \end{pmatrix} \cdot \begin{pmatrix} \mathbf{e}(\mathbf{x}) \\ \mathbf{h}(\mathbf{x}) \end{pmatrix} = \nabla \mathbf{u}(\mathbf{x}) \cdot \boldsymbol{\sigma}(\mathbf{x}) - \nabla V(\mathbf{x}) \cdot \mathbf{d}(\mathbf{x}) - \nabla \psi(\mathbf{x}) \cdot \mathbf{b}(\mathbf{x}) = \nabla \cdot \mathbf{Q}(\mathbf{x}),$$

$$\mathbf{Q}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x})\mathbf{u}(\mathbf{x}) - V(\mathbf{x})\mathbf{d}(\mathbf{x}) - \boldsymbol{\psi}(\mathbf{x})\mathbf{b}(\mathbf{x}),$$

$$\int_{\Omega} \begin{pmatrix} \epsilon(\mathbf{x}) \\ \mathbf{d}(\mathbf{x}) \\ \mathbf{b}(\mathbf{x}) \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{\sigma}(\mathbf{x}) \\ \mathbf{e}(\mathbf{x}) \\ \mathbf{h}(\mathbf{x}) \end{pmatrix} = \int_{\partial \Omega} \mathbf{n} \cdot [\boldsymbol{\sigma}(\mathbf{x})\mathbf{u}(\mathbf{x}) - V(\mathbf{x})\mathbf{d}(\mathbf{x}) - \boldsymbol{\psi}(\mathbf{x})\mathbf{b}(\mathbf{x})].$$

Time Harmonic Equations:

 $\underbrace{\begin{pmatrix} -i\mathbf{v}\\ -i\nabla\cdot\mathbf{v} \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}} = \underbrace{\begin{pmatrix} -(\omega\rho) & i & 0\\ 0 & \omega/\kappa \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}} \underbrace{\begin{pmatrix} \nabla P\\ P \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}},$ Acoustics: $\mathcal{G}(\mathbf{x})$ $\mathbf{Z}(\mathbf{x})$ $\mathcal{F}(\mathbf{x})$ Elastodynamics: $\begin{pmatrix} -\sigma(\mathbf{x})/\omega \\ i\mathbf{p}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} -\mathbf{c}/\omega & \mathbf{0} \\ \mathbf{0} & \omega \rho \end{pmatrix} \begin{pmatrix} \mathbf{v}\mathbf{u} \\ \mathbf{u} \end{pmatrix}$ $\mathbf{Z}(\mathbf{x})$ $\mathcal{F}(\mathbf{x})$ $G(\mathbf{x})$ $\begin{pmatrix} -i\mathbf{h} \\ i\nabla \times \mathbf{h} \end{pmatrix} = \begin{pmatrix} -[\omega\mu(\mathbf{x})]^{-1} & 0 \\ 0 & \omega\varepsilon(\mathbf{x}) \end{pmatrix} \underbrace{\begin{pmatrix} \nabla \times \mathbf{e} \\ \mathbf{e} \end{pmatrix}},$ Maxwell: \mathbf{Z} Schrödinger equation, $\begin{pmatrix} \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{q}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} -\mathbf{A} & 0 \\ 0 & E - V(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla \psi(\mathbf{x}) \\ \psi(\mathbf{x}) \end{pmatrix}$, $\mathbf{Z}(\mathbf{x})$

Thermoacoustics: (s = 0)



$$\begin{pmatrix} i\boldsymbol{\sigma} \\ i\nabla\cdot\boldsymbol{\sigma} \\ \mathbf{q} \\ \nabla\cdot\mathbf{q} \\ -iP \end{pmatrix} \cdot \begin{pmatrix} \nabla\mathbf{v} \\ \mathbf{v} \\ \nabla\theta/T_0 \\ \theta/T_0 \\ s \end{pmatrix} = \nabla\cdot[i\boldsymbol{\sigma}\mathbf{v} + \mathbf{q}\theta/T_0].$$

Acoustics in the time domain:

$$\begin{pmatrix} \frac{\partial \mathbf{v}}{\partial t} \\ \nabla \cdot \mathbf{v} \end{pmatrix} = \underbrace{\begin{pmatrix} -\rho(\mathbf{x})^{-1} & 0 \\ 0 & \kappa(\mathbf{x})^{-1} \end{pmatrix}}_{\mathbf{Z}(\mathbf{x})} \begin{pmatrix} \nabla P \\ -\frac{\partial P}{\partial t} \end{pmatrix}.$$

$$\begin{pmatrix} \frac{\partial \mathbf{v}}{\partial t} \\ \nabla \cdot \mathbf{v} \end{pmatrix} \cdot \begin{pmatrix} \nabla P \\ -\frac{\partial P}{\partial t} \end{pmatrix} = (\nabla P) \cdot \left(\frac{\partial \mathbf{v}}{\partial t} \right) - \left(\frac{\partial P}{\partial t} \right) (\nabla \cdot \mathbf{v}) + P \frac{\partial \nabla \cdot \mathbf{v}}{\partial t} - P \frac{\partial \nabla \cdot \mathbf{v}}{\partial t}$$

$$= \begin{pmatrix} \nabla \\ -\frac{\partial}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} P \frac{\partial \mathbf{v}}{\partial t} \\ P \nabla \cdot \mathbf{v} \end{pmatrix}$$

$$= \overline{\nabla} \cdot \mathbf{Q},$$

Elastodynamics in the time domain:

