Mth 255 Calculus V: Supplementary Lecture Notes

Applications to Physics and Mechanics

Dacian N. Daescu
Portland State University, daescu@pdx.edu

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Contents

1 Introduction

Vector calculus provides the mathematical foundations for modeling various physical processes and problems from applied sciences. These lecture notes introduce some of the fundamental applications to conservation laws, including conservation of mass, conservation of energy, and conservation of momentum, and their mathematical representation through *partial differential equations (PDEs).*

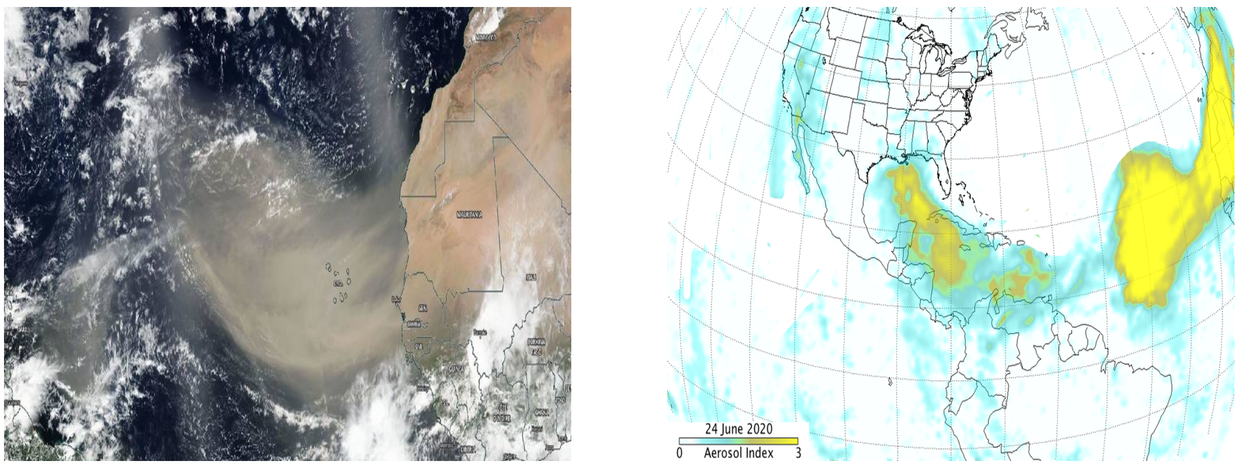


Figure 1. PDEs are used to study processes of high-impact to our society and environment. On June 2020, NASA-NOAA's satellites captured images of the large light brown plume of Saharan dust over the North Atlantic Ocean. The dust was transported across the Atlantic and, eventually reached North and South America. Credits: NASA/NOAA.

1.1 Notation and terminology

In many practical applications we consider processes that evolve in a spatial region represented by variables x, y, z (such as a ball, the interior of the classroom, Earth's atmosphere) and time represented by the variable t, $u = u(x, y, z, t)$. For example, we may be interested in the time-evolution of the temperature of a heated object or inside a classroom, atmospheric pollutant concentrations over the Portland metro area, air humidity or wind velocity.

Notational convention: the partial derivatives of the function u are denoted

$$\frac{\partial u}{\partial x} = u_x, \qquad \frac{\partial u}{\partial t} = u_t, \qquad \frac{\partial^2 u}{\partial x^2} = u_{xx}, \qquad \frac{\partial^2 u}{\partial x \partial t} = u_{xt} \qquad , \dots \tag{1}$$

A *partial differential equation (PDE)* is an equation that involves an unknown function u of several variables $(x, y, z, t, ..)$ and some of its partial derivatives

$$\mathcal{E}(x, y, z, t; u, u_x, u_y, u_z, u_t, u_{xx}, \dots) = 0 \tag{2}$$

The *order* of the PDE is the order of the highest partial derivative in the equation and a function u that satisfies equation (2) is called a solution to the PDE.

An example of a first order PDE for a function of two variables $u(x, t)$ is

$$u_t + 3u_x = 0 \tag{3}$$

HW: Notice that $u(x, t) = x - 3t$ is a solution to (3). Find other solutions to this PDE.

An example of a second order PDE for a function of two variables $u(x, t)$ is

$$u_t = u_{xx} \tag{4}$$

HW: Notice that $u(x, t) = e^{-t} sin(x)$ is a solution to (4). Find other solutions to this PDE.

Equation (3) may be used to model transport of substance at a constant speed, whereas (4) may be used to model diffusion processes such as movement of substance or energy from a region of high density to a region of low density, as illustrated in Fig. 2 below.

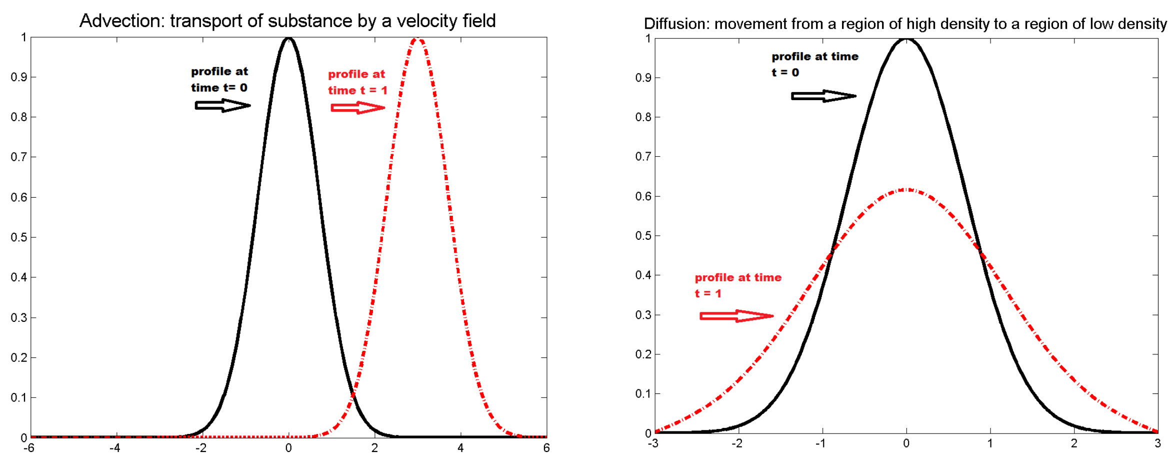


Figure 2. Left figure: Illustration of the transport process modeled by PDE (3). Right figure: illustration of the diffusion process modeled by PDE (4).

1.2 Some concepts from vector calculus and integral identities

For a function $u = u(x, y, z)$ defined on a region $\mathcal{V} \subset \mathbb{R}^3$, the *gradient* of u is the vector of partial derivatives,

$$\nabla u = \frac{\partial u}{\partial x}\,\hat{\mathbf{i}} + \frac{\partial u}{\partial y}\,\hat{\mathbf{j}} + \frac{\partial u}{\partial z}\,\hat{\mathbf{k}} \tag{5}$$

If $\boldsymbol{\alpha} = \alpha_1\hat{\mathbf{i}} + \alpha_2\hat{\mathbf{j}} + \alpha_3\hat{\mathbf{k}}$ denotes a unit vector in $\mathbb{R}^3$, $(|\boldsymbol{\alpha}| = 1)$, the *directional derivative of u* in direction $\boldsymbol{\alpha}$ is given by

$$\frac{\partial u}{\partial \boldsymbol{\alpha}} = \alpha \cdot \nabla u = \alpha_1 \frac{\partial u}{\partial x} + \alpha_2 \frac{\partial u}{\partial y} + \alpha_3 \frac{\partial u}{\partial z} \tag{6}$$

If θ denotes the angle between the vectors $\boldsymbol{\alpha}$ and ∇u then

$$\frac{\partial u}{\partial \boldsymbol{\alpha}} = |\nabla u| \cos\theta \tag{7}$$

where $|\nabla u| = \sqrt{u_x^2 + u_y^2 + u_z^2}$ is the norm (length) of the gradient vector. The largest rate of change of u (the largest directional derivative) is equal to $|\nabla u|$ and occurs in the direction of the gradient (that is when the angle $\theta = 0$).

