Title: The Tyranny of Scales

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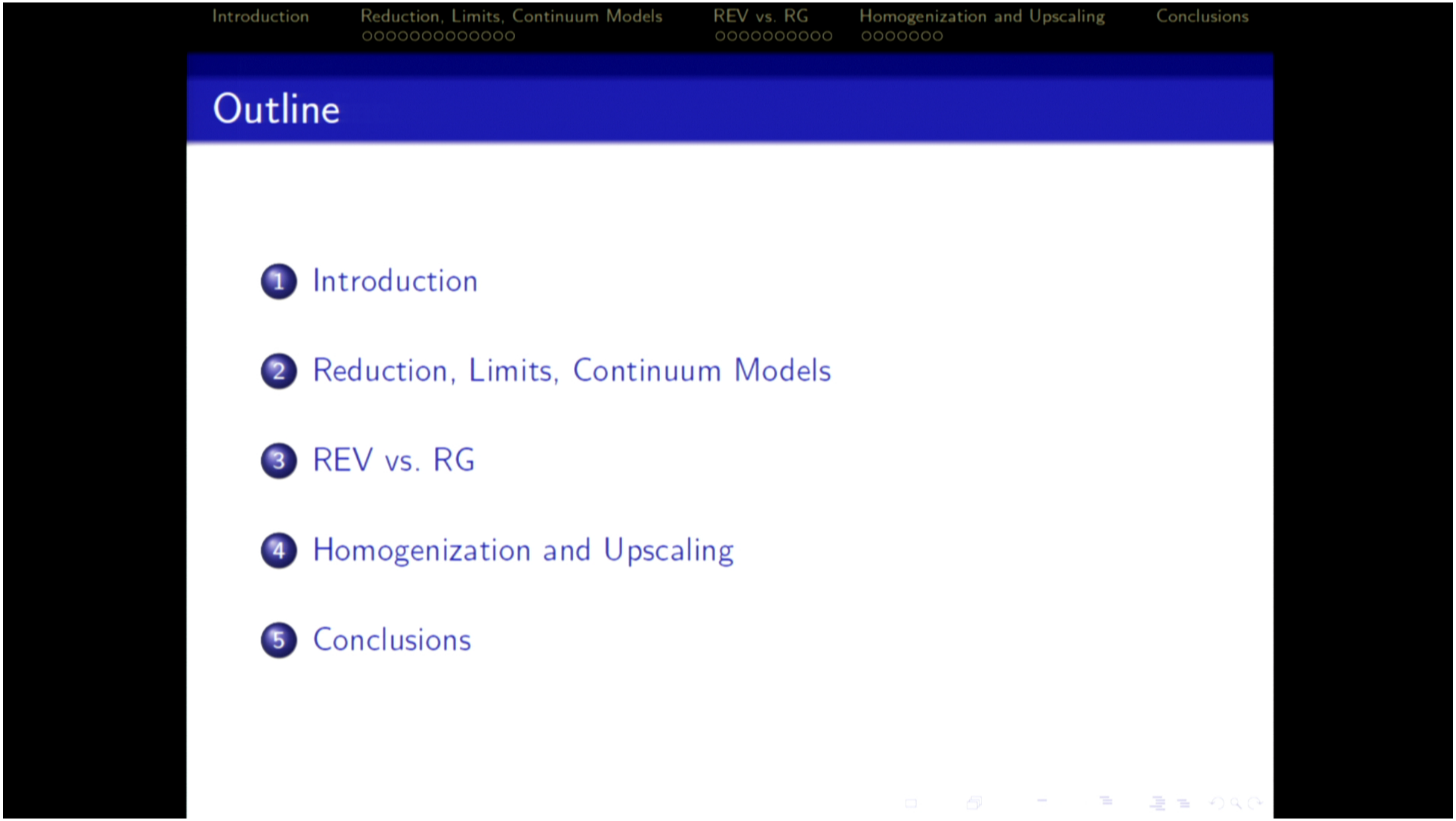
Abstract: How can one model the behavior of materials that display radically different, dominant behaviors at different length scales. Although we have good models for material behaviors at small and large scales, it is often hard to relate these scale-based models to one another. Macroscale (effective) models represent the integrated effects of very subtle factors that are practically invisible at the smallest, atomic, scales. For this reason it has been notoriously difficult to model realistic materials with a simple bottom-up-from-the-atoms strategy. The widespread failure of that strategy forced physicists interested in overall macro-behavior of materials toward completely top-down modeling strategies familiar from traditional continuum mechanics. The problem of the ``tyranny of scales" asks whether we can exploit our rather rich knowledge of intermediate micro- (or meso-) scale behaviors in a manner that would allow us to bridge between these two dominant methodologies. Macroscopic scale behaviors often fall into large common classes of behaviors such as the class of isotropic elastic solids, characterized by two phenomenological parameters---so-called elastic coefficients. Can we employ knowledge of lower scale behaviors to understand this universality---to determine the coefficients and to group the systems into classes exhibiting similar behavior?



Outline

1. Introduction
2. Reduction, Limits, Continuum Models
3. REV vs. RG
4. Homogenization and Upscaling
5. Conclusions

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- To design materials like steel girders one must attempt to deal with phenomena across 10+ orders of magnitude in spatial scales.

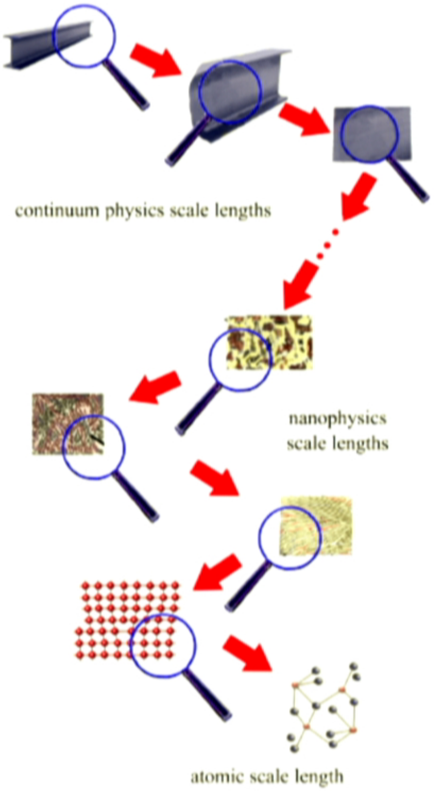
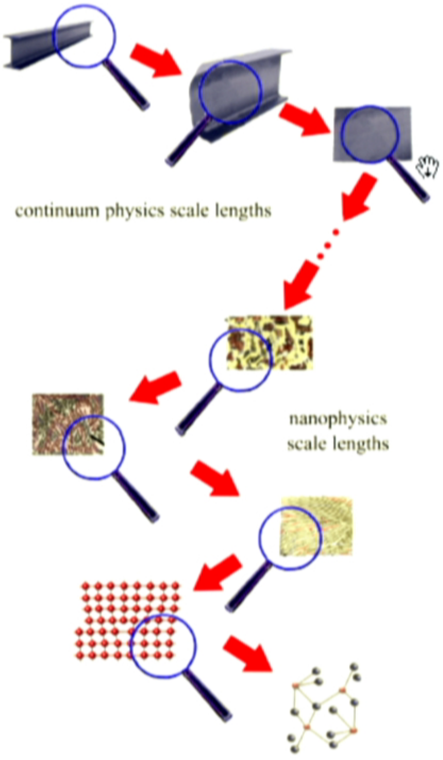


Figure: Steel—Widely Separated Scales



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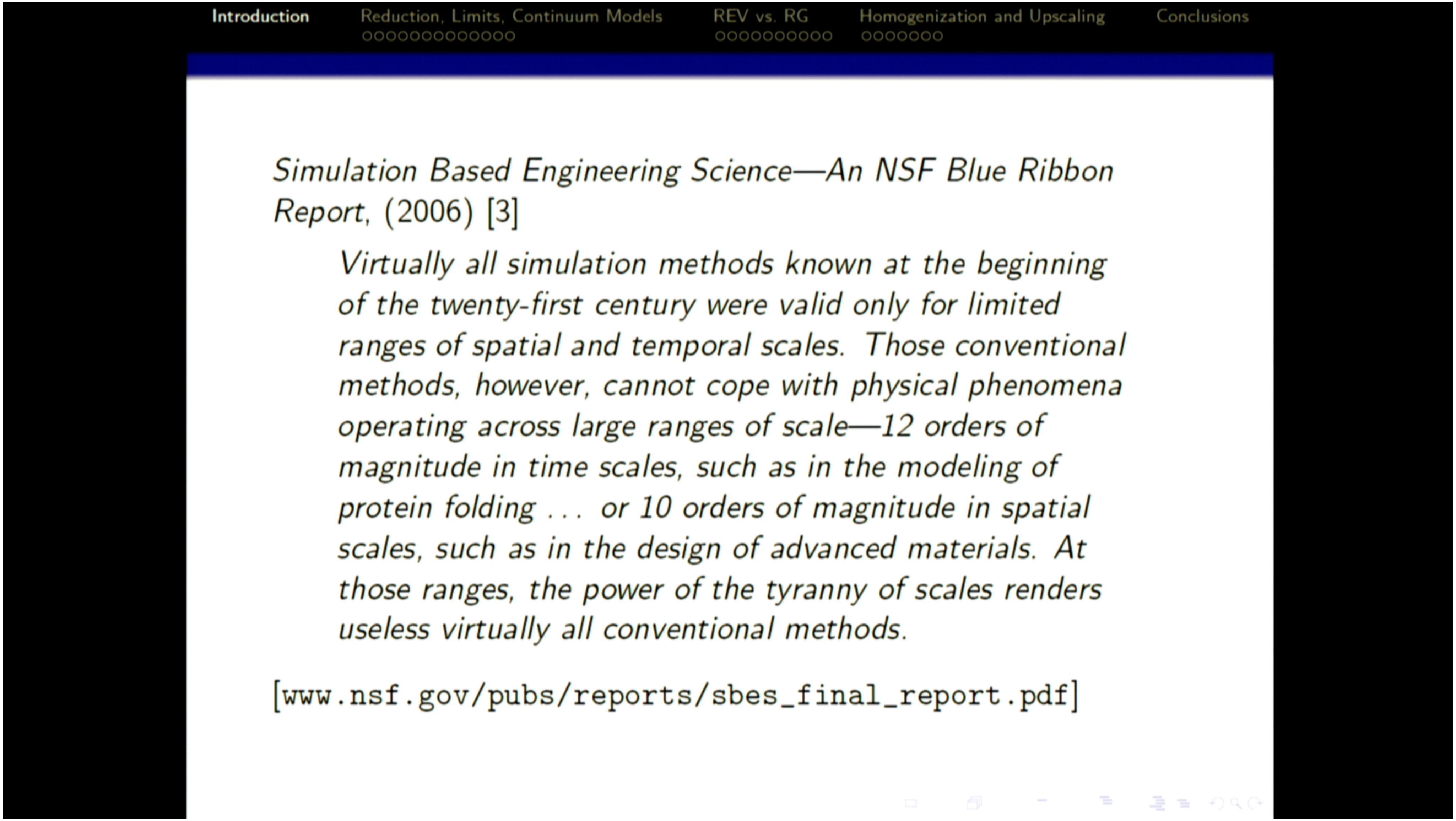

Simulation Based Engineering Science—An NSF Blue Ribbon Report, (2006) [3]

> *Virtually all simulation methods known at the beginning of the twenty-first century were valid only for limited ranges of spatial and temporal scales. Those conventional methods, however, cannot cope with physical phenomena operating across large ranges of scale—12 orders of magnitude in time scales, such as in the modeling of protein folding . . . or 10 orders of magnitude in spatial scales, such as in the design of advanced materials. At those ranges, the power of the tyranny of scales renders useless virtually all conventional methods.*

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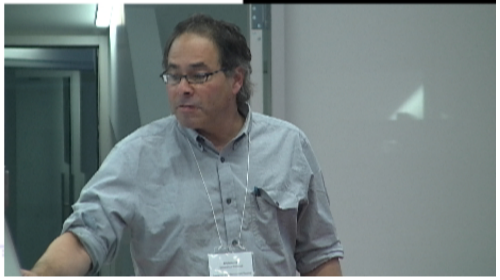
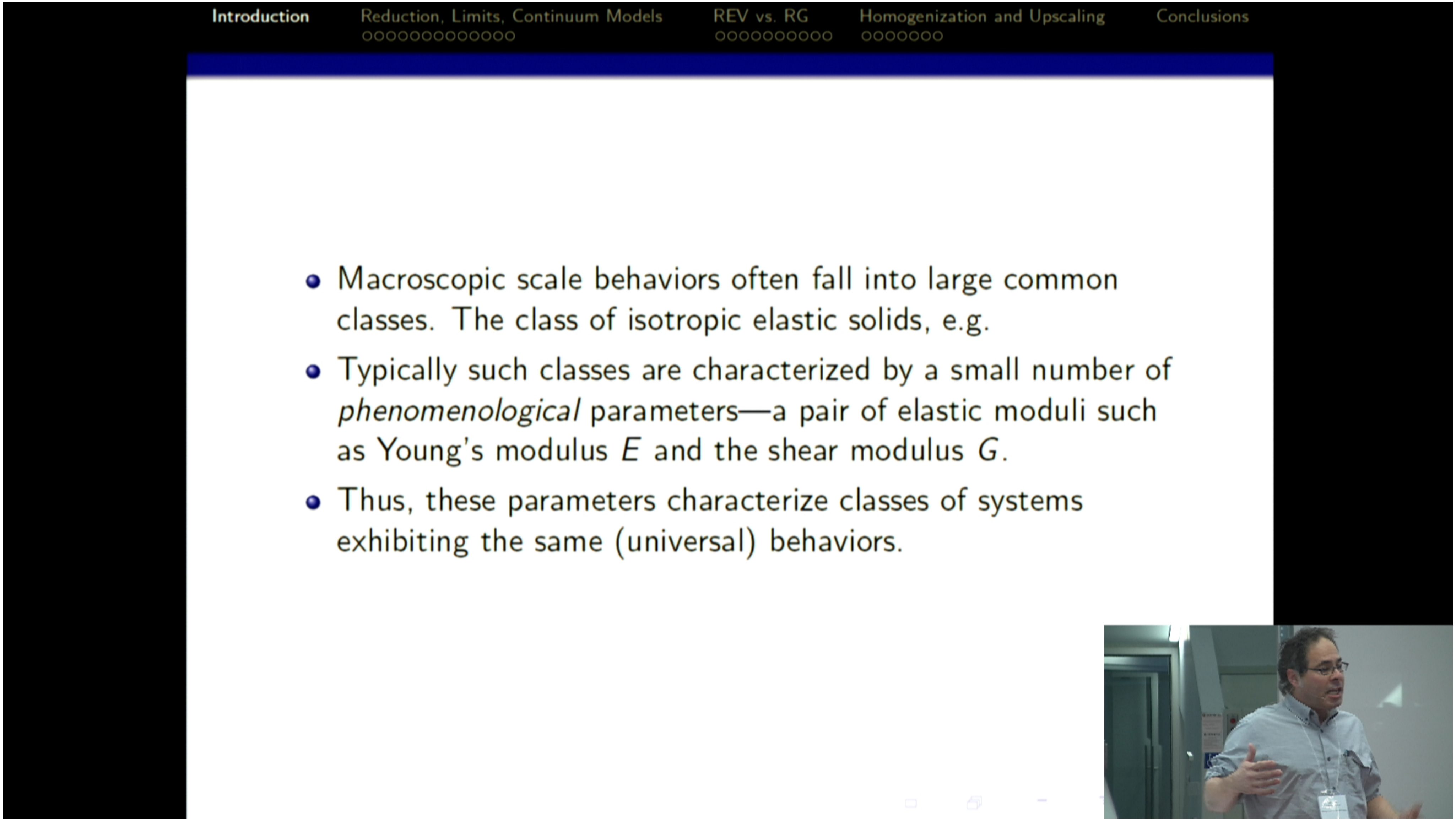
- Macroscopic scale behaviors often fall into large common classes. The class of isotropic elastic solids, e.g.





- Macroscopic scale behaviors often fall into large common classes. The class of isotropic elastic solids, e.g.
- Typically such classes are characterized by a small number of *phenomenological* parameters—a pair of elastic moduli such as Young's modulus E and the shear modulus G.
- Thus, these parameters characterize classes of systems exhibiting the same (universal) behaviors.

Universality Classes

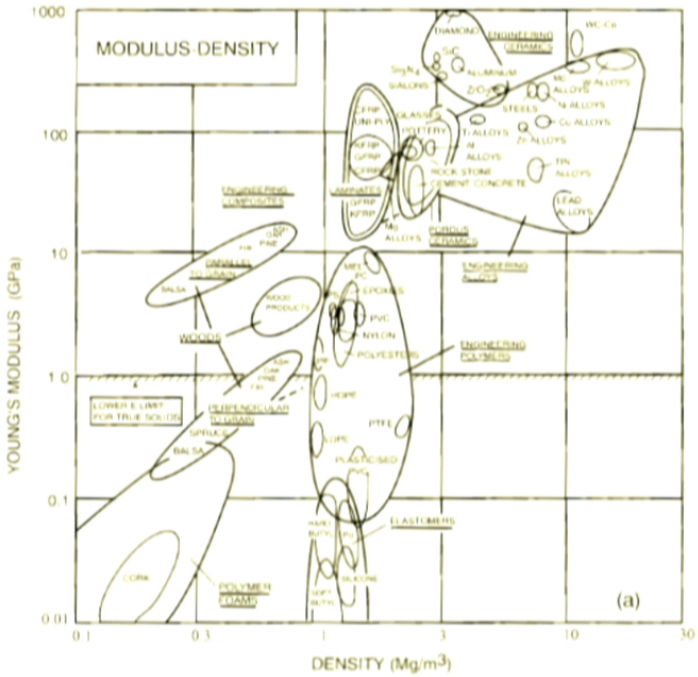
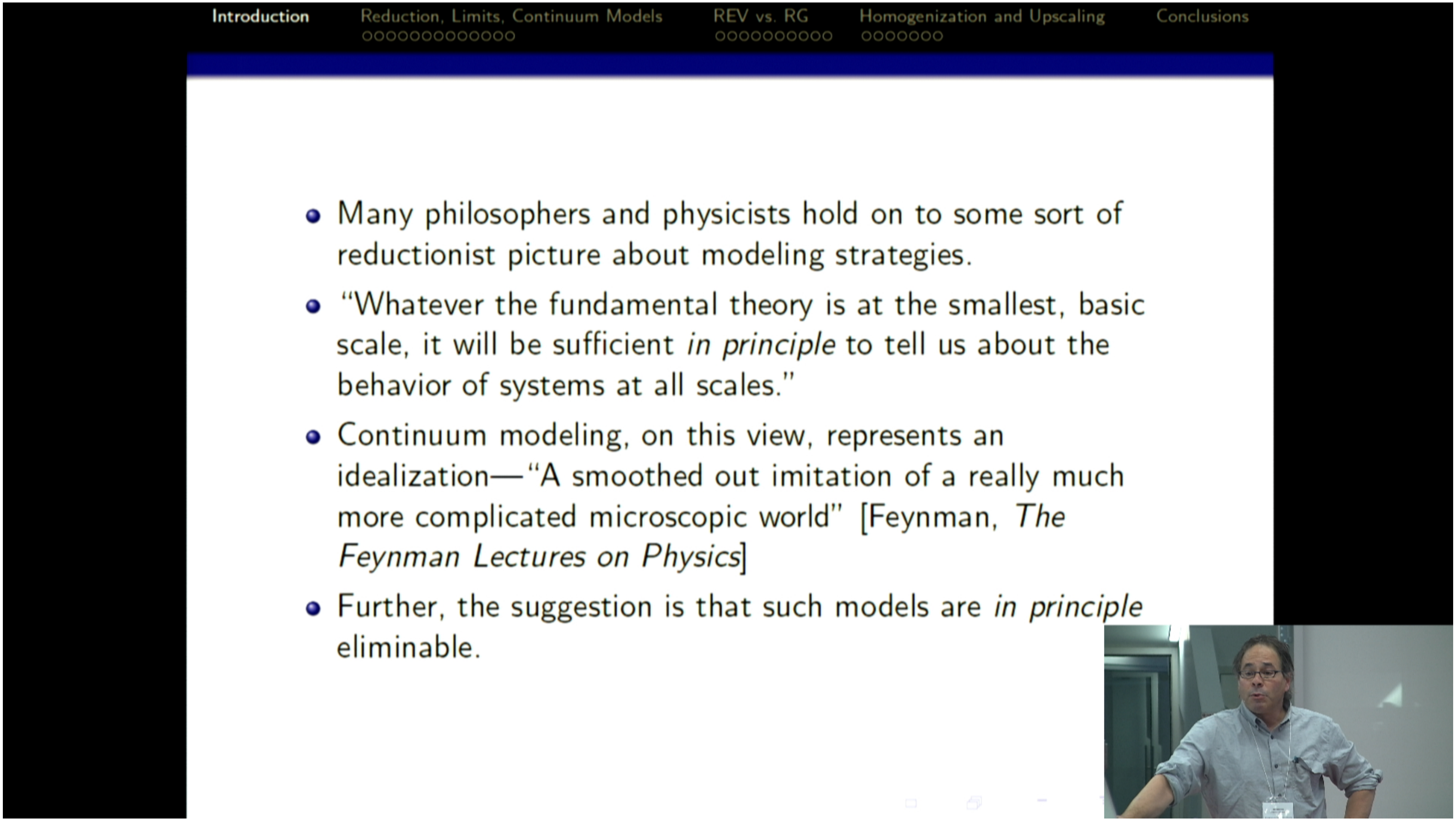


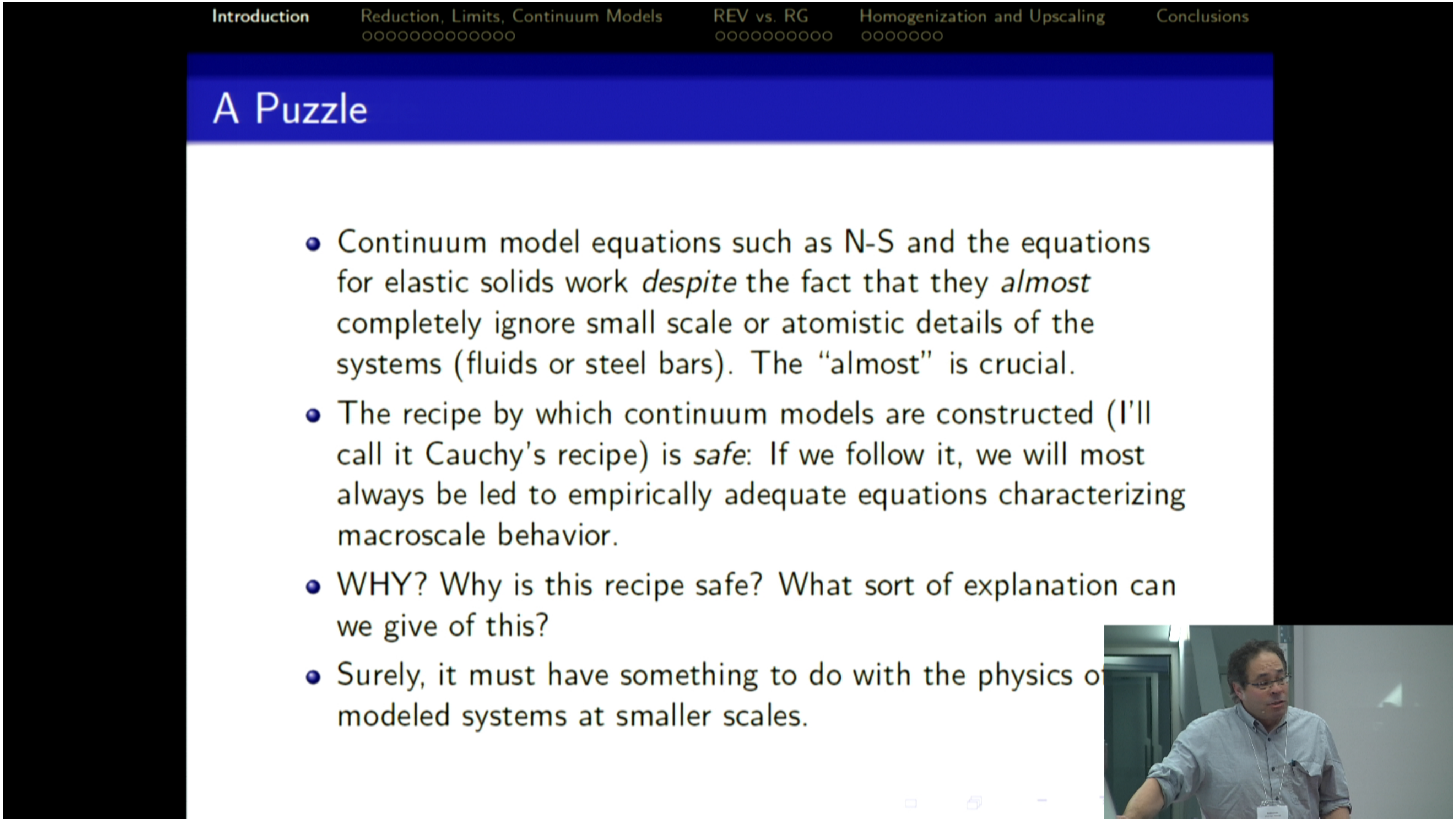
Figure: Elastic Properties of Materials. [After Ashby, [1]]

Fundamental Question

- How can we model and understand systems that exist across *extremely wide ranges of scale*?

