Partial Differential Equations and Multiphysics Simulations

Chap 1. Intro. to Partial Differential Equations (PDEs)

Jung Y. Huang

www.jyhuang.idv.tw

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◯ 1.1 Conservation laws for governing equations of multiphysics simulations

Many PDEs for mathematical simulations come from a variety of conservation laws, which state that a particular measurable property of an isolated physical system does not change as the system evolves.

Here are some conservation laws that are useful to generate governing PDEs for simulations:

1) Conservation of mass: the total mass of a closed system of substances remains constant.

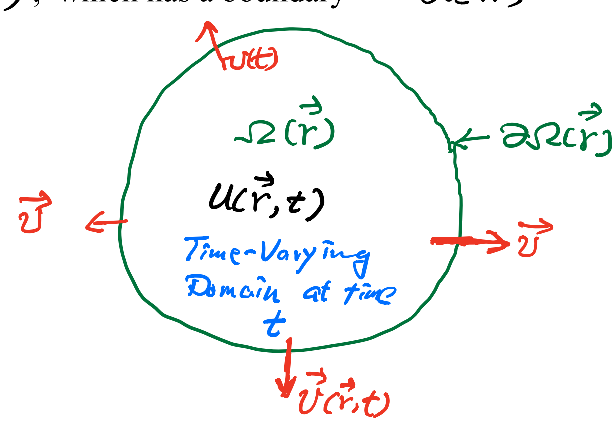
2) Conservation of energy

3) Conservation of linear momentum

4) Conservation of electric charge

◯ 1.2 Using conservation law to generate governing equations of multiple physics simulations: A General Formalism

Consider a spatio-temporal scalar field variable $u(\vec{r},t)$ defined in a domain $\Omega(\vec{r})$, which has a boundary $\partial\Omega(\vec{r})$



The conservation law of the scalar can be expressed as

$$\frac{d}{dt}\int_{\Omega(t)} u(\vec{r},t)\,d\Omega + \oint_{\partial\Omega} \vec{J}\cdot\hat{n}\,dA = \int_{\Omega(t)} q\,dV,$$

where the first term indicates the change of scalar quantity enclosed in $\Omega(\vec{r})$, the second term denotes the gain/loss of the quantity via flow across the boundary $\partial\Omega(\vec{r})$. The term on the right-hand side is the generative source q of u(r, t) in the domain.

We can invoke the Reynolds transport Theorem on the first term

$$\frac{d}{dt}\int_{\Omega(t)} u(\vec{r},t)\,d\Omega = \int_{\Omega(t)} \frac{\partial u}{\partial t}\,d\Omega + \int_{\partial\Omega} (u\vec{v})\cdot\hat{n}\,dA$$

The first term on the right-hand side reflects the direct change of the time-varying quantity u inside the domain at time t; whereas the second term indicates the gain/loss of u through the moving boundary in the time interval of (t, t+dt).

We want to rewrite the second term of a surface integral to a volume integral. This can be done by using Gauss (divergence) law:

$$\oint_{\partial\Omega(t)} \vec{J}\cdot\hat{n}\,dA = \int_{\Omega(t)} \nabla\cdot J\,dV$$

Thus, we can have $\displaystyle\int_{\Omega(t)} \frac{\partial u(t)}{\partial t}\,dV + \int_{\Omega(t)} \nabla\cdot(u\vec{v})\,dV + \int_{\Omega(t)} \nabla\cdot J\,dV = \int_{\Omega(t)} q\,dV$

$$\int_{\Omega(t)} \left[\frac{\partial u(t)}{\partial t} + \nabla\cdot(u\vec{v}) + \nabla\cdot J\right] dV = \int_{\Omega(t)} q(\vec{r},t)\,dV$$

From DuBois-Reynolds lemme, at every position in $\Omega(t)$, the u satisfies the PDE

$$\underbrace{\frac{\partial u(\vec{r},t)}{\partial t}}_{\text{accumulation in } \Omega(\vec{r},t)} + \underbrace{\nabla\cdot(u\vec{v})}_{\text{advection}} + \underbrace{\nabla\cdot J}_{\text{Diffusion term}} = \underbrace{q(\vec{r},t)}_{\text{source}}$$

