
Model PDEs and Basic Numerical Methods

2.1 Some classical equations

In this section, we introduce some classical equations.

2.1.1 Heat equations

$$\left\{ \begin{array}{l} \frac{\partial u}{\partial t} - \nabla \cdot (k \nabla u) = f \\ u(x, 0) = u_0(x) \\ u = g \quad \text{on } \Gamma_D \subset \partial\Omega \\ \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_N \subset \partial\Omega \end{array} \right.$$

where $\nabla = \text{grad} = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d})^T$, $d = 1, 2, 3$.

2.1.2 Poisson equation

Poisson equation is the steady state of heat equations with $\kappa = 1$.

$$\left\{ \begin{array}{l} -\Delta u = f \\ u = g \quad \text{on } \Gamma_D \subset \partial\Omega \\ \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_N \subset \partial\Omega \end{array} \right.$$

2.1.3 Linear elasticity

We consider a homogeneous isotropic elastic body occupying a bounded domain $\Omega \in \mathbb{R}^3$ with boundary Γ decomposed into two parts Γ_D and Γ_N such that Γ_D has a positive area. Let the elastic body be acted upon by a volume load $f = (f_1, f_2, f_3)$ and boundary load $g = (g_1, g_2, g_3)$ on Γ_N . Furthermore, we assume that the body is fixed along Γ_D .

Let $u = (u_1, u_2, u_3)$ be the displacement of the elastic body. We assume that u is small. The linear elasticity theory shows that the displacement u should satisfy the following equilibrium equation:

$$(2.1) \quad \sigma = \lambda \operatorname{div} u + 2\mu \epsilon(u) \quad \text{in } \Omega$$

$$(2.2) \quad -\operatorname{div} \sigma = f \quad \text{in } \Omega$$

$$(2.3) \quad u = 0 \quad \text{on } \Gamma_D$$

$$(2.4) \quad 2\mu \sigma n = g \quad \text{on } \Gamma_N.$$

Here σ is stress and $\epsilon(u) = (\epsilon_{ij}(u))_{ij}$ with

$$\epsilon_{ij}(u) = \frac{1}{2}(\partial_j u_i + \partial_i u_j).$$

Alternatively the partial differential equation can be written as

$$-\mu \Delta u - \lambda \nabla \operatorname{div} u = f.$$

2.1.4 N-S equations

$$\begin{cases} \frac{\partial u}{\partial t} + (u \cdot \nabla)u - \nu \Delta u + \nabla p = f \\ \operatorname{div} u = 0 \end{cases}$$

with some proper boundary conditions. Combining the linear elasticity problem with the N-S problem, we will get the Fluid Structure Interaction(FSI) problem.

2.1.5 Maxwell equations

$$\begin{cases} \frac{\partial B}{\partial t} + \nabla \times E = 0 \\ \frac{\partial \epsilon_0 E}{\partial t} - \nabla \times (\epsilon_0 E) = \rho \\ \nabla \cdot (\epsilon_0 E) = \rho \\ \nabla \cdot B = 0 \end{cases}$$

with some proper boundary conditions. Combining the Maxwell problem with the N-S problem, we will get the Magnetohydrodynamics(MHD) problem.

2.1.6 Kirchhoff plate bending equation

$$\Delta^2 u = f.$$

Kirchhoff plate bending equation is a fourth order elliptic problem.

2.1.7 Darcy's law

For the model problem,

$$\begin{cases} -\Delta u = f, & \in \Omega, \\ u = 0, & \in \partial\Omega. \end{cases}$$

It is equivalent to the weak form: Find $u \in V \equiv H_0^1(\Omega)$, s.t.

$$a(u, v) = \langle f, v \rangle, \quad \forall v \in V,$$

where $a(u, v) = \int_{\Omega} \nabla u \nabla v$.

It can also be written as

$$u = \arg \min_{\phi \in V} E(\phi),$$

where

$$E(\phi) = \frac{1}{2} \int_{\Omega} |\nabla \phi|^2 - \int_{\Omega} f \phi$$

which means u is the minimizer of $E(\phi)$, i.e.

$$E(u) = \min_{\phi \in V} E(\phi), \quad E(u) \leq E(\phi), \quad \forall \phi \in V.$$

In particular, $E(u) = \min_{t \in \mathbb{R}} E(u + tv)$, for all $v \in V$. Denote $F(t) = E(u + tv)$, so

$$F(0) = \min_{t \in \mathbb{R}} F(t).$$

Since

$$\begin{aligned} E(u + tv) &= \frac{1}{2} \int_{\Omega} |\nabla u + t\nabla v|^2 - \int_{\Omega} f(u + tv) \\ &= \frac{1}{2} \int_{\Omega} |\nabla u|^2 - \int_{\Omega} f(u) + \frac{t^2}{2} \int_{\Omega} |\nabla v|^2 + t \left(\int_{\Omega} (\nabla u, \nabla v) - \int_{\Omega} f v \right). \end{aligned}$$

It is a quadratic function of t , by the Frechet derivative: $\langle \partial_u E(u), v \rangle = \frac{d}{dt} E(u + tv)|_{t=0}$ and

$$\partial_u E(u) = 0 \iff \langle \partial_u E(u), v \rangle = 0,$$

the minimizer satisfies

$$F'(0) = 0 \iff \int_{\Omega} (\nabla u, \nabla v) - \int_{\Omega} f v = 0.$$

u is called the critical "point".

