Chapter 2

Origin of Partial Differential Equations

2.1 Individual Particle Motion

To model a physical or any other system (chemical, biological, financial, etc.) system it is necessary to translate the system behavior into a set of mathematical equations which describe the system appropriately. Many physical systems consist on an elementary level of discrete particles, e.g., molecules, atoms, ions, electrons, etc. In many cases these elemental particle follow concise equations of motion subject to external or internal forces. Thus an elementary approach to model such systems is to model all individual particle. For the case of charged particles or particles (electrons and ions) subject to gravitational forcing (molecules, dust, satellites, planets, stars, galaxies etc.) these equations of motion are

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i \tag{2.1}$$

$$\frac{d\mathbf{v}_i}{dt} = \frac{1}{m}\mathbf{F}_i. \tag{2.2}$$

with

$$\mathbf{F}_i = \begin{cases} q_i(\mathbf{E}+\mathbf{v}\times\mathbf{B})_{\mathbf{r}_i,t} & \text{for EM forces} \\ -m\nabla\Psi|_{\mathbf{r}_i,t} & \text{for gravitational forces} \end{cases}$$

where $\mathbf{E}$ and $\mathbf{B}$ are electric and magnetic fields and Ψ is the gravitational potential.

If the forces are external, the corresponding equations of motion are complete and the particle motion is often called test particle motion. However, if the other particle contribute to the force on a particular particle the forces have to be evaluated. Examples are electromagnetic forces in a plasma where current and charge densities are determined by the collective particle or a gravitationally interacting system like a galaxy or the universe where the forces are the gravitational drag from all other stars or galaxies. In those cases the forces are determined from the corresponding field equations for electromagnetic interaction (Maxwell's equations)

$$
\begin{aligned}
\nabla \cdot \mathbf{E} &= \frac{1}{\varepsilon_0}\rho_c && (2.3)\\
\nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} &= \mu_0 \mathbf{j} && (2.4)\\
\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= 0 && (2.5)\\
\nabla \cdot \mathbf{B} &= 0. && (2.6)
\end{aligned}
$$

with $c = 3 \cdot 10^8 \mathrm{ms}^{-1}$, $\varepsilon_0 = 8.85 \cdot 10^{-12} \mathrm{Fm}^{-1}$, and $\mu_0 = 4\pi \cdot 10^{-7} \mathrm{Hm}^{-1}$. For computational purposes it is convenient to express the electromagnetic fields in terms of an electric potential Φ and a vector potential $\mathbf{A}$ such that

$$
\begin{aligned}
\mathbf{E}(\mathbf{r},t) &= -\nabla\Phi(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}\\
\mathbf{B}(\mathbf{r},t) &= \nabla \times \mathbf{A}(\mathbf{r},t)
\end{aligned}
$$

which requires to solve the electromagnetic field equations for the potentials for instance in the form

$$
\begin{aligned}
\frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} - \nabla^2 \Phi &= \frac{1}{\varepsilon_0}\rho_c(\mathbf{r},t) && (2.7)\\
\frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} &= \mu_0 \mathbf{j}(\mathbf{r},t) && (2.8)
\end{aligned}
$$

where Φ and $\mathbf{A}$ satisfy the Lorentz Gauge $\partial\Phi/\partial t + c\nabla \cdot \mathbf{A} = 0$. If particle interact through their mutual gravitational force, it is necessary to solve the equation for the gravitational potential

$$\Delta\Psi = 4\pi G \rho_m. \tag{2.9}$$

As outlined in section 1.3.1 the number of particles in a physical system is usually rather large. In addition the overwhelming majority of problems deal with the collective particle behavior rather than the individual one. Discrete particle dynamics can be important in some areas of plasma physics for sufficiently small (‘microscopic’) length or time scales. The collective behavior is usually well described in a fluid approximation.