If $\mathbf{F} = F_1(x, y, z)\hat{\mathbf{i}} + F_2(x, y, z)\hat{\mathbf{j}} + F_3(x, y, z)\hat{\mathbf{k}}$ is a vector field on $\mathcal{V}$, the *divergence* of $\mathbf{F}$ is defined to be the *scalar* field

$$\operatorname{div} \mathbf{F} \equiv \nabla \cdot \mathbf{F} = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z} \tag{8}$$

In particular, by taking $\mathbf{F} = \nabla u$ in (8), we have

$$\boxed{\nabla \cdot \nabla u \equiv \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = u_{xx} + u_{yy} + u_{zz}} \tag{9}$$

The expression $\nabla^2 u$ is called the *Laplacian* of u and is obtained by taking the divergence of the gradient. Often, the *Laplacian* it also denoted Δu.

HW: For smooth scalar functions $u(x, y, z)$ and $v(x, y, z)$, verify the following identity

$$\nabla \cdot (u \nabla v) = \nabla u \cdot \nabla v + u \nabla^2 v \tag{10}$$

Recall the **vector form of Green's theorem for flux**

$$\boxed{\oint_{\partial \mathcal{D}} \mathbf{F} \cdot \mathbf{n} \, \mathrm{d}s = \iint_{\mathcal{D}} \nabla \cdot \mathbf{F} \, \mathrm{d}A} \tag{11}$$

where $\mathcal{D}$ is a region in the two dimensional space whose boundary $\partial \mathcal{D}$ is a simple closed curve, $\mathbf{n}$ denotes the outward unit normal vector to the boundary, and $\mathbf{F}$ is a vector field whose domain contains $\mathcal{D}$. In particular, given a smooth function u defined in $\mathcal{D}$, we take $\mathbf{F} = \nabla u$ in Green's theorem (11) and use (9) to obtain the following identity:

$$\boxed{\oint_{\partial \mathcal{D}} \nabla u \cdot \mathbf{n} \, \mathrm{d}s = \iint_{\mathcal{D}} \nabla \cdot \nabla u \, \mathrm{d}A = \iint_{\mathcal{D}} \nabla^2 u \, \mathrm{d}A} \tag{12}$$

Notice that the left side term in (12) is the integral of the directional derivative $\nabla u \cdot \mathbf{n}$ (also known as the outer normal derivative) over the closed curve $\partial \mathcal{D}$, whereas the right side term in (12) is the area integral of the Laplacian $\nabla^2 u$ over the region enclosed by $\partial \mathcal{D}$.

We also recall the **Divergence Theorem**

$$\boxed{\iiint_{\mathcal{V}} \nabla \cdot \mathbf{F} \mathrm{d}V = \iint_S \mathbf{F} \cdot \mathrm{d}\mathbf{S} = \iint_S \mathbf{F} \cdot \mathbf{n} \, \mathrm{d}S} \tag{13}$$

where S is a closed and piecewise smooth surface that encloses the three-dimensional region $\mathcal{V} \in \mathbb{R}^3$, oriented by normal vectors pointing outward of $\mathcal{V}$ and $\mathbf{n}$ is the outward unit normal vector to S. In particular, given a smooth function $u(x, y, z)$ defined in $\mathcal{V}$, we take $\mathbf{F} = \nabla u$ in the Divergence theorem (13) and use (9) to obtain the following identity:

$$\boxed{\iiint_{\mathcal{V}} \nabla^2 u \, \mathrm{d}V = \iint_S \nabla u \cdot \mathbf{n} \, \mathrm{d}S} \tag{14}$$

Therefore, for any smooth function u, the flux of the gradient of u through a closed surface S is equal to the volume integral of the Laplacian of u over the region $\mathcal{V}$ inside the surface.

HW: Use identity (10) and the divergence theorem (13) to derive *Green's first and second integral identities:* If u and v are smooth scalar functions then

$$\boxed{\iiint_{\mathcal{V}} u \nabla^2 v \, \mathrm{d}V = \iint_S u \nabla v \cdot \mathbf{n} \, \mathrm{d}S - \iiint_{\mathcal{V}} \nabla u \cdot \nabla v \, \mathrm{d}V} \tag{15}$$

$$\boxed{\iiint_{\mathcal{V}} (u \nabla^2 v - v \nabla^2 u) \, \mathrm{d}V = \iint_S (u \nabla v - v \nabla u)) \cdot \mathbf{n} \, \mathrm{d}S} \tag{16}$$

By taking $v = u$ in the equation (15) above we obtain the following identity:

$$\boxed{\iiint_{\mathcal{V}} u \nabla^2 u \, \mathrm{d}V = \iint_S u \nabla u \cdot \mathbf{n} \, \mathrm{d}S - \iiint_{\mathcal{V}} |\nabla u|^2 \, \mathrm{d}V} \tag{17}$$

HW: Given a region $\mathcal{V} \subset \mathbb{R}^3$ with boundary represented by the closed surface S, show that there is at most one smooth function $u(x, y, z)$ that has prescribed values of its Laplacian inside $\mathcal{V}$ and has prescribed values on the boundary S

$$\nabla^2 u(x, y, z) = f(x, y, z), \quad \text{for} \quad (x, y, z) \in \mathcal{V} \tag{18}$$
$$u(x, y, z) = g(x, y, z), \quad \text{for} \quad (x, y, z) \in S \tag{19}$$

where $f : \mathcal{V} \to \mathbb{R}$ and $g : S \to \mathbb{R}$ are given functions.

Hint: Use (17) to show that the difference $u = u_1 - u_2$ between any two functions u_1 and u_2 that satisfy both (18) and (19) must be the null (identically zero) function.

The vector calculus concepts and differential and integral identities reviewed in this section provide the necessary tools for deriving the partial differential equations of mathematical physics. Fundamental examples are provided next.

2 Conservation Laws

"Nothing comes from nothing." (Aristotle's Physics).

Fundamental conservation laws of nature such as conservation of mass, conservation of energy, and conservation of momentum are mathematically expressed through an equation known as the *continuity equation*.

2.1 Conservation of mass

"For any system closed to all transfers of matter and energy, the quantity of mass is conserved over time."

$$\boxed{\rho_t + \nabla \cdot (\rho \mathbf{v}) = 0} \tag{20}$$

We begin the presentation with the conservation of mass first derived for a one-dimensional gas dynamics problem and then extended to regions in two- and three-dimensional space.

2.1.1 One-dimensional model

Consider a gas flowing in a tube where properties such as the gas density and velocity may change in time and space but are assumed to be constant through each cross section of the tube, as illustrated in Fig. 3.

