FLUID MECHANICS SERIES

Discrete Mechanics

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Contents

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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

•	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
$\frac{d}{dt}$	material derivative
$\frac{\partial}{\partial t}$	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
φ	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
γ	acceleration
ε	strain tensor

ω	vector potential
ω^o	equilibrium vector potential
σ	stress tensor
τ	viscous stress tensor
Γ	curvilinear contour
Φ	scalar potential
Σ	surface of a domain
Ω	volume of a domain
Ω	rotation rate tensor
(x, y, z)	Cartesian coordinates
(r, θ)	polar coordinates
(r, θ, z)	cylindrical coordinates
(r, θ, φ)	spherical coordinates
(e_1, e_2, 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_υ	volume flowrate
r	perfect gas constant
s	specific entropy, curvilinear abscissa
t	time
υ	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
f	body volume force
g	acceleration due to gravity
n	outward normal
q	momentum
t	tangential unit vector
v′	fluctuation of velocity
v	perturbation of velocity
D	strain rate tensor
F	force
I	identity matrix or tensor
K	permeability tensor
M	mobility tensor
N	outward normal to a free surface
T	stress
V	velocity component
|W|	velocity modulus

W	velocity
$\overline{\mathbf{W}}$	averaged velocity
B_i	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 $T = \sigma \cdot n$, 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.

The continuum formalism is essentially linked to the relations between stresses and strains (also known as deformations), which are represented by a stress tensor, of varying degrees of complexity. The most complete tensors, such as the Green–Lagrange tensor, enable us to take account of significant deformations, whilst certain tensors found by linearization, such as the Cauchy tensor, are limited to small transformations. The displacement field gradient thus introduces the notion of a tensor which can be decomposed into symmetric and antisymmetric parts. The purpose of this operation is to filter out the rigid translational motion which does not give rise to any force within the material.

The issue that we tackle in the area of Discrete Mechanics is based on the laying aside of the idea of a continuum, where all the scalar and vectorial variables are defined at a single point. In a discrete medium, the scalar values are associated with a point, whereas the vectorial values are defined on an edge which can be as short as it needs to be, provided its direction is preserved. To begin with, we shall work in the context of small displacements, and in order to counter the disadvantages that come with that approach, we shall introduce the principle of accumulation, whereby each equilbrium state is conserved so as to represent the evolution of the physical system.

There are a certain number of principles which seem indispensable in order to model all the mechanical effects:

– the medium is at equilibrium in space if it is not subject to any force, body or contact;

– the principle of action and reaction must be borne in mind, although the surface stress does not have the same meaning here as it does in Continuum Mechanics;

– the rigidifying overall translational and rotational motions may lead to the inadequacy of the formulation where rotation plays an important role. We shall suppose that the rotation rate is zero at infinity, which is one of the use conditions for the Stokes theorem. The only essential condition is that any rigid or rigidifying translational or rotational motion must not affect the acceleration;

– the dissipation of the mechanical effects, wave propagation and viscous effects must be positive.

The theory taking shape in this book is founded upon the fundamental law of dynamics and on some elementary experiments, using these as bases upon which to construct coherent and balanced models of the observed effects – in particular the diffusion of momentum and the propagation of waves. It also draws on certain elements which were established in a previous publication by this author on the subject [CAL 01] to specify and supplement the derivation of the scalar and vectorial conservation equations without using tensors whose order is equal to or higher than two.

Next, we go on to discuss the general properties of these equations. In particular, the differences between the Navier–Stokes equation and the momentum balance equation stemming from this theory will be illustrated; also, the two forms of the dissipation term will be compared.

1

Framework of Discrete Mechanics

1.1. Frames of reference and uniform motions

Any change in the position of a particle defined by its position x, at time *t*, depends on the frame of reference in relation to which the motion is observed. As no absolute rest state exists, it is possible to choose an inertial frame of reference, wherein a body remains at rest or animated with uniform rectilinear motion when not subjected to any external force. In view of the principle of relativity, the physical laws take the same form in all inertial frames of reference. This principle holds true for velocity values which are much lesser than the speed of light. Herein, we shall not take account of the relativistic effects, and our discussion fits into the context of mechanics at moderate velocities, far lesser than the celerity of light. We are left with the fundamental principles of restricted (special) relativity theory or of general relativity in the presence of gravitational forces, which apply for all velocity levels.

The case of a uniform rotational motion is similar in nature: an observer at rest in the rotating frame of reference is subject to a centripetal force which is equal and opposite to the centrifugal force deriving from a scalar potential $\Phi = \rho/2\ (\Omega \times r)^2$, where Ω is the constant speed of rotation of the frame of reference.

