Algebraic Formulation of Elastodynamics: the Cell Method

E. Tonti and F. Zarantonello¹

Abstract: This paper completes a preceeding paper on the algebraic formulation of elastostatics [Tonti, Zarantonello (2009)]. It shows how to obtain a numerical formulation for elastodynamics by avoiding any process of discretization of differential equations, i.e. PDE-free formulation. To this end, we must analyse in more detail the discretization of time by highlighting the need to introduce a dual subdivision of the time axis, as we did for a space cell complex. The mass matrix obtained with the direct algebraic formulation is diagonal.

Keywords: Cell Method, Discrete, Finite, Algebraic, Elastostatics, Elastodynamics.

1 Computational physics from PDE ?

In computational physics, the algebraic equations needed for the numerical solution are usually obtained through different discretization methods of differential equations, such as FVM, FEM, FDM, etc. In all these methods it is taken for granted that the differential equations contain *all* the information on the physical law which they describe. But, are we sure that *the differential formulation is the best starting point for the algebraic or discrete or finite formulation? Are we sure that the differential formulation channels all the physical and geometric features of the physical phenomenon?* The answer is no and the source of this absence lies upstream from the differential equations. In fact, some physical features are lost in the very moment in which we introduce the physical variables. In other words, we must ask whether the differential formulation, which is only one of the tools which mathematics has to offer, the other being algebra, is the most suitable for thoroughly describing the physical phenomenon.

The main information lost in the differential formulation are

• the distinction between configuration, source and energy variables;

¹ University of Trieste, Italy. E-mail: tonti@units.it; f_zarantonello@libero.it

- the introduction of global variables at the outset;
- the notion of the two kinds of orientation of space elements: inner and outer;
- the association of global variables with oriented space elements;
- in time-dependent phenomena it is not often taken into account that some physical variables must be evaluated at the instant in between the initial and final instants. This fact is relevant because in the algebraic formulation, hence in the numerical formulation, the lack of this distinction implies a loss of accuracy, instability and the violation of energy conservation.

Configuration and source variables. Recalling the subdivision of *physical quantities* into *physical constants* and *physical variables*, we can see that in all physical theories, physical variables can be divided into three classes: configuration, source and energy variables. For example, in the electric field we have electric potential (configuration) and electric charge (source); in solid mechanics we have displacement (configuration) and force (source). This fundamental distinction, based on the role that physical variables play in a theory, is usually ignored and this yields a loss of information.

Global variables. Since the differential formulation makes use of field functions, it does not give importance to the global variables from which the field functions, in general, are deduced. Instead of reconstructing global variables by the integration of field variables, as in FVM, obtaining the so-called integral variables, it is more natural to deduce field variables from global variables. Since global variables are associated with extended space elements, they are rich in geometric information. The field functions do not contain the same information as the global variables because the passage to the limit loses the link with geometry. We remark that when writing a balance law in the differential form, even if the volume element is infinitesimal, we must use global variables (e.g. surface forces not stresses).

Oriented space elements. Space elements, i.e. points, lines, surfaces, volumes, can have two kinds of orientation: inner and outer orientation. The most natural way to use the two types of orientation is to make use of two cell complexes, with one being the dual of the other. If we provide all elements of the primal complex with internal orientation, automatically all the elements of the dual complex will be endowed with outer orientation.

Global variables and space elements. Global physical variables are naturally associated with oriented space and time elements the last being instants and intervals. In fact, from the analysis of a great number of physical variables of classical fields one can infer the

ASSOCIATION PRINCIPLE. In spatial description, global configuration variables are associated with space elements endowed with inner orientation. In contrast, global source variables and global energy variables are associated with space elements endowed with outer orientation.

This principle offers a rational criterion for associating global variables of every physical theory to space and time elements and, as such, it is useful in computational solid mechanics, as we will explain later.

Let us give an example of the role of this space association by considering the two Maxwell equations of electromagnetism

$$\nabla \times \vec{E} + \partial_t \vec{B} = 0 \qquad \nabla \times \vec{H} - \partial_t \vec{D} = \vec{J} \tag{1}$$

which describe Faraday's and Ampère's laws, respectively. Even though the two equations appear very similar in the differential formulation, in an algebraic formulation they are very different because of the different association with space elements. In fact, the two equations must be associated with edges and faces of the primal complex and edges and faces of the dual complex, respectively. The reason for this loss of information is that, during the discretization process, it is not usually taken into consideration that \vec{B} is an axial vector while \vec{D} is a polar vector. This difference is the clue that the corresponding global variables, i.e. the magnetic flux Φ and the electric flux Ψ , are associated with a surface endowed with inner and outer orientation respectively [Tonti (2001b)]. Hence, in an algebraic formulation, the variables of the first equation must be associated with the primal complex, while those of the second equation must be associated with the dual complex.

