
Introduction to Aspects of Multiscale Modeling as Applied to Porous Media

Part I

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Importance of Subsurface Flow

Groundwater:

- Groundwater provides over 50% of the water used in the US, and over 90% in many European countries.
- San Antonio, the seventh largest US city, is entirely dependent on groundwater.
- World population growth of 2 billion in the next 25 years will require 17% increase in water just to grow food.
- By 2025, 2/3 of the world's population is likely to experience moderate to severe water shortages.
- EPA estimates \$100 billion cost over the next 15 years to ensure safe drinking water in US.

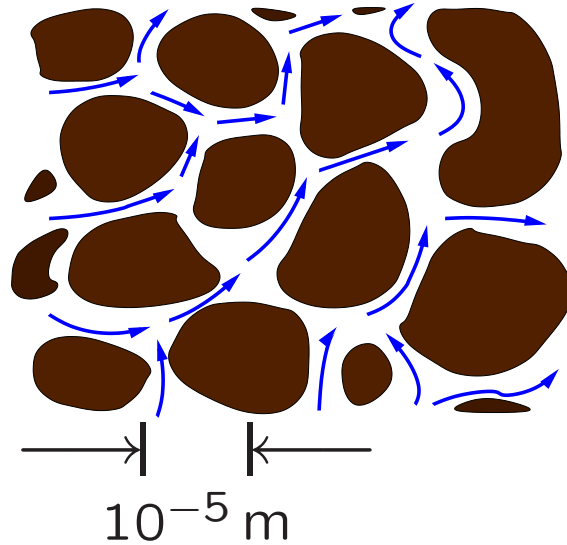
Petroleum:

- Petroleum and natural gas will continue to play a major role in meeting the world's energy needs.
- Economic expansion, especially in Asia, will increase fossil fuel demand.
- A promising technique to reduce greenhouse gasses is to sequester CO₂ in deep saline aquifers.

Flow in Porous Media

Microstructure

A natural porous medium is a rock with void or *pore* space between the rock grains. The pore scale is around 10^{-5} to 10^{-4} meter (0.01 to 0.1 millimeter).

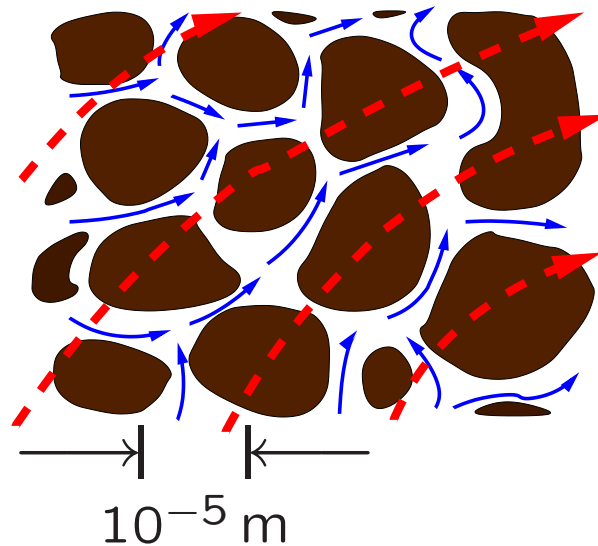


Problem: Too much detail!

- Requires too much information to characterize.
- Generates too much information to analyze.
- Computationally intractable (requires $\sim 10^{23}$ resolution).