Note for a) $U(\vec{r},t) \propto C(\vec{r},t) \equiv$ Concentration

$$\begin{cases} \vec{J}(\vec{r},t) = -D\,\nabla C(\vec{r},t) & \text{for concentration flux} \\ \nabla\cdot\vec{J} = -D\,\nabla^2 C(\vec{r},t) \end{cases}$$

b) $u = T(\vec{r}, t) =$ temperature

$$\begin{cases} J(\vec{r}, t) = -K \nabla T(\vec{r}, t) \\ \nabla \cdot J = -K \nabla^2 T(\vec{r}, t) \end{cases} \quad \text{and}$$

for thermal flux

Let $u = \rho C_v T$ = internal energy

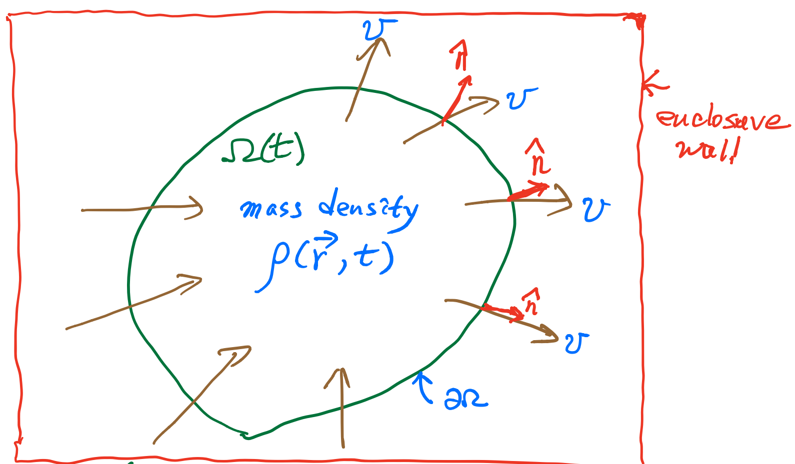
$$\rho C_v \frac{\partial T}{\partial t} + \rho C_v \nabla \cdot (T \vec{v}) - K \nabla \cdot \underbrace{(\nabla T)}_{J = -K\nabla T} = \delta_T$$

is the governing PDE for thermal conduction phenomenon.

○ 1.3 Specific example of mass balance

Conservation of mass can be extended to a mass balance for an accounting of material entering and leaving a system.

Consider a system



Total mass in Ω $= \int_\Omega \rho(\vec{r}, t)\, dV \equiv \rho * \Omega = M$

Net mass change due to net flow $= \oint \rho\, \vec{v} \cdot \hat{n}\, dt\, dA = \left(\oint_{\partial\Omega} \rho \vec{v} \cdot \hat{n}\, dA \right) dt$

$\Rightarrow \Delta t \cdot \partial_t M = \Delta t \cdot \partial_t \int_\Omega \rho(\vec{r}, t)\, dV$ = total mass change in Ω

$$\Rightarrow \int_{\Omega} \partial_t \rho \, dV + \underbrace{\oint_{\partial\Omega} \rho \vec{v} \cdot \hat{n} \, dA}_{\text{transform into volume integral over } \Omega(t)} = 0$$

From integration by part

$$\int_{\Omega} \underbrace{(\nabla \cdot v)}_{dv} \underbrace{\phi}_{u} \, dV = \oint_{\partial\Omega} \underbrace{\vec{v} \cdot \hat{n}}_{v} \underbrace{\phi}_{u} \, dA - \int_{\Omega} \underbrace{\vec{v}}_{v} \cdot \underbrace{\nabla\varphi}_{du} \, dV$$

Let $\phi = \rho$, The conservation of mass:

$$dM/dt = 0 \Rightarrow \frac{d}{dt} \int_{\Omega} \rho \cdot dV = 0$$

$$\therefore \int_{\Omega} \partial_t \rho \, dV + \int_{\Omega} (\nabla \cdot \vec{v}) \rho \, dV + \int_{\Omega} \vec{v} \cdot \nabla\rho \, dV = 0$$