A uniform rectilinear motion “eludes” definition by the law of Mechanics; the acceleration is zero and the sum of the forces at work is also null. In the presence of an external force, such as constant gravity, an observer is at rest in a frame of reference linked to the Earth when a different force is exerted upon him/her – in this case, the gravitational pull of the ground; the body forces, in this scenario, derive from a scalar potential Φ. The fundamental law of dynamics therefore becomes $-\nabla\Phi + \rho\,\mathbf{g} = 0$, which is the equation of static of fluids.

In both cases, the acceleration due to gravity and the centripetal acceleration are compensated by the gradient of a scalar potential. If the corresponding forces could no longer be described on the basis of true potentials, the medium would be subject to acceleration, and therefore would lose the state of relative rest. These two examples illustrate that forces which derive from a scalar potential do not give rise to motion: they simply contribute to a modification of the definition of the potential. The Hodge–Helmholtz decomposition, which separates the two components of a vector into a gradient of scalar potential and a rotational of a vector potential, suggests that for a medium at rest, the acceleration vector is null, and therefore, with the exception of the sign, the gradient of the scalar potential is equal to the rotational of the vector potential. The Hodge–Helmholtz theorem predicts, for a simply-connected domain, that a field such that $\nabla a = \nabla \times \mathbf{b}$ is a constant. This constant is, simultaneously, the gradient of a scalar potential and the rotational of a vector potential; it is a harmonic field which corresponds to a decomposition into three Hodge–Helmholtz terms. Generally speaking, the third term V_h is practically impossible to extract directly, and its existence probably needs to be linked to the uniform motions.

A constant introduced on the right-hand side of the motion balance equation can be interpreted as a gradient of a scalar potential, or as the rotational of a vector potential; in both cases, all that changes is the definition of the existing potentials. The directional aspect of the gradient operator suggests that the uniform rectilinear motions will be carried by a scalar potential, whilst the uniform rotational motions will be contained in a vector potential.

The Law of Dynamics formulated by Newton cannot be used to find the uniform motions – be they rectilinear or rotational. The model of the physical phenomena constructed here in order to take account of the numerous effects observed for a continuum – e.g. viscosity, capillarity, rotation, dissipation, etc. – will therefore not take account of these uniform motions. However, if they are present, it is essential that they do not give rise to any artifact for the model; such is the case of the rotational motion, which must be prevented from engendering mechanical dissipation. Note that, at a small timescale, a uniform rotational motion can be considered to be a uniform rectilinear motion.

If we cannot find out the acceleration, why then are we interested in the position of a point of the medium as a function of time? In any case, our knowledge of the particle's absolute position at a later moment in time will be altered by errors, because we can always superimpose a uniform velocity field V′ to calculate it using the formula $x = x^{o} + (V + V')\, dt$. In solid mechanics, the problem can be resolved by adopting a Lagrangian approach using a reference state. As for fluid mechanics, where we are only interested in the velocities and their variations, the question simply does not arise. A more unified approach to mechanics – both fluid and solid – would lead us to consider only the velocities; the displacements would then be deduced by an incremental process based on the evolution from one state of mechanical equilibrium to another.

Another important question merits particular attention: do we actually need a frame of reference? If we consider that the velocity is a vector **W**, then it is necessary to perform elementary operations such as the scalar product, which uses the components of the vector. In this case, we introduce a frame of reference anchored to a given system of coordinates. If we now consider that the velocity is an oriented scalar, following a fixed direction Γ, it can be considered either as a new vector **V** = (**W** · t) **t** or as a scalar *V* = (**W** · t), where **t** is the unit vector over Γ. Evidently, merely knowing **V** and **t** is insufficient to find the local vector **W**, but is it really necessary to do so? If we replace the scalar product with a geometric projection, and differential geometry can be used to write all the operators on the basis of the components of **V** alone, then knowing the velocity vector **W** is no longer useful, in the same way as a frame of reference is no longer needed. It is the concept of a continuum, where all the values are defined at a single point, which creates the need for a frame of reference. Certainly, the lengths, surface areas, volumes, normals, etc. of the topologies need to be known, and therefore calculated previously, in order to be able to apply the differential operators.

Based on this observation, it is possible to do away with the notion of a vector and that of a tensor, instead using the concept of a component associated with elementary topology – that of the oriented bipoint. Hence, by simply knowing the scalars *V* on all of the oriented edges Γ, we are able to define a motion on a discrete topology made up of edges and points. The aim of Discrete Mechanics is to construct physical models on that basis. To find the starting point for this theory, we need to go back to the primary