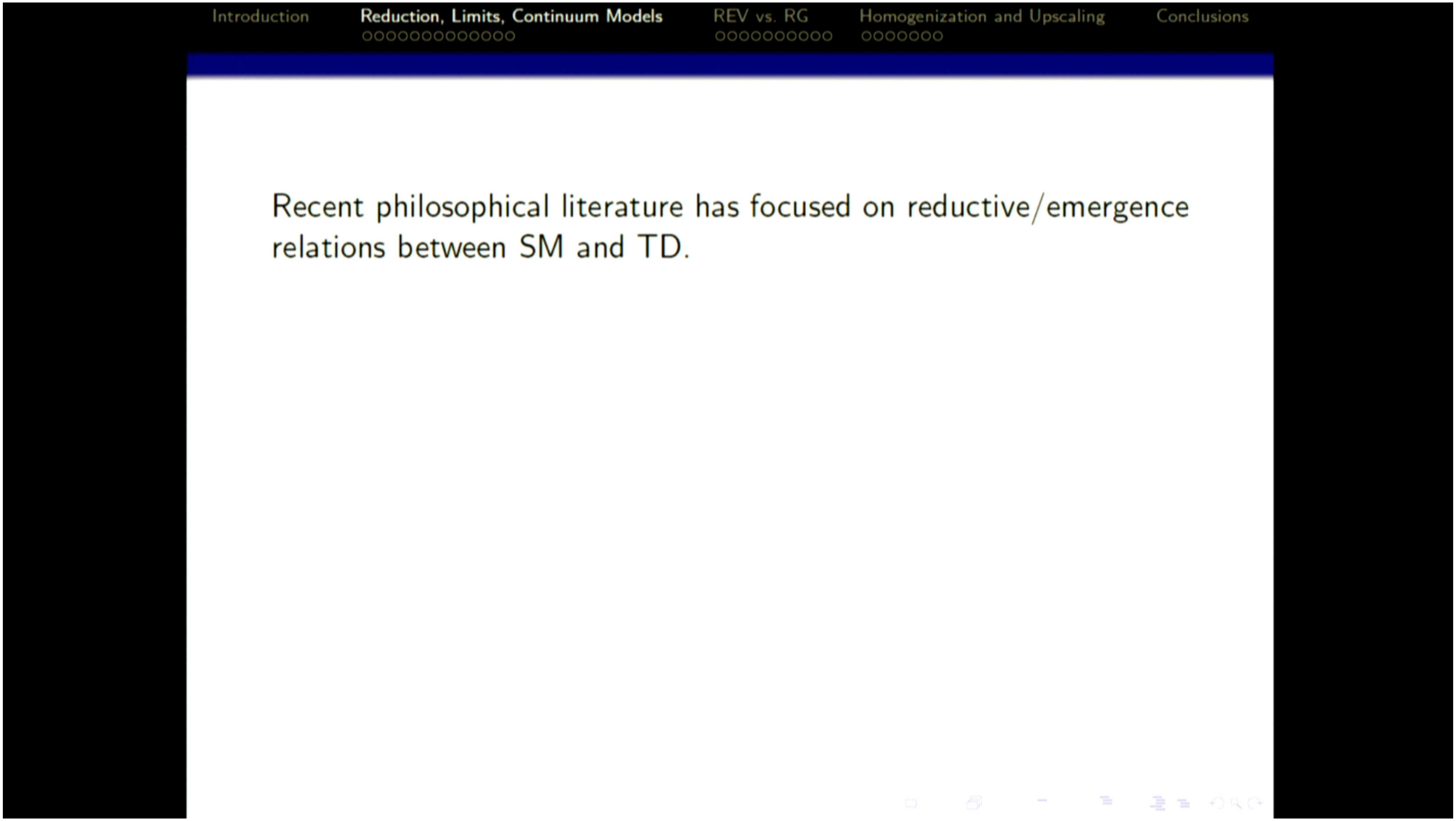


- Many philosophers and physicists hold on to some sort of reductionist picture about modeling strategies.
- “Whatever the fundamental theory is at the smallest, basic scale, it will be sufficient *in principle* to tell us about the behavior of systems at all scales.”
- Continuum modeling, on this view, represents an idealization—“A smoothed out imitation of a really much more complicated microscopic world” [Feynman, *The Feynman Lectures on Physics*]
- Further, the suggestion is that such models are *in principle* eliminable.



A Puzzle

- Continuum model equations such as N-S and the equations for elastic solids work *despite* the fact that they *almost* completely ignore small scale or atomistic details of the systems (fluids or steel bars). The “almost” is crucial.
- The recipe by which continuum models are constructed (I'll call it Cauchy's recipe) is *safe*: If we follow it, we will most always be led to empirically adequate equations characterizing macroscale behavior.
- WHY? Why is this recipe safe? What sort of explanation can we give of this?
- Surely, it must have something to do with the physics o
  modeled systems at smaller scales.



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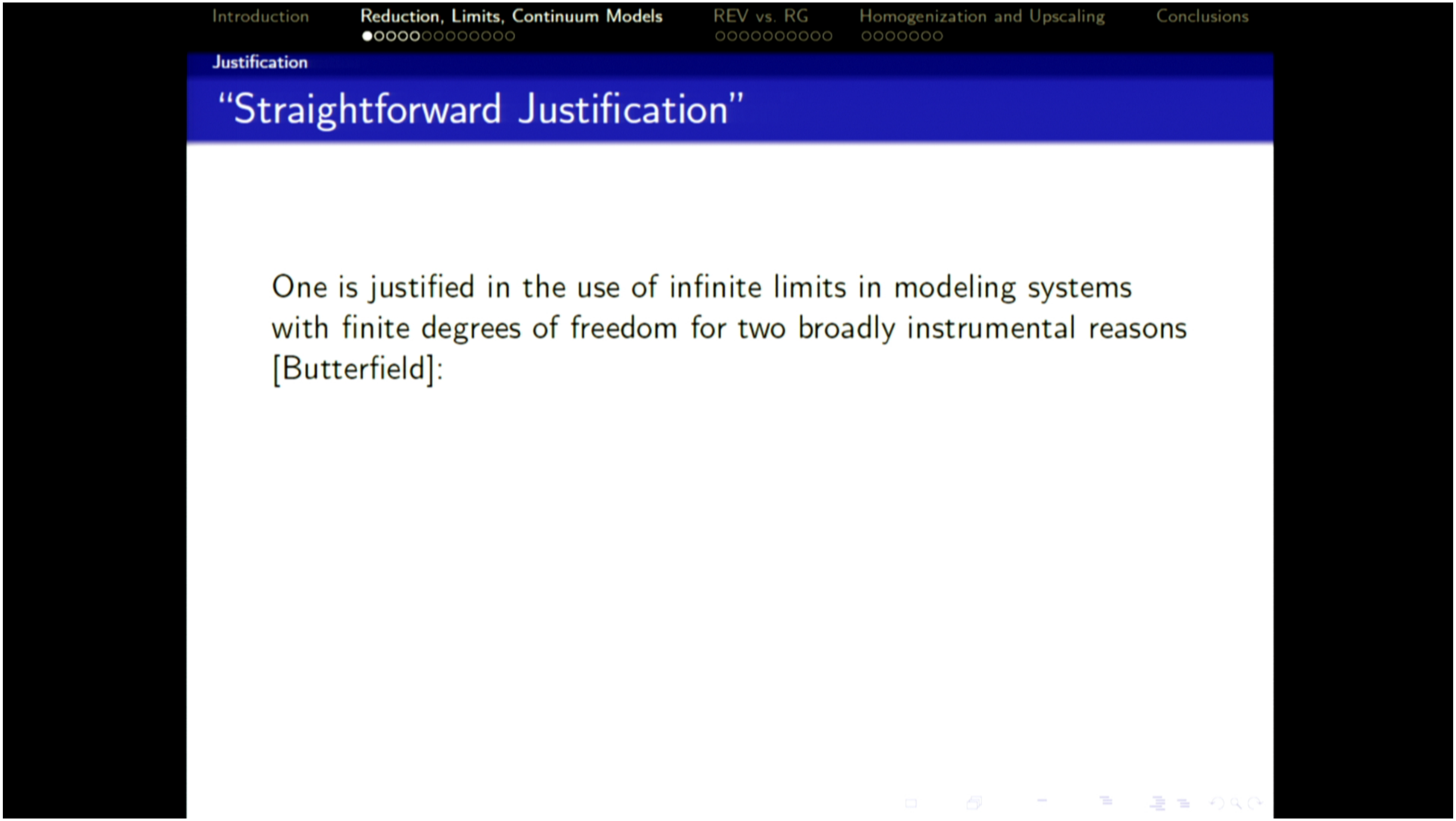
- One key component of this is the role of the thermodynamic limit in connecting these theories and in providing an understanding of phase transitions and critical phenomena.
- Kadanoff: “The existence of a phase transition requires an infinite system. No phase transtions occur in systems with a finite number of degrees of freedom.” [5, p. 238]

Here I consider the role of the thermodynamic limit in a more general context:

- How can one connect (upscale) from the finite statistical micro-theory to the continuum macro-theory.
- One prominent view (largely driven by this philosophical confusion, I think) is that the use of the continuum limit is to be justified *solely* on pragmatic grounds—it is a matter of convenience.



"Straightforward Justification"

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- Mathematical convenience.
- Empirical adequacy (up to a required accuracy).
    - Abstract from finitary effects—transients and edge/boundary effects.

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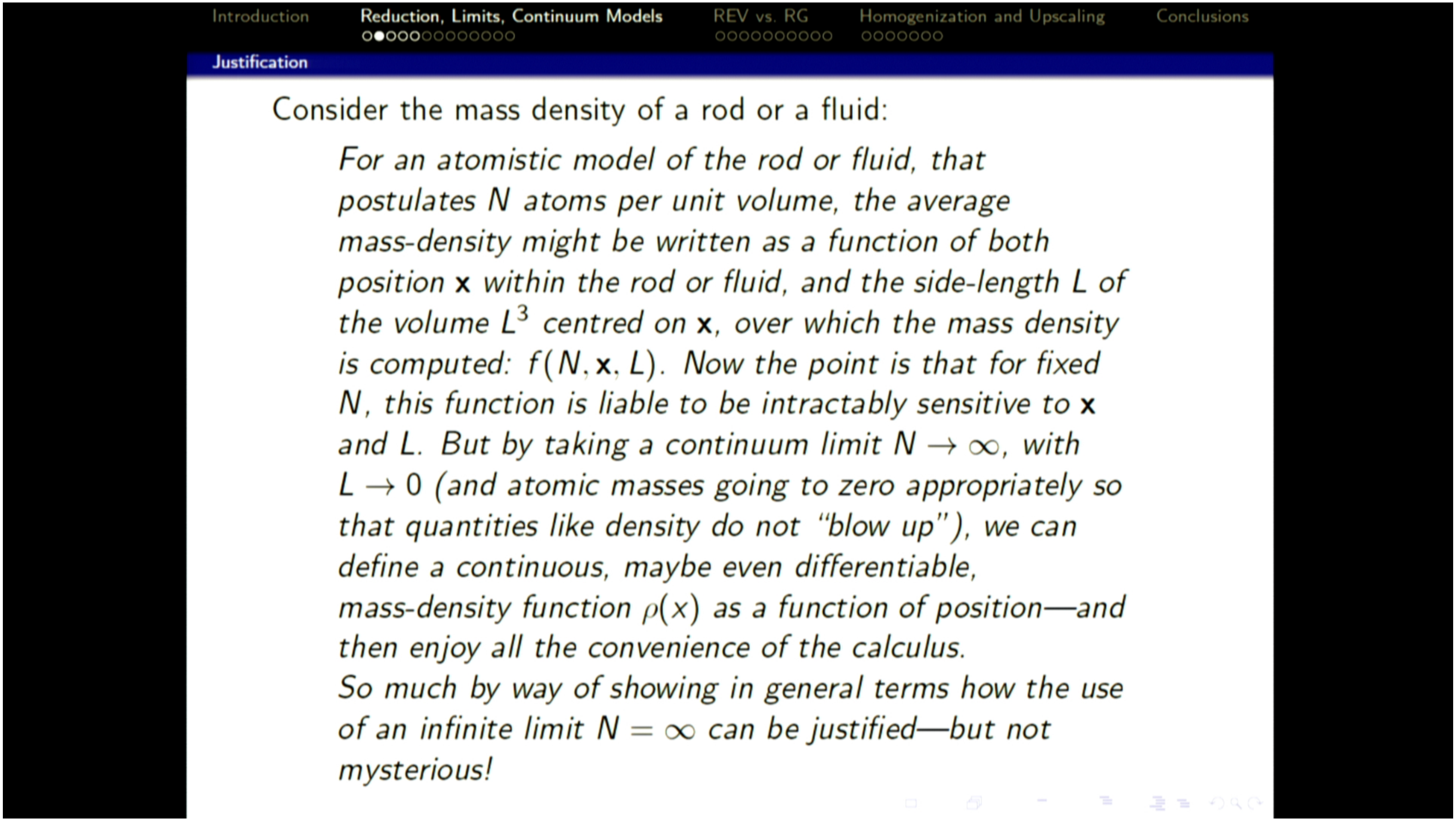
- Mathematical convenience.
- Empirical adequacy (up to a required accuracy).
  - Abstract from finitary effects—transients and edge/boundary effects.
  - Mathematics of infinity—calculus—is more convenient than mathematics of the large finite.



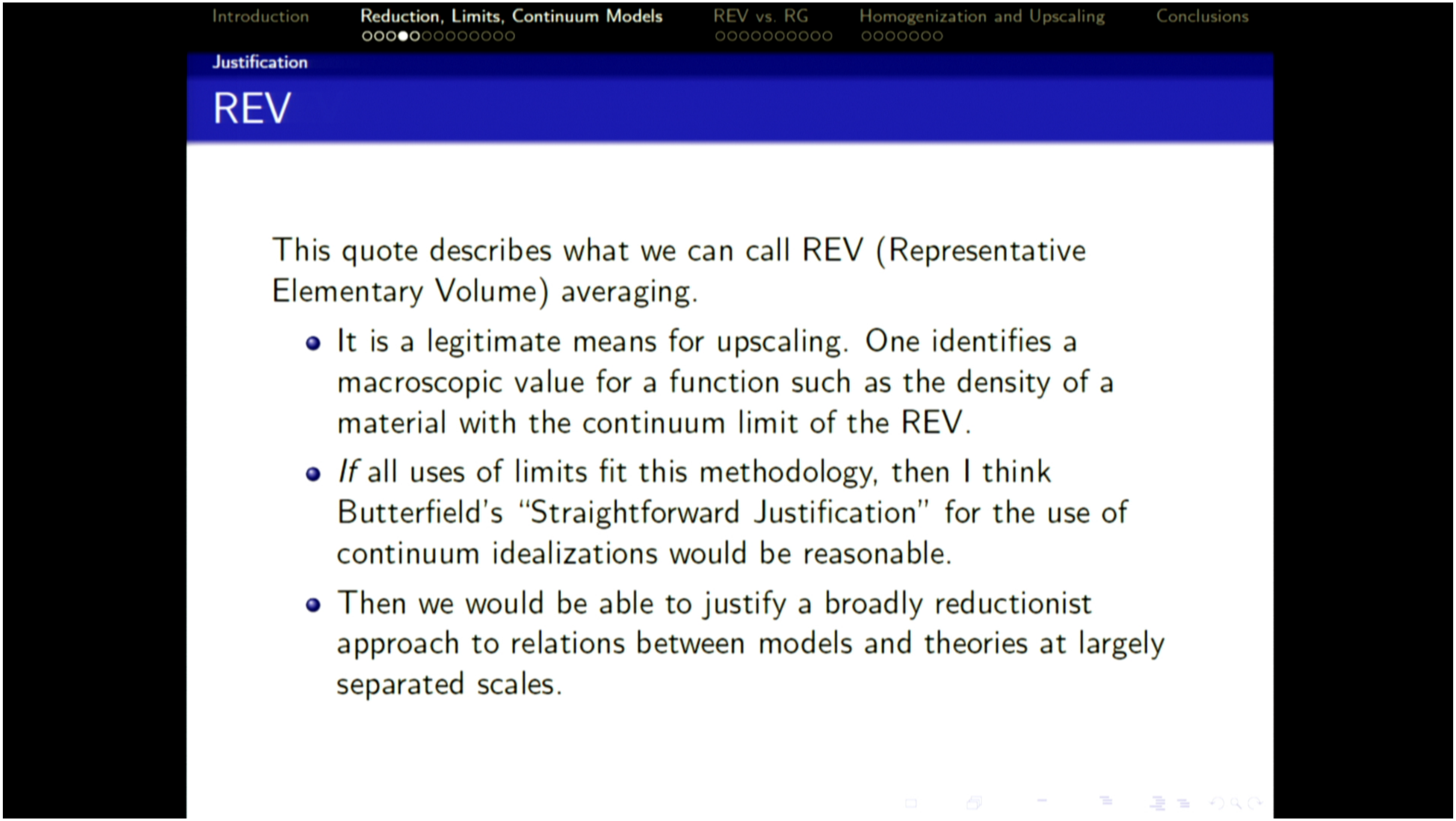
Justification

Consider the mass density of a rod or a fluid:

> *For an atomistic model of the rod or fluid, that postulates* N *atoms per unit volume, the average mass-density might be written as a function of both position* $\mathbf{x}$ *within the rod or fluid, and the side-length* L *of the volume* L^3 *centred on* $\mathbf{x}$*, over which the mass density is computed:* $f(N, \mathbf{x}, L)$*. Now the point is that for fixed* N*, this function is liable to be intractably sensitive to* $\mathbf{x}$ *and* L*. But by taking a continuum limit* $N \to \infty$*, with* $L \to 0$ *(and atomic masses going to zero appropriately so that quantities like density do not "blow up"), we can define a continuous, maybe even differentiable, mass-density function* $\rho(x)$ *as a function of position—and then enjoy all the convenience of the calculus.*
> *So much by way of showing in general terms how the use of an infinite limit* $N = \infty$ *can be justified—but not mysterious!*

REV

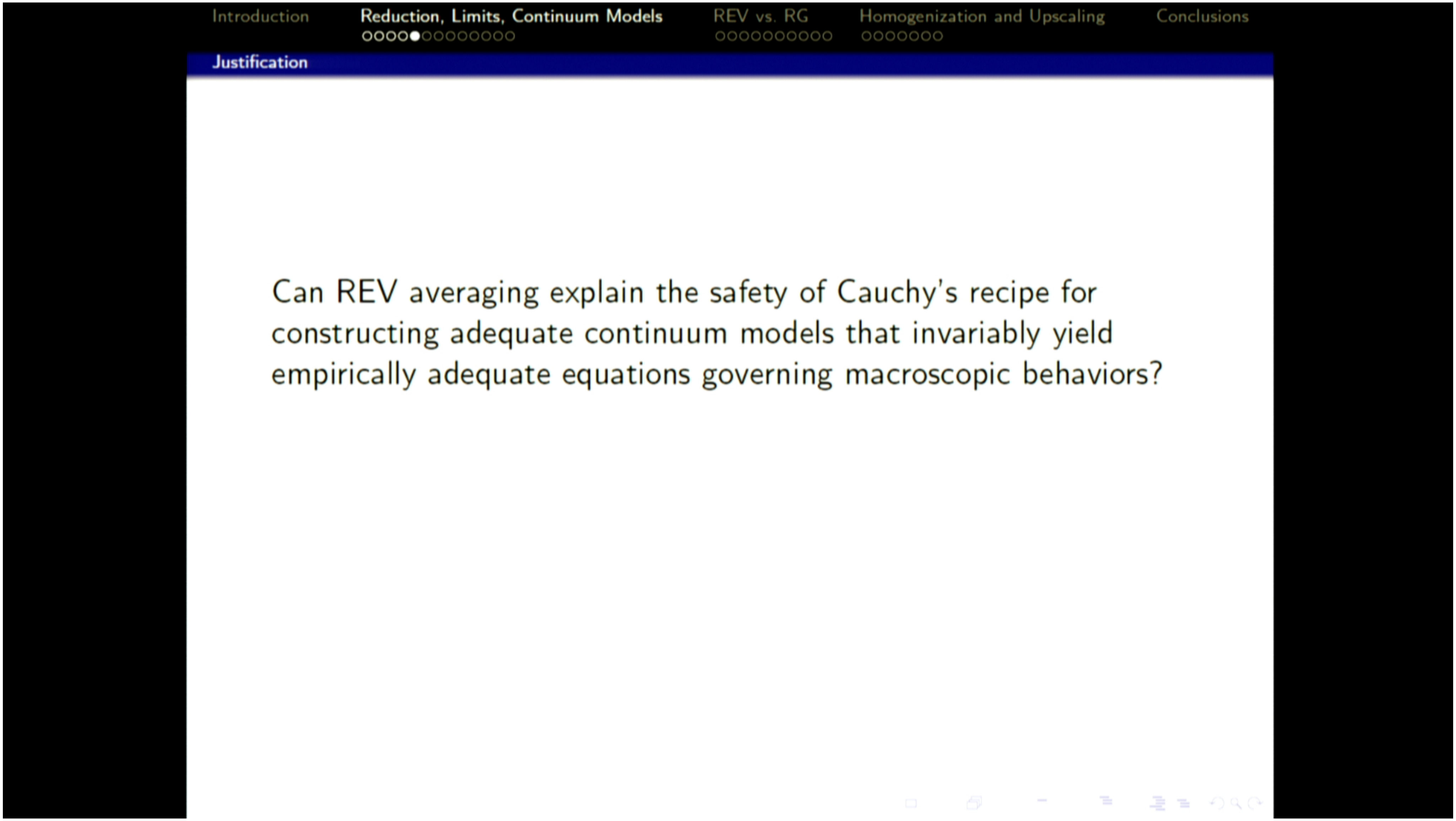
This quote describes what we can call REV (Representative Elementary Volume) averaging.