The use of staggered grids enables the recovery of this lost information. Historically, the introduction of staggered grids in the middle of the 1960s in fluid dynamics [Harlow-Welch (1965)] and in electromagnetism [Yee (1966)] constituted a major advance in computational physics. Staggered grids are preferable to nonstaggered grids. In fact, in fluidynamics, one of the advantages of staggered grids is to prevent non-physical pressure oscillations that may occur on the non-staggered grid [Ferziger-Peric (1997), p.157]. Moreover, in electromagnetism the use of staggered grids avoids spurious solutions [Jiang-Wu-Povinelli, (1996)]. This shows that the introduction of staggered grids was dictated by an attempt to improve the accuracy of the solution and avoid some of the inconvenient features of FEM. Hence this choice was not induced from the natural association of global physical variables with oriented space elements and, as a consequence, with the primal and dual cell complexes.

FVM, which starts from the differential formulation using field variables, has no rule linked with physical reasons for the association of variables with space elements: take for example velocity and pressure. In contrast, the natural association of global variables with oriented space elements provides a rule for avoiding a trial and error procedure. Moreover, starting from field variables, the global variables, which are nedeed to express conservation laws, must be reconstructed by an approximate integration, which introduces a further approximation in the algebraic formulation. The direct use of the global variables makes avoiding this approximation possible. By itself FVM is unable to indicate the best placement of field variables in space and time because it tries to satisfy a numerical requirement and not a physical demand. In contrast, if the mathematical formulation of physical laws starts from global variables rather than their densities, the right association with the extended space elements can be immediately seen.

The direct algebraic formulation permits higher order of convergence [Tonti (2001a)] than has been obtained with FVM [Ferziger-Peric (1997), p.229].

Time dependent phenomena. To give another example of *information loss* with regard to evolution problems, let us consider two adjacent rooms separated by a wall, as shown in Fig. (1). If the temperatures in the two rooms are different, they will tend to level off because of heat transmission. Let us now mathematically describe the law which regulates the heat balance, preserving the physical content.



Figure 1. Temperature behavior in unsteady heat conduction.

The drawings refer to two situations, one at a starting instant t_i , the other at a final instant t_f . By indicating with T_1 and T_2 the temperatures, which are supposedly uniform in the two rooms, the temperature differences at the initial and final instants

are

$$T_1(t_i) - T_2(t_i)$$
 $T_1(t_f) - T_2(t_f)$. (2)

Clearly, the amount of heat Q moved from left to right in the interval (t_i, t_f) does not depend *only* on the initial temperature difference nor *only* on the final temperature difference, but, intuitively, on the difference evaluated at an instant in between. For small time intervals, we can consider the middle instant t_m of the interval, i.e.

$$t_m = \frac{t_f + t_i}{2} \,. \tag{3}$$

Denoting by A the area of a piece of the wall and with d the thickness of the wall, λ thermal conductivity, the heat Q crossing this surface during the time interval (t_i, t_f) will be approximately

$$Q(t_i, t_f) = -\lambda A (t_f - t_i) \frac{T_2(t_m) - T_1(t_m)}{d} .$$
(4)

In fact, since the initial temperature difference is different from the final temperature difference, it is unreasonable to choose the initial or the final temperature difference to evaluate the heat flow.

