# Coarse-Graining and Homogenization

## Two Years of Headaches

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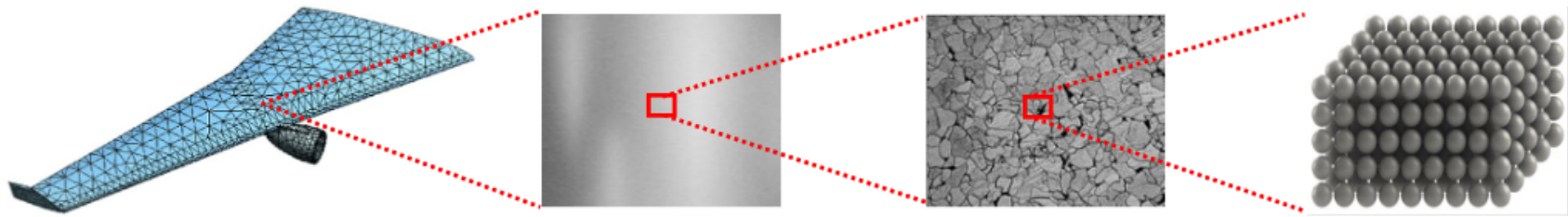
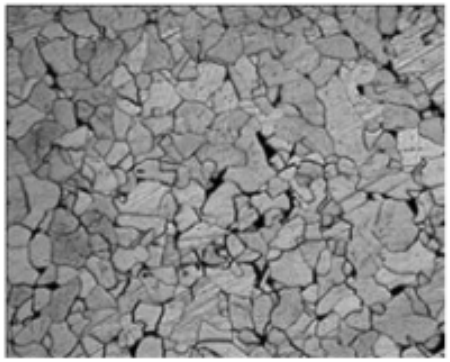
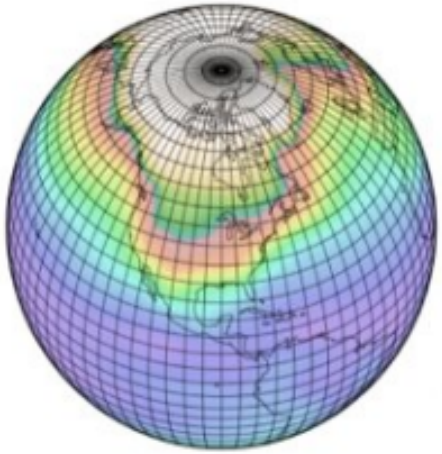
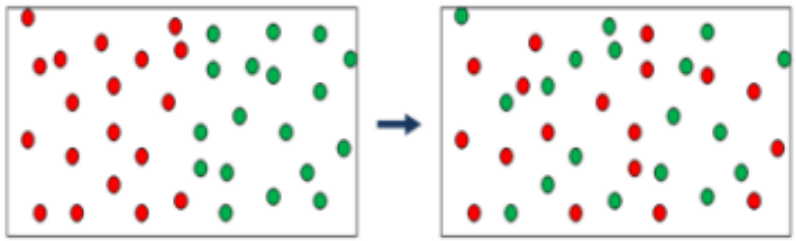


# What do the following problems have in common?

- Modeling a structure with heterogeneous microstructure
- Numerically simulating the weather on the scale of kilometers
- Making sense of diffusion processes







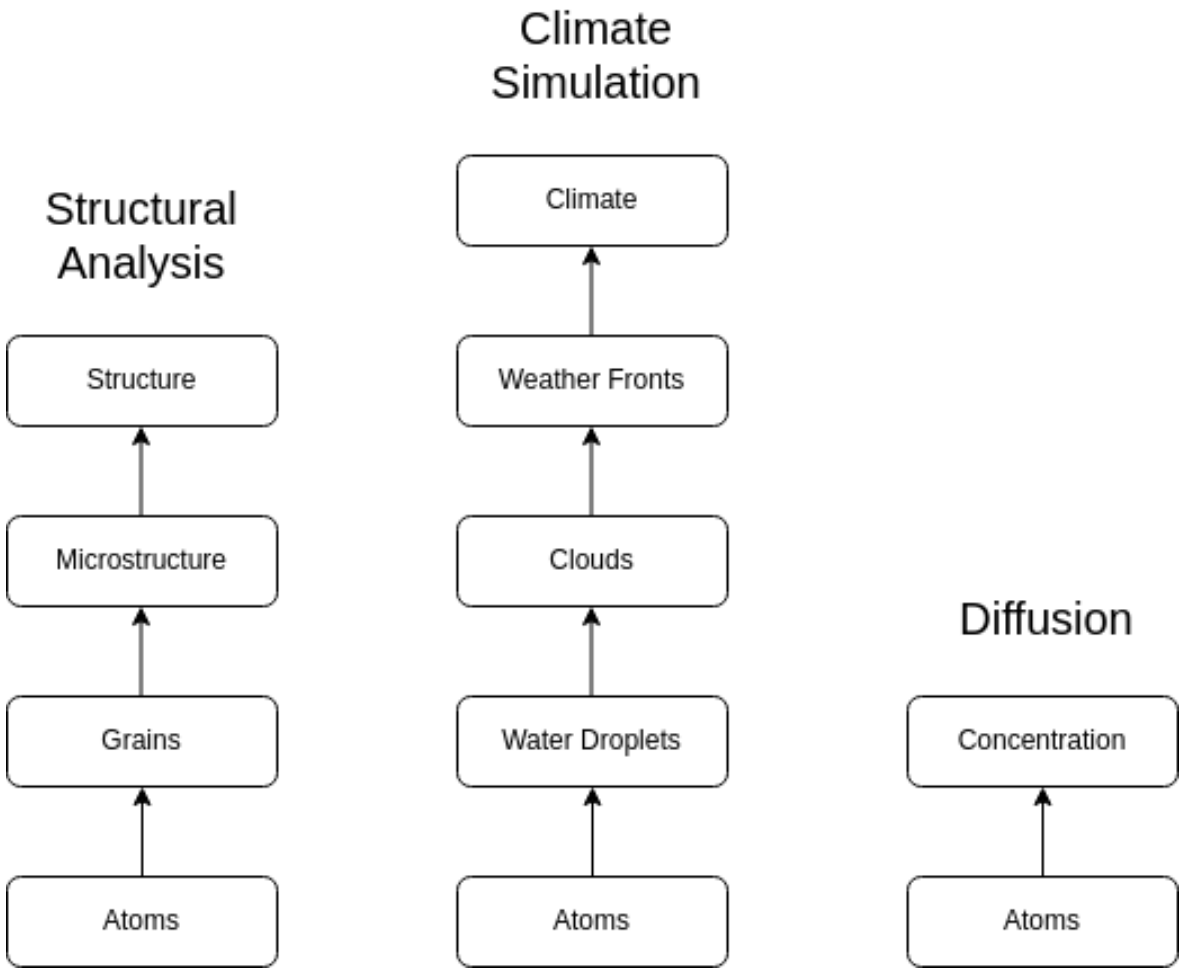
# Micro governs the macro

- Physical phenomena are governed by dynamics at the microscopic level
- This is cumbersome or impossible to model explicitly
- Experience suggests that this level of specificity is not needed
- **Are there systematic ways to ignore irrelevant details? How do we determine what is relevant? Why should simplifications like this be possible?**

# Coarse-grained models

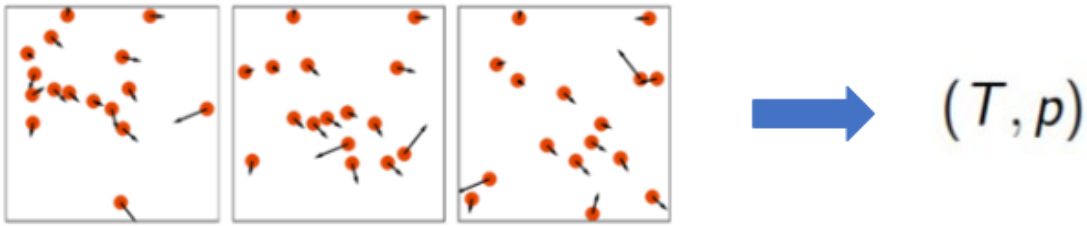
- Often care only about "macroscopic" quantities like maximum displacement, total heat flux, average global temperature, etc.
- **Good models are as simple (or inexpensive) as possible while remaining accurate**
- Coarse-graining is the process of throwing out unnecessary information
- Homogenization is a specific example of coarse-graining

