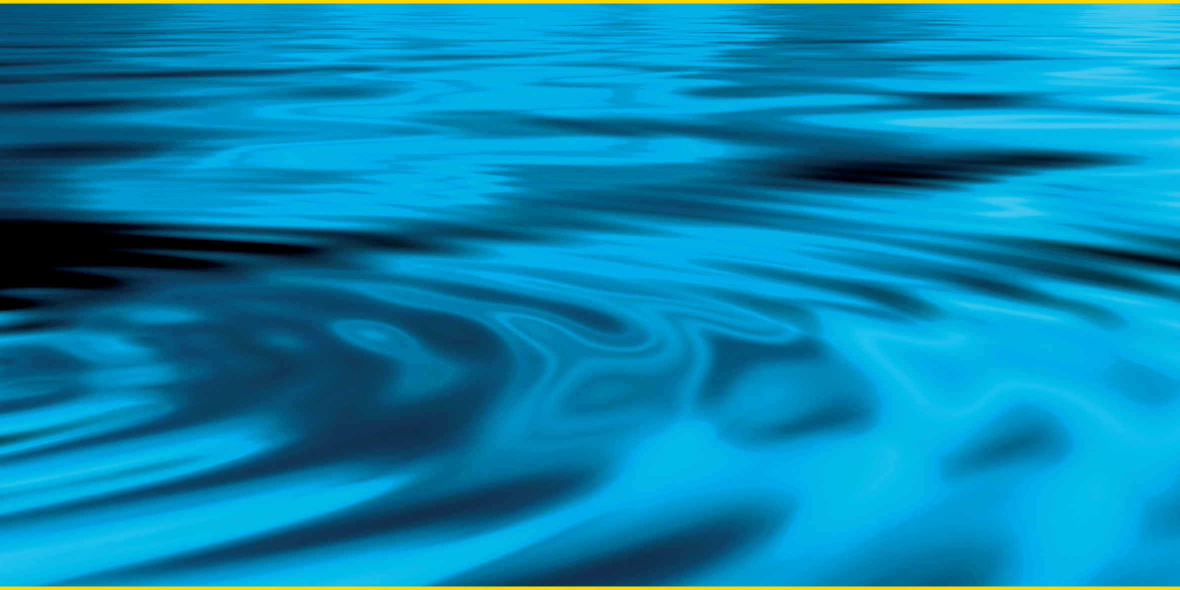
FLUID MECHANICS SERIES



Discrete Mechanics

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Preface

The law of dynamics stated by Isaac Newton in 1686 in his treatise *Philosophiæ Naturalis Principia Mathematica* [NEW 87] introduces the vectorial nature of both sides of that law: the force and the quantity of acceleration. For Newton and his contemporaries, the concepts of vectors and scalars applied to rectilinear trajectories were not so different. The composition of the motions helps to extend those motions along their plane or in space, and Newton himself adds forces to them (see Corollaries I and II of the *Principia*).

The establishment of the equations of general motions in around 1740 by Euler, Lagrange and MacLaurin, introduced the concept of fixed directions in space, where the vectors, velocity and acceleration could be expressed in the form of coordinates. In the field of Mechanics today, we still use the fundamental bases introduced by these concepts. The work of Truesdell illustrates the rise and trajectory of this discipline, to which Truesdell himself contributed greatly during the last century, bringing together the concepts of mechanics with those of thermodynamics; up until that point, the two disciplines had developed in parallel, independently of one another.