REV

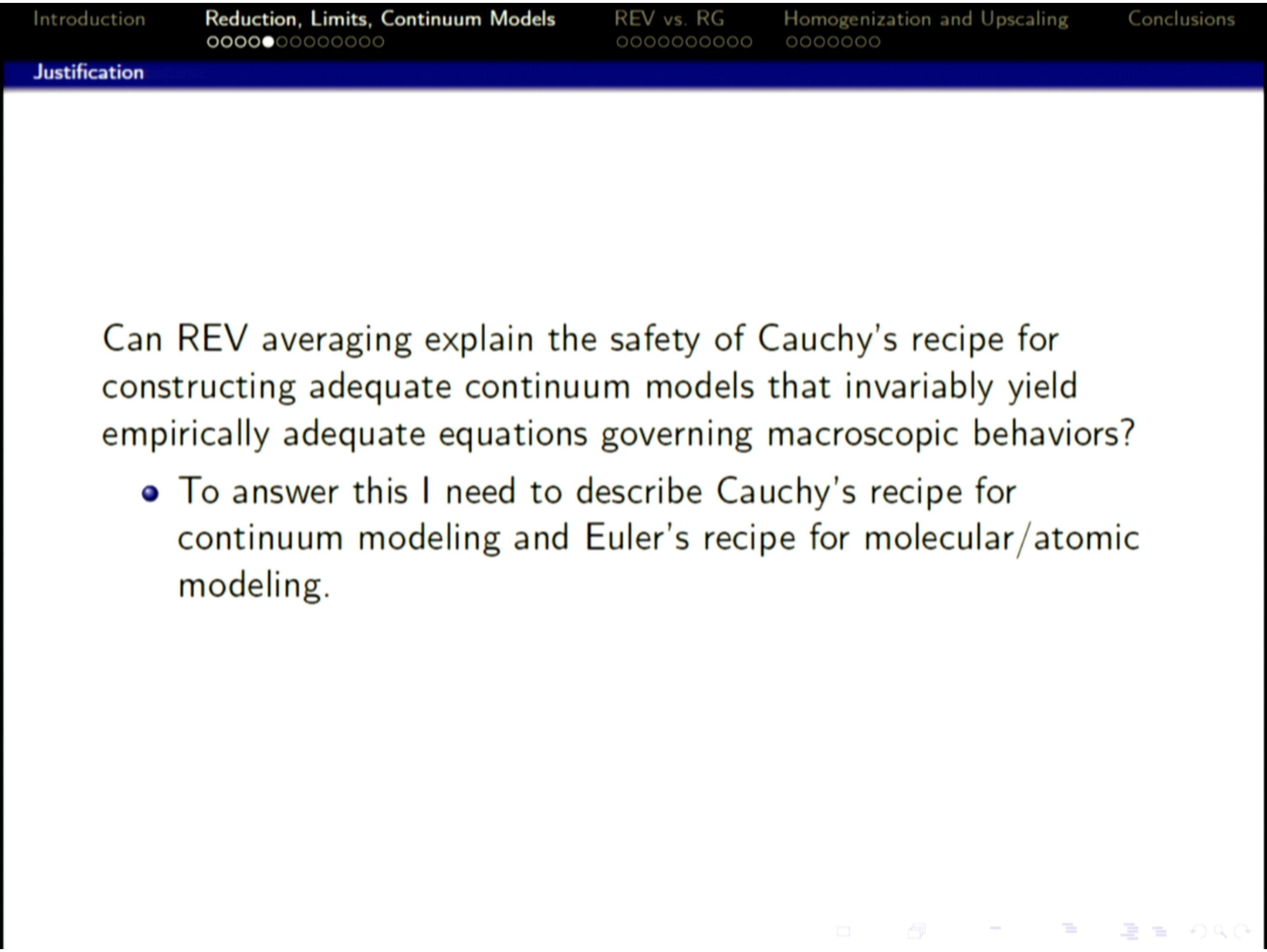
This quote describes what we can call REV (Representative Elementary Volume) averaging.

- It is a legitimate means for upscaling. One identifies a macroscopic value for a function such as the density of a material with the continuum limit of the REV.
- *If* all uses of limits fit this methodology, then I think Butterfield's "Straightforward Justification" for the use of continuum idealizations would be reasonable.
- Then we would be able to justify a broadly reductionist approach to relations between models and theories at largely separated scales.



Justification

Can REV averaging explain the safety of Cauchy's recipe for constructing adequate continuum models that invariably yield empirically adequate equations governing macroscopic behaviors?



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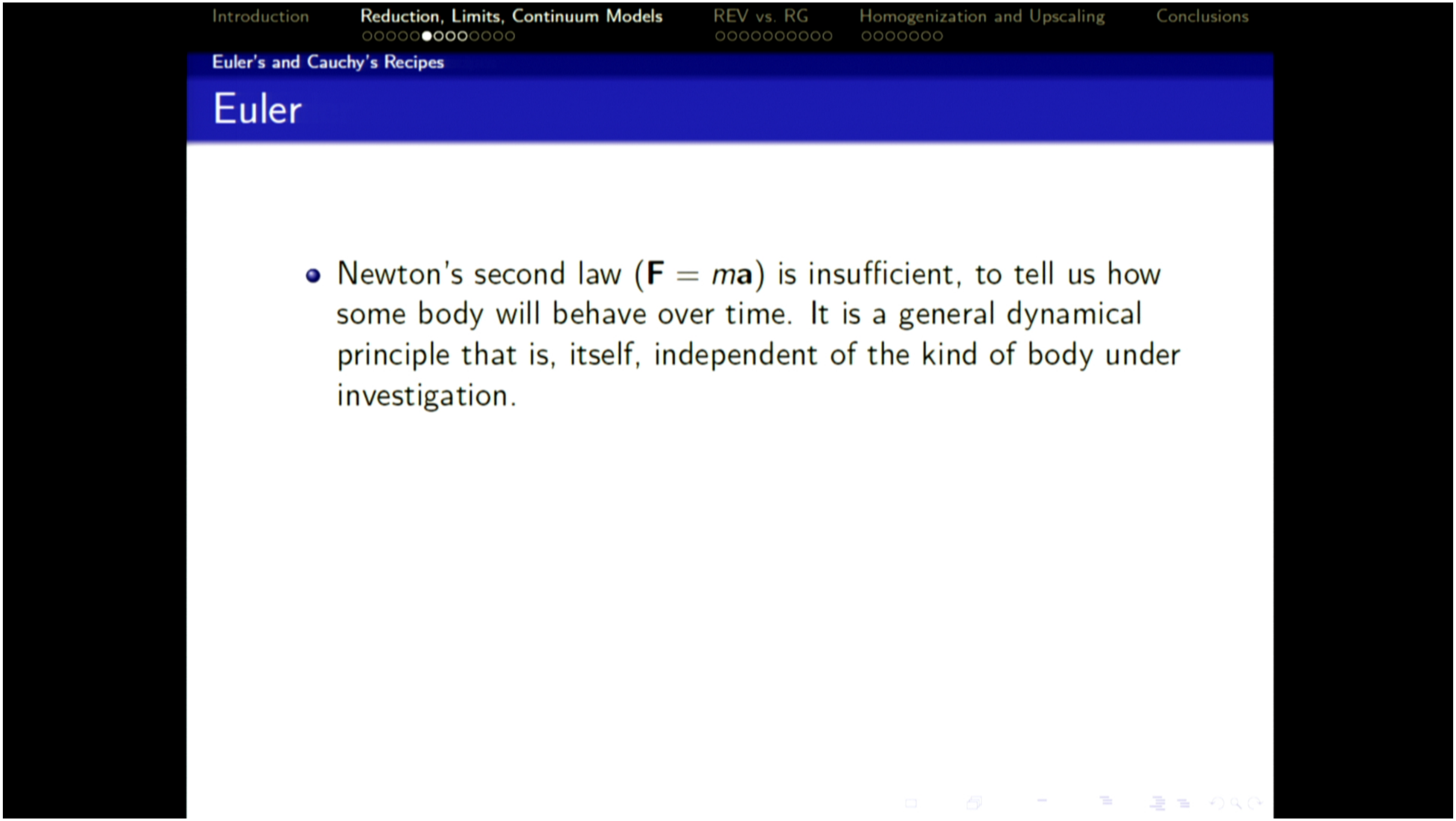
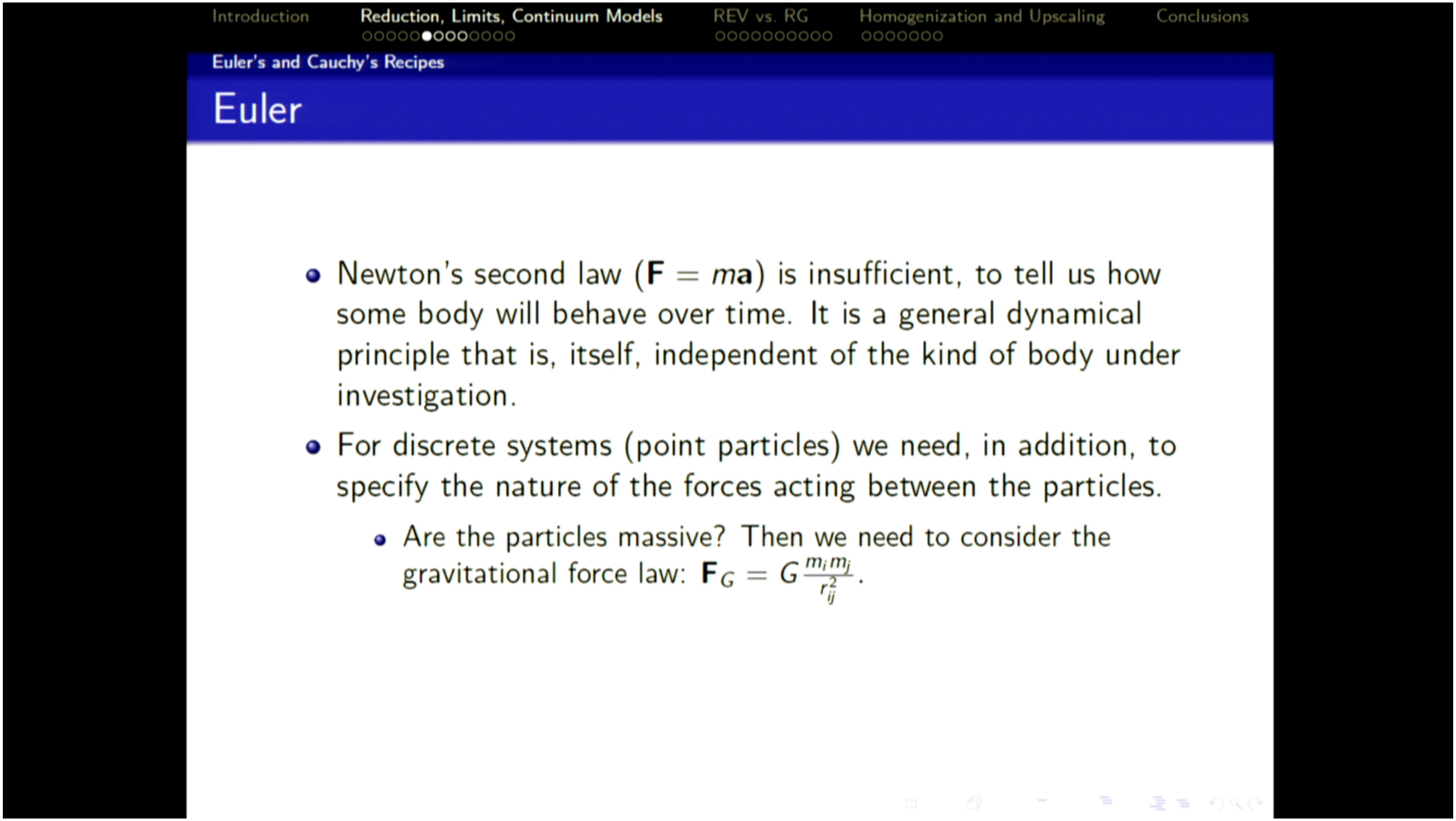
- To answer this I need to describe Cauchy's recipe for continuum modeling and Euler's recipe for molecular/atomic modeling.



Euler

- Newton's second law ($\mathbf{F} = m\mathbf{a}$) is insufficient, to tell us how some body will behave over time. It is a general dynamical principle that is, itself, independent of the kind of body under investigation.



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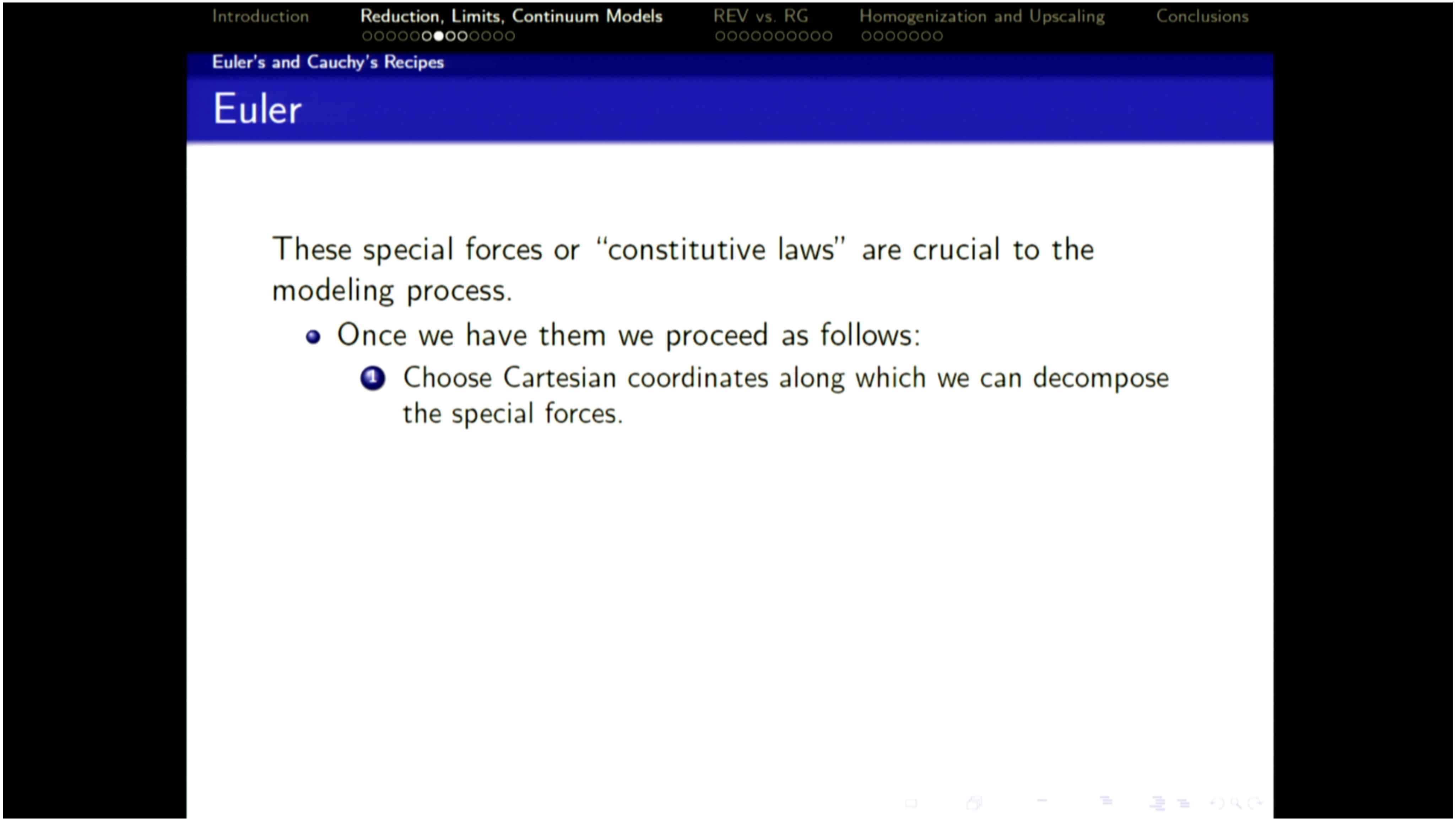
- For discrete systems (point particles) we need, in addition, to specify the nature of the forces acting between the particles.
  - Are the particles massive? Then we need to consider the gravitational force law: $\mathbf{F}_G = G\frac{m_i m_j}{r_{ij}^2}$.

Euler

These special forces or “constitutive laws” are crucial to the modeling process.



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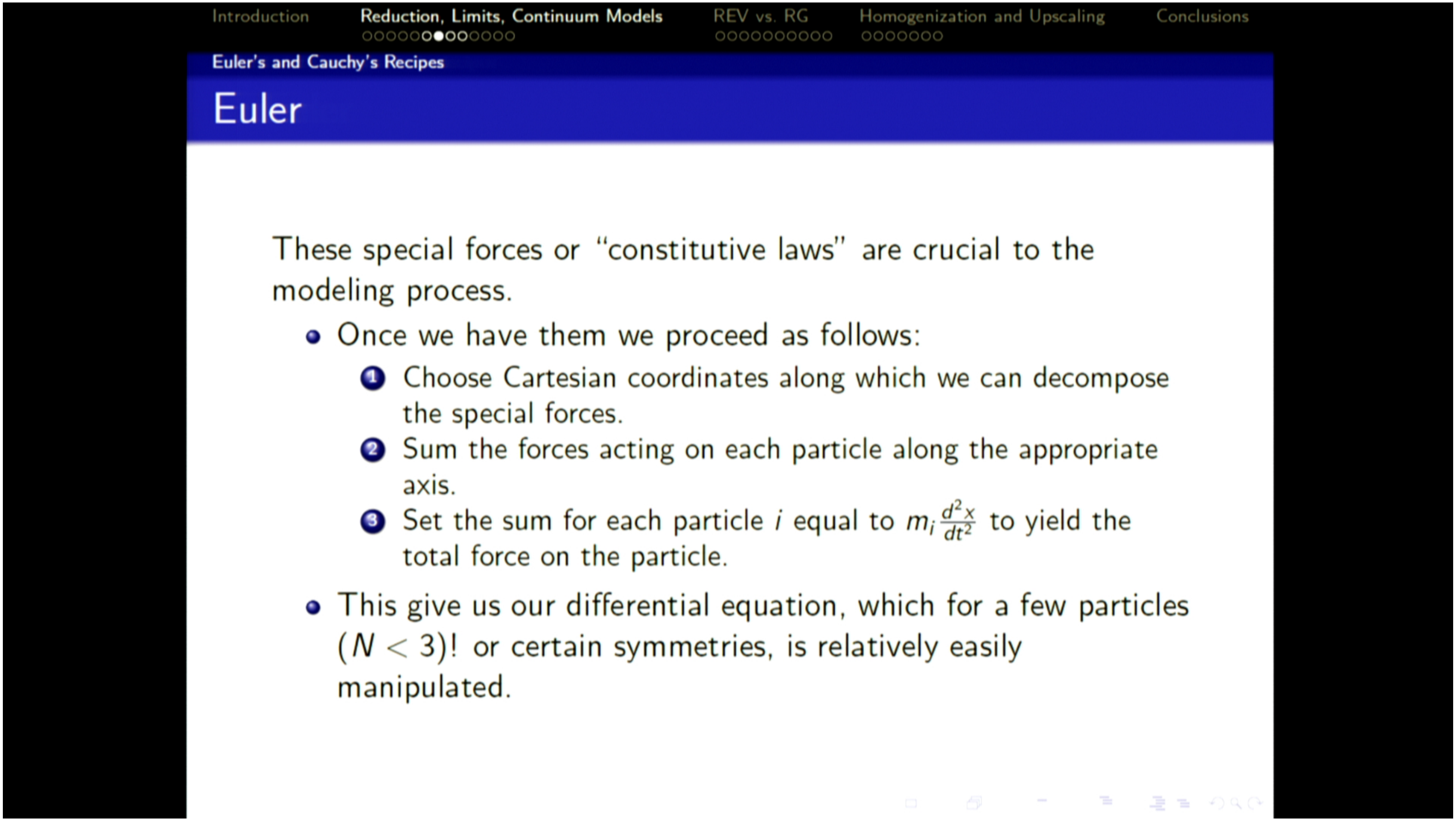

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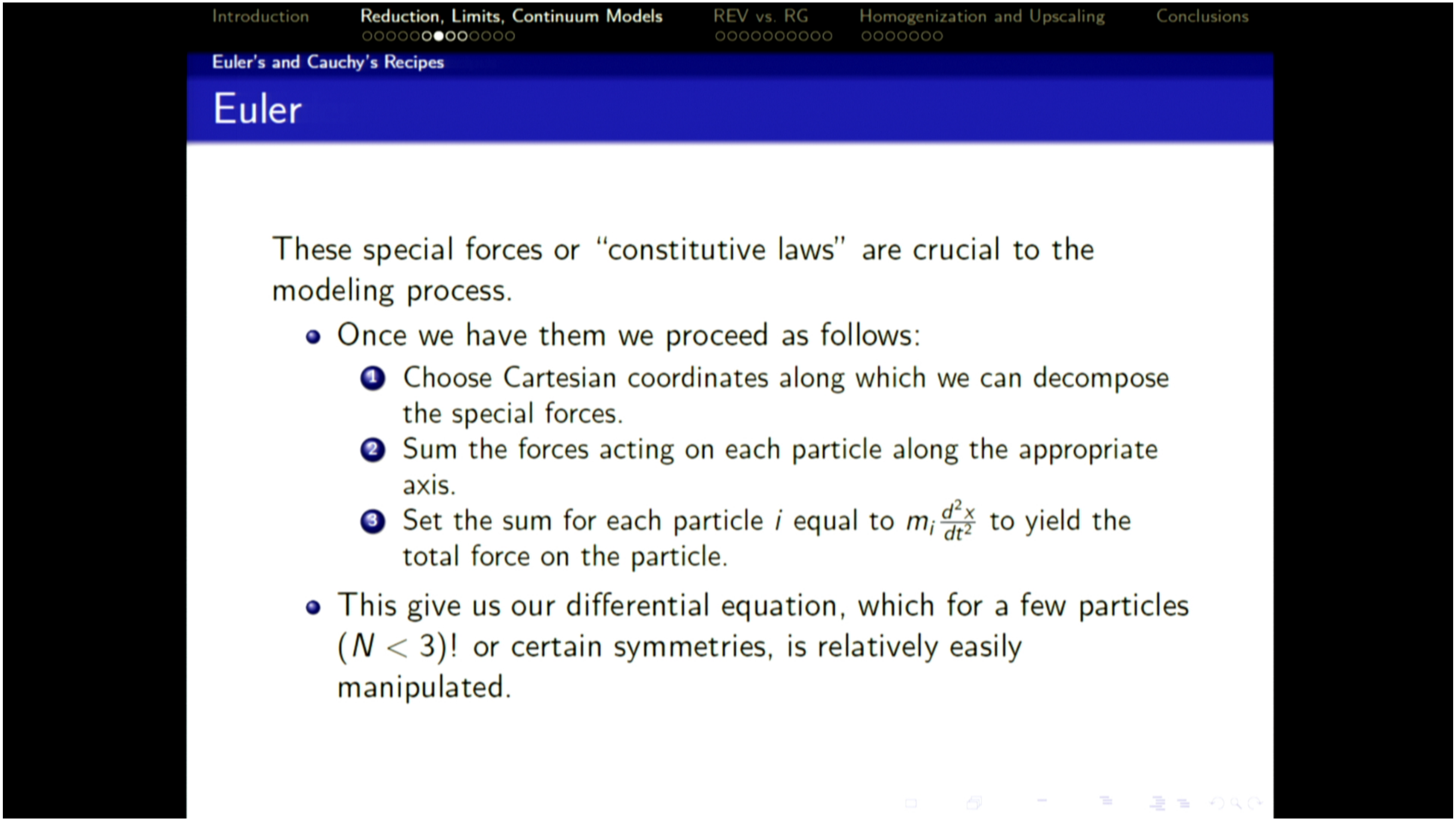
  3. Set the sum for each particle i equal to $m_i \frac{d^2x}{dt^2}$ to yield the total force on the particle.
- This give us our differential equation, which for a few particles $(N < 3)$! or certain symmetries, is relatively easily manipulated.