Upscaling

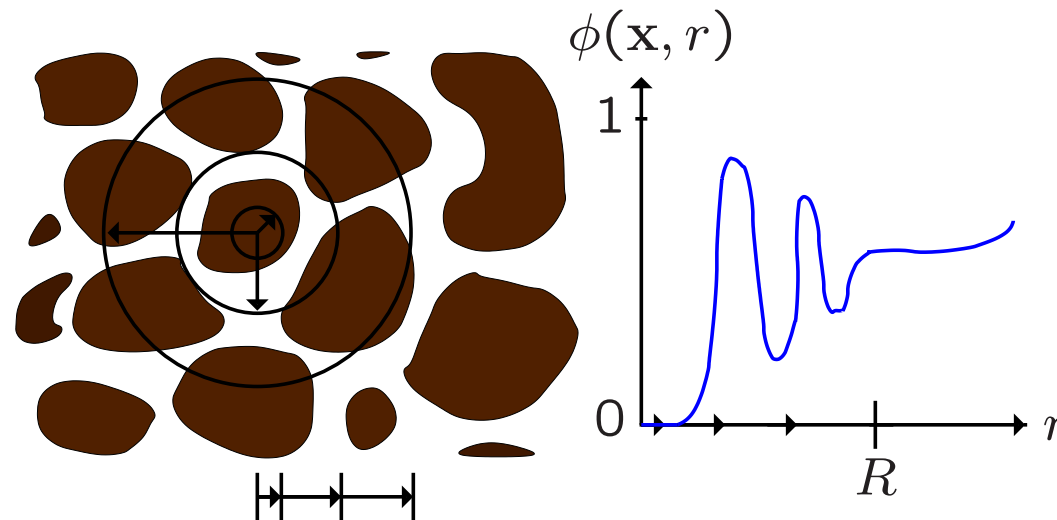
Question: Can we find the “average” macroscale flow without finding the microscale flow? That is, can we **change scale** from 10^{-5} meter to about 0.1–1 meter?



The system must be represented on a larger scale by incorporating the finer details in an **average** sense only.

Representative Elementary Volume and Porosity

Definitions: The *porosity*, ϕ , at a point \mathbf{x} is the ratio of pore volume to total volume in a *representative elementary volume* (REV). The REV is a ball of radius $R > 0$ centered at \mathbf{x} , where R is the smallest so that porosity is “well defined,” i.e., ϕ does not change (much) for r greater than but near R .



If V is the volume of the ball of radius R and V_{pore} is the volume of the ball intersected with the void space, then

$$\phi(\mathbf{x}) = \phi(\mathbf{x}, R) = \frac{V_{\text{pore}}}{V}.$$

Question: Will this quantity always “settle down”?

Continuum Modeling Hypothesis

The **continuum modeling hypothesis** is that the REV is well defined. That is, things act as a continuum on scales greater than R . We do not model (directly) anything below this scale.

Micromodel: At the microscale, we have fluid flowing in pore space around rock grains. The fluid obeys the Navier-Stokes equations (this is a continuum hypothesis on fluids!).

Macromodel: How do we define the governing system at the macroscale? By the three **pillars of science**: experiments, theory, and computation!

Pillar 1: Experiments

Experimental observations: Does the system behave consistently in terms of measurement devices at least the size of R ? Can we discover empirically the governing equations of the macromodel? Is what we see consistent with what we know about other systems?

Pillar 2: Theory

Theoretical upscaling: We begin with the system as defined at the microscale. This is assumed to be the true or correct model of the system. The theoretical (i.e., mathematical) technique is used to obtain the macroscale model, with the deviation between the two models bounded by some small parameter, such as R (so the error is small).

Many techniques are available, such as:

- Probabilistic/statistical (thermodynamics, statistical mechanics);
- Volume averaging/effective properties (solid and fluid mechanics);
- Dimensional/scaling analysis;
- Mathematical homogenization (limits of operators);
- Mixture theory;
- Distributed microstructure models;
- Multiscale numerical techniques;
- and others!

Pillar 3: Computation

Computations: These allow a detailed comparison of the macromodels and experiments. Moreover, we can test hypotheses about the form of the macromodel.

More directly, computational investigation allow us to simulate the flow at the microscale, which we can average and compare to the macroscale model computations.