Newton's vision, which some might consider to be restrictive, is, in fact, remarkable. He considered a vector as an oriented bipoint – i.e. two points connected by an edge, with its direction being clearly defined. The intensity of the velocity vector can then be calculated, if we introduce the concept of time. A more commonplace and contemporary view can be constructed by considering a road, running between two roundabouts. The driver of a vehicle traveling on that road does not need to know the direction of the journey at a large scale – the local direction of travel is clearly determined by the road itself. Until the driver reaches the next roundabout, his/her direction of travel will be the direction of that particular road, and his/her speed can be calculated as being the distance between the two roundabouts over the travel time. When the next roundabout is reached, the driver will need to continue the journey in a particular direction by choosing the most appropriate exit. Hence, the vehicle's speed on the portion of road between the two roundabouts can be considered to be the component of the velocity vector, projected along the direction of the piece of road. The mean velocity along that portion of road can be calculated as the integral of the vehicle's acceleration over that stretch of road. Furthermore, the journeys made over several successive stretches of road can be added together in the same way that vectors can. Based on these elementary considerations, it is possible to construct a discrete theory of motion, based on Newton's law.

In a Galilean frame of reference, a single material point is at rest or has uniform rectilinear motion, and the laws of mechanics are invariant, regardless of whether the frame of reference changes. The motion of uniform rotation is, *a priori*, a particular case, set apart from the category of Galilean frames of reference, in that an additional force of inertia, stemming from the centrifugal acceleration, is also present. Yet the fundamental law of dynamics still remains valid and applicable to this type of motion. As is the case with gravity, the centrifugal forces derive from a scalar potential which, at all times and at all points, compensates for these purely kinematic effects. Such is the case for an object or person on a carousel, subject simultaneously to centrifugal and centripetal forces, which balance one another out exactly to keep the subject stationary within a rotating frame of reference. An isolated observer on Earth's surface does not feel the effects of the planet's rotation. Hence, in the presence of a force deriving from a scalar potential, a Galilean frame of reference can be deemed to be inertial; such is the case with gravity if density is constant. Other types of force do not contribute directly to acceleration; for instance, a spherical drop subject to capillary forces deriving from a potential (the capillary pressure) will not be subject to acceleration, and will remain in a state of static equilibrium. Hence, not all the forces contribute to the modification of the state of a system; some of them – those which derive from a scalar potential – are counteracted exactly by that potential, and the resulting acceleration is null. Generally speaking, a force derives from two potentials: one scalar and the other vectorial. The vectorial potential alone is responsible for the acceleration of the medium. For a closed system, animated with a uniform translational or rotational motion, the total energy contained in the system must be conserved as that system evolves. In particular, if the system were stationary to begin with, it could not spontaneously begin to move. This physical principle is, at once, a curse and a blessing: uniform motions defy any description by Newton's law of dynamics, but by that token, we are able to "forget" about the kinematic history of the system; in particular, we do not need to know where a particle has come from if we know its current position. It is, however, important to know the history of the stresses undergone by the system during the course of its motion, so as to be able to predict the restitution of any energy that has been accumulated. The immediate consequence of this is that these uniform motions do not contribute to the accumulation of the aforementioned stresses.

Thus, here, the idea of using a fixed, absolute frame of reference to construct a vectorial representation is no longer useful. The velocity and acceleration are, at once, directed vectors and scalars, which represent the measurement of the vectors. The question then arises of which frame of reference to choose; strictly speaking, in that the scalar product is the same regardless of the chosen base, the choice of the frame of reference is unimportant. It is possible to express all the forces involved in the fundamental law of dynamics using solely the velocity components defined on each edge. Hence, even if the velocity vector exists in a particular frame of reference, there is absolutely no need to represent it. Similarly, the acceleration will only be observed by way of its projection onto the edge in question. Stokes' theorem leads us to expect such a possibility; indeed, the rotational of a vector on a surface is equal to the circulation of that same vector, projected onto the path underlying the surface, i.e. the circulation of its components. Those components can be considered to be the geometric projection of the velocity, which it is not necessary to know.