# Hierarchy of scales




- Each level in hierarchy is a different "scale"
- Separation into discrete scales is often a convenient simplification

# Micro- and macrostates




- A microstate is a description of the system at small scale, macrostate is a simplified ("coarse-grained") description
- Terminology comes from statistical thermodynamics
- For a box of gas, microstate is vector of positions and momenta for each particle
- Macrostates are thermodynamic variables like temperature and pressure

# Why does this work?

The pressure $p$ is proportional to the number of random collisions of particles with the wall. Collision probabilities for labeled particles are random variables $X_i$ with $\langle X_i \rangle = \mu$ and $Var(X_i) = \sigma^2$. The pressure is then a random variable:

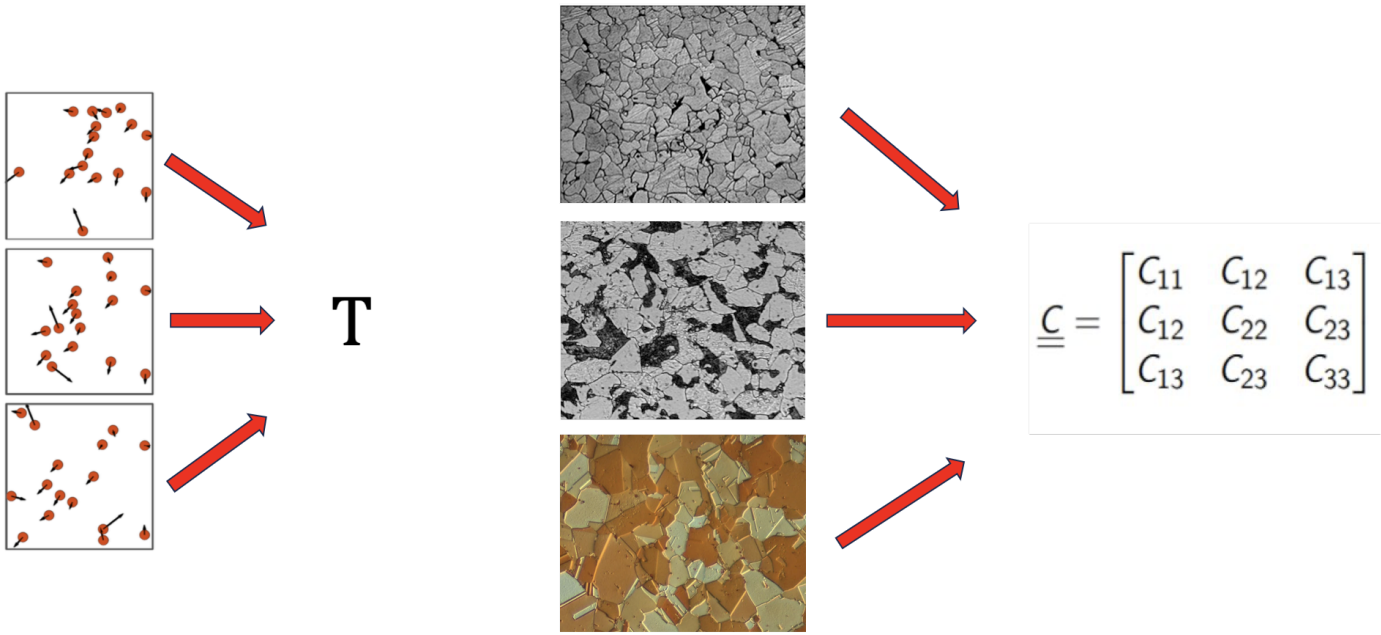
$$p \sim X_1 + X_2 + \cdots + X_N$$

The central limit theorem says that

$$p \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{N}\right)$$

When $N$ is large, the variance of the pressure approaches zero and it can be treated as a (new) deterministic quantity. Temperature is related to the total kinetic energy of the particles and energy is a conserved quantity.

# Entropy




- Not a unique relation between macrostates and microstates
- Entropy is a concept arising from coarse-graining operations in thermodynamics
- Measures the number of microstates that map onto the same macrostate
- Possible to define this for any coarse-graining operation

# Equivalence of thermodynamic and statistical entropy

Consider a gas with fixed volume being heated from initial temperature $T_1$ to a final temperature $T_2$. The thermodynamic entropy change is

$$\Delta S = \int \frac{\delta Q}{T} = \int_{T_1}^{T_2} \frac{3}{2} Nk \frac{dT}{T} = \frac{3}{2} Nk \ln\left(\frac{T_2}{T_1}\right)$$

where we have used that $\delta Q$ is the change in internal energy $dE = \frac{3}{2} NkdT$. The definition of entropy change from statistical mechanics for the constant volume heating is

$$\Delta S = k \ln\left(\frac{\Omega(T_2)}{\Omega(T_1)}\right)$$

where $\Omega$ is the volume of phase space consistent with the total energy of the gas. Each point in phase space describes a particular configuration of positions and momenta for all of the gas particles.

# Equivalence of thermodynamic and statistical entropy

The gas has energy from the motion of the particles. The total kinetic energy of all the particles must equal the internal energy, which is specified by the temperature.

$$\frac{1}{2m}\sum_{i=1}^{N}\sum_{j=1}^{3}p_{ij}^2 = E = \frac{3}{2}NkT \implies \sum_{i=1}^{N}\sum_{j=1}^{3}p_{ij}^2 = 3mNkT$$

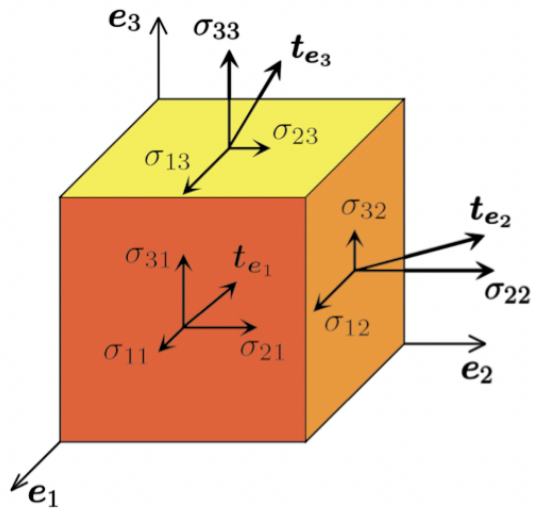
$$\Omega(T) \propto (3mNkT)^{(3N-1)/2}$$

$$\Delta S = k\ln\left(\frac{\Omega(T_1)}{\Omega(T_2)}\right) = k\ln\left(\frac{T_2}{T_1}\right)^{3(N-1)/2} = \frac{3}{2}Nk\ln\left(\frac{T_2}{T_1}\right) - \frac{1}{2}k\ln\left(\frac{T_2}{T_1}\right)$$

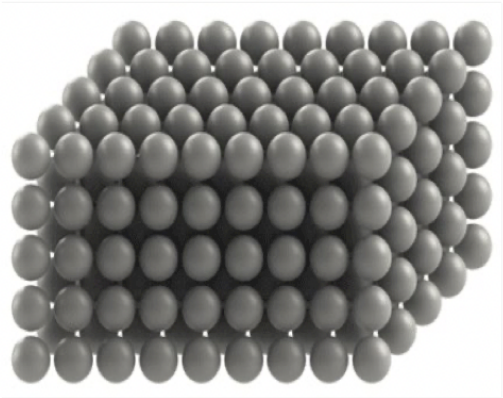
Not clear why the second term appears but it is very, very small when the number of particles $N$ is large ($> 10^{20}$ in practice).