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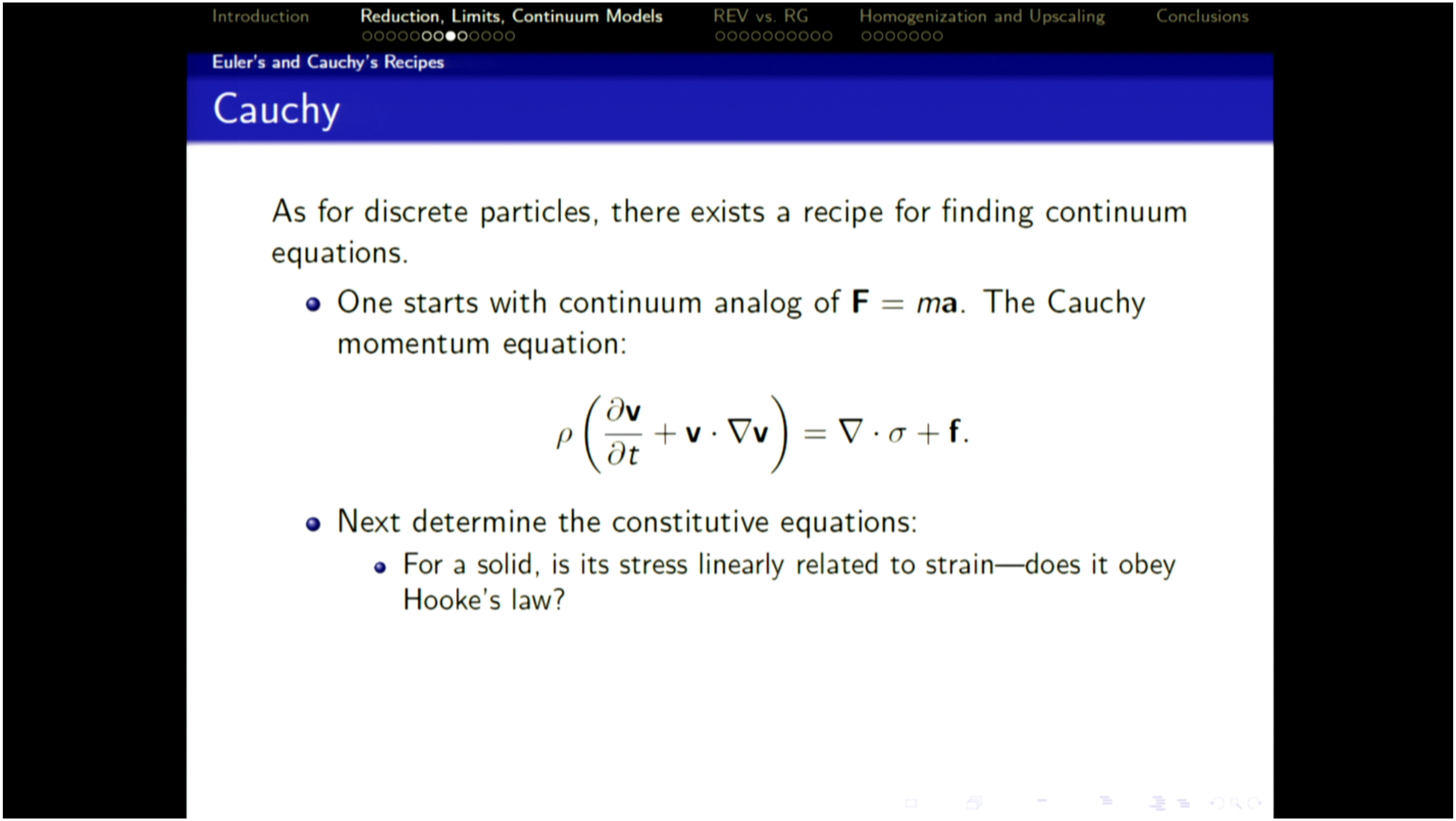


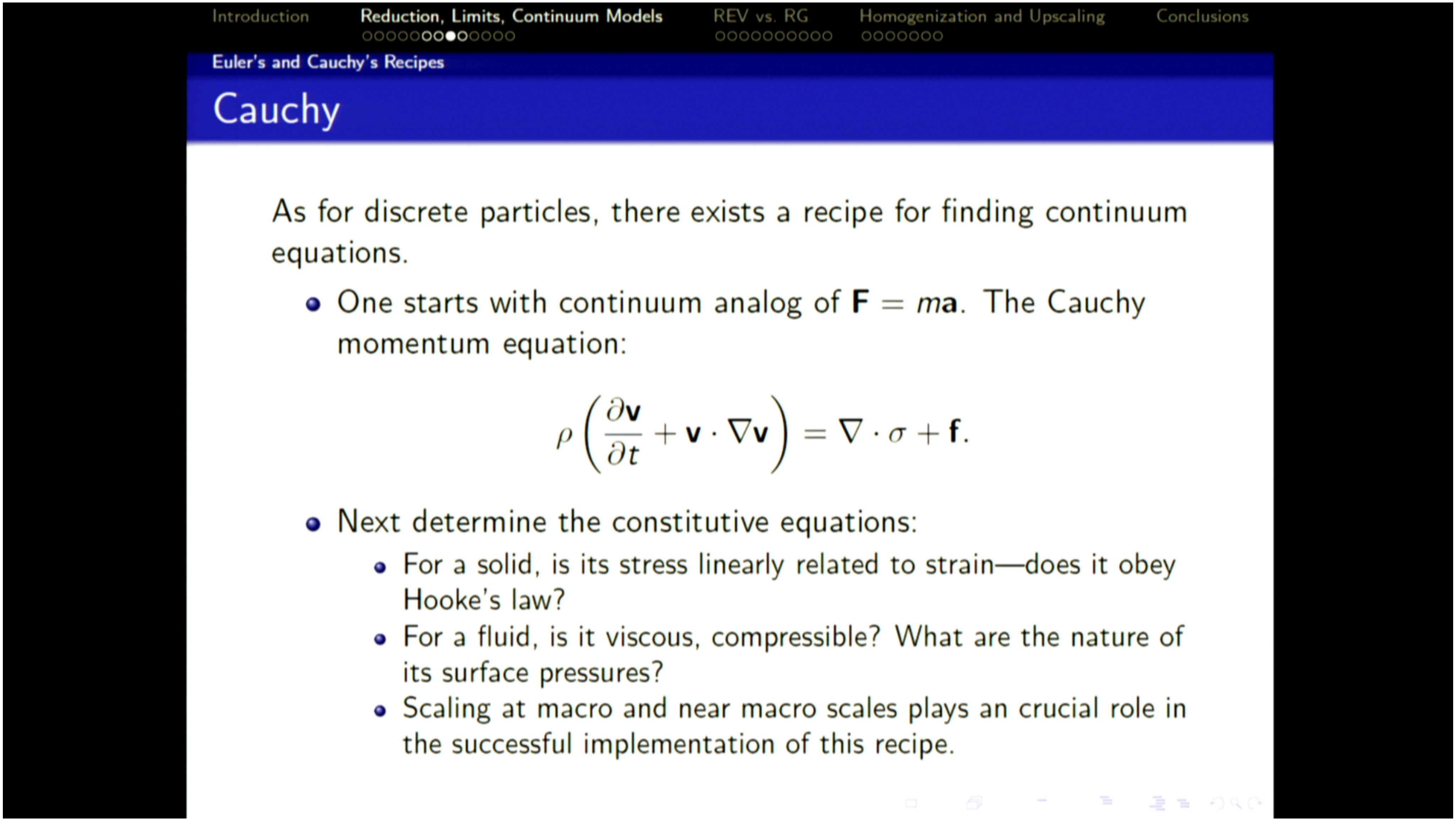
Cauchy

As for discrete particles, there exists a recipe for finding continuum equations.

- One starts with continuum analog of $\mathbf{F} = m\mathbf{a}$. The Cauchy momentum equation:

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \nabla \cdot \sigma + \mathbf{f}.$$

- Next determine the constitutive equations:
  - For a solid, is its stress linearly related to strain—does it obey Hooke's law?



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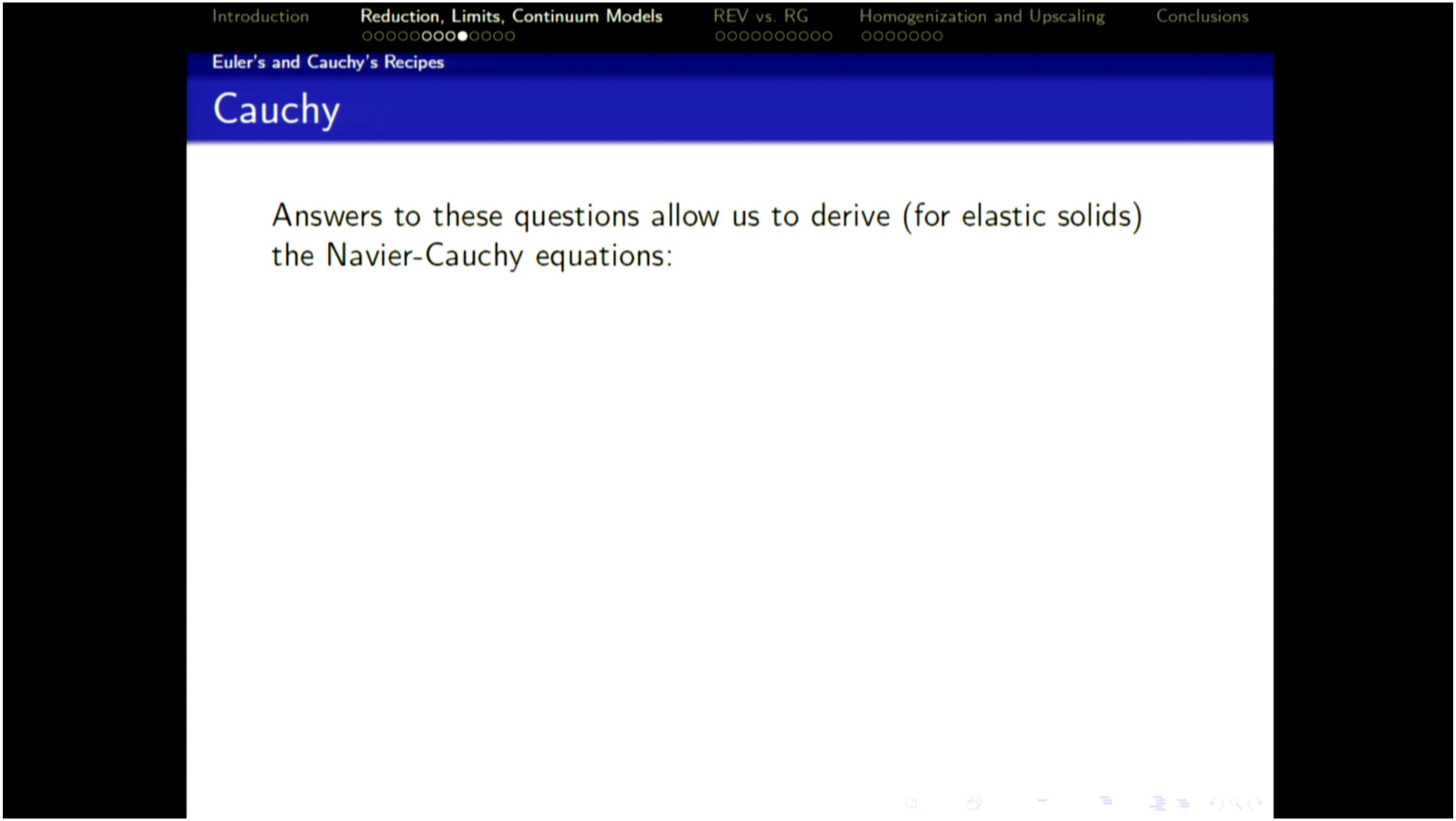
- Next determine the constitutive equations:
  - For a solid, is its stress linearly related to strain—does it obey Hooke's law?
  - For a fluid, is it viscous, compressible? What are the nature of its surface pressures?
  - Scaling at macro and near macro scales plays an crucial role in the successful implementation of this recipe.



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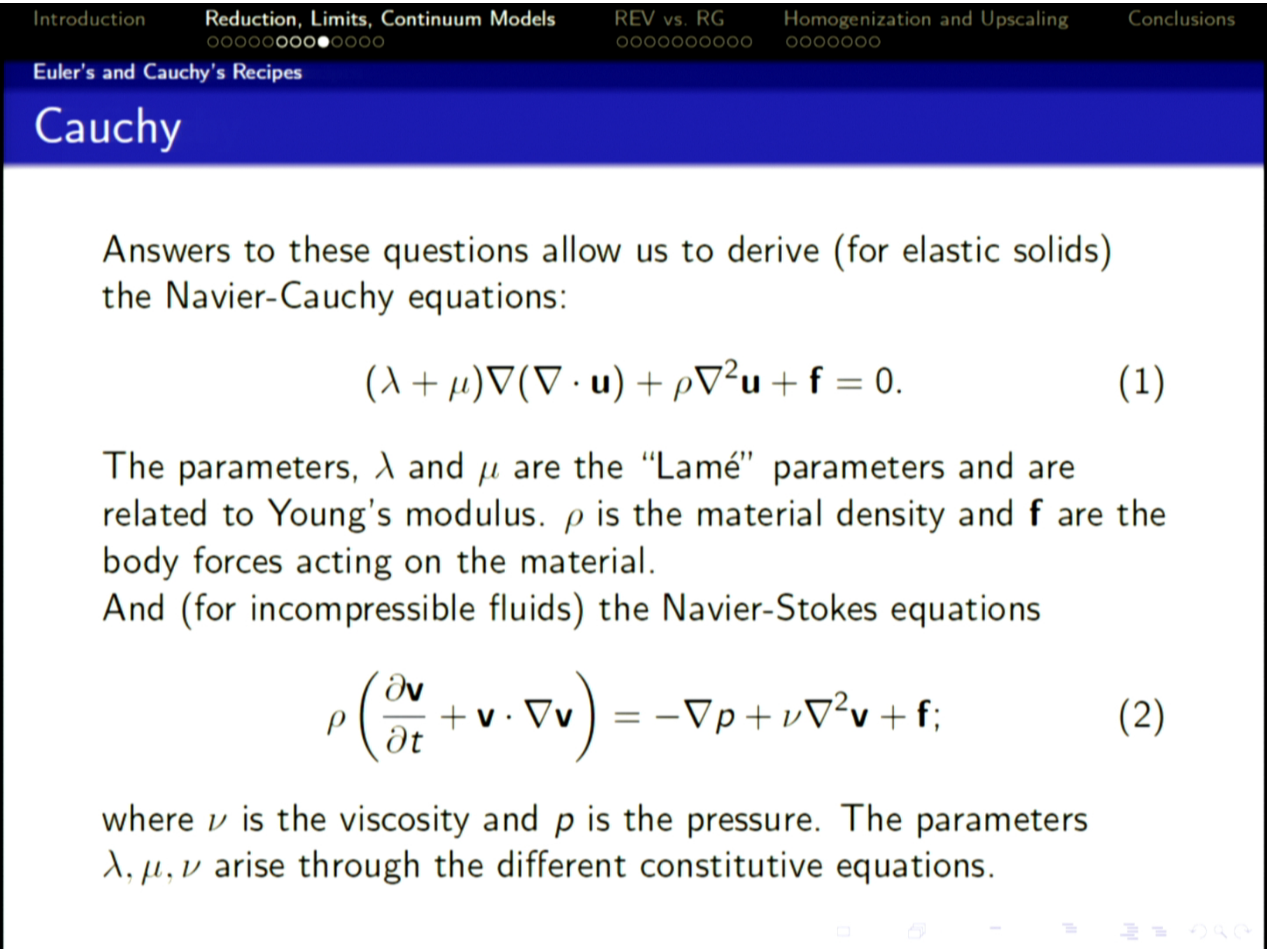
Answers to these questions allow us to derive (for elastic solids) the Navier-Cauchy equations:



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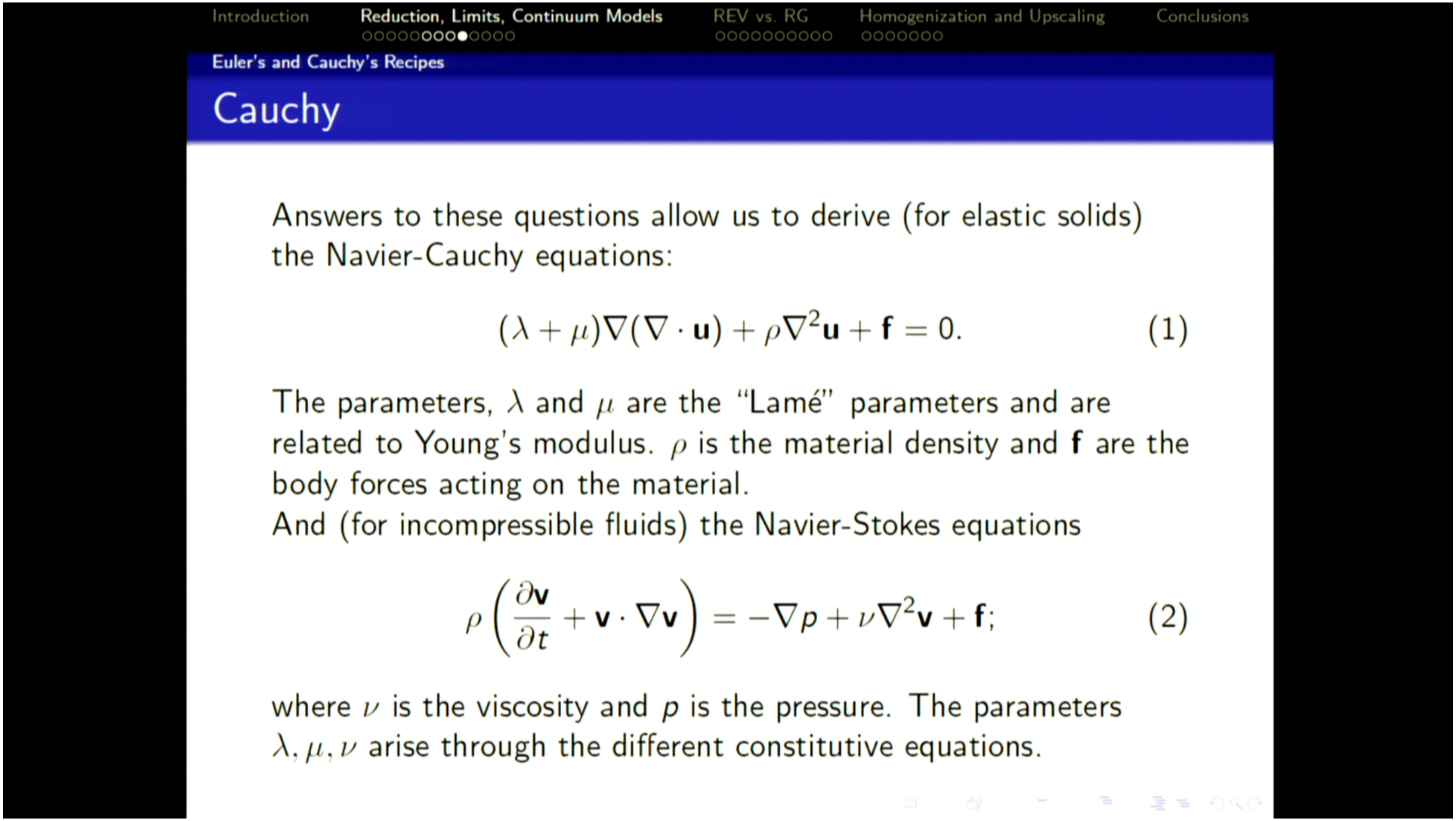
$$(\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}) + \rho\nabla^2\mathbf{u} + \mathbf{f} = 0. \tag{1}$$

The parameters, λ and μ are the "Lamé" parameters and are related to Young's modulus. ρ is the material density and $\mathbf{f}$ are the body forces acting on the material.