The differential nature of the law of dynamics precludes any representation of the uniform rectilinear motion. Similarly, a uniform block rotation of a body around an axis must not give rise to any acceleration other than that corresponding to the centrifugal acceleration. These uniform motions therefore must not come into play when establishing the conservation of momentum equation. This is one of the rules from which it is possible to derive the motion equation. For these states of rest or of uniform translational or rotational motion (with the exception of a scalar potential), the acceleration is zero. The definition of mechanical equilibrium adopted will be associated with any motion which obeys the fundamental law of dynamics, where the acceleration is equal to the sum of the forces.

In Continuum Mechanics, all values, be they vectorial or tensorial, are reduced to a single point once they have been evaluated for an elementary control volume. This reduction entails a loss of information about the concept of direction; thus, in order to define a single-point vector or tensor, it is necessary to introduce a frame of reference so as to be able to express their components. This hypothesis of a continuum is abandoned when we switch back to the idea of a bipoint and an edge. The consequence is that the notion of a tensor vanishes, as do the plethora of approximations and hypotheses which go along with that notion, such as the principle of material frame indifference, which is closely linked to the constitutive equation.

The strong link established (notably by Truesdell) between Mechanics and Thermodynamics can also be called into question. The constitutive equation defining the links between the applied stresses and the mechanical or thermal alterations undergone by the body is not useful as an entirely separate law in its own right. The confusion which exists between conservation laws, physical properties and phenomenological relations can be alleviated; there are the laws of vectorial conservation on the one hand, and the thermophysical properties on the other. These properties are assumed to be known as a function of the variables of the problem, but the state laws and rheological constitutive equations are not used to calculate one of these physical characteristics.

This vision of Mechanics, which is similar to the concepts introduced by Newton using Geometry, is known as “Discrete Mechanics”. It corresponds simply to an attempt to revisit the equations of Mechanics using elementary concepts from differential geometry.

Jean-Paul CALTAGIRONE
November 2014

List of Symbols

$\cdot$	scalar product
$\otimes$	tensorial product
$:$	contracted tensorial product
∇	nabla operator, gradient 0
$\nabla\times$	rotational
$\nabla^2(*)$	$\nabla\cdot\nabla(*)$, Laplacian
tr	trace of a tensor
$\dfrac{d}{dt}$	material derivative
$\dfrac{\partial}{\partial t}$	partial derivative in relation to time
α	isothermal expansion coefficient
β	thermal expansion coefficient
χ_T	isothermal compressibility coefficient
γ	specific heat ratio

δ_{ij}	Kronecker delta
ε_{ij}	components of the stress tensor
κ	curvature of an interface
λ	compression viscosity
ϕ	dissipation function
$\boldsymbol{\varphi}$	heat flux density
μ	shear viscosity
μ_{sm}	subgrid viscosity
μ_t	turbulent viscosity
ν	kinematic viscosity
ρ	density
σ	surface tension, Poisson coefficient
ψ	stream function
$\boldsymbol{\gamma}$	acceleration
$\boldsymbol{\varepsilon}$	strain tensor
$\boldsymbol{\omega}$	vector potential
$\boldsymbol{\omega^o}$	equilibrium vector potential
$\boldsymbol{\sigma}$	stress tensor
$\boldsymbol{\tau}$	viscous stress tensor
Γ	curvilinear contour
Φ	scalar potential
Σ	surface of a domain
Ω	volume of a domain

$\boldsymbol{\Omega}$	rotation rate tensor
(x, y, z)	Cartesian coordinates
(r, θ)	polar coordinates
(r, θ, z)	cylindrical coordinates
(r, θ, φ)	spherical coordinates
$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$	unit vectors
$\mathcal{A}$	area of a surface
$\mathcal{D}$	domain, control volume
$\mathcal{L}$	linear operator
$\mathcal{M}$	molar mass
$\mathcal{N}$	nonlinear operator
$\mathcal{P}$	power
$\mathcal{V}$	volume
a	heat diffusivity
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
d	distance
d_{ij}	components of the strain rate tensor
e	specific internal energy
f	scalar function
k	heat conductivity, turbulent kinetic energy
h	specific enthalpy
m	mass

p	pressure, scalar potential
p^o	equilibrium scalar potential
p^*	driving pressure
p_B	Bernouilli pressure
q	heat production per volume
q_m	mass flowrate
q_v	volume flowrate
r	perfect gas constant
s	specific entropy, curvilinear abscissa
t	time
v	specific volume
D	flowrate
D_h	hydraulic diameter
E	Young's modulus, total energy
J	Jacobian of the transformation
R	molar constant of gases
L	reference distance
S	entropy
T	temperature
T^o	equilibrium temperature