# Micro- and macrostates in continuum mechanics

macrostates

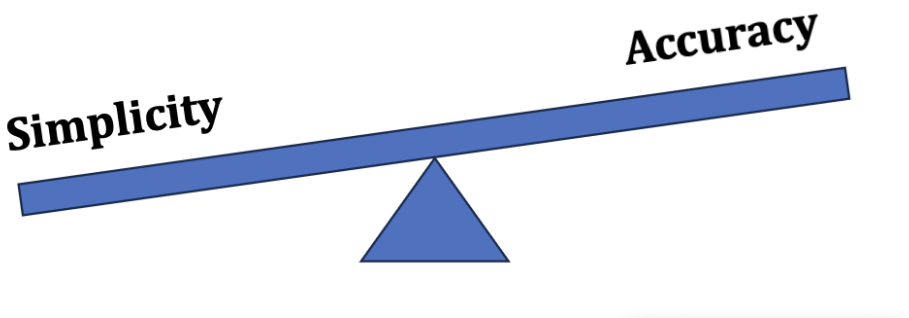



microstates



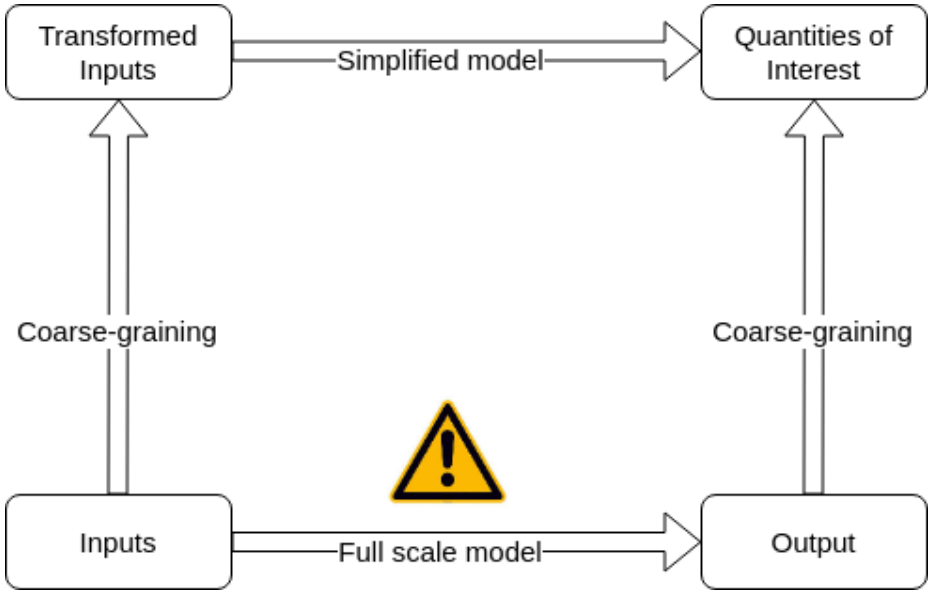
scale

# Information loss



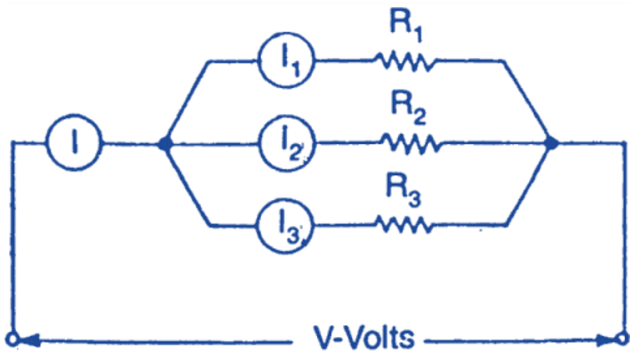

- High entropy macrostates correspond to large uncertainty about what is going on at small scale
- Balance between model simplicity and specificity of the system description
- Accuracy depends on what we ask of the model; it may be totally unnecessary to know the microstates in detail

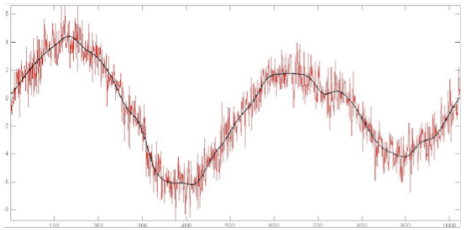
# Commutation diagram




- Avoid complex/expensive full scale model by coarsening problem
- In general, we need to find a coarse-graining operation for the problem input parameters and a new model which governs their evolution
- If microstates are of interest, there is no point in trying to carry out this process

# Other examples of coarse-graining



- Finding effective resistance in a circuit
- Denoising a signal, dimensionality reduction
- Modeling a discrete probabilistic process over multiple steps
- Breaking history up into periods


# Review

- Physical phenomena can be described at different scales
- Macrostates are high-level description, microstates are descriptions of system at small scales
- Want models which use the minimum amount of information necessary to predict quantities of interest
- Coarse-graining is the process of ignoring irrelevant information at small scales
- This involves defining macrostates and their evolution

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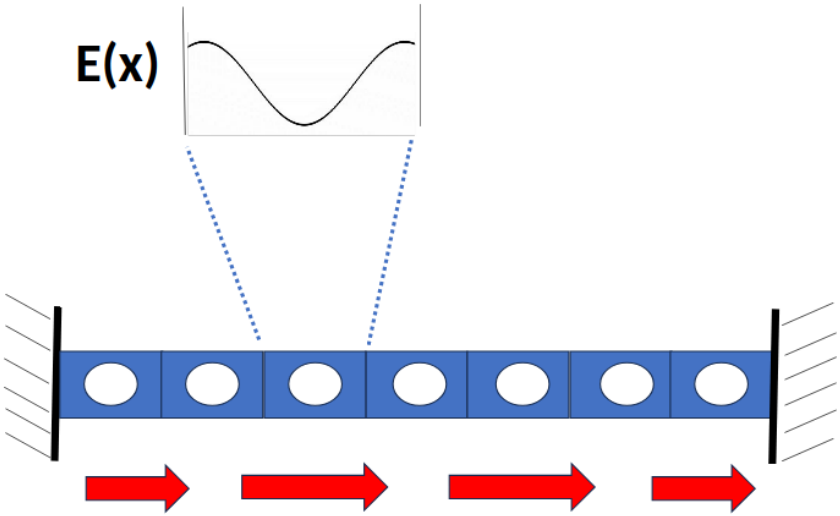
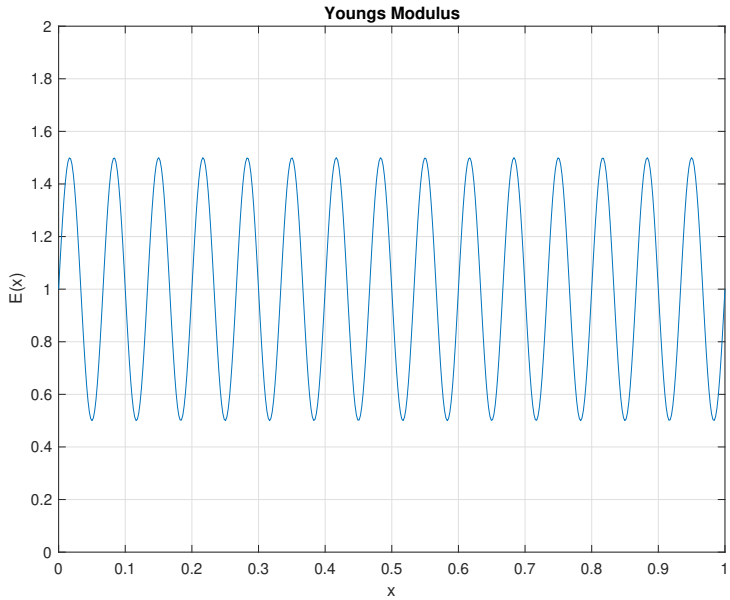
# Illustrative example




1D elliptic boundary value problem

$$\frac{\partial}{\partial x}\left(E(x)\frac{\partial u}{\partial x}\right) = -\sin(\pi x), \quad E(x) = 1 + \frac{1}{2}\sin(30\pi x), \quad u(0) = u(1) = 0$$

# Exact and approximate solutions

The analytical solution is given by

$$u(x) = \int_0^x \frac{\cos(\pi y)}{\pi E(y)} dy + C \int_0^x \frac{1}{E(y)} dy$$

where $C$ is an integration constant. We can approximate the solution with

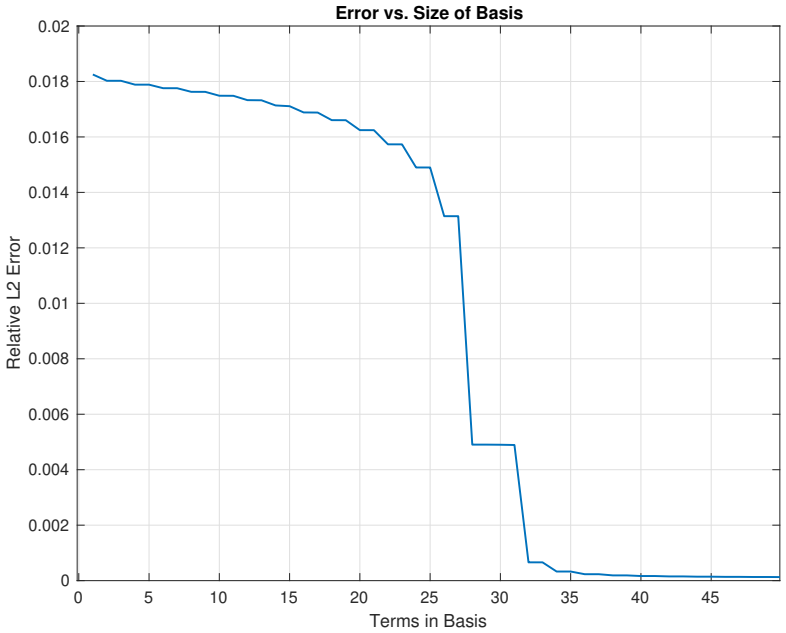
$$u(x) \approx \sum_{n=1}^{N} u_n \sin(n\pi x)$$