2.2 Kinetic Equations

The first step toward a fluid description is the introduction of a phase fluid with the phase space consisting of the set of ordinary coordinates and velocities $(\mathbf{r}, \mathbf{u})$. The entire ensemble of n particle has $3n$ spatial and $3n$ velocity degrees of freedom. By integrating the corresponding Liouville equation (see statistical mechanics) over $3(n-1)$ spatial coordinate and $3(n-1)$ coordinates one obtains the Boltzmann equation for the so-called single particle distribution function $f(\mathbf{r}, \mathbf{u}, t)$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f = \left.\frac{\partial f}{\partial t}\right|_{collisions} \tag{2.10}$$

In the case of thermal equilibrium f assumes locally a Maxwell distribution in velocity space and the collision term on the rhs of 2.10 vanishes. Equation 2.10is clearly a fluid (advection) equation though in a 6 dimensional space. The lhs can be interpreted as the total derivative of $f(\mathbf{r}, \mathbf{u}, t)$ along a trajectory given by the 6 dimensional velocity $(\mathbf{v}, \frac{\mathbf{F}}{m})$. In the absence of collisions

$$\frac{df}{dt} = 0$$

implies that the value of f is conserved along this trajectory. This particularly means that any maximum of the distribution remains exactly the same. If in addition the force is conservative the 6 dimensional flow is incompressible, that means that the phase space volume of a contour with any constant value of f is conserved during the evolution as illustrated in Figure 2.1.

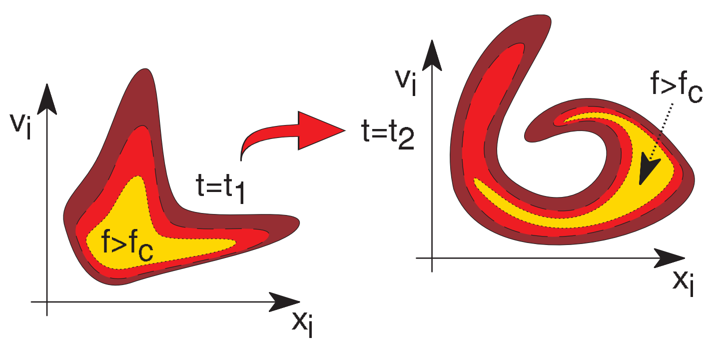

Figure 2.1: Illustration of the evolution of a collisionless distribution conserving the area inside contours of constant f.

Equation 2.10 is complemented with Maxwell's equations or the equation for the gravitational potential for self-consistent electromagnetic respectively gravitational forces. The collision term on the rhs can consider many different physical or chemical processes. Chemical reactions, ionization or recombination, friction, diffusion, and energy exchange collisions are contained in the collision term. Details depend on the corresponding processes.

The description with the single particle distribution function 2.10 and the actual equations of motion 2.1 and 2.2 are in many respects equivalent. Each description has its particular advantages and disadvantages. It is usually rather difficult or impossible to compute realistic particle number. However, the particle approach that densities can never become negative which is a problem common to most fluid simulation methods.

The simulation of the Boltzmann equation may be easier than the discrete particle model because it does not have the enormous ($6N$, N =number of particles) number of degrees of freedom. However, it is still quite challenging to compute a 6 dimensional space as required by the Boltzmann equation. For instance a resolution of each direction with 100 grid points, or modes requires 10^{12} real numbers which is beyond todays computer capabilities. While there are many important applications for which the Boltzmann equation is necessary many fluid and plasma problems involve collective phenomena which do not depend an kinetic scales or processes. In those cases a much more efficient approach is needed to model macroscopic large scale systems. This is the traditional fluid approach illustrated in the next section.

2.3 Fluid Equations

Fluid equations are probably the most widely used equations in numerical modeling and simulation. While the phase fluid which is governed by the Boltzmann equation represents a first example, the overwhelming majority of applications does not require the precise velocity distribution at any point in space. Ordinary fluid equations for gases and liquids can be obtained from the Boltzmann equation or can be derived using properties like the conservation of mass, momentum, and energy of the fluid.

2.3.1 Definitions and derivation

The equations of ordinary fluids and gases as well as those for magneto-fluids (plasmas) can be obtained from equation 2.10 in a systematic manner. Defining the 0th, 1st, and 2nd moment of the integral over the distribution function f as mass density ρ, fluid bulk velocity $\mathbf{u}$, and pressure tensor $\underline{\underline{\Pi}}$

$$\rho(\mathbf{x},t) = m\int_{\infty}^{\infty} d^3v f(\mathbf{x},\mathbf{v},t) \tag{2.11}$$

$$\mathbf{u}(\mathbf{x},t) = \frac{1}{n}\int_{\infty}^{\infty} d^3v\mathbf{v} f(\mathbf{x},\mathbf{v},t) \tag{2.12}$$

$$\underline{\underline{\Pi}}(\mathbf{x},t) = m\int_{\infty}^{\infty} d^3v(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u}) f(\mathbf{x},\mathbf{v},t). \tag{2.13}$$