And (for incompressible fluids) the Navier-Stokes equations

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}\right) = -\nabla p + \nu\nabla^2\mathbf{v} + \mathbf{f}; \tag{2}$$

where ν is the viscosity and p is the pressure. The parameters λ, μ, ν arise through the different constitutive equations.



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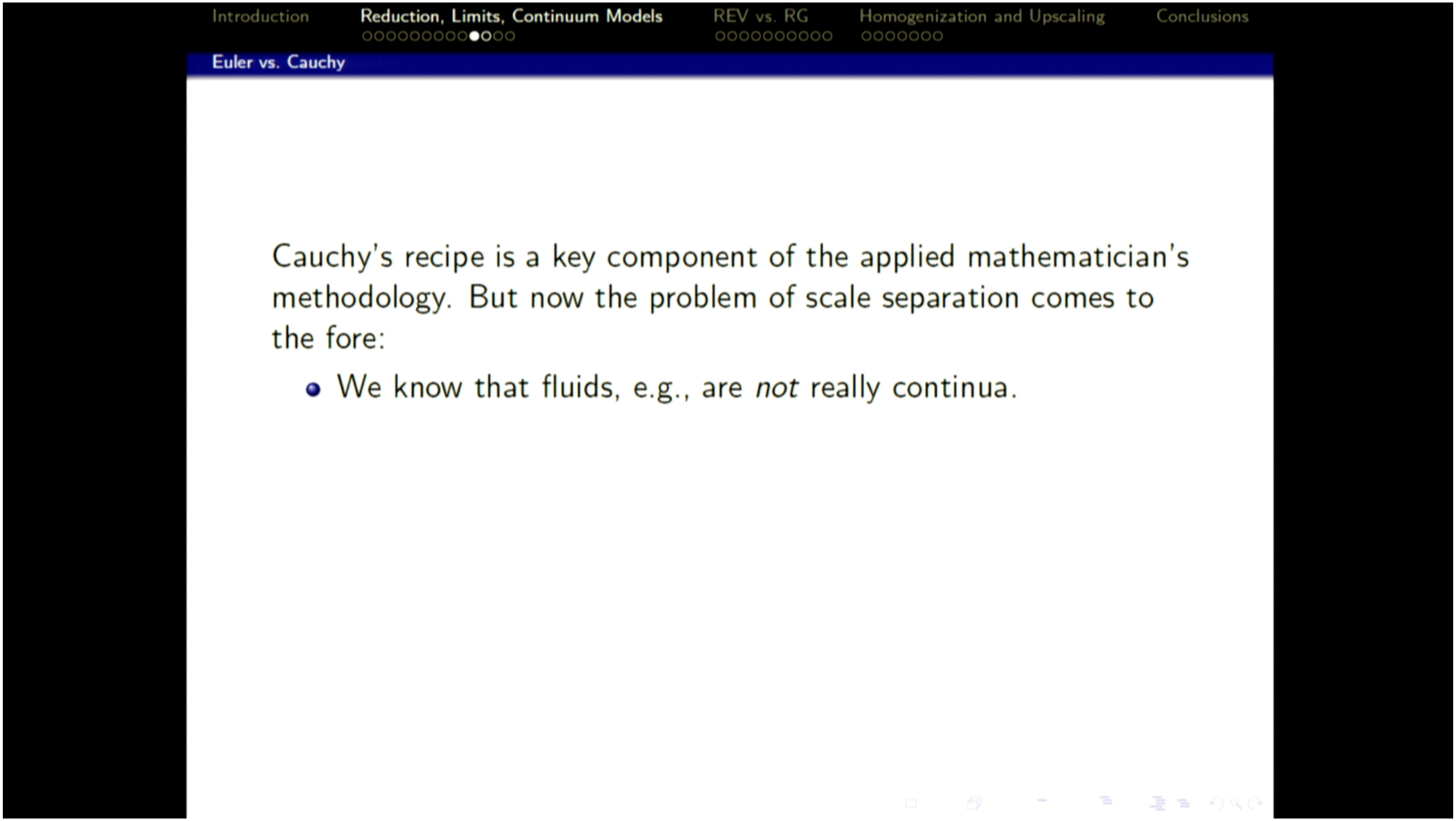
Cauchy's recipe is a key component of the applied mathematician's methodology. But now the problem of scale separation comes to the fore:



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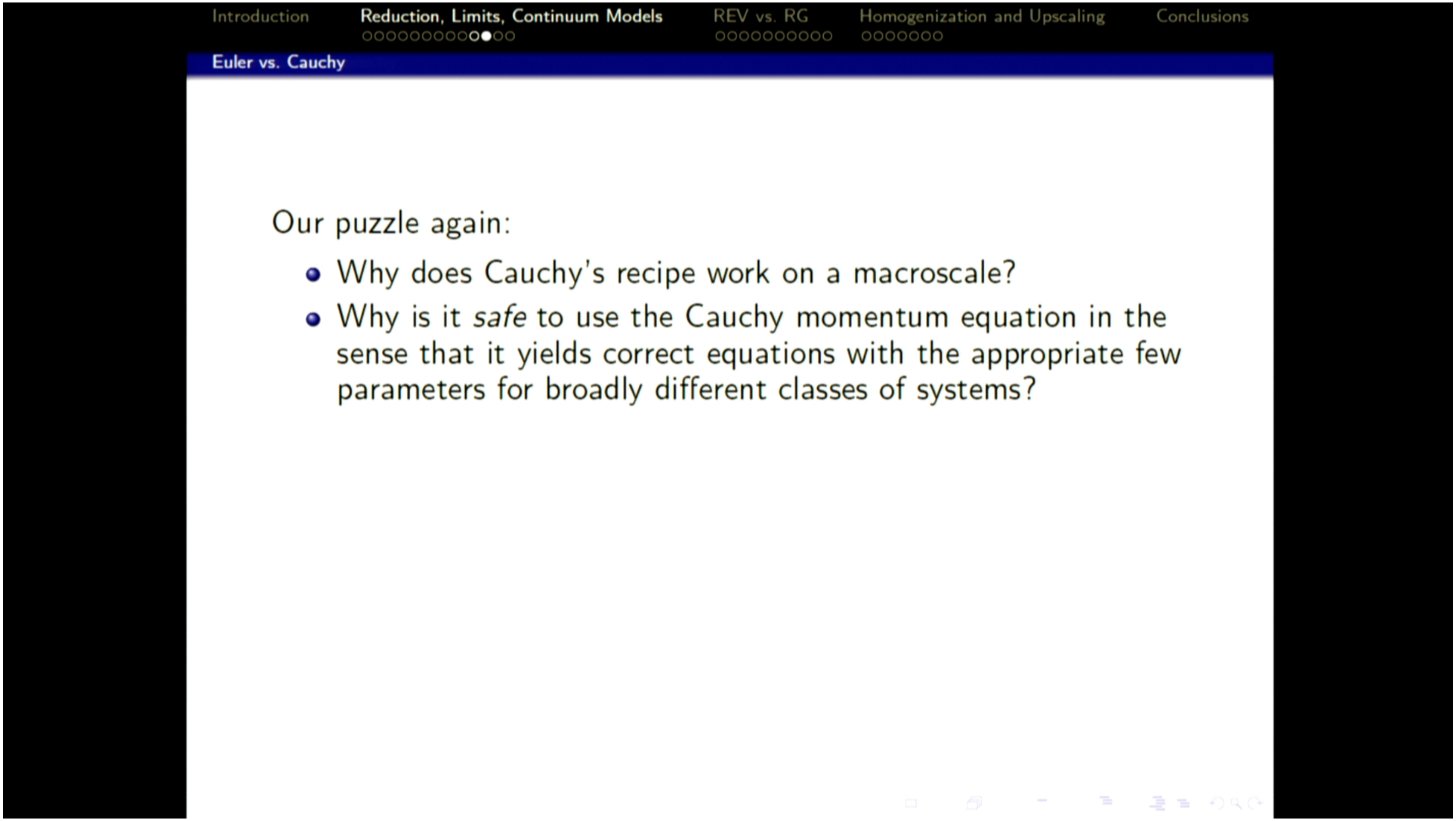
- We know that fluids, e.g., are *not* really continua.
- What is the relation between molecular dynamical models that track individual molecular behavior at the scale of nanometers, and equations like those of Navier-Stokes that apply at the scale of millimeters?

Euler vs. Cauchy

Our puzzle again:



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- Why does Cauchy's recipe work on a macroscale?
- Why is it *safe* to use the Cauchy momentum equation in the sense that it yields correct equations with the appropriate few parameters for broadly different classes of systems?
    - The answers to these questions involve telling a story about how *properly* to connect a statistical atomic theory to a continuum theory—how to connect statistical mechanics to hydrodynamics.
    - This is the story of the so-called renormalization group and related homogenization strategies.

Generalized Conception of a Fixed Point

- From the point of view of Cauchy's recipe, one derives the N-S and Navier-Cauchy equations independently of any views about the molecular or atomic makeup of the medium.
- In the nineteenth century there were doubts about whether matter was atomistic! Interesting controversy pitting Navier and Cauchy against Green and Stokes—rari-constancy vs. multi-constancy theories.

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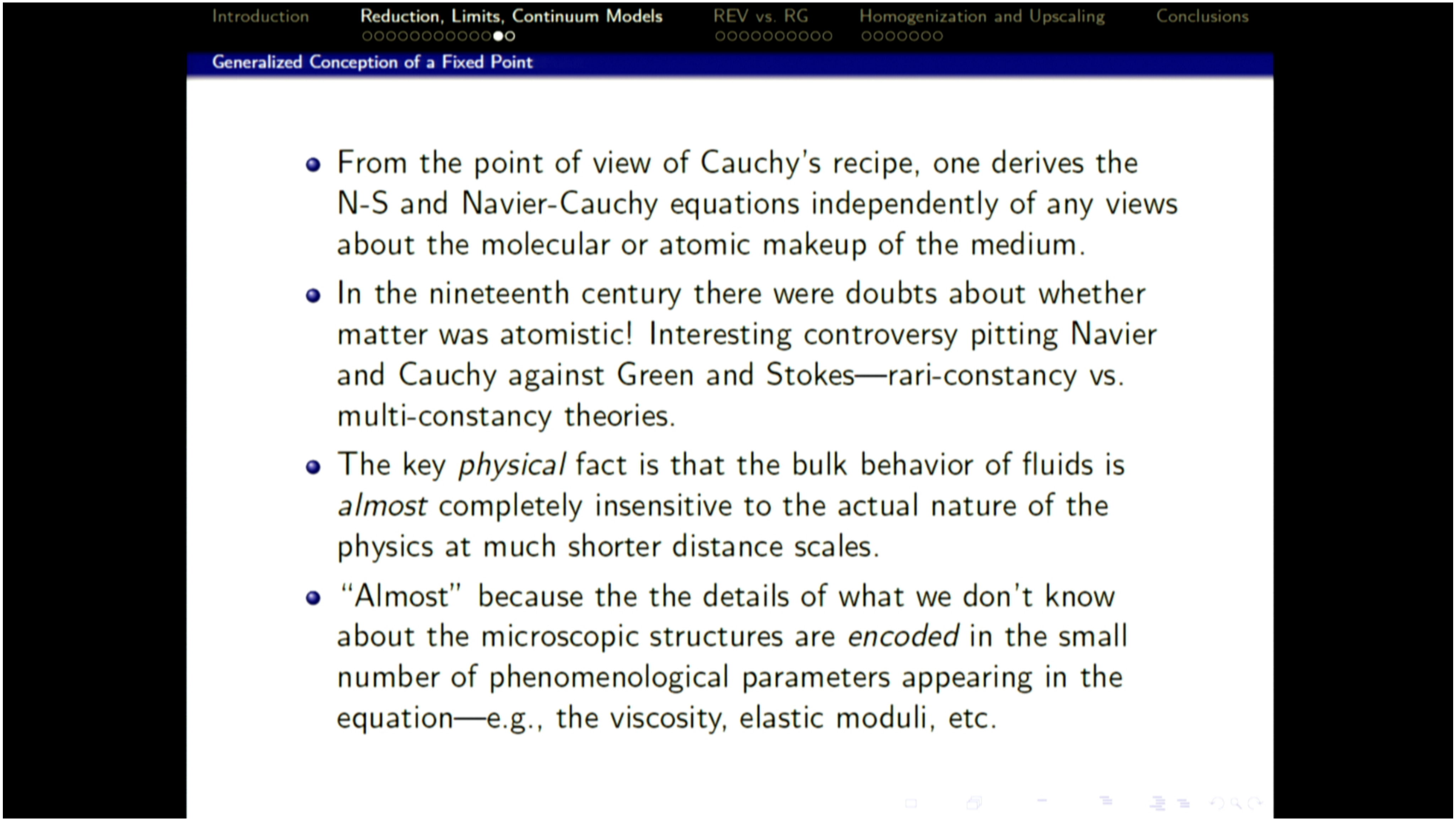
- The key *physical* fact is that the bulk behavior of fluids is *almost* completely insensitive to the actual nature of the physics at much shorter distance scales.



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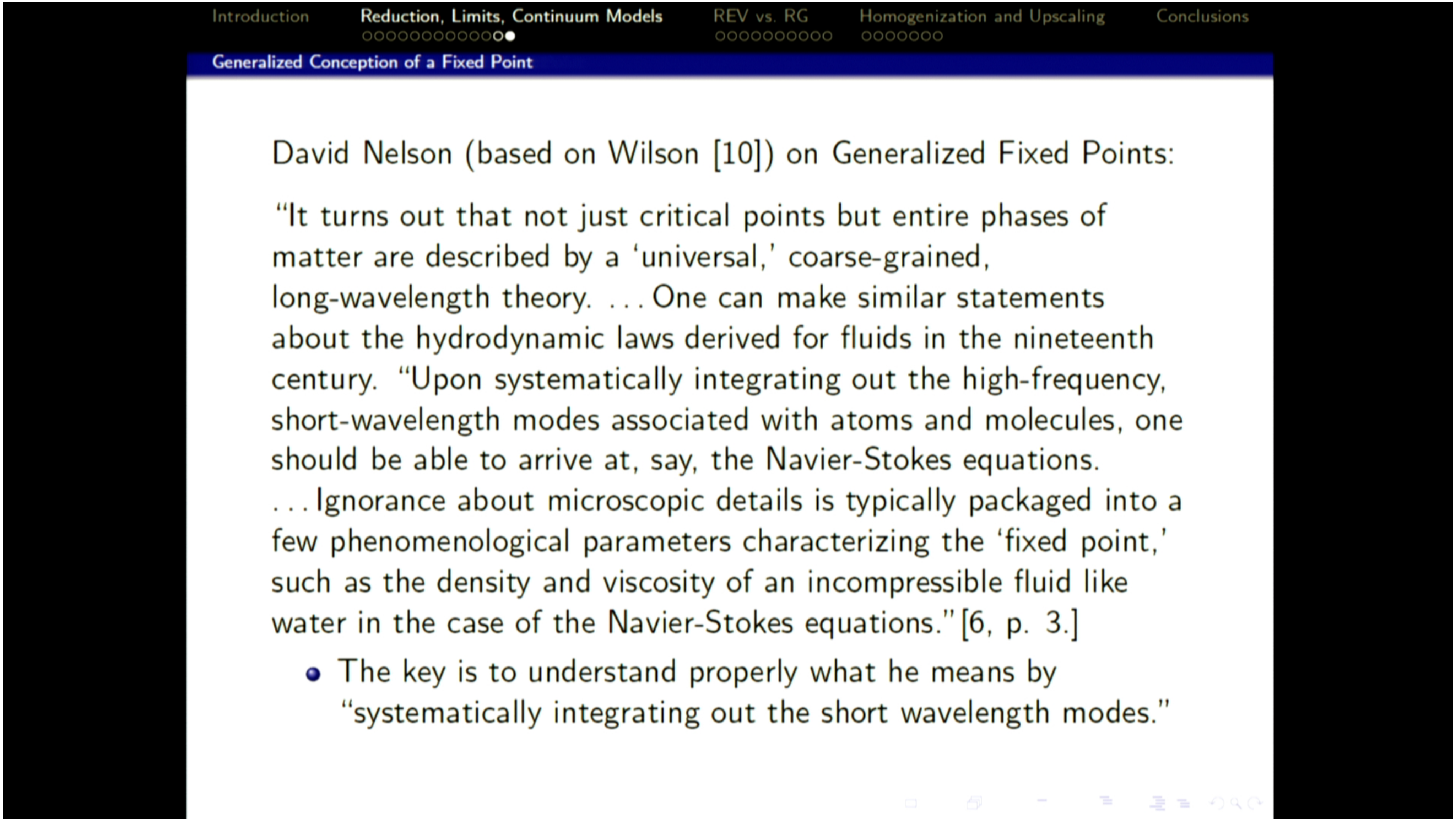
- The key *physical* fact is that the bulk behavior of fluids is *almost* completely insensitive to the actual nature of the physics at much shorter distance scales.
- "Almost" because the the details of what we don't know about the microscopic structures are *encoded* in the small number of phenomenological parameters appearing in the equation—e.g., the viscosity, elastic moduli, etc.



Generalized Conception of a Fixed Point

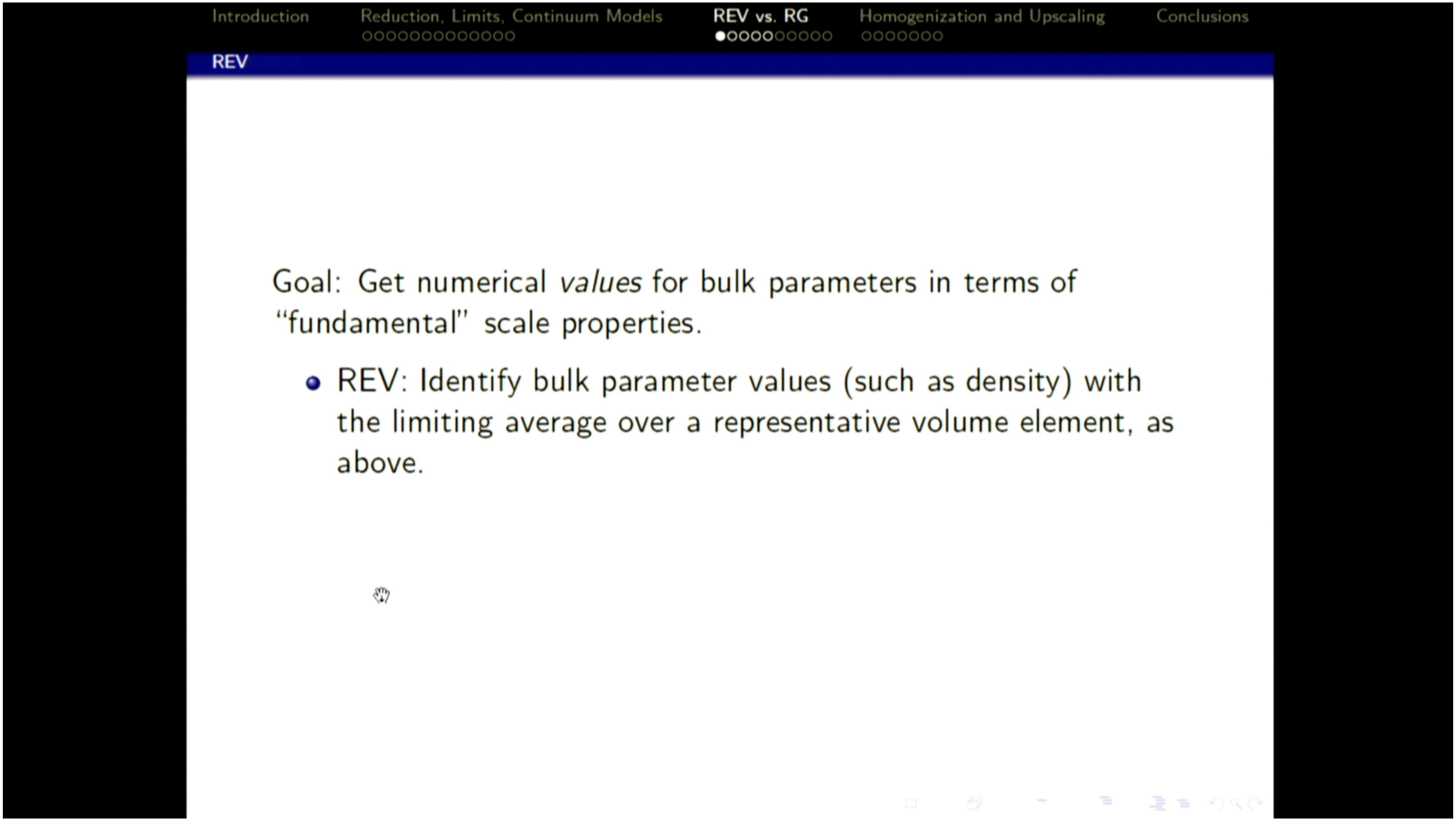
David Nelson (based on Wilson [10]) on Generalized Fixed Points:

"It turns out that not just critical points but entire phases of matter are described by a 'universal,' coarse-grained, long-wavelength theory. . . . One can make similar statements about the hydrodynamic laws derived for fluids in the nineteenth century. "Upon systematically integrating out the high-frequency, short-wavelength modes associated with atoms and molecules, one should be able to arrive at, say, the Navier-Stokes equations. . . . Ignorance about microscopic details is typically packaged into a few phenomenological parameters characterizing the 'fixed point,' such as the density and viscosity of an incompressible fluid like water in the case of the Navier-Stokes equations."[6, p. 3.]

- The key is to understand properly what he means by "systematically integrating out the short wavelength modes."

REV

Goal: Get numerical *values* for bulk parameters in terms of "fundamental" scale properties.



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- REV: Identify bulk parameter values (such as density) with the limiting average over a representative volume element, as above.
- This often fails completely.

REV

Consider a composite material consisting of a disconnected phase and a connected phase in a 50–50 mixture. Suppose the red phase is a conductor and the white phase is an insulator.

