Fundamentals of multiphase flow in porous media
From the molecular scale to the REV scale
Averaging-thermodynamic approach for development of basic equations

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Materials have a fundamentally discrete nature, consisting of particles (for example, molecules, ions, and/or atoms), with spatially discrete and temporally random (in fact enormously fluctuating) properties. However, we commonly observe and describe them as continua. We employ concepts such as pressure, viscosity, temperature, and mass density that even don’t exist at the particulate level. Given the fact that the behavior of a material at a given scale derives ultimately from its structure at lower scale(s), one may ask the question whether we can link the continuum description of materials to their fundamentally discrete nature. One may ask questions such as:
- What is the origin of pressure?
- What is the origin of viscous stress?
- What is the origin of diffusion and diffusivity?
- What is the origin of internal energy?
Can we derive Navier-Stokes equations, Fick’s law, or Darcy’s law starting from a molecular description of the matter? How about equations governing flow and transport in more complex systems, such as a porous medium? In this lecture series, we use principles and methods of continuum mechanics and rational thermodynamics to derive governing equations for flow and transport in fluids, solids, and in porous media.

We start with a particulate description of the matter. We assume that a material system consists of a set of fundamentally discrete particles (point masses), each having a mass \( m \) and a position vector \( \mathbf{x}(t) \). We also assume that there are attraction/repulsion forces among them and there are long-range forces acting on particles. The second Law of Newton is assumed to apply to each and every particle.

With this very limited set of assumptions, we follow an upscaling procedure that allows us to derive equations of conservation of mass, momentum, and energy at larger scales. Next, we present a procedure for deriving constitutive laws for various materials (deforming solids, gasses, viscous liquids, diffusing solutes, porous media, and even a river catchment). Following this systematic procedure, we derive well-known equations such as Navier-Stokes equations, Fick’s law, and Darcy’s law.

Participants only need to have a basic knowledge of mathematics and physics. Familiarity with concepts of derivation and integration would be sufficient.

Plan of lectures could be as follows (12 hours of lectures in two days):
- From molecular to pore or grain scale; derivation of conservation equations for a single phase; 3 hours
- Derivation of constitutive equations for solids (e.g., Hooke’s law of elasticity) and fluids (e.g., Newton’s law of viscosity) using Rational thermodynamic approach; 3 hours
- From molecular to core scale; derivation of conservation eqs. for a porous medium (Averaging); 1 hour
- Derivation of constitutive equations for single-phase flow in a porous medium (Rational thermodynamic approach); 1 hour
- Derivation of equations for multiphase flow in a porous medium (Rational thermodynamics); 2 hours
- Advanced theories of two-phase flow in porous media; combining conservation laws and constitutive equations; 2 hours