Note that the macroscopic fluid velocity $\mathbf{u}(\mathbf{x},t)$ is a dependent variable not to be confused with the microscopic independent variable $\mathbf{v}$ (which represents a coordinate in the 6 dimensional phase space of the distribution function $f(\mathbf{x},\mathbf{v},t)$. With the above definitions one also obtains number density $n(\mathbf{x},t) = \rho/m$, charge density $\rho_c(\mathbf{x},t) = qn$, momentum density $\mathbf{p}(\mathbf{x},t) = \rho\mathbf{u}$, current density $\mathbf{j}(\mathbf{x},t) = q\mathbf{u}$, and scalar pressure (the isotropic portion of the pressure) $p(\mathbf{x},t) = \frac{1}{3}Tr(\underline{\underline{\Pi}})$ where the individual particle mass m and charge q are used. The fluid equations are then determined by the moments of the Boltzmann equation, i.e.,

$$\int_{\infty}^{\infty} d^3v\,\mathbf{v}^{\mathbf{i}}(Boltzmann\,Equ.)$$

To account for the collision term in (2.10) we define

$$Q^{\rho}(\mathbf{x},t) = m\int_{\infty}^{\infty} d^3v \left.\frac{\partial f}{\partial t}\right|_c \tag{2.14}$$

$$\mathbf{Q}^{p}(\mathbf{x},t) = m\int_{\infty}^{\infty} d^3v(\mathbf{v}-\mathbf{u}) \left.\frac{\partial f}{\partial t}\right|_c \tag{2.15}$$

$$Q^{E}(\mathbf{x},t) = \frac{1}{2}m\int_{\infty}^{\infty} d^3v(\mathbf{v}-\mathbf{u})^2 \left.\frac{\partial f}{\partial t}\right|_c \tag{2.16}$$

The precise form of these terms depends on the particular properties of the systems and will not be specified at this point. To provide an example for the evaluation of the moments of the Boltzmann equations let us evaluate the 0th moment of the integral. Note that the distribution function has to satisfy $f_{\mathbf{v}\hookrightarrow\infty} \hookrightarrow 0$ because there can be no mass at infinite velocities. The first term of the equation becomes

$$\int_{\infty}^{\infty} d^3v\frac{\partial f}{\partial t} = \frac{\partial}{\partial t}\int_{\infty}^{\infty} d^3v f(\mathbf{x},\mathbf{v},t) = \frac{\partial n(\mathbf{x},t)}{\partial t}.$$

The second term is

$$\int_{\infty}^{\infty} d^3v\mathbf{v}\cdot\nabla f = \int_{\infty}^{\infty} d^3v\nabla\cdot(\mathbf{v}f(\mathbf{x},\mathbf{v},t)) = \nabla\cdot\int_{\infty}^{\infty} d^3v\mathbf{v}f(\mathbf{x},\mathbf{v},t) = \nabla\cdot(\mathbf{u}(\mathbf{x},t)n(\mathbf{x},t))$$

and the third term is

$$\int_{\infty}^{\infty} d^3v\frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}} f = \sum_i \int_{\infty}^{\infty} d^3v\frac{F_i}{m}\frac{\partial f}{\partial v_i} = \sum_i \int_{\infty}^{\infty} d^2v\left[\frac{F_i}{m}f\right]_{v_i=-\infty}^{v_i=\infty} - \sum_i \int_{\infty}^{\infty} d^3v\frac{f}{m}\frac{\partial F_i}{\partial v_i}$$

The terms on the rhs. in the above equation are 0 because the $f=0$ for $v_i = \left\{\begin{array}{c} +\infty \\ -\infty \end{array}\right.$ for each component v_i and in because $\partial F_i/\partial v_i = 0$ (see homework for the Lorentz force). Therefore

$$\int_{\infty}^{\infty} d^3v\frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}} f = 0$$

The collision term of the Boltzmann equation reduces to Q^{ρ} (see equation 2.14) such that in summary the 0th moment of the Boltzmann equation reduces to

$$\frac{\partial n(\mathbf{x},t)}{\partial t} + \nabla\cdot(n\mathbf{u}) = \frac{1}{m}Q^{\rho}. \tag{2.17}$$

This is the usual continuity equation for the particle number density with a source term on the right side. Multiplying (2.17) with the particle mass yields the continuity equation for mass density

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = Q^{\rho} \tag{2.18}$$

The source term describes production or annihilation of mass for instance through chemical reactions or ionization or recombination. It is noted that (2.18) is for one species only. In the case of several neutral constituents or ion species a corresponding continuity equation is obtained for each species. The total production rate of mass has to be zero.