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \end{pmatrix} = \underbrace{\begin{pmatrix} -\mathcal{C}(\mathbf{x}) & 0 \\ 0 & \boldsymbol{\rho}(\mathbf{x}) \end{pmatrix}}_{\mathbf{Z}(\mathbf{x})} \begin{pmatrix} -\frac{1}{2} \begin{bmatrix} \nabla \mathbf{v} + \nabla \mathbf{v}^T \end{bmatrix} \\ \frac{\partial \mathbf{v}}{\partial t} \end{bmatrix},$$

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \end{pmatrix} \cdot \begin{pmatrix} -\frac{1}{2} \left[\nabla \mathbf{v} + \nabla \mathbf{v}^T \right] \\ \frac{\partial \mathbf{v}}{\partial t} \end{pmatrix} = - \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} \right) : \nabla \mathbf{v} + (\nabla \cdot \boldsymbol{\sigma}) \cdot \left(\frac{\partial \mathbf{v}}{\partial t} \right) + \boldsymbol{\sigma} : \frac{\partial (\nabla \mathbf{v})}{\partial t} \\ - \boldsymbol{\sigma} : \frac{\partial (\nabla \mathbf{v})}{\partial t} \\ = \begin{pmatrix} \nabla \\ -\frac{\partial}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{\sigma} \frac{\partial \mathbf{v}}{\partial t} \\ \boldsymbol{\sigma} : \nabla \mathbf{v} \end{pmatrix} = \overline{\nabla} \cdot \mathbf{Q},$$

Elastodynamics in a moving frame: Galilean transformation

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}'}{\partial t'} \\ \nabla' \cdot \boldsymbol{\sigma}' \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathcal{I}} & \mathbf{w}\mathbf{I} \\ 0 & \mathbf{I} \end{pmatrix} \begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \end{pmatrix} = \begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{w}(\nabla \cdot \boldsymbol{\sigma})^T \\ \nabla \cdot \boldsymbol{\sigma} \end{pmatrix},$$

$$\begin{pmatrix} -\nabla' \mathbf{v}' \\ \frac{\partial \mathbf{v}'}{\partial t'} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathcal{I}} & 0 \\ \mathbf{I}\mathbf{w}^T & \mathbf{I} \end{pmatrix}^{-1} \begin{pmatrix} -\nabla \mathbf{v} \\ \frac{\partial \mathbf{v}}{\partial t} \end{pmatrix} = \begin{pmatrix} -\nabla \mathbf{v} \\ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{w}^T \nabla \mathbf{v} \end{pmatrix},$$

Matrix in the constitutive law now has Willis type couplings:

$$\begin{aligned} \mathbf{Z}'(\overline{\mathbf{x}}') &= \begin{pmatrix} \mathbf{\mathcal{I}} & \mathbf{w}\mathbf{I} \\ 0 & \mathbf{I} \end{pmatrix} \mathbf{Z}(\mathbf{x}) \begin{pmatrix} \mathbf{I} & 0 \\ \mathbf{I}\mathbf{w}^T & \mathbf{I} \end{pmatrix} \\ &= \begin{pmatrix} -\mathcal{C}(\mathbf{x}) + \mathbf{w}\rho(\mathbf{x})\mathbf{w}^T & \mathbf{w}\rho(\mathbf{x}) \\ \rho(\mathbf{x})\mathbf{w}^T & \rho(\mathbf{x}) \end{pmatrix}. \end{aligned}$$



Yellow=Compliant, Blue=Stiff Red=Rubber, Black=Lead

Time harmonic acceleration with no strain gives stress: Example of a Willis material



Electric dipole array generates polarization field

Force dipole array generates stress field Piezoelectricity in the time domain:

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \\ \frac{\partial \mathbf{d}}{\partial t} \end{pmatrix} = \underbrace{ \begin{pmatrix} -\mathcal{C}(\mathbf{x}) & 0 & -\mathbf{a}(\mathbf{x}) \\ 0 & \rho(\mathbf{x}) & 0 \\ -\mathbf{a}^T(\mathbf{x}) & 0 & \varepsilon(\mathbf{x}) \end{pmatrix}}_{\mathbf{Z}(\mathbf{x})} \begin{pmatrix} -\frac{1}{2} \left[\nabla \mathbf{v} + \nabla \mathbf{v}^T \right] \\ \frac{\partial \mathbf{v}}{\partial t} \\ \frac{\partial \mathbf{e}}{\partial t} \end{pmatrix} ,$$

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \\ \frac{\partial \mathbf{d}}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} -\frac{1}{2} \left[\nabla \mathbf{v} + \nabla \mathbf{v}^T \right] \\ \frac{\partial \mathbf{v}}{\partial t} \\ \frac{\partial \mathbf{e}}{\partial t} \end{pmatrix} = \overline{\nabla} \cdot \mathbf{Q},$$

$$\mathbf{Q} = \begin{pmatrix} \boldsymbol{\sigma} \frac{\partial \mathbf{v}}{\partial t} - \frac{\partial V}{\partial t} \frac{\partial \mathbf{d}}{\partial t} \\ \boldsymbol{\sigma} \nabla \cdot \mathbf{v} \end{pmatrix},$$

Biot equations in the time domain (s=0)