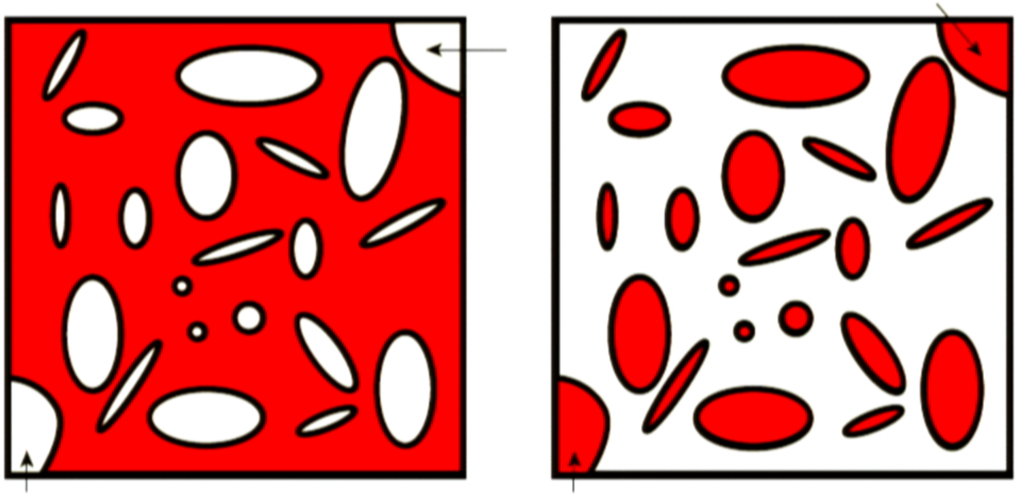
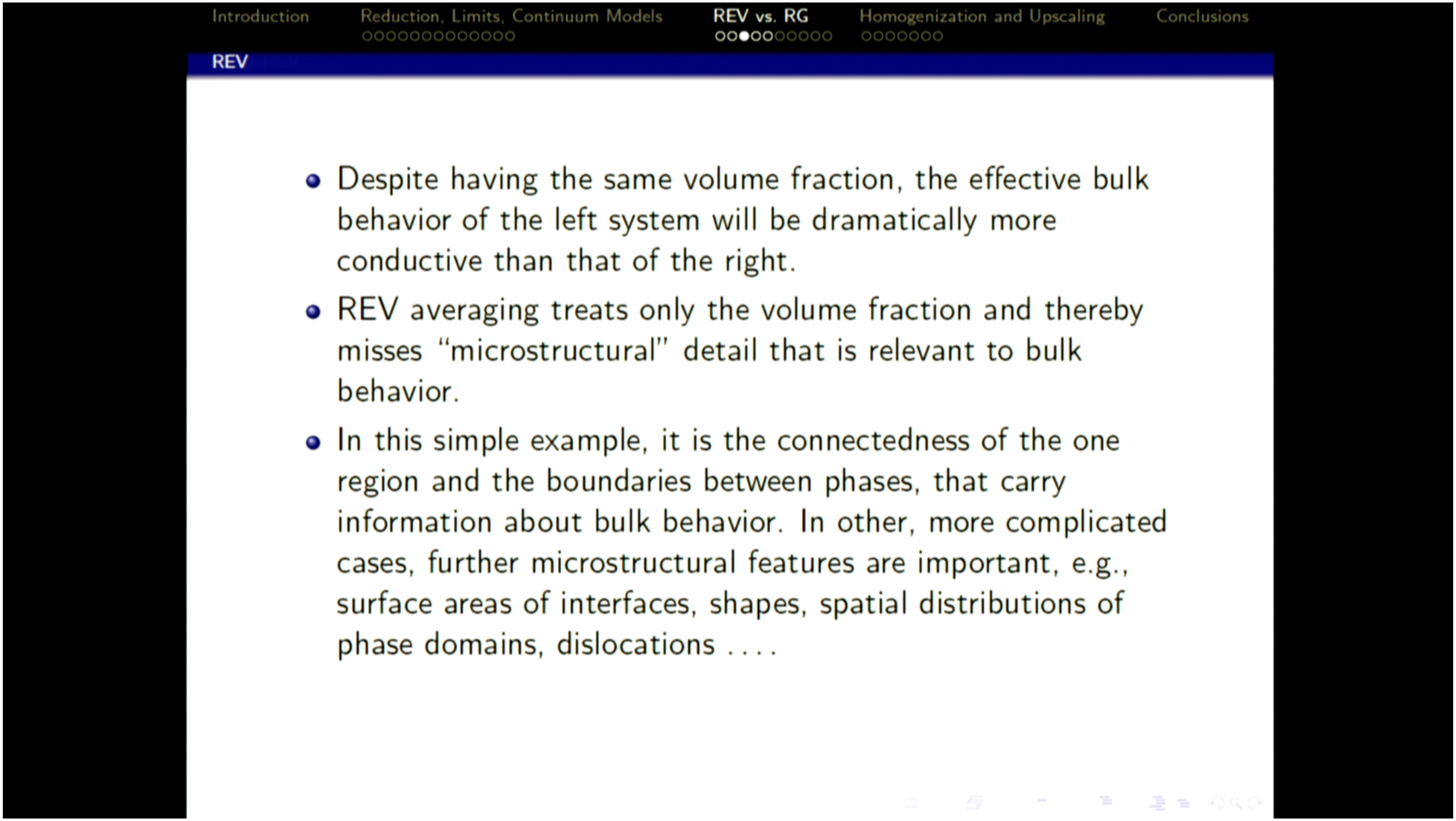
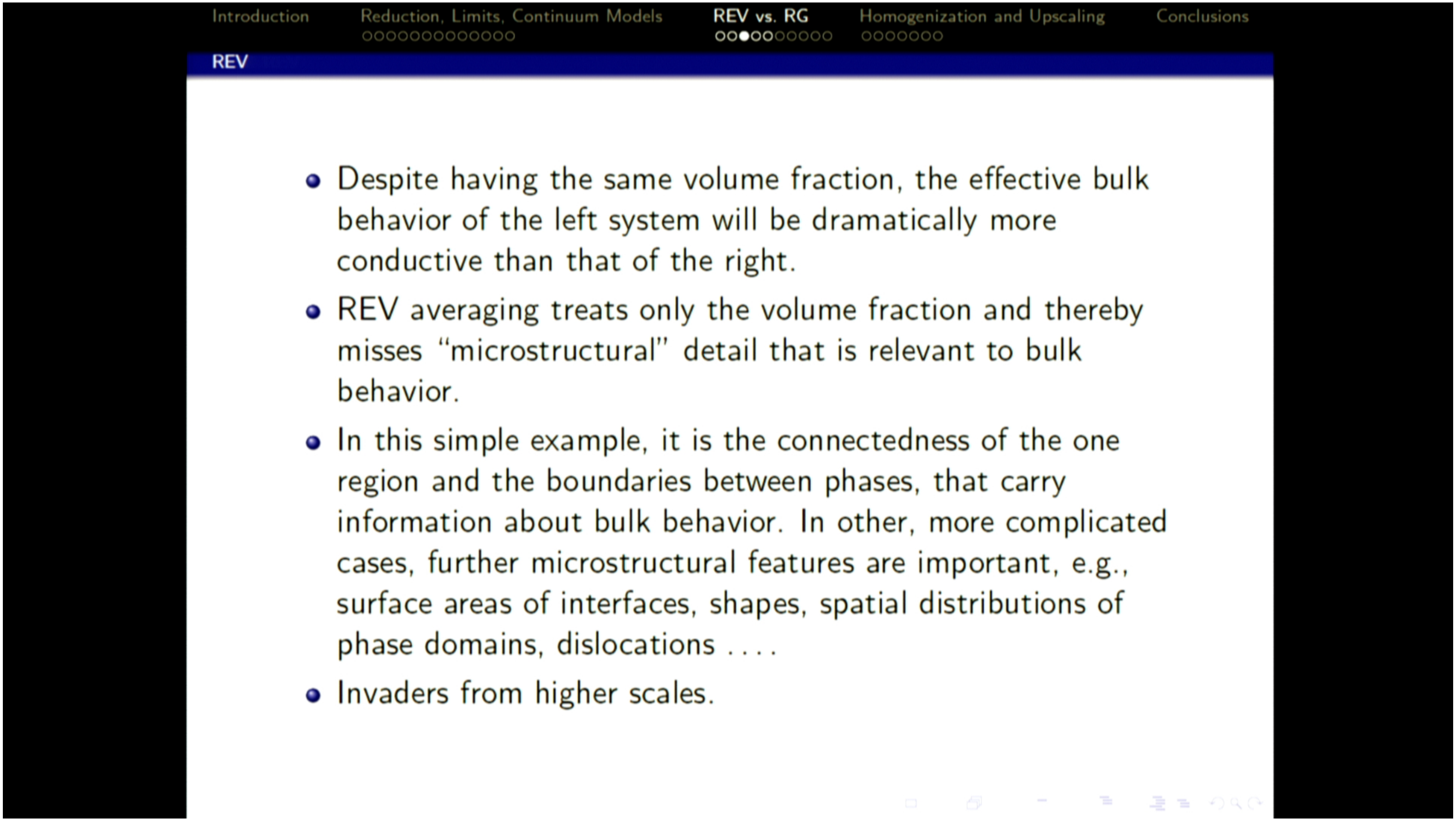


Figure: 50-50 Composites



REV

- Despite having the same volume fraction, the effective bulk behavior of the left system will be dramatically more conductive than that of the right.
- REV averaging treats only the volume fraction and thereby misses “microstructural” detail that is relevant to bulk behavior.
- In this simple example, it is the connectedness of the one region and the boundaries between phases, that carry information about bulk behavior. In other, more complicated cases, further microstructural features are important, e.g., surface areas of interfaces, shapes, spatial distributions of phase domains, dislocations . . . .



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- Invaders from higher scales.

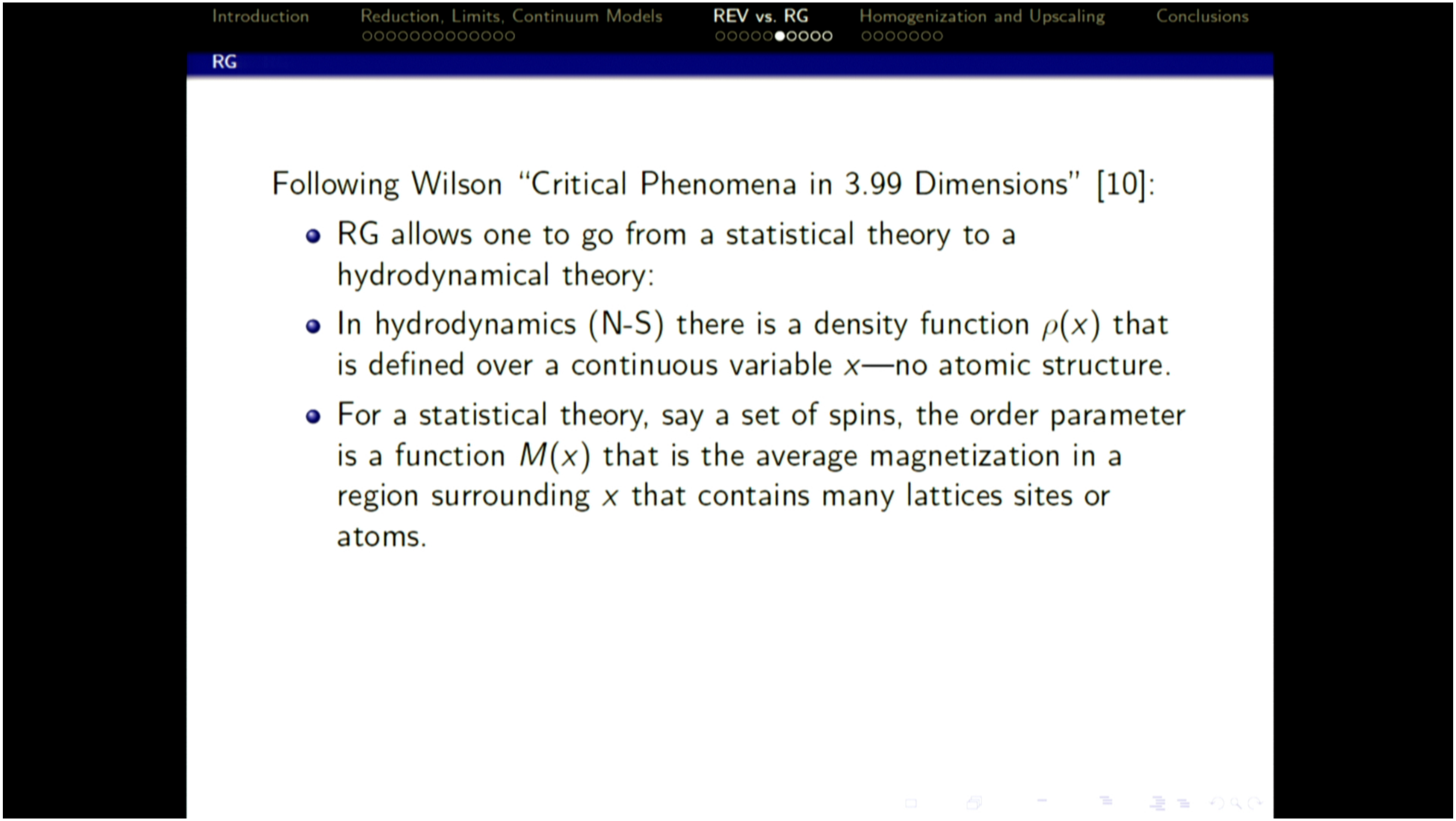
REV

Compare the picture of composites with a picture of a system near criticality.

Figure: Connecting Scales: Bubbles within bubbles within bubbles . . . [After Kadanoff, [4]]

REV

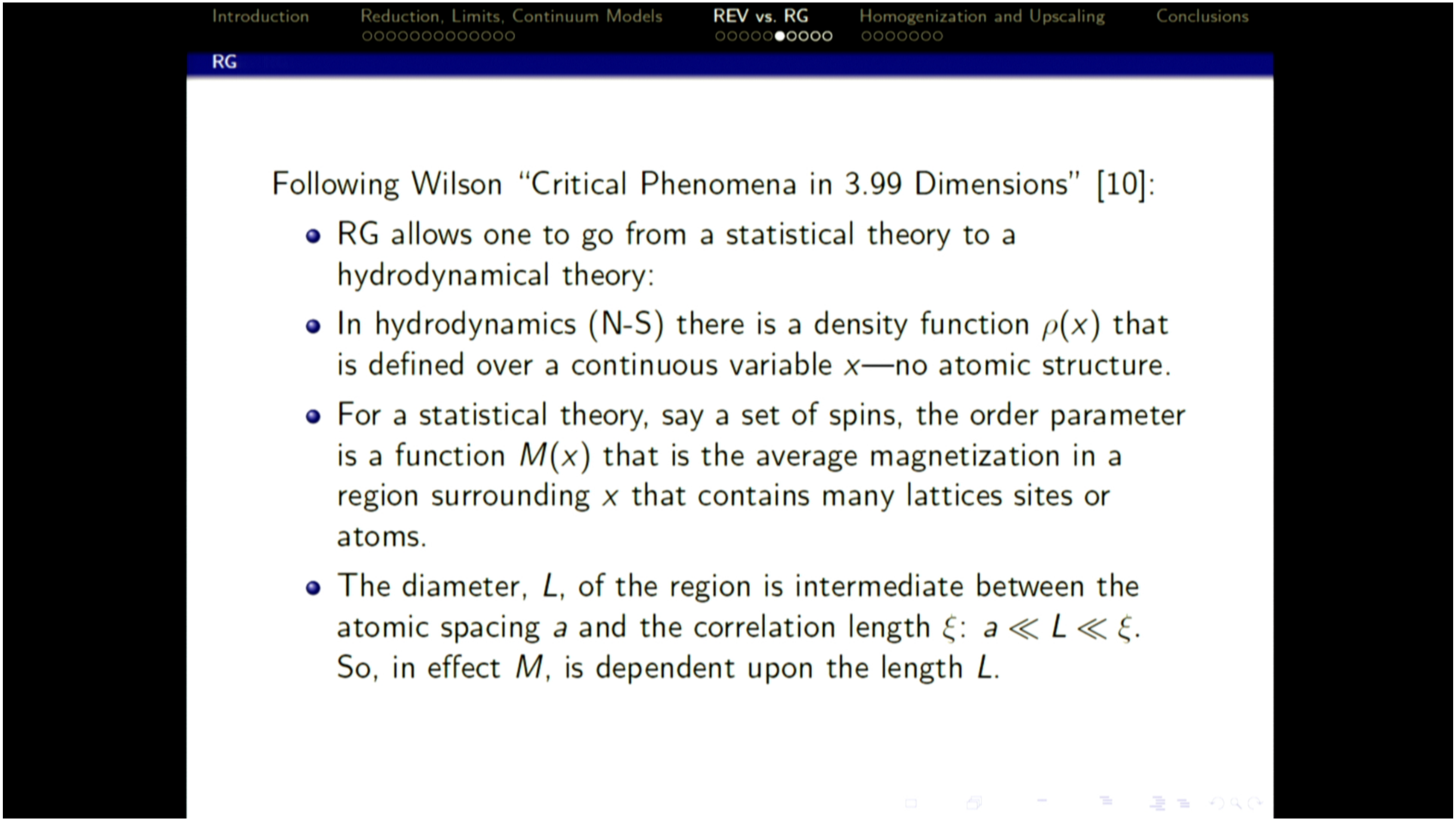
For near critical systems, REV averaging is not going to work.



RG

Following Wilson “Critical Phenomena in 3.99 Dimensions” [10]:

- RG allows one to go from a statistical theory to a hydrodynamical theory:
- In hydrodynamics (N-S) there is a density function $\rho(x)$ that is defined over a continuous variable x—no atomic structure.
- For a statistical theory, say a set of spins, the order parameter is a function $M(x)$ that is the average magnetization in a region surrounding x that contains many lattices sites or atoms.



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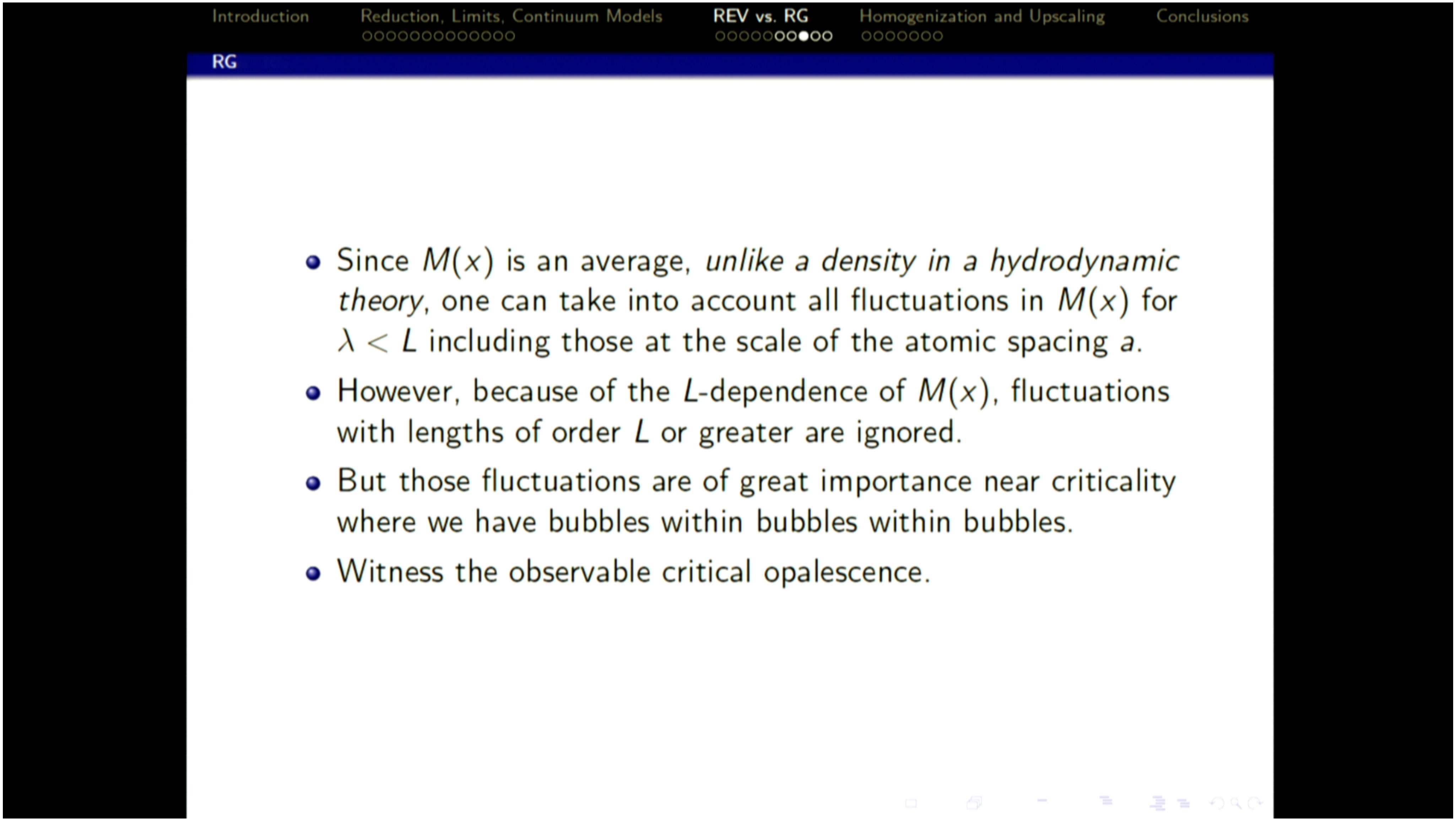
- The diameter, L, of the region is intermediate between the atomic spacing a and the correlation length ξ: $a \ll L \ll \xi$. So, in effect M, is dependent upon the length L.



RG

- Since $M(x)$ is an average, *unlike a density in a hydrodynamic theory*, one can take into account all fluctuations in $M(x)$ for $\lambda < L$ including those at the scale of the atomic spacing a.
- However, because of the L-dependence of $M(x)$, fluctuations with lengths of order L or greater are ignored.
- But those fluctuations are of great importance near criticality where we have bubbles within bubbles within bubbles.
- Witness the observable critical opalescence.

RG

Now one needs to include the contributions to the order parameter for scales/wavelengths $\lambda > L$. One does this piecewise:

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- Given the average $M(x)$ for averaging size L we must determine its value for $L + \delta L$.
- This requires examining a volume $\xi^d \gg V \gg L^d$ (d, the spatial dimension).
- Divide $M(x)$ in V into two parts:

$$M(x) = M_H(x) + mM_{fl}. \tag{3}$$

M_H (a hydrodynamic part with wavelengths of order ξ); M_{fl} (a fluctuating part with wavelength between L and $L + \delta L$).