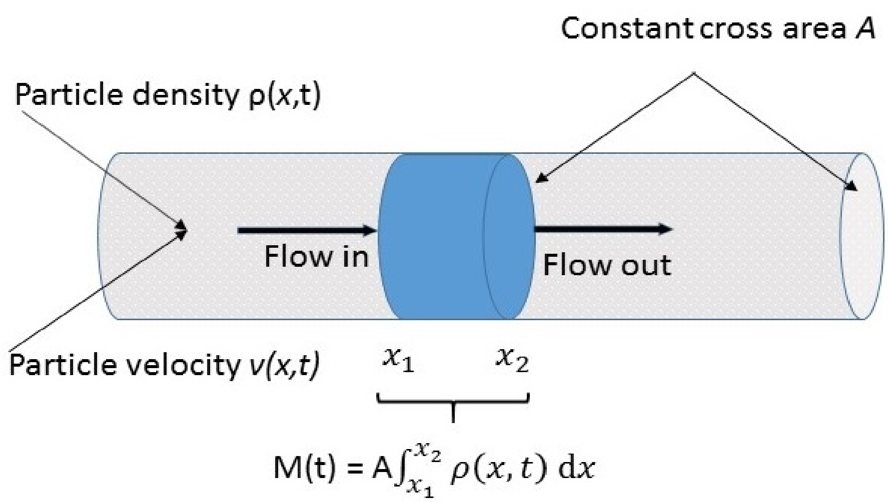


Figure 3. Illustration of the one dimensional mathematical model for gas flow in a tube with constant cross section area A. The density and velocity are functions of time and the x-coordinate only and, at any given time, are constant through each cross section.

Let $\rho(x,t)$ and $v(x,t)$ denote the density of the gas and the velocity of the gas respectively, at location point x and time t and let A denote the area of the cross section of the tube. The mass of gas in any region of the tube determined by the horizontal segment $[x_1, x_2]$ at time t is

$$\text{mass in } [x_1, x_2] \text{ at time } t = M(t) = A \int_{x_1}^{x_2} \rho(x,t)dx$$

At any given time t, the rate of flow, or *flux* of gas past the cross section at point x is

$$\text{mass flux at } (x,t) = A\rho(x,t)v(x,t)$$

Assuming that mass can change only because of gas flowing across the endpoints x_1 or x_2, the rate of change in the mass of gas within the region from x_1 to x_2 is

$$\frac{dM}{dt} = \frac{d}{dt}\left\{A \int_{x_1}^{x_2} \rho(x,t)dx\right\} = A\rho(x_1,t)v(x_1,t) - A\rho(x_2,t)v(x_2,t) \tag{21}$$

and after simplification by the constant A, we obtain the *integral form* of the one-dimensional mass conservation law,

$$\boxed{\frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t)dx = \rho(x_1,t)v(x_1,t) - \rho(x_2,t)v(x_2,t)} \tag{22}$$

By integrating (22) in an arbitrary fixed time interval $[t_1, t_2]$

$$\int_{x_1}^{x_2} \rho(x,t_2)dx - \int_{x_1}^{x_2} \rho(x,t_1)dx = \int_{t_1}^{t_2} [\rho(x_1,t)v(x_1,t)dt - \rho(x_2,t)v(x_2,t)]dt \tag{23}$$

In addition, we assume that both $\rho(x,t)$ and $v(x,t)$ are continuously differentiable functions. Using the integration rules

$$\rho(x,t_2) - \rho(x,t_1) = \int_{t_1}^{t_2} \frac{\partial}{\partial t}\rho(x,t)dt \tag{24}$$

$$\rho(x_2,t)v(x_2,t) - \rho(x_1,t)v(x_1,t) = \int_{x_1}^{x_2} \frac{\partial}{\partial x}(\rho(x,t)v(x,t))dx \tag{25}$$

and after replacing in (23) we obtain

$$\int_{t_1}^{t_2}\int_{x_1}^{x_2} \left[\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}\left(\rho(x,t)v(x,t)\right)\right] dxdt = 0 \tag{26}$$

Since the time interval $[t_1, t_2]$ and the region $[x_1, x_2]$ are arbitrary, the equation above implies that at any time t and point x we must have

$$\boxed{\rho_t(x,t) + \left(\rho(x,t)v(x,t)\right)_x = 0} \tag{27}$$

which is the *differential form* of the one-dimensional mass conservation law.

2.1.2 Conservation of mass in higher dimensions

Consider the problem of modeling the time and space evolution of the density $\rho(x, y, t)$ of a substance flowing in a two dimensional domain $\Omega \in \mathbb{R}^2$ with a velocity field $\mathbf{v} = (v_1(x, y, t), v_2(x, y, t))$. For example, in weather prediction we are interested in the transport of the water vapor density in the atmosphere at a given altitude level and over geographical region, as illustrated in Figure 4.

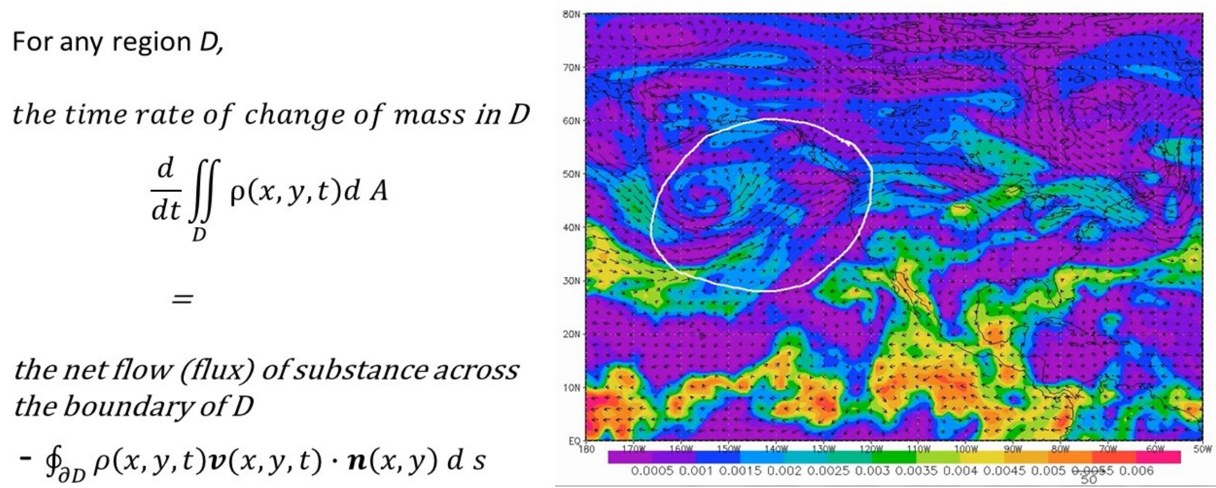


Figure 4. Conservation of mass may be used to study the time evolution of moisture in the atmosphere transported by the wind velocity field. At any given time, the rate of change in the mass inside any region D is equal to the flux of mass across the boundary ∂D.

For any selected subregion $\mathcal{D}$ of the domain Ω, the total amount (mass) of substance in $\mathcal{D}$ at a given time t is expressed as the area integral of the density,

$$M(t) = \iint_{\mathcal{D}} \rho(x, y, t)\, \mathrm{d}A \tag{28}$$

The time rate of change of the mass in the domain D must be equal to the mass flux across the boundary ∂D (entering or leaving the domain), as illustrated in Figure 4,

$$\boxed{\frac{d}{dt}\iint_{\mathcal{D}} \rho(x, y, t)\, \mathrm{d}A = -\oint_{\partial D} \rho(x, y, t)\mathbf{v}(x, y, t)\cdot \mathbf{n}(x, y)\, \mathrm{d}s} \tag{29}$$

where $\mathbf{n}(x, y)$ denotes the outward unit normal vector to the boundary ∂D. Notice that the flux is outward (loss of mass) across those boundary regions where $\mathbf{v}(x, y, t)\cdot\mathbf{n}(x, y) > 0$ and inward (gain of mass) across those boundary regions where $\mathbf{v}(x, y, t)\cdot\mathbf{n}(x, y) < 0$, thus we have inserted the minus sign in front of the boundary integral.