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \\ -\nabla P \\ -\frac{\partial P}{\partial t} \\ M\zeta_{,t} \end{pmatrix} = \begin{pmatrix} -\boldsymbol{\mathcal{C}} & 0 & 0 & \mathbf{M} & 0 \\ 0 & \rho & \rho_f & 0 & 0 \\ 0 & \rho_f & \hat{m}_{ij} \ast & 0 & 0 \\ \mathbf{M} & 0 & 0 & M & M \\ 0 & 0 & 0 & M & M \end{pmatrix} \begin{pmatrix} -\nabla \mathbf{v} \\ \frac{\partial \mathbf{v}}{\partial t} \\ \frac{\partial \mathbf{w}_t}{\partial t} \\ -\nabla \cdot \mathbf{w}_t \\ \mathbf{s} \end{pmatrix}.$$

$$\begin{pmatrix} \frac{\partial \boldsymbol{\sigma}}{\partial t} \\ \nabla \cdot \boldsymbol{\sigma} \\ -\nabla P \\ -\frac{\partial P}{\partial t} \\ M\zeta, t \end{pmatrix} \cdot \begin{pmatrix} -\nabla \mathbf{v} \\ \frac{\partial \mathbf{v}}{\partial t} \\ -\frac{\partial \mathbf{w}_t}{\partial t} \\ -\nabla \cdot \mathbf{w}_t \\ s \end{pmatrix} = \begin{pmatrix} \nabla \\ -\frac{\partial}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{\sigma} \frac{\partial \mathbf{v}}{\partial t} - P \frac{\partial \mathbf{w}_t}{\partial t} \\ \boldsymbol{\sigma} \nabla \cdot \mathbf{v} - P \nabla \cdot \mathbf{w}_t \end{pmatrix}$$

Thermal Conduction and Diffusion:

$$\begin{pmatrix} \mathbf{q}_{x} \\ q_{t} \\ \nabla \cdot \mathbf{q}_{x} + \frac{\partial q_{t}}{\partial t} \end{pmatrix} = \underbrace{\begin{pmatrix} i\mathbf{k}(\mathbf{x}) & 0 & 0 \\ 0 & 0 & -\frac{i\alpha(\mathbf{x})}{2} \\ 0 & \frac{i\alpha(\mathbf{x})}{2} & 0 \end{pmatrix}}_{\mathbf{Z}(\mathbf{x})} \begin{pmatrix} \nabla T \\ \frac{\partial T}{\partial t} \\ T \end{pmatrix}.$$

$$\begin{pmatrix} \mathbf{q}_{x} \\ q_{t} \\ \nabla \cdot \mathbf{q}_{x} + \frac{\partial q_{t}}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \nabla T \\ \frac{\partial T}{\partial t} \\ T \end{pmatrix} = \mathbf{q}_{x} \cdot \nabla T + q_{t} \frac{\partial T}{\partial t} + T \nabla \cdot \mathbf{q}_{x} + T \frac{\partial q_{t}}{\partial t}$$
$$= \begin{pmatrix} \nabla \\ -\frac{\partial}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{q}_{x} T \\ -T q_{t} \end{pmatrix}$$

Thermoelasticity in the time domain:



$$\begin{pmatrix} \frac{i\partial\boldsymbol{\sigma}}{\partial t} \\ i\nabla\cdot\boldsymbol{\sigma} \\ i\mathbf{q} \\ i\rho S\theta_0 \\ i\left(\nabla\cdot\mathbf{q} + \frac{\partial\rho S\theta_0}{\partial t}\right) \end{pmatrix} \cdot \begin{pmatrix} -\nabla\mathbf{u} \\ \frac{\partial\mathbf{u}}{\partial t} \\ -\nabla\theta/\theta_0 \\ -\frac{1}{\theta_0}\frac{\partial\theta}{\partial t} \\ -\theta/\theta_0 \end{pmatrix} = \begin{pmatrix} \nabla \\ -\frac{\partial}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} i\boldsymbol{\sigma}\frac{\partial\mathbf{u}}{\partial t} - i\mathbf{q}\theta/\theta_0 \\ i\boldsymbol{\sigma}\nabla\cdot\mathbf{u} + i\rho S\theta \end{pmatrix}.$$

Maxwell's equations in the time domain:

$$\begin{pmatrix} -\mathbf{h} \\ \mathbf{d} \end{pmatrix} = \underbrace{\begin{pmatrix} -[\boldsymbol{\mu}(\mathbf{x})]^{-1} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\varepsilon}(\mathbf{x}) \end{pmatrix}}_{\mathbf{z}} \begin{pmatrix} \mathbf{b} \\ \mathbf{e} \end{pmatrix},$$