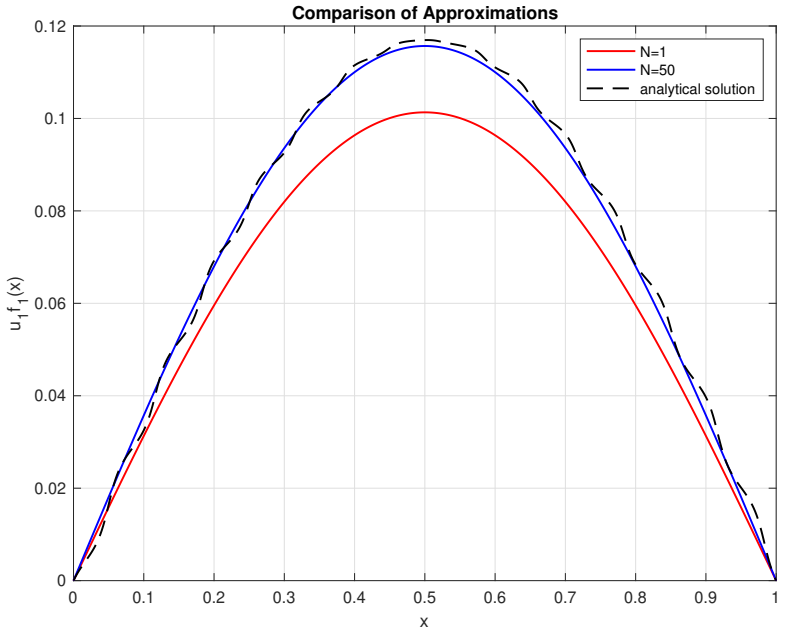
Discretized weak form is $u_i = K_{ij} F_j$ with

$$K_{ij} = \pi^2 \int_0^1 E(x) \cos(i\pi x) \cos(j\pi x) dx, \quad F_j = \int_0^1 \sin(\pi x) \sin(j\pi x) dx$$

Investigate the accuracy of the approximation with varying $N$...

# Results




- Error is relatively stationary until seeing sudden improvement
- **Don't get low frequency part of solution correct until resolving high frequency behavior**
- Oscillations are small, analytical solution well approximated by lowest frequency basis function
- **This corresponds to a constant but unknown modulus!**

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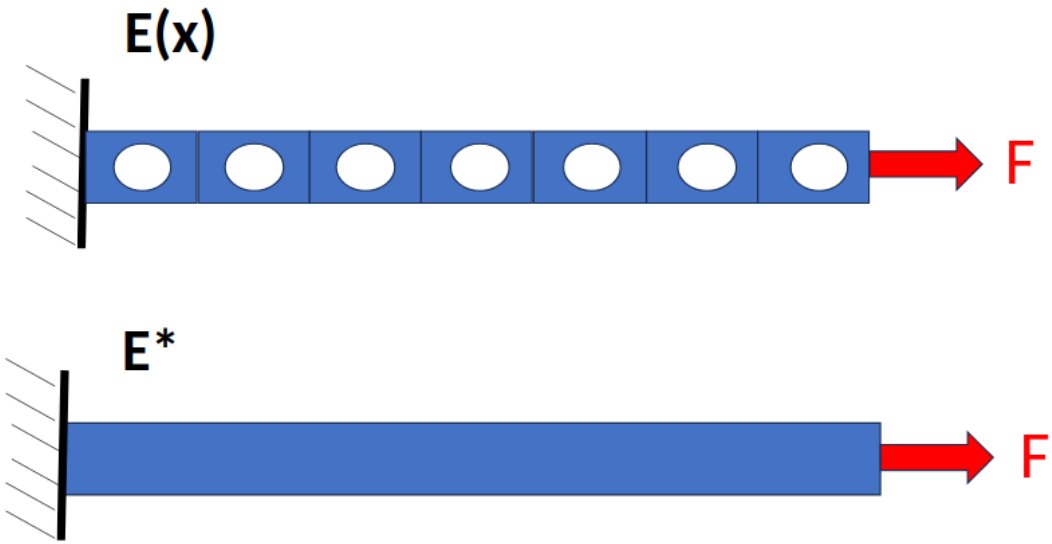
# Coarse-graining criterion




- Want to find "coarse-grained" modulus $E^*$ which approximates solution with fast oscillating $E(x)$
- Need a coarse-graining criterion $f\Big(E(x)\Big) = E^*$ such that $E(x) = E^*$ **in some sense**
- One idea would be to choose $E^*$ such that the force-displacement relations of the whole structure are in agreement

# Equivalent end displacements

$$\frac{\partial}{\partial x}\left(E(x)\frac{\partial u}{\partial x}\right) = 0, \quad u(0) = 0, \quad E(1)\frac{\partial u}{\partial x}(1) = F$$

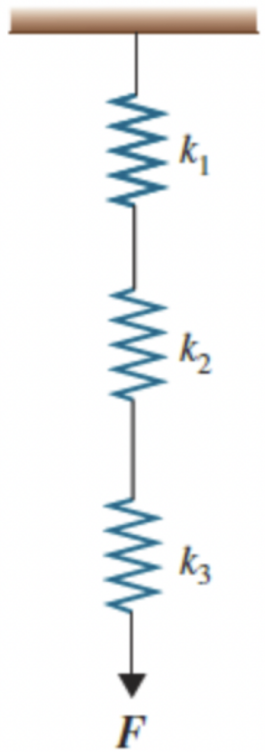
$$\implies u(x) = \int_0^x \frac{F}{E(y)}dy$$

$$\frac{F}{E^*} = F\int_0^1 \frac{dy}{E(y)} \implies E^* = \frac{1}{\int_0^1 \frac{dy}{E(y)}}$$

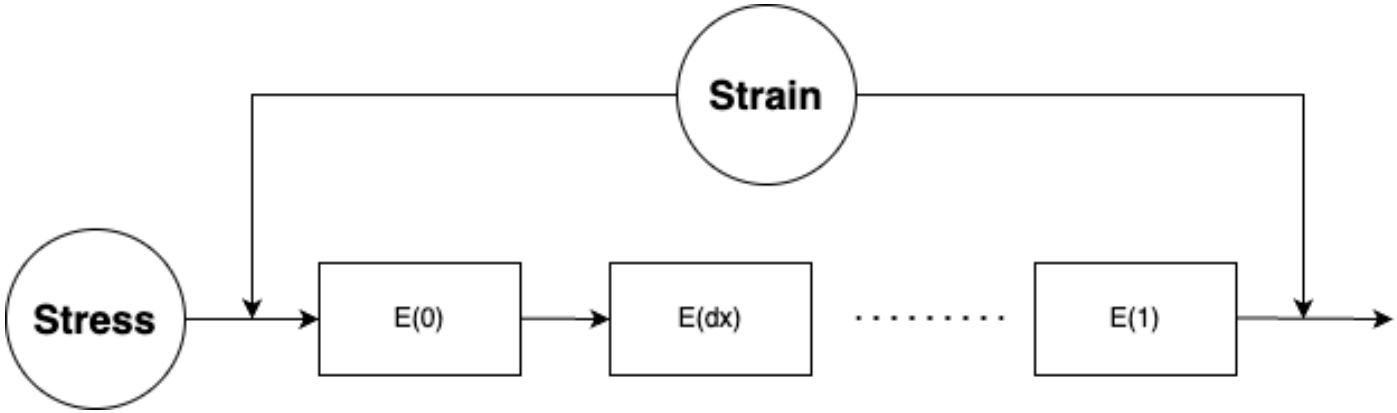
- Linearity ensures that the value of the force does not influence the coarse-grained (homogenized) modulus
- We have no control of how good the approximation is inside the bar, only that "macroscopic" response is captured
- See this plot for illustration
- This turns out to be the right answer for general loading, but not obvious why