Equation (29) is the *the integral form of the mass conservation law.* Using the Green's theorem for flux (11), we may express the right side term in (29) as an area integral over $\mathcal{D}$,

$$\frac{d}{dt}\iint_{\mathcal{D}} \rho(x, y, t)\, \mathrm{d}A = -\iint_{\mathcal{D}} \nabla\cdot(\rho(x, y, t)\mathbf{v}(x, y, t))\, \mathrm{d}A \tag{30}$$

If we further assume that the density $\rho(x, y, t)$ is continuously differentiable function, then using Leibniz integral rule we may write (30) as

$$\iint_{\mathcal{D}} \frac{\partial}{\partial t}\rho(x, y, t)\,\mathrm{d}A = -\iint_{\mathcal{D}} \nabla \cdot (\rho(x, y, t)\mathbf{v}(x, y, t))\,\mathrm{d}A \tag{31}$$

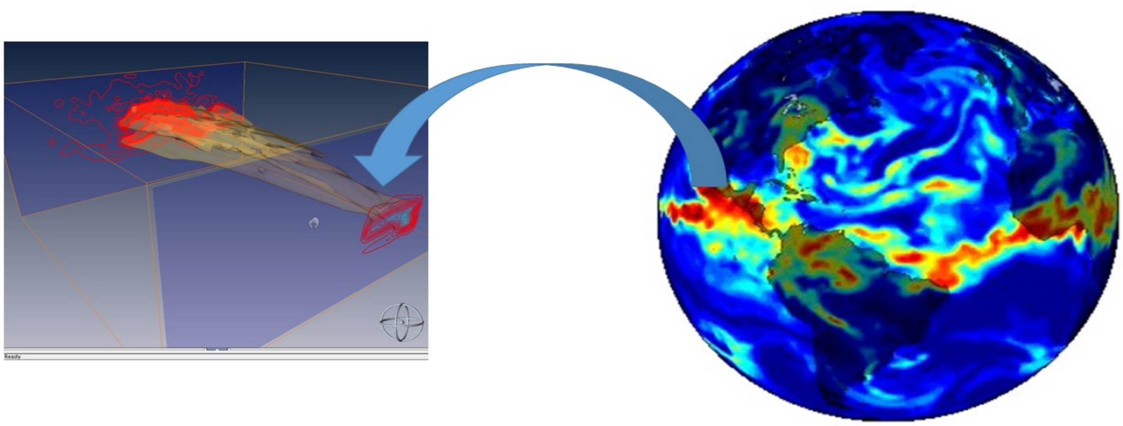
and since the equality above holds for any region $\mathcal{D}$, we obtain the *differential form of the conservation of mass in two dimensions* expressed as the *partial differential equation*

$$\boxed{\frac{\partial}{\partial t}\rho(x, y, t) + \nabla \cdot (\rho(x, y, t)\mathbf{v}(x, y, t)) = 0} \tag{32}$$

The three-dimensional case

The derivation of the PDE for the conservation of mass in a three-dimensional domain $\Omega \in \mathbb{R}^3$ proceeds in a similar fashion as above. In the 3D case, the density is a function of four variables (3D space and time), $\rho = \rho(x, y, z, t)$, and the velocity field includes a vertical component, $\mathbf{v} = (v_1(x, y, z, t), v_2(x, y, z, t), v_3(x, y, z, t))$. For any selected subregion $\mathcal{V} \in \Omega$, the mass of substance in $\mathcal{V}$ at a given time t is given by the volume integral of the density,

$$M(t) = \iiint_{\mathcal{V}} \rho(x, y, z, t)\,\mathrm{d}V \tag{33}$$



For any 3D region V, the time rate of change in mass = flux across the boundary surface S

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\iiint_V \rho(x, y, z, t)\,\mathrm{d}\,V = -\iint_S \rho(x, y, z, t)\boldsymbol{v}(x, y, z, t)\,\cdot d\,\boldsymbol{S}$$

Figure 5. Conservation of mass has very important applications in geosciences and environmental studies. At any given time, the rate of change in the mass inside a region $\mathcal{V}$ is given by the flux of mass across the closed boundary surface S.

The time rate of change of the mass in the domain $\mathcal{V}$ is equal to the mass flux across the closed surface S representing the boundary of the domain $\mathcal{V}$,

$$\boxed{\frac{d}{dt}\iiint_{\mathcal{V}} \rho(x,y,z,t)\,\mathrm{d}V = -\iint_S \rho(x,y,z,t)\mathbf{v}(x,y,z,t)\cdot\mathbf{n}(x,y,z)\,\mathrm{d}S} \tag{34}$$

where $\mathbf{n}(x,y,z)$ denotes the unit normal vector to the boundary S pointing outward of $\mathcal{V}$. Equation (34) is the *integral form of the equation for conservation of mass in three dimensions.*

Using the divergence theorem (13), the surface integral in the right side of (34) is expressed as the volume integral of the divergence of the mass flux vector,

$$\iint_S \rho(x,y,z,t)\mathbf{v}(x,y,z,t)\cdot\mathbf{n}(x,y,z)\,\mathrm{d}S = \iiint_{\mathcal{V}} \nabla\cdot\left(\rho(x,y,z,t)\mathbf{v}(x,y,z,t)\right)\,\mathrm{d}V \tag{35}$$

By replacing (35) in (34) we obtain

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho(x,y,z,t)\,\mathrm{d}V = -\iiint_{\mathcal{V}} \nabla\cdot\left(\rho(x,y,z,t)\mathbf{v}(x,y,z,t)\right)\,\mathrm{d}V \tag{36}$$

Assuming that the density $\rho(x,y,z,t)$ has continuous partial derivatives in time and space, we may express (36) as

$$\iiint_{\mathcal{V}} \frac{\partial}{\partial t}\rho(x,y,z,t)\,\mathrm{d}V = -\iiint_{\mathcal{V}} \nabla\cdot\left(\rho(x,y,z,t)\mathbf{v}(x,y,z,t)\right)\mathrm{d}V \tag{37}$$

and since the equality above holds for any region $\mathcal{V}$ of the domain Ω, we obtain the *differential form of the conservation of mass in three dimensions* expressed as the *PDE*

$$\boxed{\frac{\partial}{\partial t}\rho(x,y,z,t) + \nabla\cdot\left(\rho(x,y,z,t)\mathbf{v}(x,y,z,t)\right) = 0} \tag{38}$$

HW: Use the product rule to show that (38) may be expressed as

$$\boxed{\rho_t + \mathbf{v}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{v} = 0} \tag{39}$$

The *material (substantial, total) derivative* is defined as

$$\frac{D\rho}{Dt} \equiv \frac{\partial\rho}{\partial t} + \mathbf{v}\cdot\nabla\rho \tag{40}$$

and with this notation we may write the conservation of mass equation (38)/(39) as

$$\boxed{\frac{D\rho}{Dt} + \rho\nabla\cdot\mathbf{v} = 0} \tag{41}$$

A flow is called *incompressible* if the total derivative is zero, $\frac{D\rho}{Dt} = 0$. Since $\rho > 0$, from (41) it follows that an incompressible flow must have a divergence-free velocity field

$$\boxed{\frac{D\rho}{Dt} = 0 \quad \Leftrightarrow \quad \nabla \cdot \mathbf{v} = 0} \tag{42}$$

HW: Consider two densities $\rho_A(x, y, z, t) > 0$ and $\rho_B(x, y, z, t) > 0$ that are each solutions to (38). Show that the ratio $\mu = \rho_A/\rho_B$ solves the PDE

$$\mu_t + \mathbf{v} \cdot \nabla \mu = 0 \tag{43}$$

2.2 The continuity equation

In the previous section we derived the equation of the conservation of mass for a fluid with density ρ and flowing with velocity vector $\mathbf{v}$. This is a particular example of a more general equation known as the *continuity equation* that is presented next in a three dimensional domain.