RG

By performing a single integral over m—the scale factor in (3)—we get an interative expression for the free energy for the averaging size $L + \delta L$, $F_{L+\delta L}$, in terms of the free energy for the averaging size L:

$$e^{-F_{L+\delta L}} = \int_{-\infty}^{\infty} e^{-F_L} dm. \tag{4}$$

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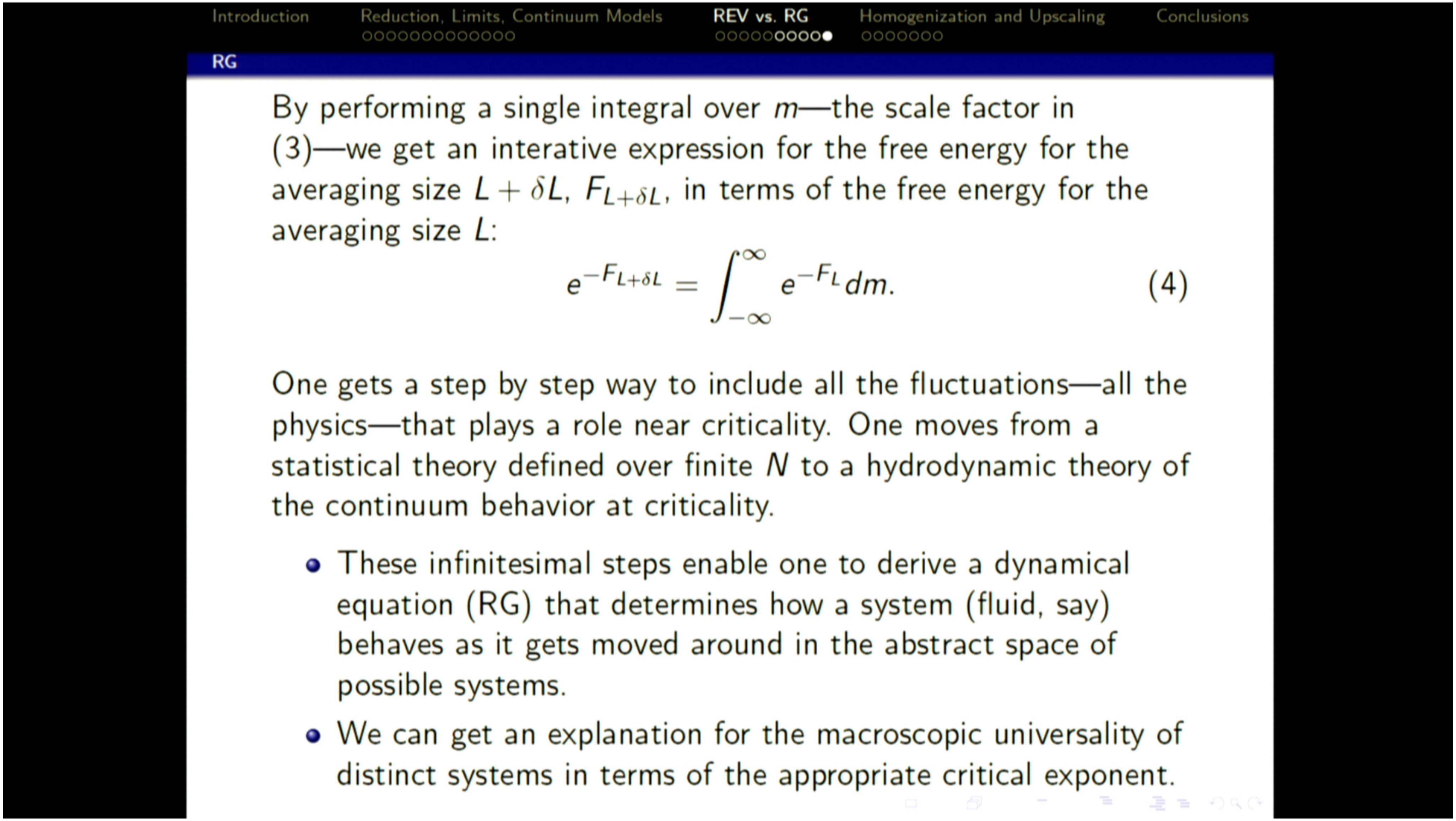

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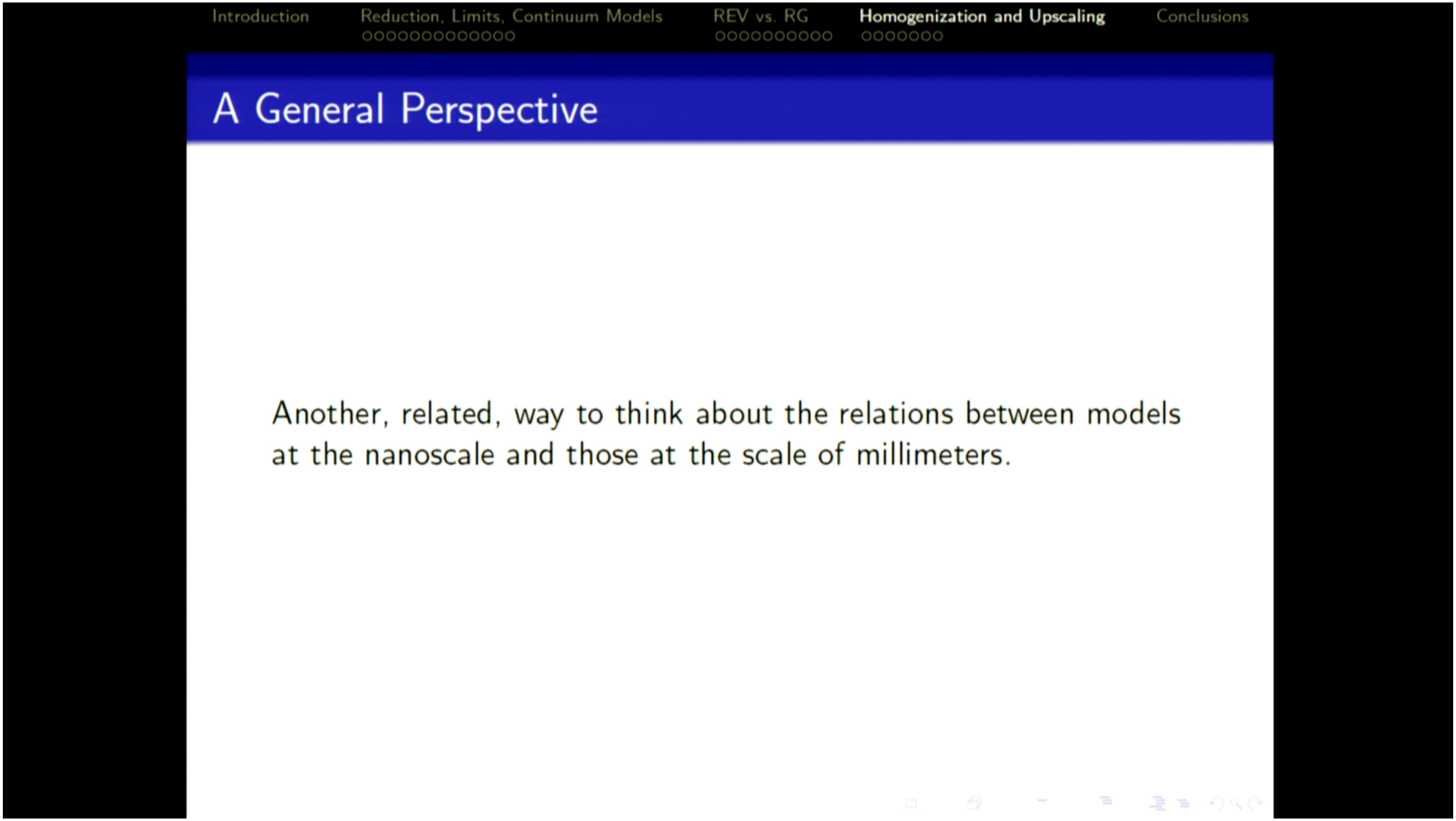
One gets a step by step way to include all the fluctuations—all the physics—that plays a role near criticality. One moves from a statistical theory defined over finite N to a hydrodynamic theory of the continuum behavior at criticality.

- These infinitesimal steps enable one to derive a dynamical equation (RG) that determines how a system (fluid, say) behaves as it gets moved around in the abstract space of possible systems.
- We can get an explanation for the macroscopic universality of distinct systems in terms of the appropriate critical exponent.



A General Perspective

Another, related, way to think about the relations between models at the nanoscale and those at the scale of millimeters.

- There are different ways one might try to “upscale” a statistical/discrete theory to a continuum theory.
    1. Standard averaging methods where one finds a *Representative Elementary Volume* (REV).
    2. Homogenization methods where one, in effect, lets the microscale go to zero.
- The RG account of universal critical behavior can be seen as an instance of the second approach.

Homogenization Methods

Consider a corporation that owns many many casinos. The CEO needs to report to her board on expected profits for the corporation. Her report will undoubtedly refer to a gaussian distribution showing the probabilities of profits and losses with standard deviations allowing for statistical predictions.

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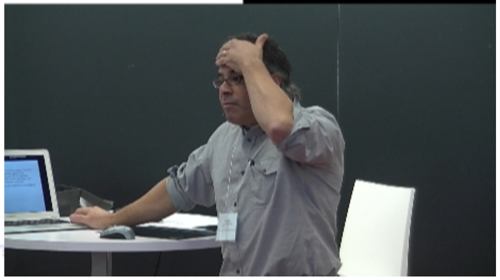

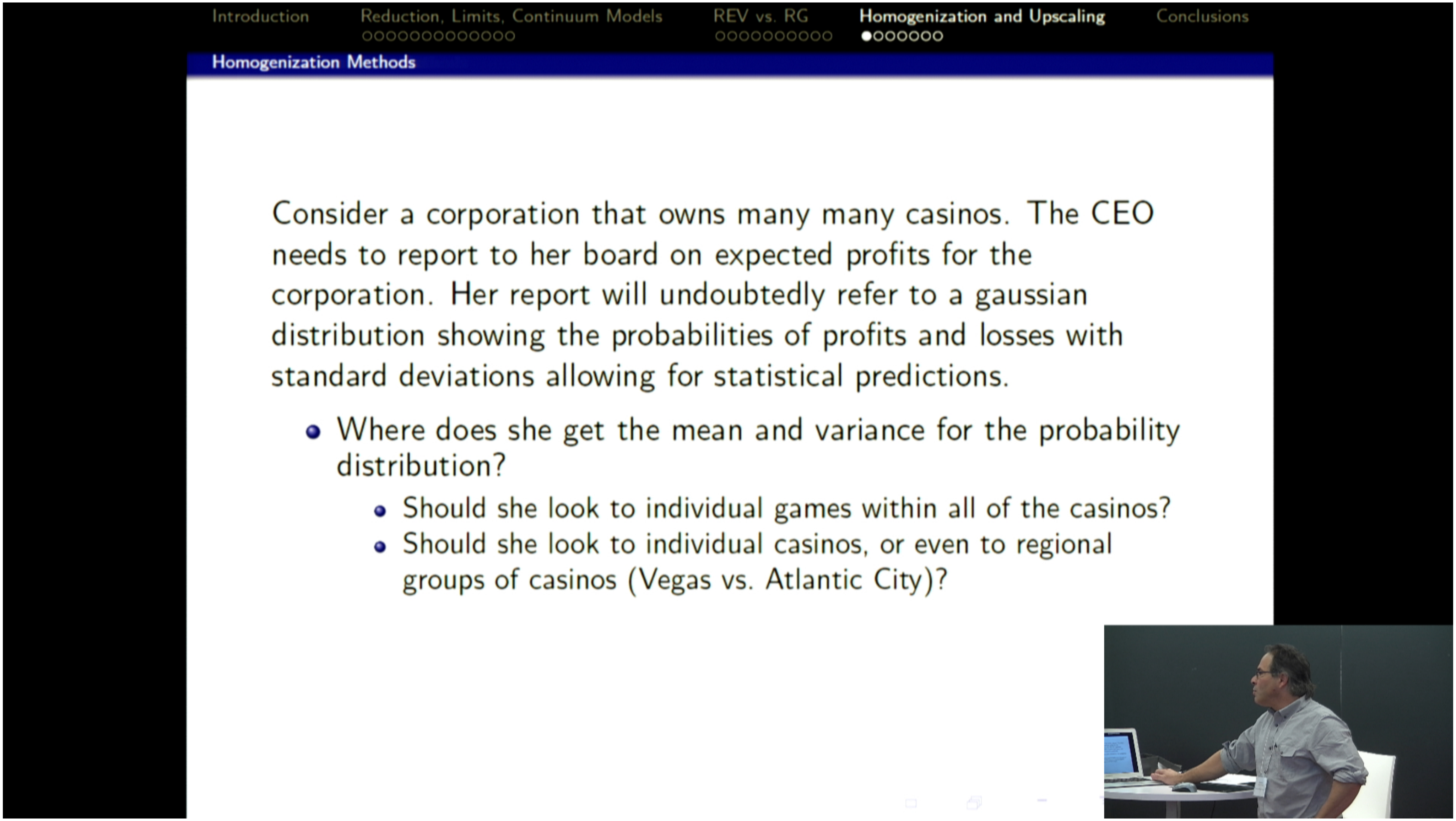

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- Where does she get the mean and variance for the probability distribution?
    - Should she look to individual games within all of the casinos?
    - Should she look to individual casinos, or even to regional groups of casinos (Vegas vs. Atlantic City)?

Homogenization Methods

Figure: Connecting Scales: Gambles within gambles within gambles . . .

Homogenization Methods

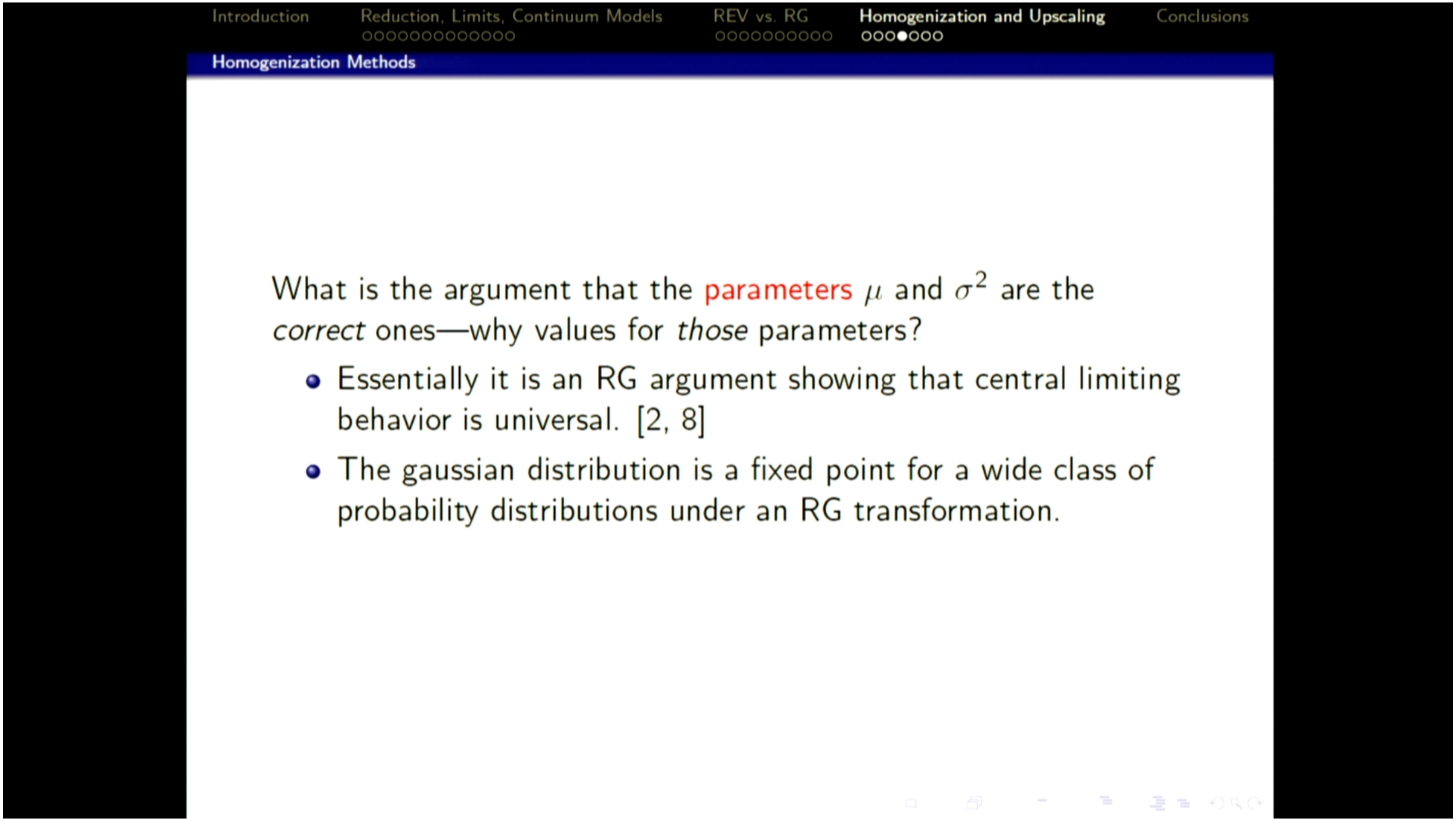
She should look to large collections of casinos where there is evident scaling and self-similarity:

- Apparent scaling at large scales is an indication of homogeneity.

Homogenization Methods

What is the argument that the parameters μ and σ^2 are the *correct* ones—why values for *those* parameters?

- Essentially it is an RG argument showing that central limiting behavior is universal. [2, 8]



Homogenization Methods

What is the argument that the parameters μ and σ^2 are the *correct* ones—why values for *those* parameters?

- Essentially it is an RG argument showing that central limiting behavior is universal. [2, 8]
- The gaussian distribution is a fixed point for a wide class of probability distributions under an RG transformation.

Homogenization Methods

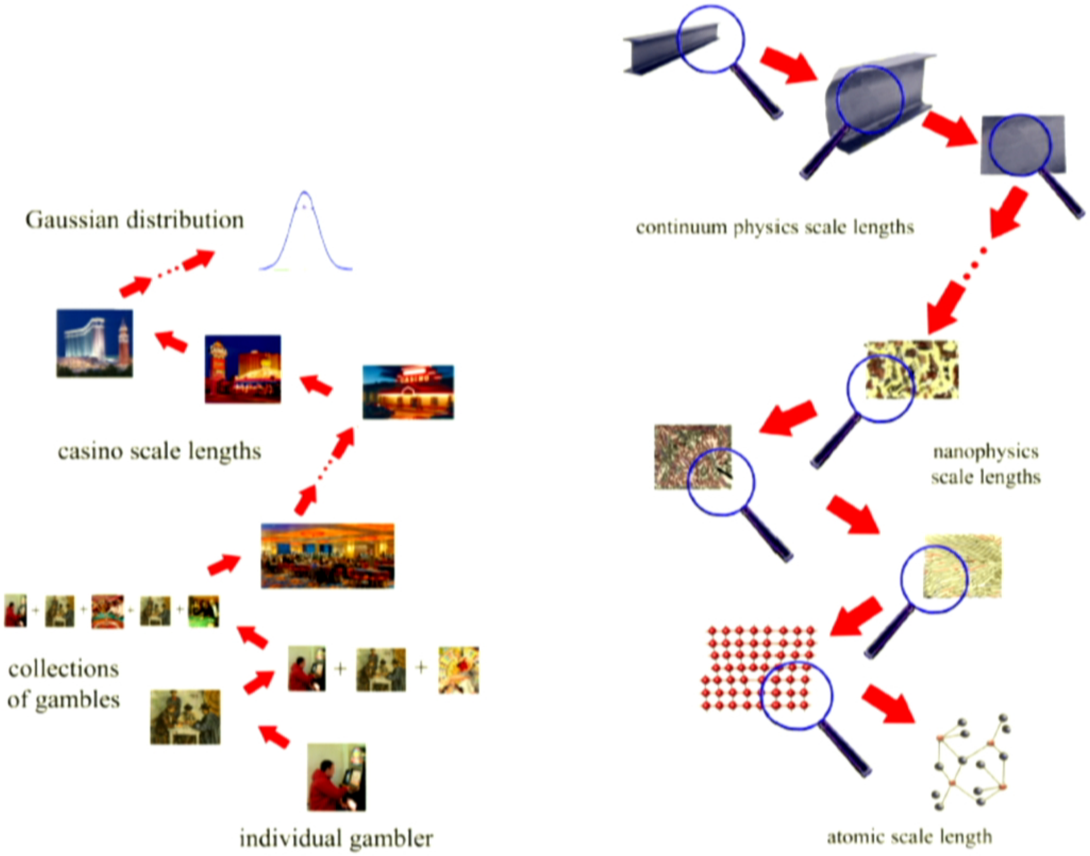
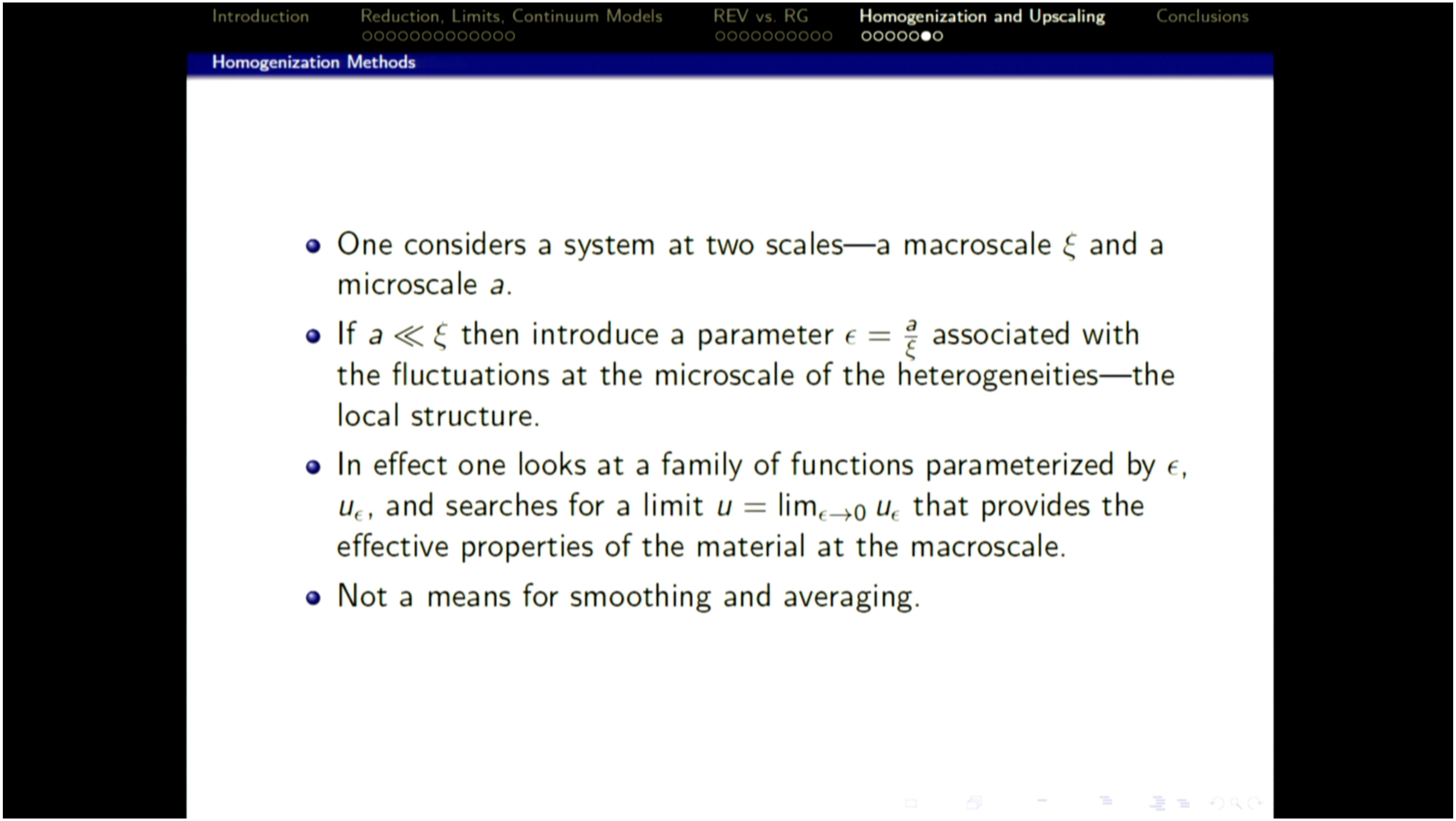


Figure: Gaussian and Steel—Few (Macro) Parameters: $[\mu,\ \sigma^2]$; $[E,\ I]$

Homogenization Methods

- One considers a system at two scales—a macroscale ξ and a microscale a.