# Harmonic mean

- The homogenized modulus is the harmonic mean of $E(x)$
- It can be shown that $E^* \leq \langle E(x) \rangle$
- A discrete version of the harmonic mean is used to coarse-grain springs in series
- The effective spring constant is $k^* = 1/(\frac{1}{k_1} + \frac{1}{k_2} + \frac{1}{k_3})$
- Lose information about "microstate" of displacement across each spring / strain field inside the bar



# Circuit analogy




- Force (like current) is constant over the spring elements
- Larger displacements over softer sections of material
- Can imagine this causing reduction in stiffness

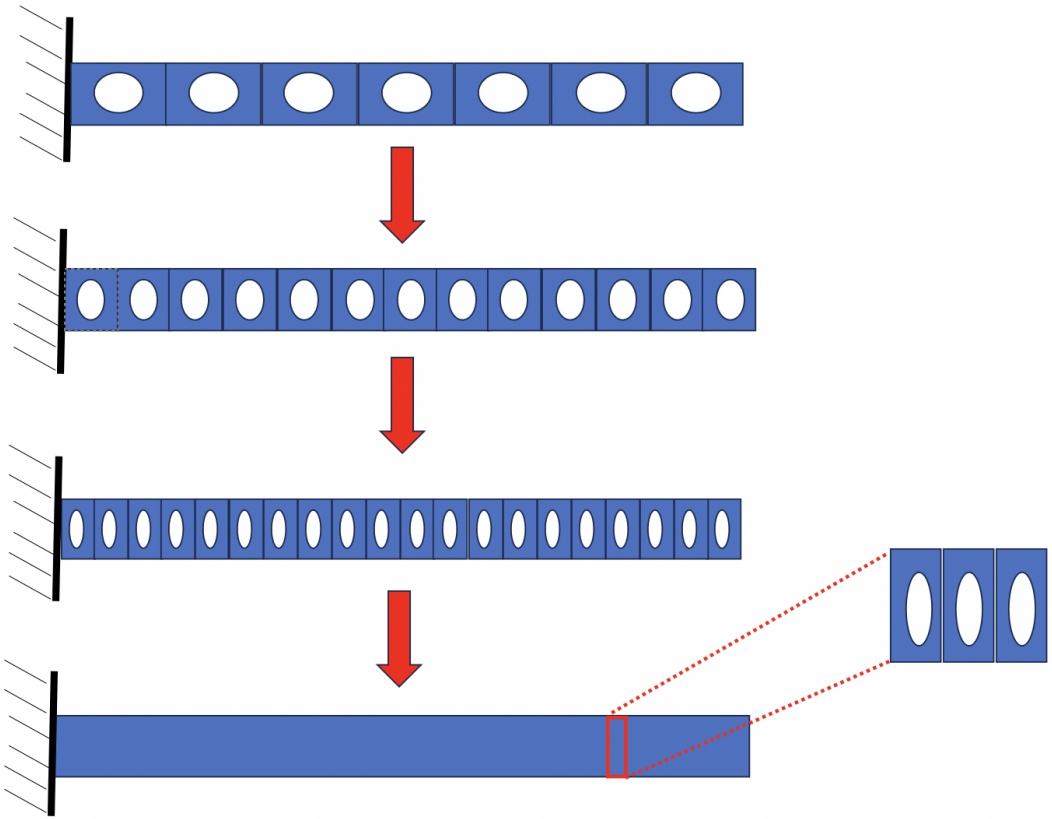
# Energy equivalence

## Clapeyron Theorem

$$\int_\Omega \frac{1}{2}\sigma_{ij}\epsilon_{ij}d\Omega = \frac{1}{2}\int_{\partial\Omega} t_i u_i dS + \frac{1}{2}\int_\Omega b_i u_i d\Omega$$

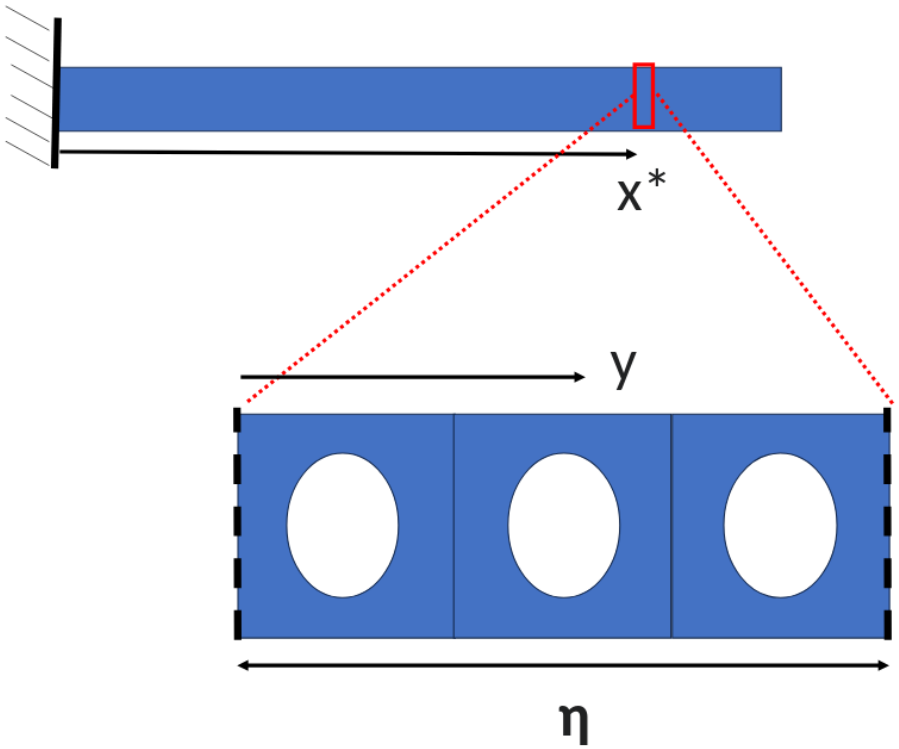
- Work done on a structure by external forces equals stored strain energy
- Matching force-displacement relation gives an energy equivalence between the response of the true and homogenized material
- Effective spring constant can also be derived from energy equivalence
- How can computation of homogenized modulus generalize to other loading conditions?

# From heterogeneous material to microstructure



- Heterogeneous material becomes a new homogeneous material in a limiting sense
- The stress-strain relation at each point is governed by a "cell" of the "microstructure"
- Apply similar analysis as above to cell as opposed to whole structure

# Cell problem




- Pick out cell with width $\eta$ at arbitrary point $x^*$
- Every point $x$ has corresponding microstructure cell
- Define a new cell coordinate $y \in [0, 1]$ such that $x = x^* + \eta y$
- Approximate the displacement with a Taylor series over the cell
  $u(x) = u(x^*) + \frac{\partial u}{\partial x}(x^*)(x - x^*) \implies u(y) = u(x^*) + \frac{\partial u}{\partial x}\eta y$

# Cell problem

Define $\epsilon = \frac{\partial u}{\partial x}(x^*)$. The displacement across the cell given this strain is $\eta\epsilon$. We want to compute the stress response of the cell. The displacement of the cell is written $U(y) = \epsilon\eta y + \Psi(y)$ where $\Psi$ accounts for displacement fluctuations induced by the microstructure. Thus,

$$\frac{\partial}{\partial y}\left(E(y)\frac{\partial}{\partial y}(\epsilon\eta y + \Psi)\right) = 0$$

$$\frac{\partial}{\partial y}\left(E(y)\frac{\partial \Psi}{\partial y}\right) = -\frac{\partial E}{\partial y}\epsilon\eta$$

Use linearity of the problem w.r.t. $\epsilon\eta$ to define a "unit response" $\chi$:

$$\frac{\partial}{\partial y}\left(E(y)\frac{\partial \chi}{\partial y}\right) = -\frac{\partial E}{\partial y}$$

$$\implies U(y) = \epsilon\eta(y + \chi(y))$$

# Effective stress response

The "corrector" $\chi(y)$ is computed with $\chi(0) = \chi(1) = 0$ which ensures that the $U(0) = 0$ and $U(1) = \epsilon\eta$. The boundary condition $U(0) = 0$ zeros a rigid body mode of the cell, as the stress only depends on the difference in displacement between the two boundaries. The stress in the cell is given by

$$\sigma(y) = E(y)\frac{\partial U}{\partial y}\frac{\partial y}{\partial x} = \epsilon E(y)\left(1 + \frac{\partial \chi}{\partial y}\right)$$