Differential constraints

$$\begin{pmatrix} \mathbf{b} \\ \mathbf{e} \end{pmatrix} = \Theta \begin{pmatrix} \Phi \\ V \end{pmatrix}, \quad \Theta^{\dagger} \begin{pmatrix} -\mathbf{h} \\ \mathbf{d} \end{pmatrix} = 0, \qquad \Theta = \begin{pmatrix} \nabla \times & 0 \\ -\frac{\partial}{\partial t} & -\nabla \end{pmatrix}, \quad \Theta^{\dagger} = \begin{pmatrix} \nabla \times & \frac{\partial}{\partial t} \\ 0 & \nabla \cdot \end{pmatrix}$$

$$\begin{split} \int_{\underline{\Omega}} \begin{pmatrix} -\mathbf{h} \\ \mathbf{d} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{b} \\ \mathbf{e} \end{pmatrix} &=& \int_{\underline{\Omega}} -\mathbf{h} \cdot (\nabla \times \Phi) - \mathbf{d} \cdot \nabla V - \mathbf{d} \cdot \frac{\partial \Phi}{\partial t} - \frac{\partial \mathbf{d}}{\partial t} \cdot \Phi + (\nabla \times \mathbf{h}) \cdot \Phi \\ &=& \int_{\partial \underline{\Omega}} \mathbf{n}_x \cdot (\mathbf{h} \times \Phi) - \mathbf{n}_x \cdot (V\mathbf{d}) - n_t \mathbf{d} \cdot \Phi, \end{split}$$

Schrödinger's equation in the time domain

$$\begin{pmatrix} \mathbf{q}_{x} \\ q_{t} \\ \nabla \cdot \mathbf{q}_{x} + \frac{\partial q_{t}}{\partial t} \end{pmatrix} = \underbrace{\begin{pmatrix} -\mathbf{A} & 0 & 0 \\ 0 & 0 & -\frac{\mathbf{i}\hbar}{2} \\ 0 & \frac{\mathbf{i}\hbar}{2} & -V \end{pmatrix}}_{\mathbf{Z}} \begin{pmatrix} \nabla \psi \\ \frac{\partial \psi}{\partial t} \\ \psi \end{pmatrix}. \qquad \mathbf{A} = \hbar^{2} \mathbf{I}/2m$$

$$\begin{split} \int_{\Omega} \begin{pmatrix} \mathbf{q}_{x} \\ q_{t} \\ \nabla \cdot \mathbf{q}_{x} + \frac{\partial q_{t}}{\partial t} \end{pmatrix} \cdot \begin{pmatrix} \nabla \psi \\ \frac{\partial \psi}{\partial t} \\ \psi \end{pmatrix} &= \int_{\Omega} \mathbf{q}_{x} \cdot \nabla \psi + q_{t} \frac{\partial \psi}{\partial t} + \psi \nabla \cdot \mathbf{q}_{x} + \psi \frac{\partial q_{t}}{\partial t} \\ &= \int_{\Omega} \nabla \cdot (\mathbf{q}_{x} \psi) + \frac{\partial}{\partial t} (\psi q_{t}) \\ &= \int_{\Omega} \overline{\nabla} \cdot \mathbf{Q}, \qquad \mathbf{Q} = (\mathbf{q}_{x}^{T} \psi, -q_{t} \psi)^{T}. \end{split}$$

Schrödinger's equation in a magnetic field ($\hbar = 1$)

$$\begin{pmatrix} \mathbf{q}_x \\ q_t \\ \nabla \cdot \mathbf{q}_x + \frac{\partial q_t}{\partial t} \end{pmatrix} = \begin{pmatrix} \frac{-\mathbf{I}}{2m} & 0 & \frac{\mathrm{i}e\mathbf{\Phi}}{2m} \\ 0 & 0 & -\frac{\mathrm{i}}{2} \\ \frac{-\mathrm{i}e\mathbf{\Phi}}{2m} & +\frac{\mathrm{i}}{2} & -eV \end{pmatrix} \begin{pmatrix} \nabla\psi \\ \frac{\partial\psi}{\partial t} \\ \psi \end{pmatrix}$$

Key identity still holds, and the above equation reduces to:

$$i\frac{\partial\psi}{\partial t} = \frac{1}{2m}[i\nabla + e\Phi]^2\psi + eV\psi,$$

Minimization principles for Schrödinger's equation with complex energies

 $E\psi(\mathbf{x}) = -\nabla \cdot \mathbf{A}\nabla\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) - h(\mathbf{x})\theta_0$ $\mathbf{A} = \hbar^2 \mathbf{I}/2m$

Minimize over ψ'

$$W(\psi', p) = \sum_{s} \int_{\Omega^{N}} \underbrace{[p(\mathbf{x})]^{2} + (E'')^{2} [\psi'(\mathbf{x})]^{2} + 2\theta_{0} p(\mathbf{x}) h(\mathbf{x})}_{I(p,\psi')} d\mathbf{r}$$

where

$$p(\mathbf{x}) = p(\mathbf{x}, \psi') = \nabla \cdot \mathbf{A} \nabla \psi' + (E' - V(\mathbf{x}))\psi',$$

subject to suitable boundary conditions on ψ'

The Desymmetrization of Schrödinger's equation

$$\begin{pmatrix} \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{v}(\mathbf{x}) + S_0 \end{pmatrix} = \begin{pmatrix} -\mathbf{A} & 0 & 0 \\ 0 & E - V(\mathbf{x}) & h(\mathbf{x}) \\ 0 & \overline{h}(\mathbf{x}) & d(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla \psi \\ \psi \\ \theta_0 \end{pmatrix} \qquad \mathbf{A} = \hbar^2 \mathbf{I}/2m$$

Replace with:

J(x) = L(x)E(x), Let Λ denote appropriate symmetrization operator:

$$\mathbf{\Lambda}\mathbf{J}(\mathbf{x}) = \begin{pmatrix} \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{v}(\mathbf{x}) \end{pmatrix} \quad \mathbf{L}(\mathbf{x}) = \begin{pmatrix} -\mathbf{A} & 0 & 0 \\ 0 & a(\mathbf{x}_1, \mathbf{x}_2) & g(\mathbf{x}_1, \mathbf{x}_2) \\ 0 & \overline{g}(\mathbf{x}_1, \mathbf{x}_2) & d(\mathbf{x}_1, \mathbf{x}_2) \end{pmatrix} \quad \mathbf{E}(\mathbf{x}) = \begin{pmatrix} \nabla \psi \\ \psi \\ \theta_0 \end{pmatrix}$$

Advantage: Can solve iteratively using FFT, and the FFT operations only need be done on (x_1, x_2) , i.e. only on two electron co-ordinates not all n electrons. A new perspective on **conservation laws**: Boundary field equalities and inequalities

If $\nabla \cdot \mathbf{Q} = 0$ in Ω then $\int_{\partial \Omega} \mathbf{n} \cdot \mathbf{Q} = 0$

If $\nabla \cdot \mathbf{Q} \ge 0$ in Ω then $\int_{\partial \Omega} \mathbf{n} \cdot \mathbf{Q} \ge 0$ Requires information about what is happening inside Ω namely that $\nabla \cdot \mathbf{Q} = 0$ or $\nabla \cdot \mathbf{Q} \ge 0$ in Ω . Are there other boundary field equalities or inequalities that use partial information about what is inside the body?

$$\begin{pmatrix} \mathbf{j}_{1}(\mathbf{x}) \\ \mathbf{j}_{2}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} a(\mathbf{x})\mathbf{I} & c(\mathbf{x})\mathbf{I} \\ c(\mathbf{x})\mathbf{I} & b(\mathbf{x})\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{e}_{1}(\mathbf{x}) \\ \mathbf{e}_{2}(\mathbf{x}) \end{pmatrix},$$

$$\nabla \cdot \mathbf{j}_{1} = 0, \quad \nabla \cdot \mathbf{j}_{2} = 0 \quad \mathbf{e}_{1} = -\nabla V_{1}, \quad \mathbf{e}_{2} = -\nabla V_{2}.$$

$$\mathbf{M}(\mathbf{x}) = \begin{pmatrix} a(\mathbf{x}) & c(\mathbf{x}) \\ c(\mathbf{x}) & b(\mathbf{x}) \end{pmatrix}, \qquad \beta \mathbf{I} \ge \mathbf{M}(\mathbf{x}) \ge \alpha \mathbf{I}, \quad \text{for some } \beta > \alpha > 0,$$

Following the ideas of Straley, Milgrom and Shtrikman suppose there is a matrix \mathbf{W} such that

$$\mathbf{W}\mathbf{M}\mathbf{W}^T = \begin{pmatrix} a'(\mathbf{x}) & 0\\ 0 & b'(\mathbf{x}) \end{pmatrix}.$$

In two dimensions suppose

$$c(\mathbf{x}) = 0$$
; $b(\mathbf{x}) = \alpha^2/a(\mathbf{x})$

Following ideas of Keller, Dykhne and Mendelson, we have the boundary field equality

$$\mathbf{n} \cdot \mathbf{j}_2(\mathbf{x}) = -\alpha \mathbf{t} \cdot \mathbf{e}_1(\mathbf{x})$$
 when $\mathbf{t} \cdot \mathbf{e}_2(\mathbf{x}) = \alpha^{-1} \mathbf{n} \cdot \mathbf{j}_1(\mathbf{x})$.

Due to the fact that the equations are satisfied with

$$\mathbf{e}_2(\mathbf{x}) = \alpha^{-1} \mathbf{R}_\perp \mathbf{j}_1(\mathbf{x}) \quad \mathbf{j}_2(\mathbf{x}) = \alpha \mathbf{R}_\perp \mathbf{e}_1(\mathbf{x})$$

where $\mathbf{R}_\perp = \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}$

Some boundary field inequalities (with D. Harutyunyan)

Look for functions $f(\mathbf{E}) = \mathbf{\overline{E}} \cdot \mathbf{TE}$ and constants f_{0} , just dependent on the boundary fields such that

$$\int_{\Omega} f(\mathbf{E}(\mathbf{x})) \geq f_{0}$$

for all fields E(x) satisfying appropriate differential constraints and the boundary conditions. To get f_0 one could solve the Euler Lagrange-equations

$$\mathbf{J}_0(\mathbf{x}) = \mathrm{TE}_0(\mathbf{x}), \quad \mathbf{J}_0 \in \mathcal{J}_\Omega, \quad \mathbf{E}_0 \in \mathcal{E}_\Omega. \qquad f_0 = \int_\Omega \overline{\mathbf{E}_0} \cdot \mathbf{J}_0,$$

To establish the inequality one needs to pick a T such that the volume average of $f(E) = \overline{E} \cdot TE$ is non-negative for any C-periodic function E(x) satisfying the appropriate differential constraints which we write as $E \in \mathcal{E}$

Find
$$c > 0$$
 such that $L(x) - cT$ is positive semidefinite for all $x \in \Omega$

Then we have the boundary field inequality:

$$0 \leq \int_{\Omega} \overline{\mathbf{E}(\mathbf{x})} \cdot \mathbf{L}(\mathbf{x}) \mathbf{E}(\mathbf{x}) - cf(\mathbf{E}(\mathbf{x})) \leq -cf_0 + \int_{\partial \Omega} \mathbf{n} \cdot \widetilde{\mathbf{Q}}(\mathbf{x}).$$

New Methods for Imaging

Key idea: making a direct link between Dirichlet-to-Neumann maps for bodies and effective tensors for composites.