Consider a quantity ψ with generic unit measure denoted SI (standard international) that evolves in time in a three dimensional region of interest Ω. For example, ψ may represent the mass (unit measure kg), energy (unit measure J) or momentum (unit measure $kg \cdot meter/s$) of an object. The amount of ψ per unit volume is given by the volume density $\rho(x, y, z, t)$ with unit measure SI/m^3. For example, a mass density may be expressed in units of kg/m^3, whereas an energy density may be expressed in units of J/m^3 (joules per cubic meter). The magnitude and direction of the flow of the quantity ψ is described by the flux vector field $\mathbf{\Phi}(x, y, z, t)$ that measures the amount of quantity ψ flowing per unit time, through a unit area. At any given time t, the amount of quantity ψ inside an arbitrary fixed region $\mathcal{V}$ is expressed as the volume integral of the density,

$$\iiint_{\mathcal{V}} \rho(x, y, z, t) \,\mathrm{d}V \tag{44}$$

The total amount of quantity ψ flowing per unit time across the boundary S of the region $\mathcal{V}$ is given by the surface integral of the flux vector field,

$$-\iint_S \mathbf{\Phi} \cdot \mathrm{d}\mathbf{S} = -\iint_S \mathbf{\Phi}(x, y, z, t) \cdot \mathbf{n}(x, y, z) \,\mathrm{d}S \tag{45}$$

where $\mathbf{n} = (n_1(x, y, z), n_2(x, y, z), n_3(x, y, z))$ denotes the unit normal vector to the boundary S pointing outward of $\mathcal{V}$. The minus sign taken in front of the surface integral in (45) reflects the fact that $\mathbf{\Phi} \cdot \mathbf{n}$ represents the flux *outward* of $\mathcal{V}$: a positive value of the integral indicates that there is a net loss of the quantity ψ over the boundary surface S and therefore, a negative time rate of change in the amount of ϕ inside the domain $\mathcal{V}$. We further assume that in Ω, the quantity ψ may be also locally generated (for example, through infusion of substance, sources of energy, or body forces) or removed (for example, through deposition or chemical reaction processes, evaporation, etc) and denote by $f(x, y, z, t)$ the rate at which ψ is produced per unit volume. The measure units for f are of $SI \cdot m^{-3}s^{-1}$; positive values $f(x, y, z, t) > 0$ indicate that ψ is locally generated at point (x, y, z) and time t (thus f is a source term) whereas negative values $f(x, y, z, t) < 0$ indicate that ψ is locally removed at point (x, y, z) and time t (thus f is a sink term). The net rate at which ψ is being generated inside the volume $\mathcal{V}$ at time t is given by the volume integral

$$\iiint_{\mathcal{V}} f(x, y, z, t)\,\mathrm{d}V \tag{46}$$

From (44), (45), and (46), the time rate of change in the amount of ψ within the volume $\mathcal{V}$ is expressed as

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\mathcal{V}} \rho\,\mathrm{d}V = -\iint_{S} \mathbf{\Phi}\cdot\mathbf{n}\,\mathrm{d}S + \iiint_{\mathcal{V}} f\,\mathrm{d}V} \tag{47}$$

which is the *integral form of the continuity equation.*

Assuming that the flux $\mathbf{\Phi}$ is a continuously differentiable vector field, the *divergence theorem* may be used to express the surface integral (45) as a volume integral

$$\iint_{S} \mathbf{\Phi}\cdot\mathbf{n}\,\mathrm{d}S = \iiint_{\mathcal{V}} \nabla\cdot\mathbf{\Phi}\,\mathrm{d}V \tag{48}$$

If we further assume that the density $\rho(x, y, z, t)$ is a continuously differentiable function, then (47) may be expressed as

$$\iiint_{\mathcal{V}} \frac{\partial\rho}{\partial t}\,\mathrm{d}V = -\iiint_{\mathcal{V}} \nabla\cdot\mathbf{\Phi}\,\mathrm{d}V + \iiint_{\mathcal{V}} f\,\mathrm{d}V \tag{49}$$

Since (49) holds at any time t and in any region $\mathcal{V}$ of the domain Ω, we obtain the PDE

$$\boxed{\rho_t + \nabla\cdot\mathbf{\Phi} = f} \tag{50}$$

which represents the *differential form of the continuity equation.*

Notice that the equation for conservation of mass (38) is a particular case of the general continuity equation (50) and corresponds to the flux specification $\mathbf{\Phi} = \rho\mathbf{v}$ and without source/sink terms ($f = 0$).

2.3 Diffusion processes, the heat equation

"diffusion: the spreading of something more widely." (Oxford Dictionary).

In this section we use conservation of thermal energy to derive a second order PDE, the heat equation that is used to model the time evolution of the temperature of an object. It is also a mathematical model to a fundamental physical process known as *diffusion* which represents the movement of a quantity from a region of higher concentration to a region of lower concentration. A one dimensional illustration of the diffusion process was given in Fig. 2 and a two dimensional illustration is shown in Fig. 6 below.

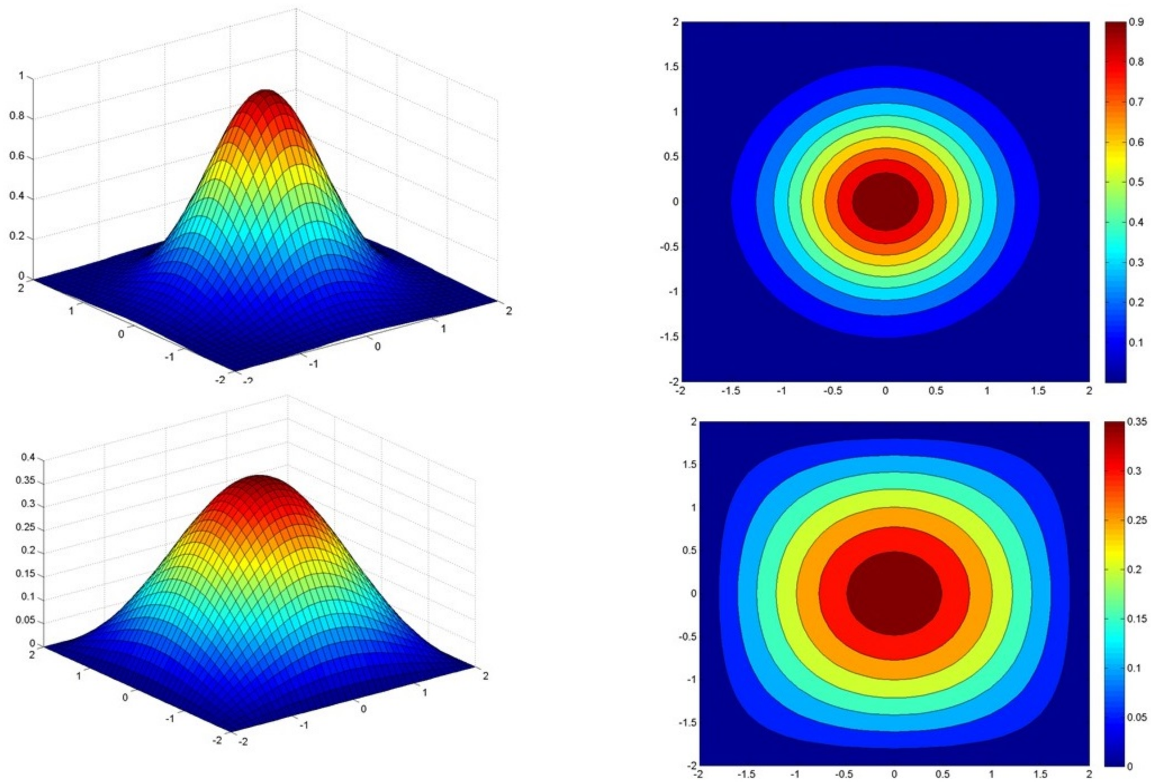


Figure 6. Diffusion represents movement of a quantity from higher density to lower density. The initial density profile is shown in the top figures as a surface (left) or contour lines (right). The bottom figures show the density profile at a later time, after diffusion started.