Note that we need to take derivatives w.r.t. $x$ to compute the strain. We claim that the effective stress response of the cell (as seen by the structure) is the cell average:

$$\sigma(x^*) = \epsilon \int_0^1 E(y)\left(1 + \frac{\partial \chi}{\partial y}\right) dy = E^*\epsilon$$

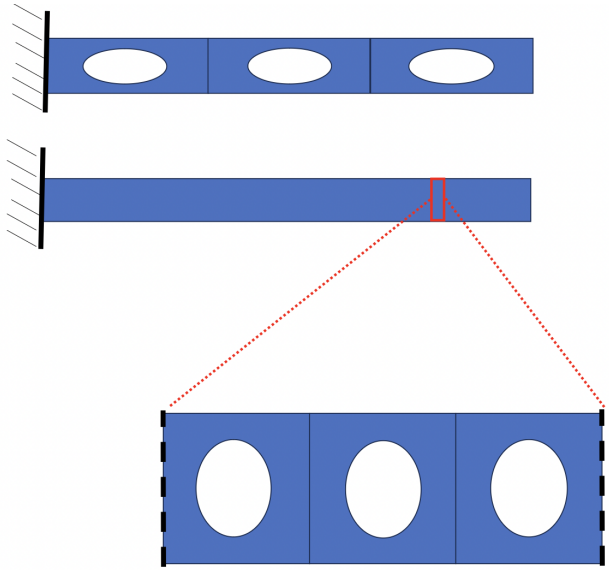
# Equivalence of approaches

When coarse-graining an entire structure with heterogeneous material, the homogenized modulus was the harmonic mean. When computing the effective stress response of the microstructure, the homogenized modulus had a different form. It can be shown that

$$E^* = \int_0^1 E(y)\left(1 + \frac{\partial \chi}{\partial y}\right) dy = \frac{1}{\int_0^1 \frac{dy}{E(y)}}$$

by using the definition of $\chi$. Thus the two methods agree. This shows that stress averaging gives rise to energy equivalence between the cell and homogenized problems.

# Scale separation

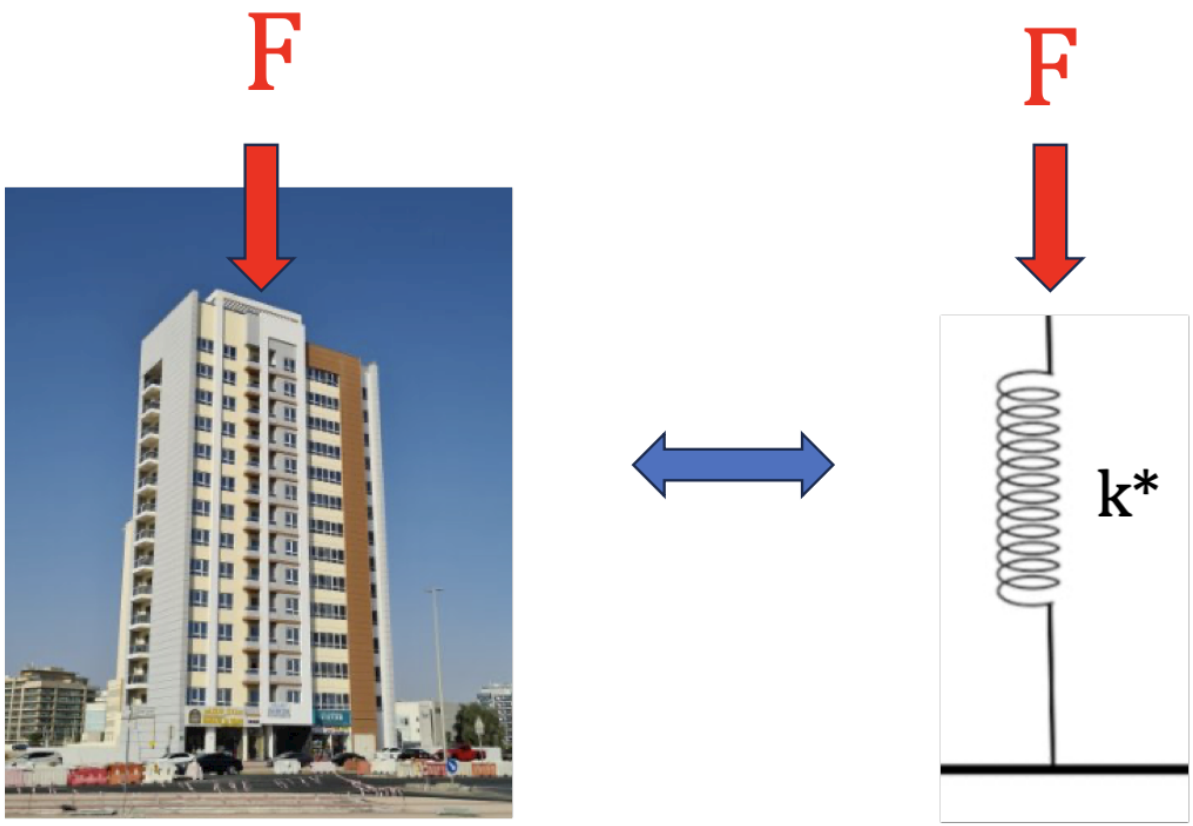


- Scale separation is the idea that structure comprises many repeating cells of microstucture ($\eta << 1$)
- The top structure does not have separated scales, the bottom does
- If the top structure is treated as a single cell, it has the same homogenized modulus as the bottom structure
- The "mean" response is always computed accurately regardless of scale separation (see this plot)
- **Fluctuations become small with separated scales**

# Why is any of this helpful?

- Still have to fully resolve the microstructure to compute the homogenized response
- Can do this in an "offline" way; if the microstructure is the same everywhere, only one solve is needed for $\chi(y)$
- Even if microstructure varies from one cell to the next, decoupling scales is advantageous from the standpoint of computational cost

# Anything can be homogenized!




- It is a question of how much information is lost in doing so...

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# Periodic homogenization / method of multiple scales

"The first move [in a multiscale expansion] . . . is really kind of bizarre. I cant give you good intuition for it, because I don't have it myself. Even though I have been thinking about this for 30 years."

— Steven Strogatz (famous mathematician), found here

- Periodic homogenization is an application of perturbation theory (for a nice introduction, check out the videos in this series)
- Strange piece of mathematics, but very formulaic once you are familiar with it
- Leads to exactly the same cell problem and homogenized modulus derived above

# Set up

Introduce a new coordinate $y = x/\eta$ where $\eta$ is a small parameter which specifies the size of the microstructure cell. The coordinate $x$ is the slow variable, or "macroscale" coordinate, whereas $y$ is the fast variable, or "microscale" coordinate. We assume that the displacement can be represented as

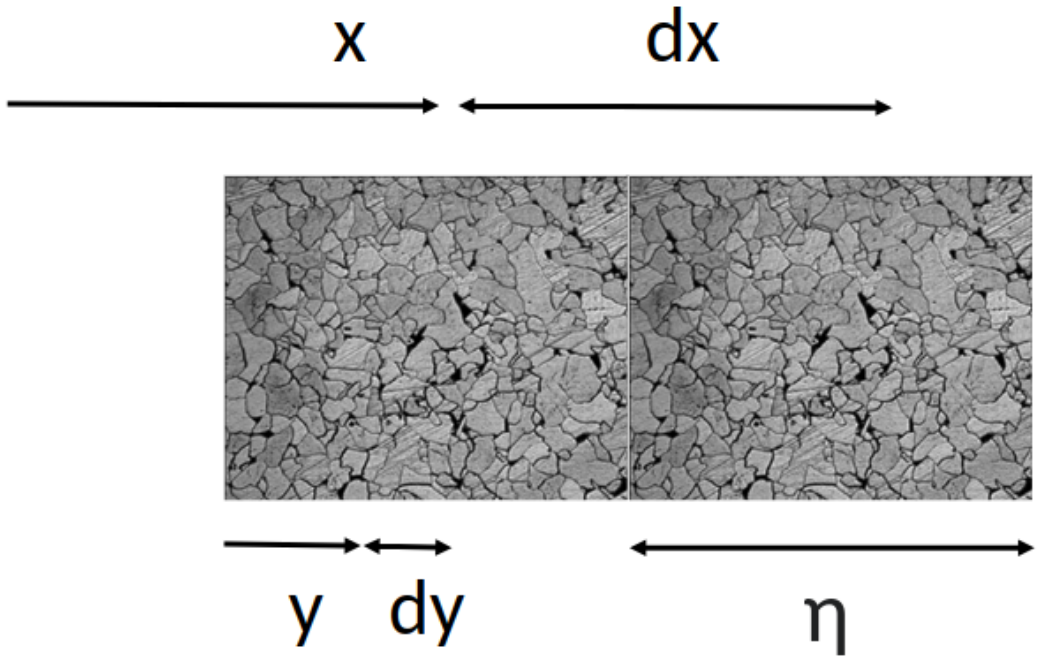
$$u^\eta(x, y) = u^0(x) + \eta u^1(x, y)$$

where the superscript $\eta$ indicates a "multiscale" quantity, meaning that it varies on both the macro and micro scale. The displacement is made up of a macroscopic part $u^0$ and a correction $u^1$ with slow and fast variations. The multiscale derivative is given by

$$\frac{d}{dx^\eta} := \frac{\partial}{\partial x} + \frac{1}{\eta}\frac{\partial}{\partial y}$$