From Du Bois-Reynolds Lemma,

$$\partial_t \rho(\vec{r}, t) + (\nabla \cdot \vec{v}) \rho + \vec{v} \cdot \nabla\rho = 0$$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \text{ Continuity equation}$$

For a constant density case (ρ = const, incompressibility) in steady-state condition ($\partial\rho/\partial t = 0$)

continuity eq. $\longrightarrow$ $\underline{\nabla \cdot \vec{v}(\vec{r}) = 0}$ incompressibility condition

1.4 Physics-related PDEs

1) Laplace's equation of a dependent field variable $\psi(\vec{r})$

$$\nabla^2 \psi(\vec{r}) = 0 \quad \text{with} \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplace's equation is an important equation occurring in studies of
a) source-free electrostatics
b) irrotational flow of perfect fluid
c) heat flow

2) Poisson's equation of a dependent field variable $\psi(\vec{r})$

$$\nabla^2 \psi(\vec{r}) = -\rho(\vec{r})/\varepsilon_0 ,$$

which describes electrostatics with a source term $-\rho(\vec{r})/\varepsilon_0$

3) Helmholtz equation $\nabla^2 \psi(\vec{r}) + k^2 \psi(\vec{r}) = 0$

which appears in describing propagation of either electromagnetic waves or elastic (i.e., acoustic) waves,

or time-independent diffusion equation $\nabla^2 Q(\vec{r}) - k^2 Q(\vec{r}) = 0$

4) Time-dependent diffusion equation

$$\nabla^2 \psi(\vec{r},t) = \frac{1}{a^2} \frac{\partial \psi(\vec{r},t)}{\partial t} , \quad \psi(\vec{r},t) = T(\vec{r},t)$$

5) Time-dependent wave equation

$$\nabla^2 \psi(\vec{r},t) = \frac{1}{v^2} \frac{\partial^2 \psi(\vec{r},t)}{\partial t^2}$$

6) Klein-Gordon equation

$$(\nabla^2 - \mu^2)\, \psi(\vec{r},t) = \frac{1}{v^2} \frac{\partial^2 \psi(\vec{r},t)}{\partial t^2}$$

which is the (Schrodinger equation related) relativistic wave equation, derivable from quantized form of relativistic energy-momentum relation.

7) Time-dependent Schrodinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r},t) + V(\vec{r})\, \psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$$

Let $\psi(\vec{r},t)=\phi(\vec{r})e^{-iEt/\hbar} \longrightarrow -\frac{\hbar^2}{2m}\nabla^2\phi(\vec{r})+V(\vec{r})\phi(\vec{r})=E\phi(\vec{r})$

8) Other equations for describing elastic wave propagation, movements of viscous fluids

1.5 Classification of PDEs

Most of the governing equations in physical models are second-order partial differential equations (PDEs). For generality, let us consider the PDE of the in a 2D domain $\Omega(x,y)$

$$(1)\quad A\frac{\partial^2 u(x,y)}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu+G=0$$

where A, B, C, ..., G are either constants or may be functions of both independent variables (i.e., x, y) and/or dependent variable u(x, y) .

Let $u_x=\partial u/\partial x$, $u_y=\partial u/\partial y$ to be continuous in

$$(2)\quad \begin{cases} du_x=\frac{\partial u_x}{\partial x}dx+\frac{\partial u_x}{\partial y}dy=\frac{\partial^2 u}{\partial x^2}dx+\frac{\partial^2 u}{\partial y\partial x}dy \\ du_y=\frac{\partial u_y}{\partial x}dx+\frac{\partial u_y}{\partial y}dy=\frac{\partial^2 u}{\partial x\partial y}dx+\frac{\partial^2 u}{\partial y^2}dy \end{cases}$$

u(x, y) forms a solution surface above/below the x-y plane.