Abstract Theory of Composites

Hilbert Space $\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J}$

Operator $\mathbf{L}:\mathcal{H} \to \mathcal{H}$

- Given $\mathbf{E}_0 \in \mathcal{U}$
- Solve $J_0 + J = L(E_0 + E)$
- With $\mathbf{J}_0 \in \mathcal{U}$, $\mathbf{J} \in \mathcal{J}$, $\mathbf{E} \in \mathcal{E}$,

Then $\mathbf{J}_0 = \mathbf{L}_* \mathbf{E}_0$ defines $\mathbf{L}_* \colon \mathcal{U} \to \mathcal{U}$

Example: Conducting Composites

- ${\cal H}$ Periodic fields that are square integrable over the unit cell
- \mathcal{U} Constant vector fields
- ${\mathcal E}\,$ Gradients of periodic potentials
- ${\mathcal J}$ Fields with zero divergence and zero average value
- $\mathbf{E}_0 + \mathbf{E}(\mathbf{x})$ Total electric field
- $\mathbf{J}_0 + \mathbf{J}(\mathbf{x})$ Total current field
- $\mathbf{L} = \boldsymbol{\sigma}(\mathbf{x})$ Local conductivity
- $\mathbf{L}_* = oldsymbol{\sigma}_*$ Effective conductivity

Variational principles if \mathbf{L} is self-adjoint and positive definite:

$$(\mathbf{J}_0, \mathbf{L}_*^{-1} \mathbf{J}_0) = \inf_{\underline{\mathbf{J}} \in \mathcal{J}} (\mathbf{J}_0 + \underline{\mathbf{J}}, \mathbf{L}^{-1} (\mathbf{J}_0 + \underline{\mathbf{J}}))$$

$$(\mathbf{E}_0, \mathbf{L}_* \mathbf{E}_0) = \inf_{\underline{\mathbf{E}} \in \mathcal{E}} (\mathbf{E}_0 + \underline{\mathbf{E}}, \mathbf{L}(\mathbf{E}_0 + \underline{\mathbf{E}}))$$

Leading to the elementary bounds:

 $\mathbf{L}_* \geq 0, \quad \mathbf{L}_* \leq \mathbf{\Gamma}_0 \mathbf{L} \mathbf{\Gamma}_0, \quad \mathbf{L}_*^{-1} \leq \mathbf{\Gamma}_0 \mathbf{L}^{-1} \mathbf{\Gamma}_0,$

 Γ_0 is the projection onto \mathcal{U}

Formula for the effective operator

$$\mathbf{L}_* = \mathbf{\Gamma}_0 \mathbf{L} [\mathbf{I} + \mathbf{\Gamma}_1 (\mathbf{L} / \sigma_0 - \mathbf{I})]^{-1} \mathbf{\Gamma}_0$$

where Γ_1 is the projection onto \mathcal{E} . Leads to series expansions:

$$\begin{split} \mathbf{L}_{*} &= \sum_{j=0}^{\infty} \mathbf{\Gamma}_{0} \mathbf{L} [\mathbf{\Gamma}_{1} (\mathbf{I} - \mathbf{L}/\sigma_{0})]^{j} \mathbf{\Gamma}_{0}, \\ \mathbf{J}_{0} &= \sum_{j=0}^{\infty} \mathbf{\Gamma}_{0} \mathbf{L} [\mathbf{I} - \mathbf{\Gamma}_{1} (\mathbf{L}/\sigma_{0})]^{j} \mathbf{E}_{0}, \\ \mathbf{E} &= \sum_{j=0}^{\infty} [\mathbf{\Gamma}_{1} (\mathbf{I} - \mathbf{L}/\sigma_{0})]^{j} \mathbf{E}_{0}, \\ \mathbf{J} &= \sum_{j=0}^{\infty} \mathbf{\Gamma}_{2} \mathbf{L} [\mathbf{\Gamma}_{1} (\mathbf{I} - \mathbf{L}/\sigma_{0})]^{j} \mathbf{E}_{0}. \end{split}$$



Specify boundary potential $V_0(\mathbf{x})$ Measure current flux $\mathbf{n} \cdot \mathbf{j}(\mathbf{x})$ We want to reformulate it as a problem in the abstract theory of composites, so we can apply the machinery of the theory of composites. Remove boundary conditions, by expressing the problem in terms of the fields that solve the problem when Ω is filled with a homogeneous material



Now let

- \mathcal{U} consist of those fields $\mathbf{j}(\mathbf{x}) = \mathbf{e}(\mathbf{x})$ that solve the equations as the boundary potential $V_0(\mathbf{x})$ varies.
- \mathcal{E} consist of fields $\mathbf{E} = -\nabla V$ with $V(\mathbf{x}) = 0$ on $\partial \Omega$
- $\mathcal{J} \quad \text{consist of fields } \mathbf{J} \text{ with } \nabla \cdot \mathbf{J} = 0 \\ \text{and } \mathbf{n} \cdot \mathbf{J} = 0 \text{ on } \partial \Omega$