Similar to the 0th moment the 1st moment of the Boltzmann equation $[m\int_{\infty}^{\infty} d^3v\,\mathbf{v}\,(Boltzmann\,equation)]$ and 2nd moment $[\frac{3}{2}m\int_{\infty}^{\infty} d^3v\,v^2\,(Boltzmann\,equation)]$ yield the equations for the fluid momentum (or velocity) and energy

$$\frac{\partial \rho \mathbf{u}}{\partial t} = -\nabla\cdot(\rho\mathbf{u}\mathbf{u}) - \nabla\cdot\underline{\underline{\Pi}} + n\mathbf{F} + \mathbf{u}Q^{\rho} + \mathbf{Q}^{p} \tag{2.19}$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{1}{\gamma-1}p + \frac{1}{2}\rho u^2\right) &= -\nabla\cdot\left(\frac{1}{2}\rho u^2\mathbf{u} + \frac{1}{\gamma-1}p\mathbf{u} + \mathbf{u}\cdot\underline{\underline{\Pi}} + \mathbf{L}\right)\\ &\quad + n\mathbf{u}\cdot\mathbf{F} + \frac{1}{2}u^2Q^{\rho} + \mathbf{u}\cdot\mathbf{Q}^{p} + Q^{E}\end{aligned} \tag{2.20}$$

where $\mathbf{L}(\mathbf{x},t) = \frac{1}{2}m\int_{\infty}^{\infty} d^3v(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})^2 f(\mathbf{x},\mathbf{v},t)$ and γ is the ratio of specific heats, i.e., $\gamma = 5/3$ if a gas has 3 degrees of freedom for motion. Note that $\gamma = 5/3$ is the value obtained by the actual integration of the Boltzmann equation. However, to mimic isothermal changes one can choose $\gamma = 1$ and to model incompressible dynamics $\gamma = \infty$ is the appropriate choice.

If there is a mixture of several different species (gases or charged particles) each species has its own separate set of basic equations. These sets are then coupled through collisions. It is customary to simplify such systems by taking the sum of the different species with appropriate definitions of the total mass density, total velocity etc.. Note that

- As before an internal force $\mathbf{F}(\mathbf{x},t)$ requires to solve the corresponding field equations (2.3) - (2.6) or (2.9).
- $\mathbf{F}(\mathbf{x},t) = \begin{cases} q(\mathbf{E}+\mathbf{u}\times\mathbf{B}) \\ m\nabla\Psi \end{cases}$
- The Lorentz force (or any velocity dependent force now depends on the bulk velocity and velocity is a dependent variable in the fluid equations rather than an independent variable as in the Boltzmann equation.
- The source terms for mass Q^{ρ}, momentum $\mathbf{Q}^{p}$, and energy Q^{E} depend on system properties and need to be specified through these or through a systematic collision operator and the corresponding velocity integrals. They can reflect mass generation and annihilation, momentum exchange through friction, and energy exchange collisions.
- The pressure tensor is often split into a scalar pressure and a viscous tensor $\underline{\underline{\Pi}} = p\underline{1} + \underline{\mathbf{w}}$, with $p = \frac{1}{3}Tr(\underline{\underline{\Pi}})$ and the viscous tensor $\underline{\mathbf{w}}$.
- Often a kinematic viscosity $\sigma_{ik} = a\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right) + b\frac{\partial u_l}{\partial x_l}\delta_{ik}$ is used on the right of the momentum equation yielding a term $\nabla\cdot\underline{\underline{\sigma}} = \eta\Delta\mathbf{u} + \left(\zeta + \frac{\eta}{3}\right)\nabla(\nabla\cdot\mathbf{u})$.

- Elimination of $\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2\right)$ in the energy equation (with the aid of (2.18) and (2.19)) yields

$$\frac{1}{\gamma-1}\left(\frac{\partial p}{\partial t}+\nabla\cdot p\mathbf{u}\right)=-(\underline{\underline{\Pi}}\cdot\nabla)\cdot\mathbf{u}-\nabla\cdot\mathbf{L}+Q^E \tag{2.21}$$

Exercise: Determine the integral of the 1st order moment for the first two terms in the Boltzmann equation.

Exercise: Derive the 1st order moment force term for a gravitational force and the Lorentz force (velocity dependent).

Exercise: Do the same for the energy equation (i.e., multiply the Boltzmann equation (2.10) with $\frac{1}{2}mv^2$ and integrate).