Equations (1) and (2) can be combined and rewrite in a matrix form

$$\begin{bmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix}\begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix}=\begin{bmatrix} H=-(Du_x+Eu_y+Fu+G) \\ du_x \\ du_y \end{bmatrix}$$

u_{xx}, u_{xy}, u_{yy} could be discontinuous (i.e., indeterminate) when

$$\begin{vmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{vmatrix}=0,\quad \text{which yields}$$

$$A(dy)^2 + C(dx)^2 - B\,dx \cdot dy = 0 \quad , \quad \text{and therefore}$$

$$(3) \quad A(dy/dx)^2 - B(dy/dx) + C = 0 .$$

Here (dy/dx) denotes the characteristic curves on the solution surface u(x, y).

Solving equation (3) gives the equation of the characteristics in physical space (x, y) as

$$\frac{dy}{dx} = \frac{B \pm \sqrt{B^2 - 4AC}}{2A} ,$$

which could be either real or imaginary (complex conjugates).

Thus, the second-order PDEs can be classified according to the sign of $B^2 - 4AC$

a) Elliptic PDEs: $B^2 - 4AC < 0$, the characteristic curves do not exist, such as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad (\text{ Laplace's equation })$$

A=1, B=0, and C=1 —> $B^2 - 4AC = -4 < 0$

In this case, the solution surface u(x, y) is bounded in $\Omega(x, y)$ with a closed boundary $\partial\Omega$ (curve or surface). Unique solution exists when specifying

u on $\partial\Omega$, or

$u_n = \partial u / \partial n$ on $\partial\Omega$

b) Parabolic PDEs: $B^2 - 4AC = 0$, only one set of characteristics exists, such as for 1-D time-dependent diffusion equation

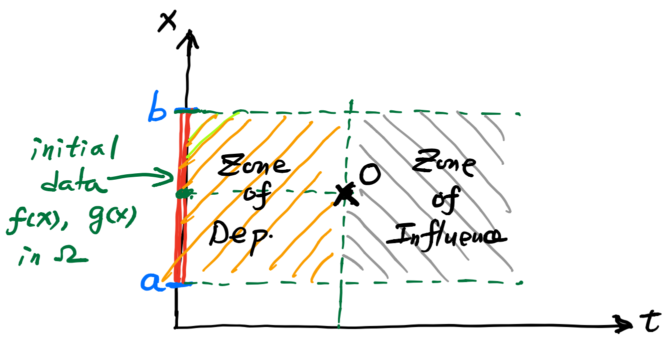
$$\frac{\partial u(x,t)}{\partial t} - \alpha \frac{\partial^2 u(x,t)}{\partial x^2} = 0 \quad , \quad (\alpha > 0)$$

$$A = -\alpha < 0 \; , \; B = 0 \; , \; C = 0 \; \longrightarrow \; B^2 - 4AC = 0$$

Solution of the problem is defined in the open region $\Omega(x, t)$ with $a \le x \le b$, $0 \le t < \infty$

Both initial condition $u(a \le x \le b, t=0) = f(x)$, and boundary conditions

$$\begin{cases} u(x=a, t) = f(t) \\ u(x=b, t) = g(t) \end{cases} \quad \text{or} \quad \begin{matrix} u_n(x=a, t) \\ u_n(x=b, t) \end{matrix}$$



are required to defined the unique solution.

For problems in which real characteristics exist, a disturbance can propagates only over a finite region. A signal at a point O in Ω can be felt only if it is originates from a finite region call "the zone of dependence" of point O. The down stream region affected by this signal at O is called "the zone of influence" of point O.

c) Hyperbolic PDEs: $B^2-4AC>0$

Two sets of characteristics exist, such as the 1-D wave equation in (x, t)

$$\frac{1}{a^2}\frac{\partial^2 u(x,t)}{\partial t^2}=\frac{\partial^2 u(x,t)}{\partial x^2}$$

$$A=1,\quad B=0,\quad C=-1/a^2<0 \longrightarrow B^2-4AC=0+4\times1\times1/a^2=4/a^2>0$$

Unique solution is defined in the open region $(x,\ -\infty<t<\infty)$

Both initial condition $u(x,t=0)=f(x)$ and $\partial_t u(x,t=0)=g(x)$
and boundary conditions

$$u(x=a,t),\ u(x=b,t) \quad \text{or} \quad u_n(x=a,t),\ u_n(x=b,t)$$

are needed to determine the unique solution.