Three spaces are orthogonal

Note that fields $\mathbf{j}(\mathbf{x}) = \mathbf{e}(\mathbf{x})$ in \mathcal{U} can be parameterized either by the boundary values of $V = V_0$ on $\partial \Omega$ or by the boundary values of $\mathbf{n} \cdot \mathbf{j}(\mathbf{x})$.
The abstract problem in composites consists in finding for a given field $\mathbf{e}(\mathbf{x})$ in \mathcal{U} (with associated boundary potential $V_0(\mathbf{x})$) the fields which solve:

$$\mathbf{j}'(\mathbf{x}) + \mathbf{J}(\mathbf{x}) = \sigma(\mathbf{x})[\mathbf{e}(\mathbf{x}) + \mathbf{E}(\mathbf{x})]$$

with

 $\mathbf{j}'(\mathbf{x})\in\mathcal{U}, \quad \mathbf{J}(\mathbf{x})\in\mathcal{J}, \quad \mathbf{E}(\mathbf{x})\in\mathcal{E}$

which is exactly the conductivity problem we would solve for the Dirichlet problem.

Furthermore if we knew the effective operator

$$\mathbf{L}_*: \mathcal{U} \to \mathcal{U}$$

Then we have

 $\mathbf{j}' = \mathbf{L}_* \mathbf{e}$

and the boundary values of $\mathbf{n} \cdot \mathbf{j}'(\mathbf{x})$ allow us to determine the Dirichlet-to-Neumann map assuming the fields in \mathcal{U} have been numerically calculated

Analyticity properties of effective tensors as functions of the moduli of the component materials (Bergman, Milton, Golden and Papanicolaou) extend to the Dirichlet-to-Neumann map

$$\sigma(\mathbf{x}) = \mathbf{R}(\mathbf{x})^T [\sum_{i=1}^n \chi_i(\mathbf{x})\sigma_i] \mathbf{R}(\mathbf{x})$$

The Dirichlet-to-Neumann map is a Herglotz function of the matrices $\sigma_1, \sigma_2, \ldots \sigma_n$ in the domain where these have positive definite imaginary parts, modulo a rotation in the complex plane. Easiest to prove using an approach of Bruno: The truncated series expansion,

$$\mathbf{L}_{*} ~pprox \sum_{j=0}^{m} \mathbf{\Gamma}_{0} \mathbf{L} [\mathbf{\Gamma}_{1} (\mathbf{I} - \mathbf{L}/\sigma_{0})]^{j} \mathbf{\Gamma}_{0}$$

with $\mathbf{L} = \boldsymbol{\sigma}(\mathbf{x})$ is a polynomial in the matrix elements of $\sigma_1, \sigma_2, \ldots, \sigma_n$ and hence \mathbf{L}_* will be an analytic function of them in the domain of convergence of the series

One obtains integral representation formulas for \mathbf{L}_* and hence for the Dirichlet to Neumann map.

Time Harmonic Equations:

 $\underbrace{\begin{pmatrix} -i\mathbf{v}\\ -i\nabla\cdot\mathbf{v} \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}} = \underbrace{\begin{pmatrix} -(\omega\rho) & i & 0\\ 0 & \omega/\kappa \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}} \underbrace{\begin{pmatrix} \nabla P\\ P \end{pmatrix}}_{-i\nabla\cdot\mathbf{v}},$ Acoustics: $\mathcal{G}(\mathbf{x})$ $\mathbf{Z}(\mathbf{x})$ $\mathcal{F}(\mathbf{x})$ Elastodynamics: $\begin{pmatrix} -\sigma(\mathbf{x})/\omega \\ i\mathbf{p}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} -\mathbf{c}/\omega & \mathbf{0} \\ \mathbf{0} & \omega \rho \end{pmatrix} \begin{pmatrix} \mathbf{v}\mathbf{u} \\ \mathbf{u} \end{pmatrix}$ $\mathbf{Z}(\mathbf{x})$ $\mathcal{F}(\mathbf{x})$ $G(\mathbf{x})$ $\begin{pmatrix} -i\mathbf{h} \\ i\nabla \times \mathbf{h} \end{pmatrix} = \begin{pmatrix} -[\omega\mu(\mathbf{x})]^{-1} & 0 \\ 0 & \omega\varepsilon(\mathbf{x}) \end{pmatrix} \underbrace{\begin{pmatrix} \nabla \times \mathbf{e} \\ \mathbf{e} \end{pmatrix}},$ Maxwell: \mathbf{Z} Schrödinger equation, $\begin{pmatrix} \mathbf{q}(\mathbf{x}) \\ \nabla \cdot \mathbf{q}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} -\mathbf{A} & 0 \\ 0 & E - V(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla \psi(\mathbf{x}) \\ \psi(\mathbf{x}) \end{pmatrix}$, $\mathbf{Z}(\mathbf{x})$

In all these examples Z has positive semidefinite imaginary part (that often can be made positive definite by a slight rotation in the complex plane)

The analog of the variational principles of Cherkaev and Gibiansky are then the variational principles of

Milton, Seppecher, and Bouchitte (2009) Milton and Willis (2010)

For acoustics, electromagnetism, elastodynamics

Minimization variational principles for electromagnetism at fixed, possibly complex, frequency in lossy materials.