Think $\frac{du^\eta}{dx^\eta} = \frac{\partial u^\eta}{\partial x} + \frac{\partial u^\eta}{\partial y}\frac{\partial y}{\partial x}$, e.g. the total rate of change of the displacement w.r.t. space involves contributions from both scales.

# What is going on?




- The additive decomposition is not too strange
- Definition of derivative more-or-less follows from treating microscale and macroscale coordinates as independent...this assumption of independence is the weirdness Strogatz is referring to!
- The argument is that $x$ and $y = x/\eta$ are such different sizes that a change in $y$ does not affect $x \implies x + dy \approx x$
- But why does changing $x$ not change $y$?

# Periodicity

- It is not the case that $y + dx \approx y$ because a small change in $x$ leads to large changes in $y$
- If all microscale quantities are periodic in $\eta$, jumping from one block of microstructure to the next does not affect their value
- Because the macroscale coordinate cannot vary within the microstructure, it is as if $dx = n\eta$ where $n$ is an integer
  $\implies mod(y + dx, \eta) = y$
- Even though the numerical value of $y$ changes with $x$, the fast quantities have no sensitivity to $x$ because of periodicity
- **Assuming that the material varies periodically on the small scale is fundamental to this approach**

# Navier equation

The usual strong form of the governing equation for linear elasticity is given by

$$\frac{\partial \sigma_{ij}}{\partial x_j} + b_i = \frac{\partial}{\partial x_j}\left( C_{ijk\ell} \frac{\partial u_k}{\partial x_\ell} \right) + b_i = 0$$

This makes use of the elastic constitutive relation, the strain-displacement relation, and symmetries of the constitutive tensor. In the multiscale setting, we say that the constitutive tensor oscillates on the microscale. The multiscale Navier (displacement) equation is

$$\frac{d}{dx_j^\eta}\left( C_{ijk\ell}(y) \frac{du_k^\eta}{dx_\ell^\eta} \right) + b_i = 0$$

$$\frac{d}{dx_i^\eta} = \frac{\partial}{\partial x_i} + \frac{1}{\eta}\frac{\partial}{\partial y_i}, \qquad u_j^\eta = u_j^0(x) + \eta u_j^1(x, y)$$

# Plug in, expand, and group terms

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

Argue that equations at given powers of $\eta$ need to be satisfied independently. This move is strange, but a central tenet of perturbation techniques. Given that $\eta << 1$, the terms have very different magnitudes. In first-order homogenization, we only look at the first two powers of $\eta$:

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

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

# Cell problem

The first equation is the cell problem. The term $\partial u_k^0/\partial x_\ell$ is the macroscopic strain and is constant over the cell (no $y$ dependence). The microscale displacement is forced by the macroscopic strain. We can use linearity to write

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

where $\chi_{imn}$ is a displacement fluctuation over the microstructure (analogous to 1D case above). The "corrector" $\chi_{imn}$ must be computed from the cell problem for each unit macroscopic strain component. We can plug this expression for $u^1$ into the $\eta^0$ (macroscale) equation and obtain

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

The body force is purely macroscopic (no $y$ dependence) but the other terms vary on the microscale. This equation cannot be satisfied for all $y$.

# Averaging

We can average this equation over the microstructure to rid of the $y$ dependence. This is analogous to averaging the cell stress in the 1D case. Note that one way to deduce the appropriateness of this averaging operation is through a technical condition called "solvability" from perturbation theory. The corrector varies on the small scale only and is periodic. Averaging over the microscale, we get

$$\left(\int C_{ijk\ell}\,dy\right)\frac{\partial^2 u_k^0}{\partial x_j \partial x_\ell} + \left(\int C_{ijk\ell}\frac{\partial \chi_{kab}}{\partial y_\ell}\,dy\right)\frac{\partial^2 u_a^0}{\partial x_j \partial x_b} + b_i = 0$$

$$\frac{\partial^2 u_a^0}{\partial x_b \partial x_\ell}\int \frac{\partial}{\partial y_j}(C_{ijk\ell}\chi_{kab})\,dy = 0$$

The latter equation follows from the periodicity of $C_{ijk\ell}$ and $\chi_{kab}$. The integral of the divergence of a periodic function is zero (shown with divergence theorem).

# Homogenized constitutive tensor

With some shuffling of indices, the macroscale equation can be written as

$$\left( \int C_{ijk\ell} \left( \delta_{ka}\delta_{\ell b} + \frac{\partial \chi_{kab}}{\partial y_\ell} \right) dy \right) \frac{\partial^2 u_a^0}{\partial x_j \partial x_b} + b_i = 0 \tag{2}$$

Recognize this as the Navier equation for a constant material. This constant material is the homogenized tensor

$$C^H_{ijab} := \int C_{ijk\ell} \left( \delta_{ka}\delta_{\ell b} + \frac{\partial \chi_{kab}}{\partial y_\ell} \right) dy \tag{3}$$

# Energy equivalence

The multiscale displacement at an arbitrary macroscale point $x^*$ is

$$u_i^\eta = u^0(x^*) + \frac{\partial u_i^0}{\partial x_j}(x^*)y_j + \chi_{imn}(y)\frac{\partial u_m^0}{\partial x_n}(x^*)$$

The corresponding stresses and strains are those which arise from these displacements. We want to show that

$$\int \sigma_{ij}^\eta \epsilon_{ij}^\eta dy = \sigma_{ij}^0 \epsilon_{ij}^0$$

where superscript 0 indicates a purely macroscale quantity and superscript $\eta$ indicates a quantity varying on both scales. Start with the LHS and use the definition of strain, stress equilibrium, and the divergence theorem:

$$\int \sigma_{ij}^\eta \epsilon_{ij}^\eta dy = \int \sigma_{ij}^\eta \frac{\partial u_i^\eta}{\partial y_j} dy = \int \frac{\partial}{\partial y_j}(\sigma_{ij}^\eta u_i^\eta) dy = \int \sigma_{ij}^\eta n_j u_i^\eta ds$$

# Energy equivalence

$$= \int \sigma_{ij}^{\eta} n_j \left( u_i^0(x^*) + \frac{\partial u_i^0}{\partial x_j}(x^*) y_j \right) ds + \left( \int \sigma_{ij}^{\eta} n_j \chi_{imn} ds \right) \frac{\partial u_m^0}{\partial x_n}(x^*)$$

Periodic boundary conditions on the corrector $\chi_{imn}$ ensure that the second integral is zero. Using the divergence theorem, the first term becomes

$$\int \frac{\partial}{\partial y_j} \left( \sigma_{ij}^{\eta} \left( u_i^0(x^*) + \frac{\partial u_i^0}{\partial x_j}(x^*) y_j \right) \right) dy = \left( \int \sigma_{ij}^{\eta} dy \right) \frac{\partial u_i^0}{\partial x_j}$$

$$\implies \sigma_{ij}^0 = \int \sigma_{ij}^{\eta} dy$$

$$\sigma_{ij}^{\eta} = C_{ijk\ell}(y) \frac{\partial u_k^{\eta}}{\partial y_\ell} = \left( C_{ijk\ell}(y) \left( \delta_{km}\delta_{\ell n} + \frac{\partial \chi_{kmn}}{\partial y_\ell} \right) \right) \frac{\partial u_m^0}{\partial x_n}$$

# Energy equivalence

- This shows that averaging the stress over the microstructure is the correct thing to do from an energy standpoint
- Also shows that homogenized tensor can be derived from energy equivalence alone
- Periodic boundary conditions were used to make an inconvenient term disappear

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# Nonlinear homogenization

The macroscale stress equilibrium equation is

$$\frac{\partial \langle \sigma \rangle}{\partial x} = 0$$

The homogenized stress $\langle \sigma \rangle$ is determined from the cell problem. The cell problem is governed by nonlinear physics

$$\mathcal{N}\Big(u(y)\Big) = 0$$

The cell has size $\eta$ and is driven by a linearized displacement and fluctuation $\Psi$:

$$\mathcal{N}(\epsilon y + \Psi) = 0$$

The cell problem is driven by the macroscopic strain $\epsilon$ and is used to determine the microscale fluctuation $\Psi(y)$.