We usually start from the traditional case of steady heat conduction

$$Q(t_i, t_f) = -\lambda A \left(t_f - t_i \right) \frac{T_2 - T_1}{d}$$
(5)

in which the time variation of temperature is not taken into account. Once the heat current density $q = Q/[(t_f - t_i)A]$ has been introduced, the elementary Fourier law, given by Eq. (5), in vector form is written as

$$\vec{q} = -\lambda \,\nabla T \,\,. \tag{6}$$

If we put this relation in the law of energy balance, we obtain the Fourier equation

$$\partial_t(c_v T) = \lambda \, \nabla^2 T + \sigma \,. \tag{7}$$

When Eq.(7) is discretized, we do not say in which time instant we should evaluate the temperature on the right hand side. In fact, in FDM on a Cartesian grid, the discrete form of Eq. (7) is usually written in one of the two forms

$$c_{\nu}\left(T_{i}^{n+1}-T_{i}^{n}\right) = \frac{\lambda \tau}{h^{2}}\left(T_{i-1}^{n}-2T_{i}^{n}+T_{i+1}^{n}\right) + \tau \sigma_{i}^{n}$$
(8)

or

$$c_{\nu}\left(T_{i}^{n+1}-T_{i}^{n}\right) = \frac{\lambda \tau}{h^{2}} \left(T_{i-1}^{n+1}-2T_{i}^{n+1}+T_{i+1}^{n+1}\right) + \tau \sigma_{i}^{n+1}$$
(9)

where *arbitrarily* the right hand side is evaluated at the initial or at the final instant of the interval [Vesely (1994), p.152; p.153][Isaacson & Keller (1966), p.501; p.505].

Discretization according to Eq. (8) leads to a scheme that is explicit, of the first order, which is stable, but rather inefficient [Vesely (1994), p.153]. Discretization according to Eq. (9) improves things, but leads to a scheme that is of the first order, stable, implicit and implies the resolution of a tridiagonal matrix at every time step.

These two discretizations do not respect the fact that the jump in temperature *must* be evaluated at an intermediate instant for evident physical reasons. This *information loss* is typical of the discretization of the differential formulation and leaves an arbitrary choice of the instant.

In contrast, using Eq.(4), we come to the following discrete form (omitting for brevity the source term)

$$c_{\nu}\left(T_{i}^{n+1}-T_{i}^{n}\right) = \frac{\lambda \tau}{2h^{2}} \left[\left(T_{i+1}^{n+1}-2T_{i}^{n+1}+T_{i-1}^{n+1}\right) + \left(T_{i+1}^{n}-2T_{i}^{n}+T_{i-1}^{n}\right) \right].$$
(10)

This approach leads *directly* to the Crank-Nicholson scheme, which is second order, by starting from physical considerations and not from a purely mathematical requirement of increasing the order of convergence.

By putting $a = (\lambda \tau)/(2h^2 c_v)$, we can write

$$T_i^{n+1} = T_i^n + a \left[\left(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1} \right) + \left(T_{i+1}^n - 2T_i^n + T_{i-1}^n \right) \right]$$
(11)

which becomes [Vesely (1994), p.155]

$$-aT_{i-1}^{n+1} + (1+2a)T_i^{n+1} - aT_{i+1}^{n+1} = +aT_{i-1}^n + (1-2a)T_i^n + aT_{i+1}^n.$$
 (12)

We see that the Crank-Nicholson method, which is implicit, requires the inversion of a tridiagonal matrix at each time step.

1.1 Algebraic formulation of elastodynamics

The direct algebraic formulation is not another method of discretization of differential equations, it is rather a *different philosophy which allows physical equations to be written directly in an algebraic form without the intermediacy of the differential formulation.* This is the essence of the *Cell Method*.

This method is opposite to the mimetic discretization methods whose objective is just to mimic the differential formulation [Bochev (2006)].

The direct algebraic formulation of a physical problem, making widespread use of global variables and their association with oriented space elements, avoids all the inconveniences described in the previous section.



Figure 2. The direct algebraic formulation: the Cell Method.

Based on the association principle we will put into square brackets the space elements associated with the variables. Thus displacement is associated with points endowed with inner orientation and we will use the notation $\vec{u}[\mathbf{P}]$. The relative displacement of two points is associated with a line, which connects the two points and which is endowed with an inner orientation because we must decide which is the previous and which is the following point, hence $\vec{h}[\mathbf{L}]$. The internal surface force is associated with a surface endowed with an outer orientation because it depends on the normal to the surface, hence we write $\vec{T}[\mathbf{\tilde{S}}]$. The body force is associated with a volume endowed with an outer orientation because we must distinguish between the inside and the outside of the volume, hence $\vec{F}[\mathbf{\tilde{V}}]$.