Darcy's law

For the incompressible fluid, it satisfies the energy minimization problem

$$\min_{\text{div} \phi = 0, \phi \in V} E(\phi),$$

where

$$E(\phi) = \frac{1}{2} \int_{\Omega} |\nabla \phi|^2 - \int_{\Omega} f \phi, \quad \text{for pure Dirichelet boundary condition}$$

$$E(\phi) = \frac{1}{2} \int_{\Omega} |\epsilon(\phi)|^2 - \int_{\Omega} f \phi, \quad \text{for others}$$

$\epsilon(\phi) = \frac{1}{2}(\nabla \phi + \nabla \phi^T)$. By introducing the Lagrangian multiplier, we can define

$$L(\phi, q) = E(\phi) - \int_{\Omega} (\operatorname{div} \phi - 0)q,$$

Let (u, p) be the critical “point” of $L(\phi, q)$,

$$\begin{cases} \partial_{\phi} L(u, p) = 0 \\ \partial_q L(u, p) = 0 \end{cases} \iff \begin{cases} a(u, v) - (\operatorname{div} v, p) = (f, v) \\ (\operatorname{div} u, q) = 0 \end{cases}$$

It can be written as the Stokes equations

$$\begin{cases} -\Delta u + \nabla p = f \\ \operatorname{div} u = 0 \end{cases}$$

For Porous media flow, the computational domain will looks like Figure2.1. $u = 0$ on the boundary of holes.

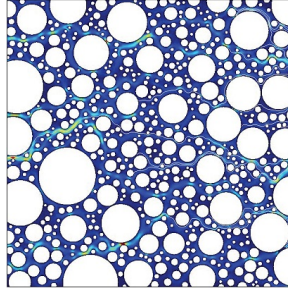


Fig. 2.1. Porous media flow

The problem can also be written as the minimization of the energy:

$$\min_{\operatorname{div} \phi = 0, \phi \in V} E(\phi),$$

where

$$E(\phi) = \frac{1}{2} \int_{\Omega} |\nabla \phi|^2 - \int_{\Omega} f \phi.$$

Since

$$\int_{\Omega} |\nabla \phi|^2 \approx \frac{1}{\delta^2} \int_{\Omega} |\phi|^2.$$

δ is the pole size. Therefore, for the porous media flow, the energy can be approximated as

$$E_\delta(\phi) = \delta^{-2} \int_{\Omega} |\phi|^2,$$

So,

$$\min_{\text{div}\phi=0, \phi \in V} E(\phi), \iff \begin{cases} -\delta^{-2}u + \nabla p = f \\ \text{div}u = 0 \end{cases}$$

When $f = 0$, we can have $u = \alpha \nabla p$, where $\alpha = \delta^2$. This is the Darcy's law.

2.2 Some classical numerical methods

In this section, we introduce some classical numerical methods.

1. **Finite difference methods** The finite difference method (FDM) is the oldest and easiest to implement. It is based upon the application of a local Taylor expansion to approximate the differential equations. The FDM uses a topologically square network of lines to construct the discretization of the PDE. This is a potential bottleneck of the method when handling complex geometries in multiple dimensions. This issue motivated the use of an integral form of the PDEs and subsequently the development of the finite element and finite volume techniques
2. **Finite volume methods** Similar to the finite difference method or finite element method, finite volume methods (FVM) solve problems in discrete places on a meshed geometry. "Finite volume" refers to the small volume surrounding each node point on a mesh. In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each finite volume. Because the flux entering a given volume is identical to that leaving the adjacent volume, these methods are conservative. Another advantage of the finite volume method is that it is easily formulated to allow for unstructured meshes. The method is used in many computational fluid dynamics packages.
3. **Finite element methods** The finite element method (FEM) is a numerical method for solving problems of engineering and mathematical physics, for example the linear elasticity equations. Typical problem areas of interest include structural analysis, heat transfer, fluid flow, mass transport, and electromagnetic potential. FEM is the most flexible one in terms of dealing with complex geometry and complicated boundary conditions. FEM also allows the adaptive/local procedure to get higher order local approximation or battling singularities. For computational fluid dynamics and electromagnetism, FEM is the way to incorporate the intrinsic geometrical properties of the solutions. It needs to point out that perhaps FEM is the most difficult among these methods to implement.
4. **Spectral methods** Spectral methods are a class of techniques used in applied mathematics and scientific computing to numerically solve certain differential equations, potentially involving the use of the fast Fourier transform. The idea is to write the solution of the differential equation as a sum of certain "basis functions". Spectral methods take on a global approach while finite element methods use a local approach. Partially for this reason, spectral methods have excellent error properties, with the so-called "exponential convergence" being the fastest possible, when the solution is smooth. However, there are no known three-dimensional single domain spectral shock capturing results. Spectral methods are computationally less expensive than finite element methods, but become less accurate for problems with complex geometries and discontinuous coefficients.
5. **Deep neural methods** Deep neural methods is part of a broader family of machine learning methods based on learning data representations, as opposed to task-specific algorithms. Learning can be supervised, semi-supervised or unsupervised. Recently some research shows the relation between the deep

neural method and the multigrid method which is a branch of FEM. This relation gives away some explanation for the high efficiency of deep neural methods.