Homogenization Methods

- One considers a system at two scales—a macroscale ξ and a microscale a.
- If $a \ll \xi$ then introduce a parameter $\epsilon = \frac{a}{\xi}$ associated with the fluctuations at the microscale of the heterogeneities—the local structure.
- In effect one looks at a family of functions parameterized by ϵ, u_ϵ, and searches for a limit $u = \lim_{\epsilon \to 0} u_\epsilon$ that provides the effective properties of the material at the macroscale.
- Not a means for smoothing and averaging.

Homogenization Methods

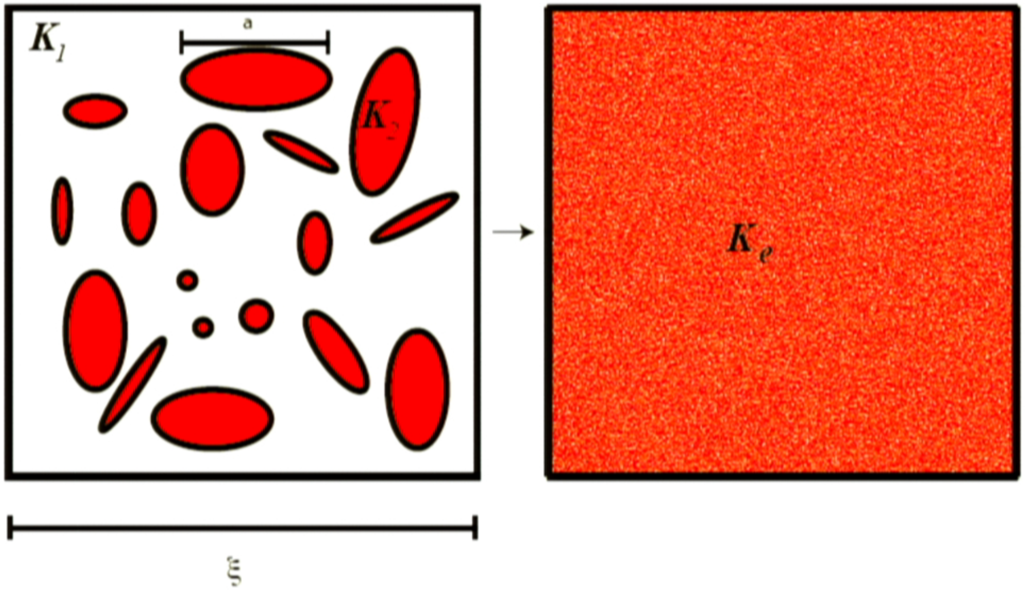


Figure: Homogenization Limit. [K_i–Different tensor quantities characterizing the different phases, K_e—effective tensor characterizing homogeneous bulk property. After Torquato [9]]

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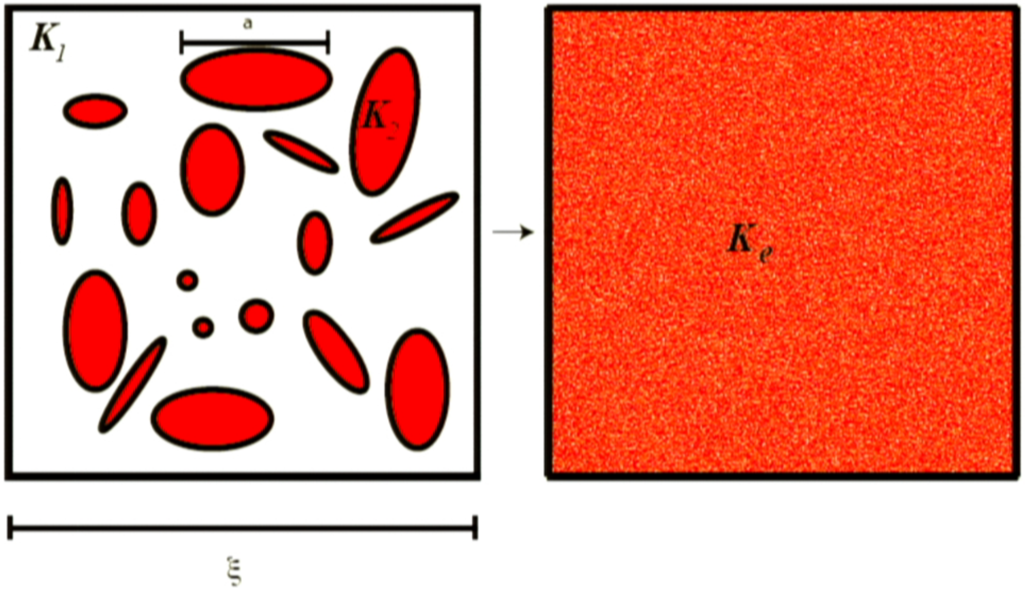

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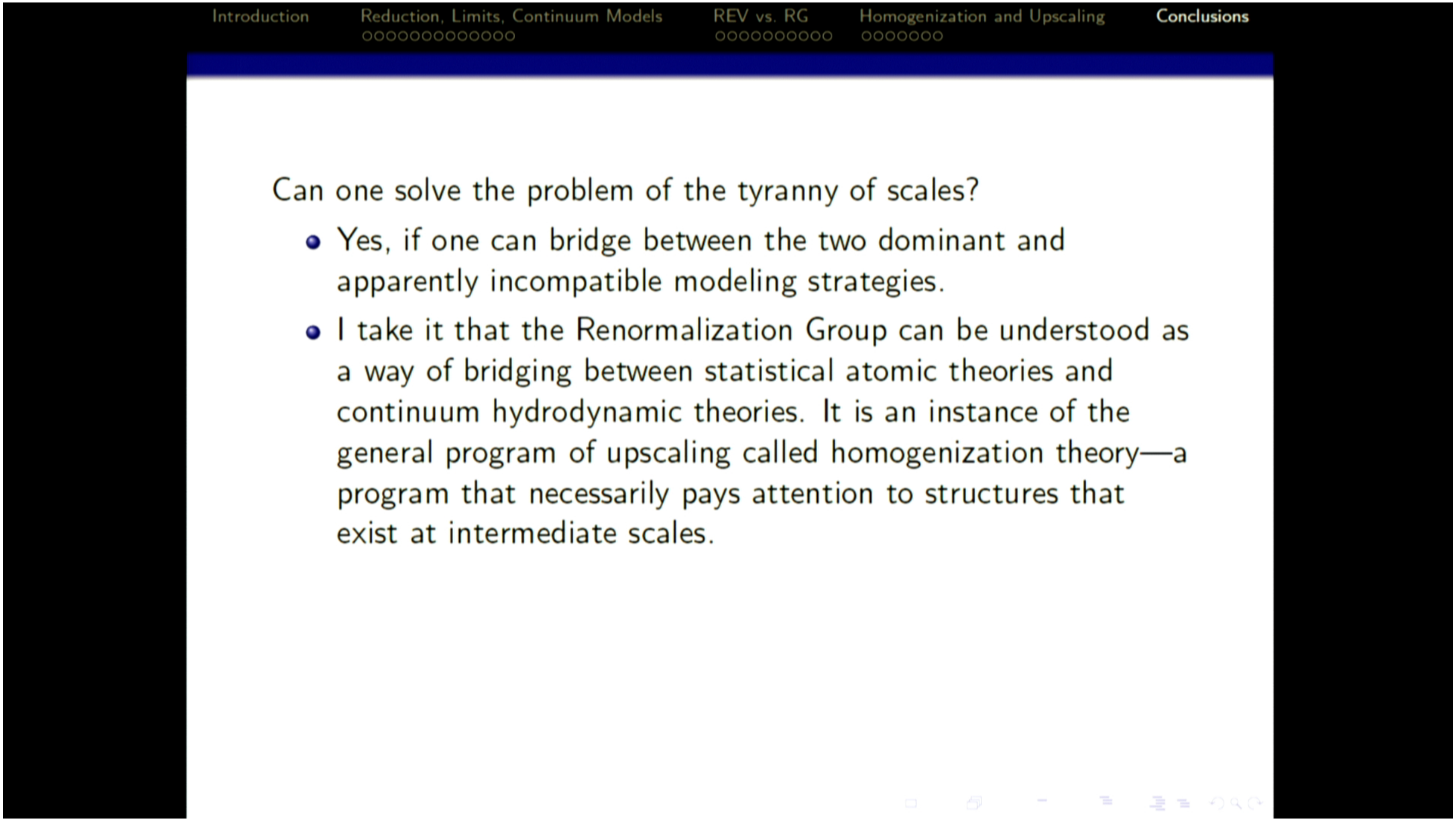
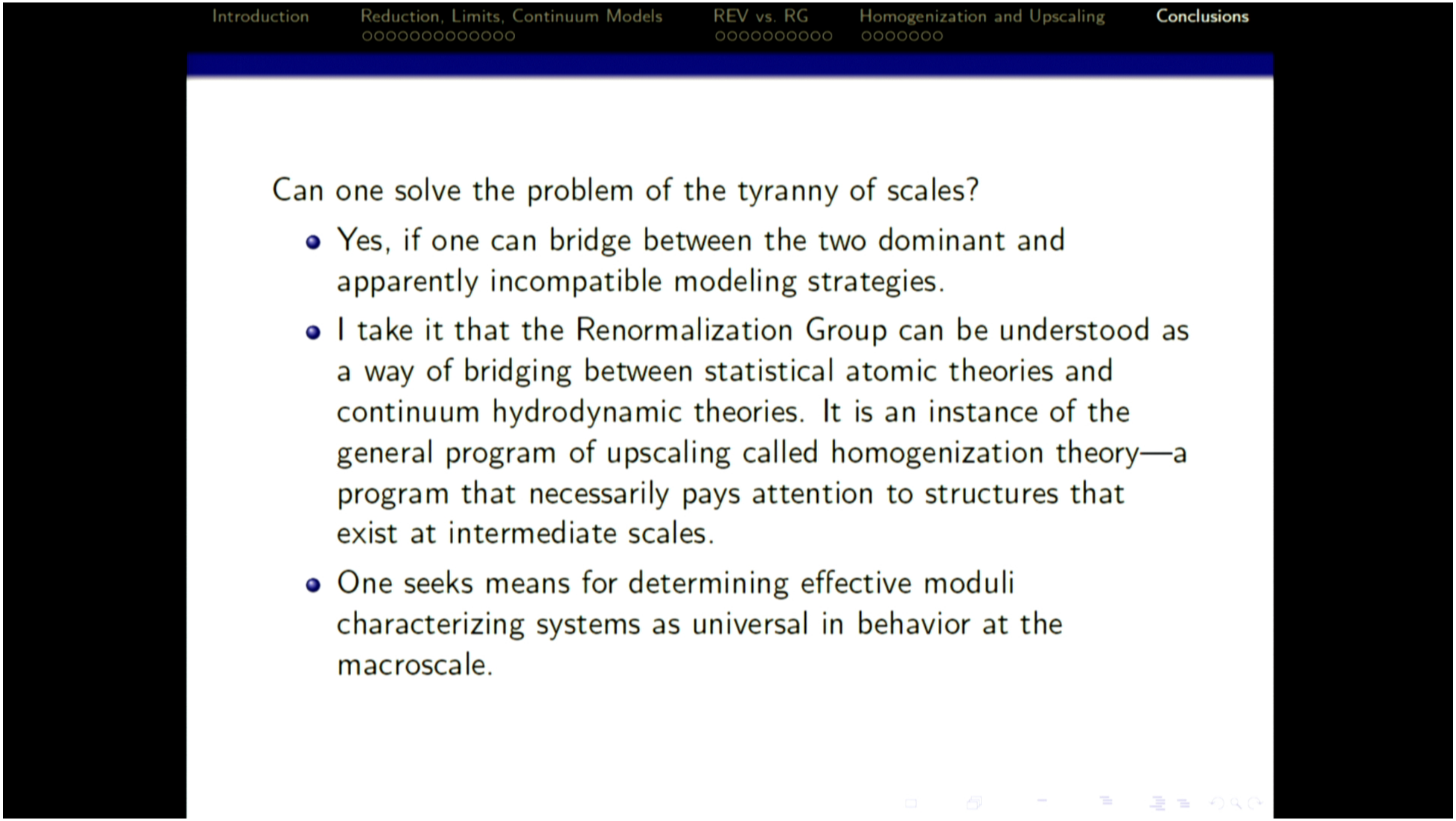


Can one solve the problem of the tyranny of scales?

- Yes, if one can bridge between the two dominant and apparently incompatible modeling strategies.
- I take it that the Renormalization Group can be understood as a way of bridging between statistical atomic theories and continuum hydrodynamic theories. It is an instance of the general program of upscaling called homogenization theory—a program that necessarily pays attention to structures that exist at intermediate scales.



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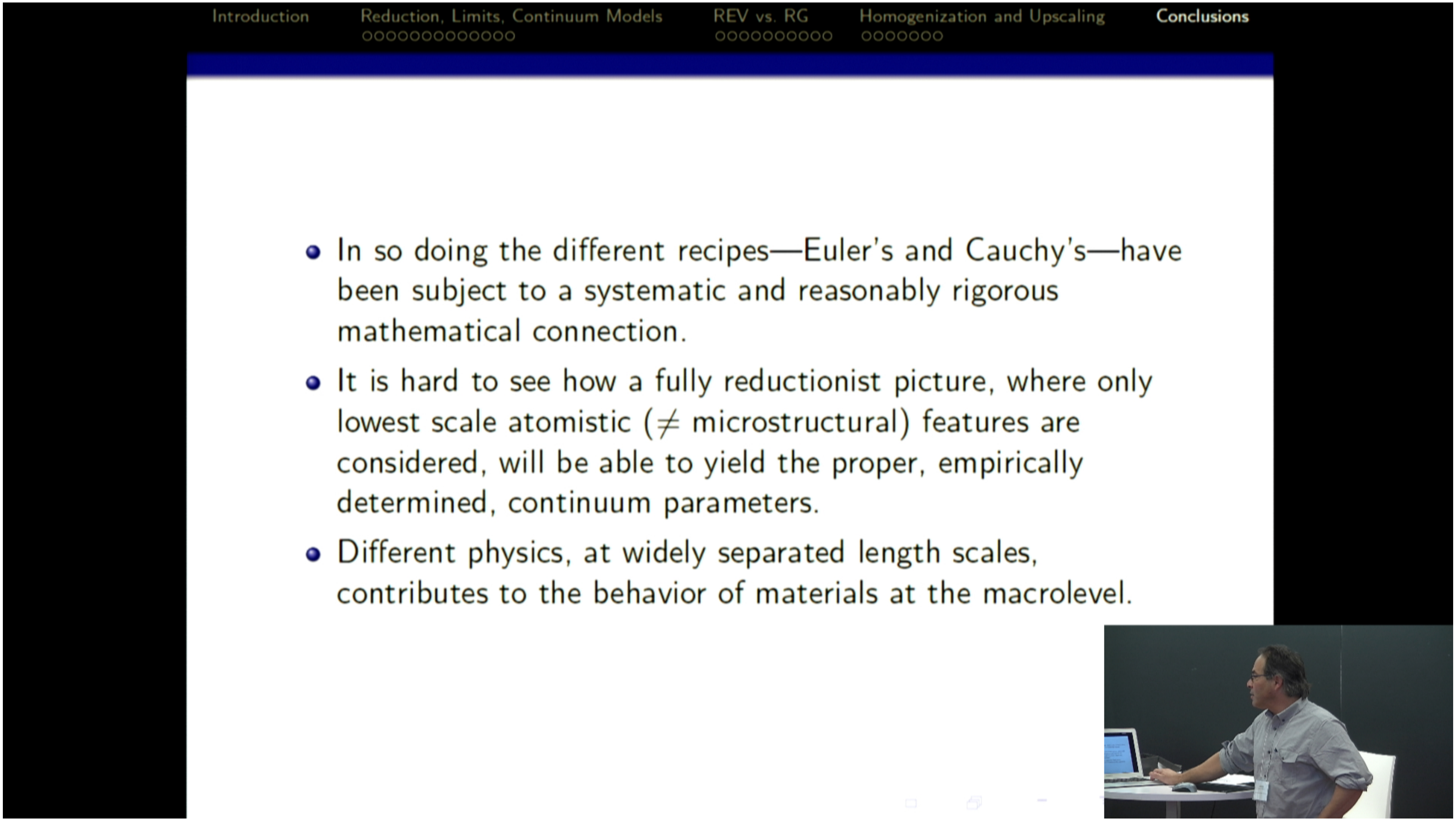
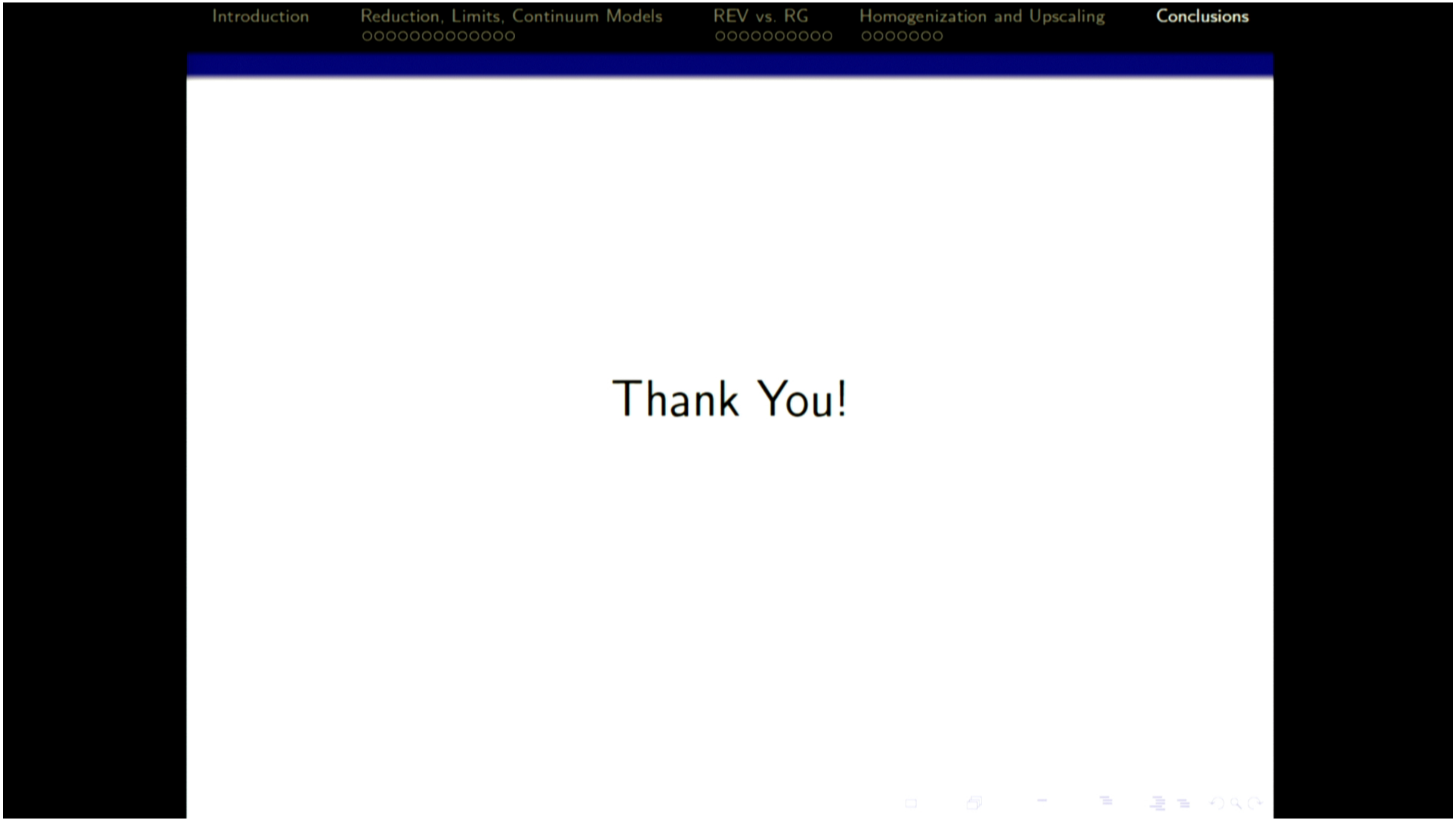
- One seeks means for determining effective moduli characterizing systems as universal in behavior at the macroscale.



- In so doing the different recipes—Euler's and Cauchy's—have been subject to a systematic and reasonably rigorous mathematical connection.
- It is hard to see how a fully reductionist picture, where only lowest scale atomistic ($\neq$ microstructural) features are considered, will be able to yield the proper, empirically determined, continuum parameters.
- Different physics, at widely separated length scales, contributes to the behavior of materials at the macrolevel.

Rob Phillips in *Crystals, Defects, and Microstructures* [7]:

"Despite the power of the idea of a material parameter, it must be greeted with caution. For many features of materials, certain 'properties' are not *intrinsic*. For example, both the yield strength and fracture toughness of a material depend upon its internal constitution. That is, the measured material response can depend upon microstructural features such as the grain size, the porosity, etc. Depending upon the extent to which the material has been subjected to prior working and annealing, these properties can vary considerably. Even a seemingly elementary property such as the density can depend significantly upon that material's life history. The significance of the types of observations given above is the realization that *many material properties depend upon more that just the identity of the particular atomic constituents that make up that material. . . . [M]icrostructural features such as point defects, dislocations, and grain boundaries can each alter the measured macroscopic 'properties' of a material.*"



Thank You!