Experiments: Darcy's Law and Permeability

Darcy's empirical law (1856). The fluid velocity is proportional to the pressure gradient

$$\mathbf{u} = -\frac{K}{\mu} \nabla p$$

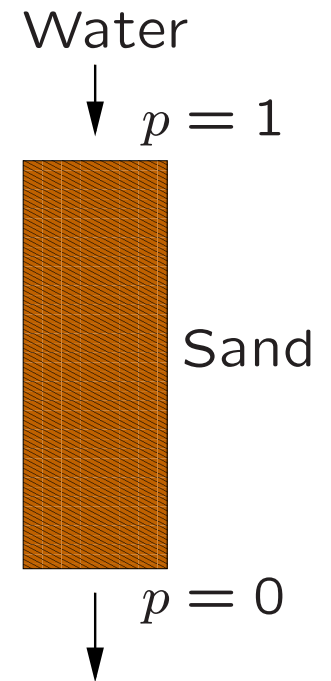
where

$\mathbf{u}(\mathbf{x})$ is the volumetric flux (the **Darcy velocity**)

$K(\mathbf{x})$ is the measured rock **permeability**

μ is the fluid viscosity

$p(\mathbf{x})$ is the fluid pressure



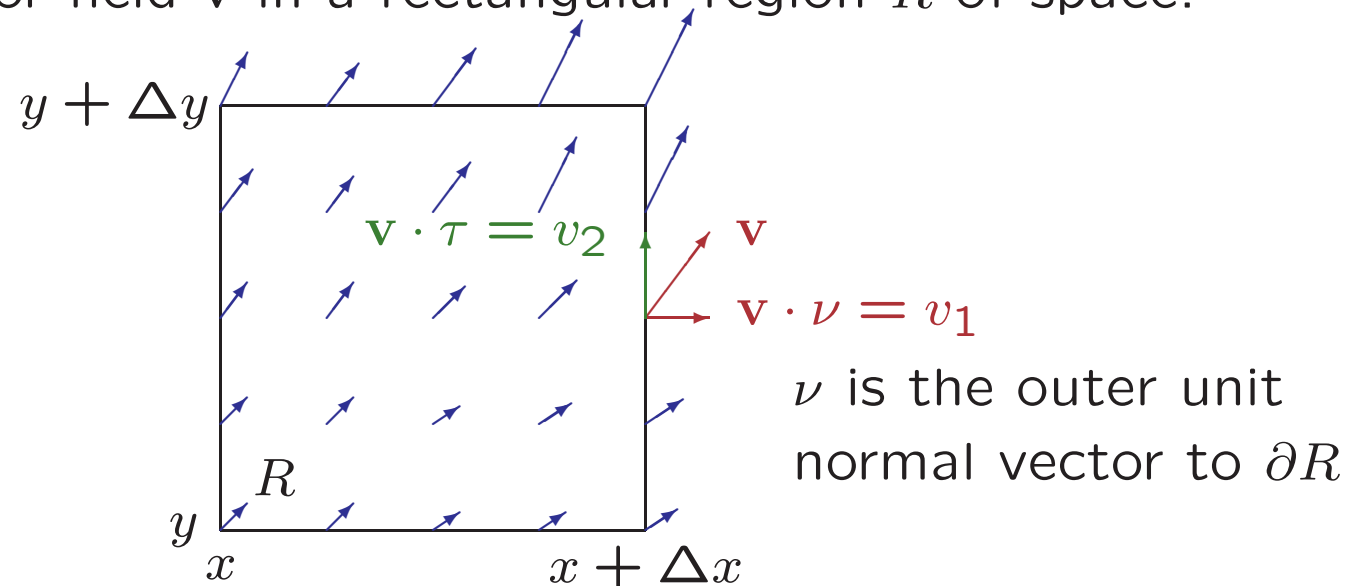
Remark: Darcy's law has been derived theoretically and computationally as well. Thus we have good empirical, theoretical, and computational scientific evidence that the law is the governing principle of subsurface flow.