Along with its fundamental applications in physics, chemistry, geosciences and engineering, diffusion is a very important process in many areas of applied sciences such as biology (spreading of a disease), sociology (diffusion of a population or ideas), economics, finance (the Black-Scholes model), or high-tech industry (signal and image processing). For example, image blurring may be achieved through diffusion, as shown in Fig. 7 below.

Figure 7. Image blurring through diffusion. Each pixel of the image has associated a value (typically from 0 to 255, or scaled to values between 0 and 1) that represents its gray scale intensity. High values are associated with "hot" (high density) regions whereas low values are associated with "cold" (low density) regions. The diffusion process applied to an image (top figure) transfers the gray scale intensity from high values to low values and produces a blurred image (bottom figure).

2.3.1 Conduction of heat in a one-dimensional rod

Consider a rod of constant cross-sectional area A, oriented in the x-direction, from $x = 0$ to $x = L$. Consider

$$e(x,t) \equiv \text{thermal energy density}$$

which represents the amount of thermal energy per unit of volume. In addition, assume that $e(x,t)$ is constant across any section and no thermal energy can pass through the lateral surface. In any finite segment $[a,b]$ of the rod, the total *heat energy* is

$$\text{total heat energy in } [a,b] = \int_a^b e(x,t)A\,dx$$

The *heat flux* is the amount of thermal energy per unit time flowing to the right per unit surface area.

$$\phi(x,t) = \text{heat flux}$$

Heat energy flowing through the side edges at time t: $\phi(a,t)A - \phi(b,t)A$.
In addition, we consider *heat sources*

$$Q(x,t) = \text{heat energy per unit volume generated per unit time}$$

Heat energy generated inside the rod region $[a,b]$ at time t: $\left(\int_a^b Q(x,t)dx\right) A$.
Conservation of heat energy

$$\frac{d}{dt}\int_a^b e(x,t)dx = \phi(a,t) - \phi(b,t) + \int_a^b Q(x,t)dx \tag{51}$$

Equation (51) represents the *integral form of the conservation law of heat energy.* If in addition, e, ϕ are differentiable, from (51) it follows that

$$\int_a^b \left(\frac{\partial e}{\partial t} + \frac{\partial \phi}{\partial x} - Q\right) dx = 0 \tag{52}$$

Continuity of the integrand in (52) implies

$$\frac{\partial e}{\partial t} = -\frac{\partial \phi}{\partial x} + Q \tag{53}$$

which represents the *differential form* of the conservation law of heat energy.

Temperature and thermal energy

Notations:
$u(x,t)$ = temperature of the rod
$c(x)$ = specific heat (the heat energy that must be supplied to a unit mass of a substance to raise its temperature one unit)
$\rho(x)$ = mass density (mass per unit volume)
The thermal energy is the energy it takes to raise the temperature from a reference temperature 0° to its actual temperature $u(x,t)$.

$$e(x,t) = c(x)\rho(x)u(x,t) \tag{54}$$

Replacing (54) in (53), it follows

$$c(x)\rho(x)\frac{\partial u}{\partial t} = -\frac{\partial \phi}{\partial x} + Q \tag{55}$$

Fourier's law of heat conduction

$$\phi = -K_0\frac{\partial u}{\partial x} \tag{56}$$

where the coefficient K_0 is the *thermal conductivity* of the material.

Heat equation

By replacing (56) in (55), it follows

$$c\rho\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(K_0\frac{\partial u}{\partial x}\right) + Q \tag{57}$$

If c, ρ, K_0 are all constants and there are no heat sources ($Q = 0$), then (57) becomes

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \tag{58}$$

where the constant

$$k = \frac{K_0}{c\rho} \tag{59}$$

is called the thermal diffusivity.
Equation (58) is called the *heat equation* and it is also known as the *diffusion equation*.

A complete mathematical model requires the specification of an *initial condition*

$$u(x,0) = f(x) \tag{60}$$

and the specification of the thermal processes through the boundary of the object, which provide *boundary conditions*. Examples of boundary conditions are as follows:

1. *Prescribed temperature*

$$u(0,t) = u_B(t) \tag{61}$$

2. *Prescribed heat flux*

$$-K_0(0)\frac{\partial u}{\partial x}(0,t) = \phi(t) \tag{62}$$

$$\frac{\partial u}{\partial x}(0,t) = 0 \qquad \textit{perfectly insulated boundary} \tag{63}$$

3. *Newton's law of cooling*

$$-K_0(0)\frac{\partial u}{\partial x}(0,t) = -H[u(0,t) - u_R(t)] \tag{64}$$

$$-K_0(L)\frac{\partial u}{\partial x}(L,t) = H[u(L,t) - u_L(t)] \tag{65}$$

HW: Show that there is *at most one solution* to the problem

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}, \;\; 0 < x < L, \;\; t > 0 \tag{66}$$

$$u(x,0) = f(x) \tag{67}$$

$$u(0,t) = T_1(t) \tag{68}$$

$$u(L,t) = T_2(t) \tag{69}$$

2.3.2 Heat equation in three dimensions

We consider an arbitrary bounded region $\mathcal{V} \subset \mathbb{R}^3$, with a closed boundary surface S. At any given time t, the heat energy in $\mathcal{V}$ is given by the volume integral

$$E(t) = \text{ heat energy } = \iiint_{\mathcal{V}} e(x, y, z, t)\,\mathrm{d}V = \iiint_{\mathcal{V}} c\rho u\,\mathrm{d}V \tag{70}$$

The time rate of change in the heat energy in $\mathcal{V}$ is given by the heat flowing across the boundary S per unit time. The three dimensional heat flux vector field is denoted $\mathbf{\Phi}$ and at any point (x, y, z) on the boundary S we consider the unit outward normal vector $\mathbf{n}$. The amount of energy flowing *out* of the region $\mathcal{V}$ per unit surface area per unit time is given by the outward normal component of the heat flux vector $\mathbf{\Phi} \cdot \mathbf{n}$. The total energy flowing over the boundary surface S per unit time is

$$-\iint_{S} \mathbf{\Phi} \cdot \mathbf{n}\,\mathrm{d}S \tag{71}$$

Notice that if $\mathbf{\Phi} \cdot \mathbf{n} > 0$ then the heat flux is directed outward (energy flows out of $\mathcal{V}$), thus the minus sign is inserted in front of the surface integral above. In addition, there may be sources of energy inside the region $\mathcal{V}$. Let Q denote the heat energy generated per unit time per unit volume. The total energy generated per unit time in the region $\mathcal{V}$ is the volume integral

$$\iiint_{\mathcal{V}} Q\,\mathrm{d}V \tag{72}$$

The conservation of heat energy in the region $\mathcal{V}$ implies

$$\frac{d}{dt} \iiint_{\mathcal{V}} c\rho u\,\mathrm{d}V = -\iint_{S} \mathbf{\Phi} \cdot \mathbf{n}\,\mathrm{d}S + \iiint_{\mathcal{V}} Q\,\mathrm{d}V \tag{73}$$

Next we use the *divergence theorem* (13) in the right side of (73) to obtain

$$\frac{d}{dt} \iiint_{\mathcal{V}} c\rho u\,\mathrm{d}V = -\iiint_{\mathcal{V}} \nabla \cdot \mathbf{\Phi}\,\mathrm{d}V + \iiint_{\mathcal{V}} Q\,\mathrm{d}V \tag{74}$$

which may be written as

$$\iiint_{\mathcal{V}} \left[c\rho \frac{\partial u}{\partial t} + \nabla \cdot \mathbf{\Phi} - Q \right] \mathrm{d}V = 0 \tag{75}$$

Since $\mathcal{V}$ was arbitrary, from (75) we obtain the *continuity equation for thermal energy*

$$\boxed{c\rho \frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{\Phi} + Q} \tag{76}$$

The *Fourier's law of heat conduction* is used to express the heat flux in terms of the temperature

$$\mathbf{\Phi} = -K_0 \nabla u \tag{77}$$

where the coefficient K_0 is given by the *thermal conductivity* of the material. Replacing (77) in (76) we obtain the PDE for the temperature

$$\boxed{c\rho\frac{\partial u}{\partial t} = \nabla\cdot(K_0\nabla u) + Q} \tag{78}$$

If $Q \equiv 0$ and the coefficients c, ρ, K_0 are constants, then (78) becomes (see definition (9))

$$\boxed{\frac{\partial u}{\partial t} = k\nabla^2 u} \tag{79}$$

where $k = K_0/c\rho$. Equation (79) is the heat (diffusion) equation in 3D.