2.3.2 Approximations

Equations (2.18) - (2.20) establish the typical set of fluid equations which are used in many simulations of fluids and gases like weather simulations, air flow around aircraft or cars, water flow in pipes or round boats, and many other research and technical applications. Using the set of equations (2.18), (2.19), and (2.21) we can derive most equations commonly used in fluid simulations:

- For a known velocity profile $\mathbf{u}$ and no sources $Q^\rho=0$ it is sufficient to model the continuity equation for instance to derive the evolution of density of a gas or the concentration of dust, aerosols, etc. in any medium like air water etc.:

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0 \tag{2.22}$$

- If the velocity profile is incompressible $\nabla\cdot\mathbf{u}=0$ the equation reduces to the common advection equation:

$$\frac{\partial\rho}{\partial t}+\mathbf{u}\cdot\nabla\rho=0 \tag{2.23}$$

- With the total derivative along the fluid path defined as $\frac{d}{dt}=\frac{\partial}{\partial t}+\mathbf{u}\cdot\nabla$ the advection equation is

$$\frac{d\rho}{dt}=0$$

- For no sources Q^ρ, $\mathbf{Q}^p=0$, no viscosity $\underline{\sigma}=0$ (scalar pressure) and gravitational acceleration for the force term one obtains Euler's equation :

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p \; (+\, \mathbf{g}) \tag{2.24}$$

- With a kinematic viscosity included the momentum equation is known as the Navier-Stokes equation:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \eta \Delta \mathbf{u} + \left(\zeta + \frac{\eta}{3} \right) \nabla (\nabla \cdot \mathbf{u}) \; (+\, \rho \mathbf{g}) \tag{2.25}$$

- Neglecting pressure and external force terms and assuming a simplified viscosity one obtains Burger's equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = 0 \tag{2.26}$$

- Diffusion and heat conduction: A diffusion equation can be obtained from the continuity equation and a redefinition of the bulk velocity in the presence of several particle species. However, the more straightforward equation for diffusion is obtained for heat conduction (i.e., diffusion of temperature). Equation (2.21) can be re-written in different forms. Defining $\frac{p}{\gamma - 1} = \rho \varepsilon$ yields an equation for the internal energy ε of a gas. More commonly used is the ideal gas law $p = nkT$ to re-write the energy equation into an equation for temperature. Assuming scalar pressure, constant density, and a heat flux driven by a temperature gradient $\mathbf{L} = -\kappa \nabla T$ on obtains

$$\frac{\partial T}{\partial t} = \mu \Delta T \tag{2.27}$$

- Steady state equation are generated from the above sets by assuming $\partial / \partial t = 0$. For steady condition the velocity is often determined from a potential which can be scalar if the flow is assumed irrotational ($\mathbf{u} = \nabla \Phi$) or incompressible flow is modeled sometimes by a vector potential ($\mathbf{u} = \nabla \times \mathbf{V}$).

- In the case of plasmas we need at least two sets of continuity, momentum, and energy equations, one for electrons and one for ions. The force equation is the Lorentz force. Usually it is assumed that the plasma is neutral, implying that number density for ions (single charged) and electrons is equal. Details on the two fluid equations and MHD equations are given in chapter 11.

- the equations of magnetohydrodynamics introduce further simplifications in the plasma description, in particular they assume that Hall term and electron inertia in Ohm's law are negligible. This assumption is correct for sufficiently large length scale. Another common assumption is that of a scalar total plasma pressure. The presence of resistivity in Ohm's law introduces diffusion of the magnetic field.

Exercise: Using the continuity equation and the stated assumptions derive Euler's equation.

Exercise: Derive the equation for heat conduction with the stated assumptions.

Exercise: Derive the heat conduction equation for nonzero velocity $\mathbf{u}$.

Exercise: Derive the continuity equation and momentum equation for irrotational flow.

Exercise: Assume a scalar pressure, $\mathbf{L} = 0$, and $Q^E = 0$ in the pressure equation (2.21). Consider a function $g = p^a \rho^b$ and determine a and b such that the resulting equation for g assumes a conservative form, i.e., $\partial g/\partial t + \nabla \cdot g\mathbf{u} = 0$.

Exercise: Assume a scalar pressure, $\mathbf{L} = 0$, and $Q^E = 0$ in the pressure equation (2.21). Consider a function $h = p^a \rho^b$ and determine a and b such that the resulting equation for h assumes a total derivative, i.e., $\partial h/\partial t + \mathbf{u} \cdot \nabla h = 0$.