Question: Are we done? What is missing from the model?

Conservation of Continuous Fluids: The Theoretical Principle of Mass Conservation

The Divergence Theorem—1

Consider a vector field \mathbf{v} in a rectangular region R of space.



The total flow through the boundary ∂R is

$$\begin{aligned}
 \int_{\partial R} \mathbf{v} \cdot \boldsymbol{\nu} \, dS &= \int_y^{y+\Delta y} \left(v_1(x + \Delta x, s) - v_1(x, s) \right) ds \\
 &\quad + \int_x^{x+\Delta x} \left(v_2(r, y + \Delta y) - v_2(r, y) \right) dr \\
 &= \int_y^{y+\Delta y} \int_x^{x+\Delta x} \frac{\partial v_1(r, s)}{\partial x} \, dr \, ds + \int_x^{x+\Delta x} \int_y^{y+\Delta y} \frac{\partial v_2(r, s)}{\partial y} \, ds \, dr \\
 &= \iint_R \left(\frac{\partial v_1(r, s)}{\partial x} + \frac{\partial v_2(r, s)}{\partial y} \right) \, dr \, ds.
 \end{aligned}$$

The Divergence Theorem—2

Definition. In 3-D, let

$$\nabla \cdot \mathbf{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z} = \sum_{i=1}^d \frac{\partial v_i}{\partial x}$$

be the **divergence** of \mathbf{v} (in 2-D, omit the partial derivative in z).

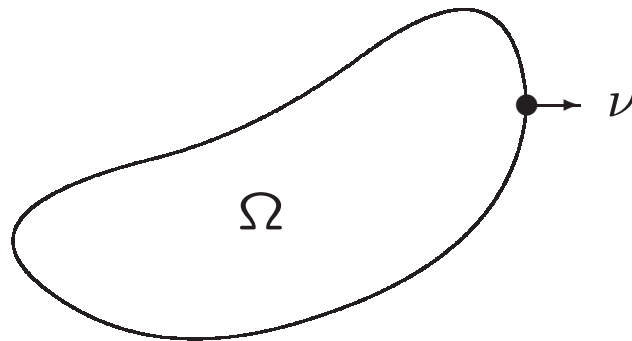
Theorem.

$$\iiint_R \nabla \cdot \mathbf{v} \, dx \, dy \, dz = \iint_{\partial R} \mathbf{v} \cdot \boldsymbol{\nu} \, dS.$$

We can fill any region with cubes and add the results above.

Theorem. For any region Ω with unit outer normal vector $\boldsymbol{\nu}$,

$$\iiint_{\Omega} \nabla \cdot \mathbf{v} \, dx \, dy \, dz = \iint_{\partial \Omega} \mathbf{v} \cdot \boldsymbol{\nu} \, dS.$$



Conservative Fluid Flow

Suppose

ξ is a conserved quantity ξ (mass/volume)

\mathbf{v} is the fluid velocity (length/time)

$\xi\mathbf{v}$ is the *flux* of ξ (mass/area/time)

f is an external source or sink of fluid (mass/volume/time)

Within a region of space R , the total amount of ξ changes in time by

$$\underbrace{\frac{d}{dt} \iiint_R \xi \, dx \, dy \, dz}_{\text{Change in } R} = - \underbrace{\iint_{\partial R} \xi \mathbf{v} \cdot \boldsymbol{\nu} \, dS}_{\text{Flow across } \partial R} + \underbrace{\iiint_R f \, dx \, dy \, dz}_{\text{Sources/sinks}}$$

\implies conservation locally on R

$$\iiint_R \xi_t \, dx \, dy \, dz = - \underbrace{\iiint_R \nabla \cdot (\xi \mathbf{v}) \, dx \, dy \, dz}_{\text{Divergence Theorem}} + \iiint_R f \, dx \, dy \, dz$$