# Nonlinear homogenization

Once we have the corrector, we can compute the stress with

$$\sigma(y) = f(\epsilon y + \Psi)$$

then average over the cell to get the effective response. Perturbation methods are not feasible to carry out for general nonlinear equations (try it, you'll see why). To construct a cell problem, take a "chunk" of heterogeneous microstructure, compute its stress response to a constant strain, then average this stress. This is the macroscopic stress that the structure sees. When there is not scale separation, constructing a cell problem amounts to linearizing the displacement over cells of finite size. This fits in nicely with typical finite element interpolations.

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# Mandel-Hill condition

The Mandel-Hill condition acts as a coarse-graining criterion for nonlinear problems. Say that we are working with hyperelasticity. Mandel-Hill requires

$$\int P_{ij}^{\eta} \delta F_{ij}^{\eta} dy = P_{ij}^{0} \delta F_{ij}^{0}$$

This is a slightly different condition than energy equivalence. It says that the variations of the macro- and averaged microscale energies agree. In a sense, this condition posits equivalent behavior in a numerical setting. n practice, it can be used to determine the boundary conditions on the microscale, and the upscaling relation $P_{ij}^{0} = f(P_{ij}^{\eta})$. Sorting out whether the Mandel-Hill condition is satisfied for a given model needs to be done on a case-by-case basis.

# Mandel-Hill for hyperelasticity

Using the definition of the deformation gradient, the product rule, stress equilibrium, and the divergence theorem, we have

$$\int P_{ij}^{\eta} \delta F_{ij}^{\eta} dy = \int \frac{\partial}{\partial y_j} (P_{ij}^{\eta} \delta x_i^{\eta}) dy = \int P_{ij}^{\eta} N_j \delta x_i^{\eta} ds$$

The quantity $x_i^{\eta}$ is the deformed position of a point in the microscale. We can write

$$\Delta x_i^{\eta} = F_{ij}^0 \Delta X_j^{\eta} + w_i$$

where $w_i$ is a microscale fluctuation. This means that

$$\delta x_i^{\eta} = \delta F_{ij}^0 X_j^{\eta} + \delta w_i$$

# Boundary conditions and upscaling

Plugging this in, we obtain

$$= \left( \int P_{ij}^{\eta} N_j X_k^{\eta} ds \right) \delta F_{ik}^0 + \int P_{ij}^{\eta} N_j \delta w_i ds$$

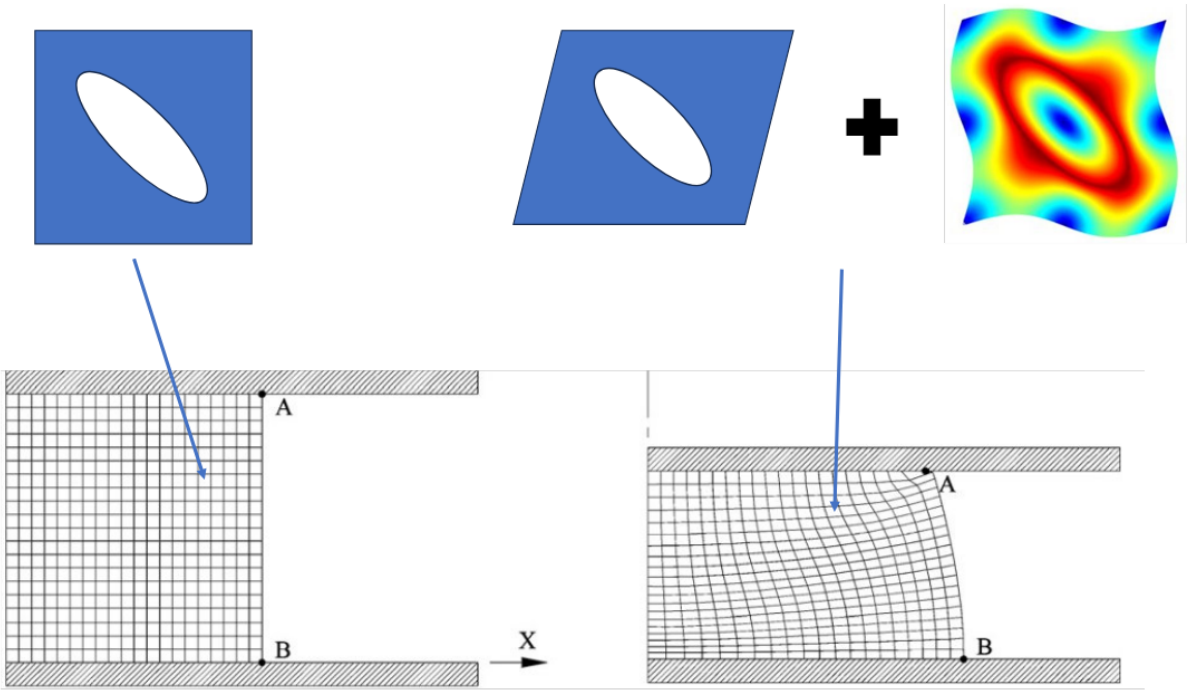
When the microscale fluctuation is zero along the boundary, we have $\delta w_i = 0$. When the stress is zero along the boundary, we have $P_{ij}^{\eta} N_j = 0$. When the displacement is periodic, we also have that $\int P_{ij}^{\eta} N_j \delta w_i ds = 0$. When any one of these three boundary conditions are used, the first term can be written as

$$= \left( \int \frac{\partial}{\partial y_j} (P_{ij}^{\eta} X_k^{\eta}) dy \right) \delta F_{ik}^0 = \left( \int P_{ik}^{\eta} dy \right) \delta F_{ik}^0$$

$$\implies P_{ik}^0 = \int P_{ik}^{\eta} dy$$

# Boundary conditions

Zero Neumann, zero Dirichlet, and periodic boundary conditions are all compatible with Mandel-Hill when upscaling with stress averages. What do we choose and why? Consider homogenizing an element of a finite element mesh. The element is driven by a constant deformation gradient and we compute the effective stress.



# Dirichlet too stiff, Neumann too soft

A constant deformation gradient corresponds to a displacement field within the element of

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} ax + by \\ cx + dy \end{bmatrix}$$

This is a combination of constant normal strains in both directions and simple shear. Each element becomes a parallelogram at the macroscale. The microscale displacement is zero at the boundary nodes but there are three choices of BC's to govern the displacement along element vertices. Remember that in reality this square of material is confined by material on all sides. Zero displacement BC's model the confinement as totally rigid. Zero Neumann models no confinement. We don't actually know what the material surrounding the element is doing when computing its effective stress response. Periodic boundary conditions are a compromise, modeling partial confinement.

# Elements don't fit together

In 1D, there is no issue with pulling a cell out of the structure, computing the effective stress as a function of macro strain, and putting it back in. In 2D and 3D, we pull an element out (say an element in a finite element mesh), drive it with a constant strain, compute its effective stress response, then put it back into the mesh. We also do this with the surrounding elements. The finite element basis functions representing the macro displacement ensure continuity along vertices, but no such condition is imposed on the microscale displacement fields. The elements don't fit together! This is because the displacements from different cell problems are not compatible with each other.

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# Conclusion

- In my experience, it is necessary to spend a lot of time thinking about these things to make any sense of it
- Learning about perturbation theory in general is helpful
- 1D problems are useful for building intuition

# Citing images in order of appearance

- Slide 1: wing, metal, microstructure, atoms
- Slide 2: earth, diffusion
- Slide 3: coffee
- Slide 6: particles
- Slide 8: microstructures
- Slide 11: stress cube
- Slide 14: circuit, denoising, Markov, history
- Slide 23: spring
- Slide 33: building
- Slide 54: mesh