A complete mathematical model to the time evolution of the temperature in a domain $\Omega \in \mathbb{R}^3$ requires the specification of the initial state as an *initial condition*

$$u(x, y, z, 0) = f(x, y, z) \tag{80}$$

and the specification of the thermal processes through the boundary surface S of the object, that provide *boundary conditions.* Some common types of boundary conditions are as follows:

1. *Prescribed temperature:* $u(x, y, z, t) = T(x, y, z, t)$ on some region of boundary surface
2. *Prescribed flux:* $-K_0\nabla u\cdot\mathbf{n} = \mathbf{\Phi}$ on some region of boundary surface

   In particular, *insulated boundary* condition is: $-K_0\nabla u\cdot\mathbf{n} = 0$
3. *Newton's law of cooling:* $-K_0\nabla u\cdot\mathbf{n} = H(u - u_b)$ on some region of boundary surface

Steady-state equation. Notice that if the temperature of the object has reached a steady-state (equilibrium), then the time derivative in (79) is zero and we obtain the *steady-state temperature equation* known as *Laplace's equation*

$$\boxed{\nabla^2 u = 0} \tag{81}$$

Changing the coordinates. In many practical applications (e.g. engineering, geophysical problems) it is more appropriate to work in a different coordinate system such as

$$\text{polar coordinates (2D)}:\quad x = r\cos\theta,\quad y = r\sin\theta \tag{82}$$
$$\text{spherical coordinates (3D)}:\quad x = r\sin\gamma\cos\theta,\quad y = r\sin\gamma\sin\theta,\quad z = r\cos\gamma \tag{83}$$
$$\text{cylindrical coordinates (3D)}:\quad x = r\cos\theta,\quad y = r\sin\theta,\quad z = z \tag{84}$$

HW: Derive the expression of the Laplacian $\nabla^2 u$ in polar, spherical, and cylindrical coordinates.

2.4 Advection-diffusion equation

Advection and diffusion are important physical processes in the study of atmospheric or water pollutants. For example, when pollutants such as smog from wild fires or a chemical plant are released in the air their spread through the atmosphere is determined both by transport with the wind field (advection) and also diffusion processes such as molecular diffusion given by particle movement from high concentrations to low concentrations or turbulent air movement (eddy diffusion).

Figure 8. The fate of atmospheric pollutants is determined by various physical processes such as advection, diffusion, emissions, chemical transformations, and soil depositions. Aircraft and NASA's Aqua satellite images show the devastating wild fires in Oregon during August - September of 2020. Credit: NASA

If $\rho(x, y, z, t)$ denotes the concentration of pollutant expressed in molecules per unit volume (e.g., molec$\cdot$m^{-3}), the combined advection and diffusion processes may be represented through the following specification of the flux vector field (unit measure of molecules per unit area per unit time (e.g., molec $\cdot$ m^{-2} $\cdot$ s^{-1})

$$\mathbf{\Phi} = \rho\mathbf{v} - K\nabla\rho \tag{85}$$

where $\mathbf{v}$ denotes the wind velocity field (unit measure of m $\cdot$ s^{-1}) and K is the diffusion coefficient (unit measure of m^2 $\cdot$ s^{-1}). [1] By replacing the flux (85) into the continuity equation (50), we obtain the *advection-diffusion equation*

$$\boxed{\rho_t + \nabla\cdot(\rho\mathbf{v}) - \nabla\cdot(K\nabla\rho) = f} \tag{86}$$

where f represents the emission (source) or deposition (removal) rate of pollutant and has unit measure of molecules per unit volume per unit time (e.g., molec $\cdot$ m^{-3} $\cdot$ s^{-1}).

[1] In practice, the diffusion coefficient is a three-dimensional matrix used to specify the diffusions coefficients in x-, y- and z-directions.

2.5 Conservation of momentum

"momentum: the quantity of movement of a moving object, measured as its mass multiplied by its speed." (Oxford Dictionary).

Momentum is defined to be the mass of an object multiplied by the velocity of the object,

$$\textit{momentum} = m\mathbf{v}$$

and has the unit measure of kilogram meter per second ($\text{kg}\cdot\text{ms}^{-1}$). Notice that momentum is a vector quantity having the same direction as the velocity vector and its magnitude directly proportional to the mass: of two objects that are moving at the same velocity, the heavier object has a greater momentum magnitude.

In section (2.1) we used the law of conservation of mass to derive the equation (38) for the evolution of the density $\rho(x, y, z, t)$ of a fluid moving at a velocity $\mathbf{v}(x, y, z, t)$. To study the fluid's motion, equation (38) must be completed with equations that describe each component of the velocity vector field $\mathbf{v}(x, y, z, t)$. This is achieved using the *law of conservation of momentum* which is a fundamental concept of physics along with the law of conservation of mass and the law of conservation of energy

"The momentum of an isolated system remains constant."

The conservation of momentum states that momentum is neither created nor destroyed, but only changed through the action of forces, as described by Newton's second law of motion

$$\mathbf{F} = m\mathbf{a} = m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \tag{87}$$

Consider an arbitrary fixed volume (control volume) $\mathcal{V} \subset \mathbb{R}^3$ of the three dimensional region of interest and let S denote the closed boundary surface of $\mathcal{V}$. At any given time t, the total momentum associated with the fluid (particles) inside $\mathcal{V}$ is given by the volume integral of the *momentum density*

$$\iiint_{\mathcal{V}} \rho\mathbf{v}\,\mathrm{d}V \tag{88}$$

When material flows through the surface S, it carries both mass and momentum. The momentum flux across the boundary surface S is the vector quantity (units of $\text{kg}\cdot\text{ms}^{-2}$)

$$\iint_S \rho\mathbf{v}(\mathbf{v}\cdot\mathbf{n})\,\mathrm{d}A \tag{89}$$

where $\mathbf{n}$ denotes the unit normal vector to the boundary S pointing outward of $\mathcal{V}$. Using Newton's second law of motion, the time rate of change in momentum inside the control volume $\mathcal{V}$ at time t is expressed as

$$\frac{d}{\mathrm{d}t}\iiint_{\mathcal{V}} \rho\mathbf{v}\,\mathrm{d}V + \iint_S \rho\mathbf{v}(\mathbf{v}\cdot\mathbf{n})\,\mathrm{d}A = \mathbf{F} \tag{90}$$

where $\mathbf{F}$ denotes the total instantaneous force acting on $\mathcal{V}$ at time t. The forces acting on the fluid are of two types: body forces and surface forces, as illustrated in Fig. 9.