This is true for each region R , so in fact

$$\boxed{\xi_t + \nabla \cdot (\xi \mathbf{v}) = f}$$

Application to Porous Media: The Macromodel

Darcy's Law

Darcy's law with gravity tells us that the fluid flux is

$$\mathbf{u} = -\frac{K}{\mu}(\nabla p + \rho \mathbf{g}),$$

where

$p(\mathbf{x}, t)$ is the fluid pressure

$\mathbf{u}(\mathbf{x}, t)$ is the Darcy velocity

$K(\mathbf{x})$ is the permeability of the medium

μ is the fluid viscosity

$\rho(\mathbf{x}, t)$ is the fluid density

\mathbf{g} is the gravitational constant vector

Remark. If we neglect gravity, Darcy's law tells us that fluid flows from high pressure to low pressure. We determine the direction of flow by taking the gradient of the pressure, and multiplying by K/μ .

Question: Why does K need to be positive?

Single Phase Darcy Flow

Conservation and Darcy's law requires that

$$\frac{\partial \phi \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = F \quad \implies \quad \frac{\partial \phi \rho}{\partial t} - \nabla \cdot \left(\rho \frac{K}{\mu} (\nabla p + \rho \mathbf{g}) \right) = F.$$

where

$p(\mathbf{x}, t)$ is the fluid pressure

$\mathbf{u}(\mathbf{x}, t)$ is the Darcy velocity ($\mathbf{v} = \mathbf{u}/\phi$)

$\phi(\mathbf{x}, t)$ is the porosity of the medium

$K(\mathbf{x})$ is the permeability of the medium

μ is the fluid viscosity

$\rho(\mathbf{x}, t)$ is the fluid density ($\xi = \phi \rho$)

\mathbf{g} is the gravitational constant vector

$F(\mathbf{x}, t)$ is the source/sink (i.e., wells)

Question: Why is $\mathbf{v} = \mathbf{u}/\phi$ and the conserved quantity $\xi = \phi \rho$?

Incompressible Single Phase Darcy Flow

If the fluid and medium are **incompressible** (ρ is constant and ϕ is constant in time), and we neglect gravity ($g = 0$), then we have

$$\nabla \cdot \mathbf{u} = f \quad \implies \quad -\nabla \cdot (k \nabla p) = f,$$

where

$f(\mathbf{x})$ is $F(\mathbf{x})/\rho$ (assuming f does not change in time)

$k(\mathbf{x})$ is $K(\mathbf{x})/\mu$

In coordinate form, this is

$$-\frac{\partial}{\partial x} \left(k \frac{\partial p}{\partial x} \right) - \frac{\partial}{\partial y} \left(k \frac{\partial p}{\partial y} \right) - \frac{\partial}{\partial z} \left(k \frac{\partial p}{\partial z} \right) = f.$$

It is convenient to write a partial derivative using a subscript. Then we have more simply

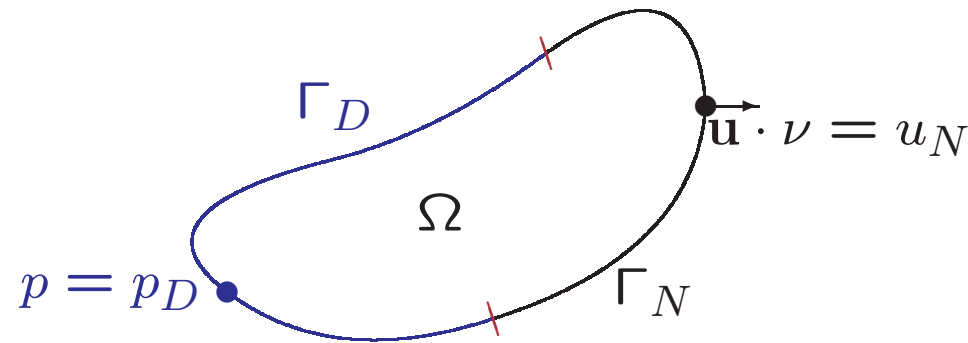
$$-(k p_x)_x - (k p_y)_y - (k p_z)_z = f.$$

Question: Is the model complete now?