T_0	reference temperature
V_0	reference velocity
$\mathbf{f}$	body volume force
$\mathbf{g}$	acceleration due to gravity
$\mathbf{n}$	outward normal
$\mathbf{q}$	momentum
$\mathbf{t}$	tangential unit vector
$\mathbf{v}'$	fluctuation of velocity
$\mathbf{v}$	perturbation of velocity
$\mathbf{D}$	strain rate tensor
$\mathbf{F}$	force
$\mathbf{I}$	identity matrix or tensor
$\mathbf{K}$	permeability tensor
$\mathbf{M}$	mobility tensor
$\mathbf{N}$	outward normal to a free surface
$\mathbf{T}$	stress
$\mathbf{V}$	velocity component
$\|\mathbf{W}\|$	velocity modulus
$\mathbf{W}$	velocity
$\overline{\mathbf{W}}$	averaged velocity
Bi	Biot number

Da	Darcy number
M	Mach number
Ma	Marangoni number
Ra	Rayleigh number
Re	Reynolds number
We	Weber number

Introduction

I.1. General points

The concept of a discrete body sets aside the notion of a continuum to establish the conservation laws of Mechanics. All of the theorems and mathematical properties are applied directly to objects of finite dimensions. Discrete Mechanics essentially takes elementary results from differential geometry to establish the laws of conservation along an edge. The Fundamental Law of Dynamics is the starting point for establishing the conservation of momentum equation.

A certain number of the concepts used in Continuum Mechanics will be abandoned; thus, the very notion of a continuum is not necessary in order to obtain discrete equations. Similarly, the hypothesis of Local Thermodynamic Equilibrium is set aside, because within the elementary volume, it is not necessary for a state equation to be satisfied. The concept of a tensor is replaced by the concepts of differential geometry and elementary operators, gradient, rotational and divergence, using which we are able to establish the link between single-point values, oriented vectors, oriented surfaces and volumes, and vice versa. Similarly, the projection onto an orthonormal axis system is not necessary to establish the conservation equations.

Although this formalism gives us a momentum balance equation which is different to the Navier–Stokes equation, their application to simple flows yields identical results. The Hodge–Helmholtz decomposition will play an essential role in showing how the momentum balance equation can be employed to separate any of the terms in this equation into a solenoidal part and an irrotational part.

In Fluid Mechanics, the pressure in the momentum balance equation cannot be reduced to the role of mechanical pressure. This equation represents an instantaneous equilibrium and the thermodynamic pressure, which plays the role of a stress accumulator, depends not only on properties such as the temperature or density, but also on the heat flux and the velocity. If we limit our discussion to mechanical and thermal effects, the role of the divergences of the flux and velocity in reading the thermodynamic pressure will become apparent.

The elements deriving from differential geometry, differential algebra, exterior calculus, and so on, will be omitted in the interests of a presentation which is as simple as possible, using the classic theorems such as those of Ostrogradski and Stokes, etc., and the properties of the standard differential operators.

I.2. Introduction

The laws of conservation in mechanics were established over two centuries ago, and have evolved very little since. The important contributions made by C. Truesdell and W. Noll [TRU 74, TRU 92] to integrate the laws of thermodynamics and the constitutive laws into the conservation of momentum- and energy laws, however, led to the establishment of the Navier–Stokes equations, which offer a very accurate representation of the physical reality of the phenomena being observed. Many more important contributions have helped construct the corpus of equations in Continuum Mechanics as it is taught today [LAN 59, BAT 67, SAL 02, GER 95, COI 07, GUY 91].