- Body forces, such as gravity, acting on all the particles throughout $\mathcal{V}$,

$$\mathbf{F}_g = \iiint_{\mathcal{V}} \rho \mathbf{g} \, \mathrm{d}V \tag{91}$$

where $\mathbf{g} = (0, 0, -g)$ denotes the gravitational acceleration vector pointing vertically downward and with magnitude given by the gravitational acceleration constant $g \approx 9.81 \mathrm{m\,s^{-2}}$.

- Surface forces that act on the surface S of the volume $\mathcal{V}$ e.g., forces caused by the fluid *pressure*, $p(x, y, z, t) > 0$ that produce a flux of momentum across the boundary, in the direction of the normal vector $\mathbf{n}$,

$$\mathbf{F}_p = -\iint_S p\mathbf{n} \, \mathrm{d}S \tag{92}$$

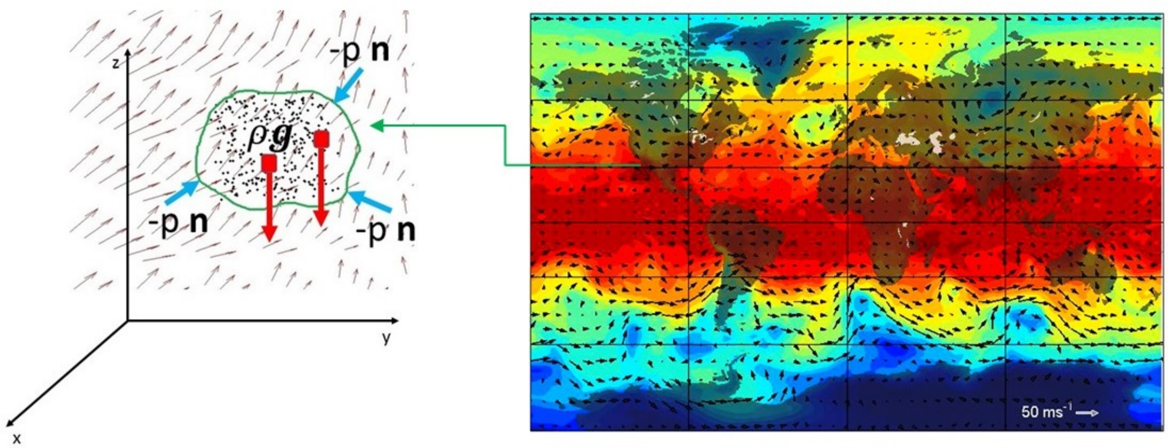


Figure 9. Body forces such as the gravity force $\rho\mathbf{g}$ act on the fluid particles inside the control volume, whereas surface forces such as the pressure force $-p\mathbf{n}$ act on its surface.

By replacing $\mathbf{F} = \mathbf{F}_g + \mathbf{F}_p$ and the force expressions (91) and (92) into equation (90), we obtain the *integral form of the conservation of momentum equation*

$$\boxed{\frac{d}{\mathrm{d}t} \iiint_{\mathcal{V}} \rho \mathbf{v} \, \mathrm{d}V + \iint_S \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A = \iiint_{\mathcal{V}} \rho \mathbf{g} \, \mathrm{d}V - \iint_S p\mathbf{n} \, \mathrm{d}S} \tag{93}$$

Notice that (93) represents a *system of three equations*, one equation associated to each component of the momentum vector. Specifically, the equation for the i^{th} component is

$$\boxed{\frac{d}{\mathrm{d}t} \iiint_{\mathcal{V}} \rho v_i \, \mathrm{d}V + \iint_S \rho v_i \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}A = \iiint_{\mathcal{V}} \rho g_i \, \mathrm{d}V - \iint_S p n_i \, \mathrm{d}S, \quad i = 1, 2, 3} \tag{94}$$

2.5.1 Euler equations and Navier-Stokes equations

The conservation of momentum may be expressed as a system of PDEs. Using the divergence theorem, the surface integrals in (94) may be expressed as volume integrals for example, in the equation for the x-component (i=1), we obtain

$$\iint_S \rho v_1 \mathbf{v}\cdot\mathbf{n}\,\mathrm{d}A = \iiint_{\mathcal{V}} \nabla\cdot(\rho v_1\mathbf{v})\,\mathrm{d}V, \qquad \iint_S p n_1\,\mathrm{d}S = \iiint_{\mathcal{V}} \frac{\partial p}{\partial x}\,\mathrm{d}V \tag{95}$$

From (94) and (95) the momentum equation associated to the x-component is written

$$\iiint_{\mathcal{V}} \frac{\partial(\rho v_1)}{\partial t} + \nabla\cdot(\rho v_1\mathbf{v})\,\mathrm{d}V = -\iiint_{\mathcal{V}} \frac{\partial p}{\partial x}\,\mathrm{d}V + \iiint_{\mathcal{V}} \rho g_1 \tag{96}$$

Since (96) holds for any control volume $\mathcal{V}$, we obtain the *partial differential equation*

$$\frac{\partial(\rho v_1)}{\partial t} + \nabla\cdot(\rho v_1\mathbf{v}) = -\frac{\partial p}{\partial x} + \rho g_1 \tag{97}$$

Using the product rule in the left side of (97) and after arranging the terms, we obtain

$$\frac{\partial(\rho v_1)}{\partial t} + \nabla\cdot(\rho v_1\mathbf{v}) = \left(\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v})\right) v_1 + \rho\left(\frac{\partial v_1}{\partial t} + \mathbf{v}\cdot\nabla v_1\right) \tag{98}$$

Recall the equation for the conservation of mass (38),

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0} \tag{99}$$

which is used to simplify (98) to

$$\frac{\partial(\rho v_1)}{\partial t} + \nabla\cdot(\rho v_1\mathbf{v}) = \rho\left(\frac{\partial v_1}{\partial t} + \mathbf{v}\cdot\nabla v_1\right) \tag{100}$$

By replacing (100) in (97), we express the conservation of momentum equation associated to the x-component as

$$\boxed{\rho\left(\frac{\partial v_1}{\partial t} + \mathbf{v}\cdot\nabla v_1\right) = -\frac{\partial p}{\partial x} + \rho g_1} \tag{101}$$

Following the same procedure, we obtain the y- and z- momentum equations[2]

$$\boxed{\rho\left(\frac{\partial v_2}{\partial t} + \mathbf{v}\cdot\nabla v_2\right) = -\frac{\partial p}{\partial y} + \rho g_2} \tag{102}$$

$$\boxed{\rho\left(\frac{\partial v_3}{\partial t} + \mathbf{v}\cdot\nabla v_3\right) = -\frac{\partial p}{\partial z} + \rho g_3} \tag{103}$$

[2] Recall that for the gravitational force we have $\mathbf{g} = (0, 0, -g)$, thus $g_1 = 0, g_2 = 0, g_3 = -g$

In summary, the conservation of momentum is expressed by the *system of nonlinear partial differential equations* (101), (102), (103). This system of equations may be written in vector format as

$$\boxed{\rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right] = -\nabla p + \rho\mathbf{g}} \tag{104}$$

The nonlinear PDE system (99) and (104) is also known as *Euler equations.*

The momentum equations (104) *neglect the fluid viscosity force*, an internal force that is caused by the molecular interactions. An extra term is introduced in the right side of (104) to account for the viscosity force $\mu\nabla^2\mathbf{v}$, where the coefficient μ denotes the viscosity of the fluid. The resulting system of equations is known as the *Navier-Stokes equations*,

$$\boxed{\rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right] = -\nabla p + \rho\mathbf{g} + \mu\nabla^2\mathbf{v}} \tag{105}$$

The following courses provide further study of PDEs and their practical applications:

- MTH 322: Applied Partial Differential Equations
- MTH 427/428: Partial Differential Equations I, II