Maxwell's equations: (here we assume real ω)

$$abla imes \mathbf{E} = i\omega \mathbf{B}, \quad \nabla \times \mathbf{H} = -i\omega \mathbf{D}$$

 $\mathbf{D} = \boldsymbol{\varepsilon} \mathbf{E}, \quad \mathbf{B} = \boldsymbol{\mu} \mathbf{H},$
Let
 $(\boldsymbol{\varepsilon}'' + \boldsymbol{\varepsilon}' (\boldsymbol{\varepsilon}'')^{-1} \boldsymbol{\varepsilon}' - \boldsymbol{\varepsilon}' (\boldsymbol{\varepsilon}'')^{-1})$

$$\mathcal{E} = \left(egin{array}{cccc} arepsilon & arepsilon &$$

When μ is real: $Y(\mathbf{E}') = \inf_{\mathbf{E}'} Y(\mathbf{E}'),$ $Y(\mathbf{E}') = \int_{\Omega} \left(\sum_{-\nabla \times \mu^{-1}(\nabla \times \mathbf{E}')/\omega} \right) \cdot \varepsilon \left(\sum_{-\nabla \times \mu^{-1}(\nabla \times \mathbf{E}')/\omega} \right) \cdot \varepsilon \left(\sum_{-\nabla \times \mu^{-1}(\nabla \times \mathbf{E}')/\omega} \right)$

The infimum is over fields with prescribed tangential components of

 $\underline{\mathbf{E}}'$ and $\mu^{-1}
abla imes \underline{\mathbf{E}}'$ at $\partial \Omega$

Unusual boundary conditions (BC), but can be replaced by more normal BC: see paper with John Willis. For electromagnetism, acoustics and elastodynamics, the Dirichlet-to-Neumann map is a Herglotz function of the matrices $\mathbf{Z}_1, \mathbf{Z}_2, \ldots, \mathbf{Z}_n$ of the component materials

For electromagnetism an alternative and rigorous proof was obtained with Maxence Cassier and Aaron Welters (in the new book) Some inverse problems for two-component bodies

Electromagnetism:

Suppose μ_1 , μ_2 are equal and frequency independent

Look for special complex frequencies where

$$\varepsilon_1(\omega) = \varepsilon_2(\omega)$$

Extrapolate (using representation formulas or bounds) measurements at different frequencies, or transient responses, to the neighborhood of these special frequencies

Quasistatic Elastodynamics:

Extrapolate to frequencies where $\mu_1(\omega_0^k) = \mu_2(\omega_0^k)$

Quasistatic Electromagnetism:

Extrapolate to ratios $\varepsilon_1/\varepsilon_2$ close to 1

Rigorous Upper and Lower Bounds on the Stress Relaxation in cylindrical composites in antiplane elasticity



Generalizing the concept of function to

Superfunctions!

Adding resistor networks



(a)

(b)



Multiplying resistor networks



Substitution of networks



We should consider a resistor network in conjunction with its batteries



Space \mathcal{H} Space \mathcal{V}

Combined Space $\mathcal{K} = \mathcal{H} \oplus \mathcal{V}$

Incidence Matrices:



 $M_{ij} = +1$ if the arrow of bond *i* points towards node *j*, = -1 if the arrow of bond *i* points away from node *j*, = 0 if bond *i* and node *j* are not connected.

Two natural subspaces:

- \mathcal{J} the null space of M^T (current vectors)
- ${\mathcal E}$ the range of M (potential drops)
- These are orthogonal spaces and $\ \mathcal{K} = \mathcal{E} \oplus \mathcal{J}$

Other spaces:

Divide the bonds in \mathcal{H} into n groups (representing the different impedances).

Define \mathcal{P}_i as the space of vectors P with elements P_j that are zero if bond j is not in group i.

The projection Λ_i onto the space \mathcal{P}_i is diagonal and has elements

 $\{\Lambda_i\}_{jk} = 1$ if j = k and bond j is in group i, = 0 otherwise.

Thus $\mathcal{K} = \mathcal{E} \oplus \mathcal{J} = \mathcal{V} \oplus \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n$,

This is an orthogonal subspace collection Y(n)

Y(n) subspace collection:

 $\mathcal{K} = \mathcal{E} \oplus \mathcal{J} = \mathcal{V} \oplus \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n,$

Z(n) subspace collection:

 $\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J} = \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n,$

Superfunction $F^{s}(n)$: Y(n) subspace collection with

 $\mathcal{V} = \mathcal{V}^I \oplus \mathcal{V}^O$

Subspace collections need not have orthogonal subspaces



Application: Accelerating some Fast Fourier Transform Methods in two-component composites

The effective conductivity σ_* is an analytic function of the component conductivities σ_1 and σ_2 With $\sigma_2 = 1$, $\sigma_*(\sigma_1)$ has the properties of a Stieltjes function: $\operatorname{Im}(\sigma_1)$

Bergman 1978 (pioneer, but faulty arguments) Milton 1981 (limit of resistor networks) Golden and Papanicolaou 1983 (rigorous proof)

Numerical scheme of Moulinec and Suquet (1994)



Numerical scheme of Eyre and Milton (1999)



Ideal scheme:



But we want to do this transformation at the level of the subspace collection, to recover the fields

At a discrete level



Problem: this substitution shortens the branch cut instead of lengthening it.

Solution:

Substitute non-orthogonal subspace collections

Model example: a square array of squares at 25% volume fraction

Obnosov's exact formula

$$\sigma_* = \sqrt{(1+3\sigma_1)/(3+\sigma_1)},$$



iteration number

error on the effective property: calculated vs theoretical (in %)





Thank you!

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