Boundary Conditions (BC's)

The equation holds in the **interior** of the porous formation, which we call $\Omega \subset \mathbb{R}^3$. We must also specify what happens on the boundary, $\partial\Omega$.

We consider two types of **boundary conditions**. Decompose $\partial\Omega$ into nonoverlapping regions Γ_D and Γ_N (so $\partial\Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$).



1. **Dirichlet.** Specify p_D , the pressure on Γ_D :

$$p = p_D.$$

2. **Neumann.** Specify u_N , the outward normal flux on Γ_N :

$$\mathbf{u} \cdot \boldsymbol{\nu} = u_N.$$

This is the fluid that enters or leaves the domain Ω . For example, $u_N = 0$ for a sealed boundary which cannot support flow.

Remark. If $p_D = 0$ and $u_N = 0$, the BC's are said to be **homogeneous**.

Compatibility Condition

If $\Gamma_N = \partial\Omega$ (i.e., $\Gamma_D = \emptyset$), then we may have a conservation problem. Recall the derivation. Within a region of space R , the total amount of $\xi = \phi\rho$ is now constant in time, so

$$0 = \underbrace{\frac{d}{dt} \iiint_R \phi\rho \, dx}_{\text{Change in } R} = - \underbrace{\iint_{\partial R} \rho \mathbf{u} \cdot \nu \, da(x)}_{\text{Flow across } \partial R} + \underbrace{\iiint_R \rho f \, dx}_{\text{Sources/sinks}}$$

If $R = \Omega$, we must have

$$\iiint_{\Omega} f \, dx = \iint_{\partial\Omega} \mathbf{u} \cdot \nu \, da(x)$$

That is, the data must satisfy the **compatibility condition**

$$\iiint_{\Omega} f \, dx = \iint_{\partial\Omega} u_N \, da(x) \text{ when } \Gamma_N = \partial\Omega.$$

Remark. If you inject some fluid through u_N on the boundary or through f in the interior, you must take it out somewhere else! This is basically what it means to have an incompressible fluid and medium.

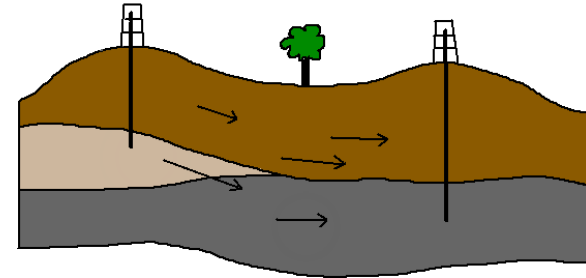
We will always assume that the compatibility condition holds in this case.

Question: Does the Dirichlet BC require a compatibility condition?

Governing Equations of Single-phase Flow

In summary, the macromodel for incompressible single phase flow is a **second order elliptic boundary value problem** of the form

$$\begin{cases} -\nabla \cdot (k \nabla p) = f, & \text{in } \Omega, \\ p = p_D, & \text{on } \Gamma_D, \\ -(k \nabla p) \cdot \nu = u_N, & \text{on } \Gamma_N, \end{cases}$$



which is also written in **mixed form** as

$$\begin{cases} \mathbf{u} = -k \nabla p, & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = f, & \text{in } \Omega, \\ p = p_D, & \text{on } \Gamma_D, \\ \mathbf{u} \cdot \nu = u_N, & \text{on } \Gamma_N. \end{cases}$$

Theorem: Under reasonable hypotheses, there exists a unique solution (\mathbf{u}, p) to the boundary value problem. Moreover, the solution exhibits continuous dependence on the data (f, p_d, u_N, k) .

Question: Why is this result important?

Question: Are we done?