However, there are a certain number of difficulties inherent to the continuum theory which need to be taken into consideration:

– the concept of a continuum itself poses a significant problem: the reduction of the elementary volume to a single point, in order to define scalars, vectors and tensors, does away with any reference to the direction and orientation. In order to restore these concepts, it is necessary to place the domain in a frame of reference – e.g. to define a point velocity on the basis of its components;

– the introduction of the Cauchy tensor to express the local stress $\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{n}$, for an isotropic fluid, brings into play two viscosity coefficients, μ and λ, which are interlinked by Stokes' law $3\lambda+2\mu \geq 0$; we shall come back to this point in greater detail later on. The value of λ is very difficult to measure for fluids in general, and varies greatly depending on the authors and the measurement methods used. This law is not valid, in gneral [GAD 95]. It should also be noted, though, that in solids, the existence of this coefficient does not pose a problem;

– the concept of a tensor first appeared in the late 19^{th} Century, and was further developed, in the context of Continuum Mechanics, before being used in other areas of physics. The absolute necessity of using tensors in the field of mechanics to describe the relations between the stresses and strains can, quite legitimately, be disputed. In fact, it was the simplistic interpretation of certain experiments in fluids and solids that guided this choice, which has remained the same ever since. The components of the Cauchy stress tensor have only been able to be reduced thanks to the principle of material frame indifference for an isotropic medium [TRU 74, SAL 02, GER 95, COI 07]. In spite of these reductions, the remaining coefficients are only linked by an inequality, which is confirmed by a thermodynamic approach;

– the formal link between the conservation equations and the Hodge–Helmholtz decomposition has not been established. Whilst Helmholtz's theorem ensures that any vectorial field can be decomposed into an irrotational part and a solenoidal part in $\mathcal{R}^3$ for a decreasing field at infinity, its application is limited to the vectorial fields themselves, such as the velocity, for instance, which can be decomposed into two terms: the scalar and vectorial potentials;

– the level of modeling of the effects of pressure and those of viscosity is not the same in the Navier–Stokes equation [SAL 02]. Whilst particular attention has been paid to viscous effects, enabling us to describe the transfers of momentum within a fluid, the effects of compression or decompression are only taken into account by means of a scalar – the pressure – without any first-order link being established between the pressure and the velocity. In order to make this connection, we have to use other conservation laws: those relating to the conservation of mass and energy;

– for a long time, thermodynamics has had an important role to play, which Trusdell [TRU 74] integrated into the equations of mechanics during the last century. It conferred the status of a law on the relation between the different measurable values, such as the density, pressure and temperature, for example. The structural coupling links between the momentum equation, the conservation of mass equation and the state law lead to confusion as to the role played by each of these relations. For example, the conservation of mass must serve to set the density as a function of the external actions, but not to calculate the pressure. In addition, there is no condition *sine qua non* which means that the state law has to be satisfied at all points and at all times;

– on its own, the conservation of energy carries the notion of flux and of energy, and the conservation of flux is completely absent from the classic formalism used in Continuum Mechanics. Although the conservation of momentum equation is associated with the conservation of mass, the heat flux can easily be introduced into this relation by a simplistic law forming the link between the flux and the temperature gradient: Fourier's law. This is considered an experimental, phenomenological law, serving to bring closure to the system of equations;

– the boundary conditions between two immiscible fluids or on the edge of a domain are written on the basis of the stresses defined by the Cauchy tensor, and are difficult to apply in practical terms; they need to be supplemented by compatibility relations – for instance in the case of shockwaves. Also, they are strongly imposed – for example, for a fluid flow entering into a domain, we impose the normal velocity, thereby violating the equilibrium conditions described by the various terms in the conservation equation.