This correspondence makes possible to build a general classification diagram of physical variables for every physical theory (see the classification diagrams on the website *discretephysics.dica.units.it*). Table 1 shows the logical relation between the physical variables of elastodynamics. The classification of global physical variables highlights the geometric content of variables. Since displacement and relative displacement, from which the notion of strain is defined, are associated with space elements endowed with *inner* orientation, they involve vertices and edges of the *primal* cell complex. In contrast, since equilibrium makes use of surface and body forces and these forces refer to volumes and surfaces endowed with an *outer* orientation, the equilibrium equation must be imposed on every cell of the *dual* complex. Hence, the use of two space cell complexes has its roots in the need to consider two kinds of orientations.

In elastodynamics there are two constitutive relations. One links the *internal sur-face forces*, which are associated with the faces of the dual complex, with the *rel-ative displacements*, which are associated with the edges of the primal complex. Another constitutive relation links *velocities*, that are associated with points of the primal complex, with *momenta* that are associated with volumes of the dual com-



 Table 1. Classification diagram of elastodynamics.

plex.

This direct algebraic formulation of elastodynamics is made possible by the use of global variables and the following requirements:

- every displacement field in a region of regularity, i.e. where it is continuous and has continuous variation, can be locally approximated by an *affine* field. We remark that even in the differential formulation the regularity requirement is needed in order to perform the partial derivatives. The definition of the strain matrix in terms of displacements can be done without making use of derivatives: in fact, displacement can be considered as having linear behavior in a *small* region. This fact opens the way to a purely algebraic formulation of the strain measure;
- 2. the equilibrium equation is a global law and, as such, needs not to be applied to infinitesimal portions of matter. The fact that the sum of the forces applied to a finite portion of matter must vanish in order to ensure equilibrium opens the way to an algebraic formulation of the equilibrium condition. The equilibrium equation is exact until we express the surface forces in terms of the Cauchy relation, which is an approximate relation. In fact, the relation between the surface forces and the area vectors, which the forces are associated with, is an approximate one when we consider a *small* region (not an necessarily infinitesimal) region. At any rate, the Cauchy relation is an algebraic relation;

3. the constitutive law, which is commonly written in a differential setting by using field variables, *is laboratory tested on specimens of finite size in con-ditions of uniform strain.* Under these conditions Hooke law is described by an algebraic relation. Therefore, their application to *small* portions of matter, even if approximate, is an immediate consequence of experiments.

By assembling these relations, we obtain the fundamental algebraic equation of elastodynamics which is, as such, necessarily approximate.

A word on approximation. Every numerical method is necessarily approximate: while the traditional methods like FEM, BEM, FDM, FVM introduce an approximation when the differential equations are discretized, the direct algebraic formulation introduces an approximation from the outset. This happens because, in small space regions, the displacement can be considered as having linear behavior in space and, in small time intervals, it can be considered as having a linear behavior in time.

1.2 Time elements

When dealing with time-dependent phenomena, computational physics discretizes time and considers a discrete set of instants and the corresponding intervals. In this way, a one-dimensional cell complex on the time axis is created.

In this cell complex there are two *time elements*, i.e. instants I and intervals T. We use boldface capital letters to render this notation uniform with the notation used for space elements and reserve the letter T to denote the measure of the time interval, i.e. its *duration*.

A more refined description of time dependent phenomena suggests considering the middle instants of each time interval as forming a second subdivision which gives rise to a second time cell complex, staggered with respect to the first one. If the first cell complex is called *primal*, the second cell complex will be called *dual*. We will call the elements of the primal time complex primal instants and primal intervals and we will denote them with a bar over the letters, i.e. \overline{I} and \overline{T} . We will call the middle instants *dual instants*, denoting them with \widetilde{I} and a time interval between two dual instants as *dual time interval*, denoting it by \widetilde{T} (Fig. 3).



Figure 3. A primal cell complex in time and its dual.

1.3 Global variables in time

An algebraic formulation of time dependent phenomena requires not only a space classification, but also a time classification of the variables involved. As we shall see in the following, all variables of a physical field are *associated* with one of the four time elements, i.e. $\overline{I}, \overline{T}, \widetilde{I}, \widetilde{T}$. This implies that the direct algebraic formulation naturally assigns the correct instant where the physical variable must be evaluated, i.e. it is not an arbitrary choice, but the reason of this choice has a physical motivation.

Among the physical variables which are functions of time instants there are those which are *rates* of variables associated with time intervals and those which are not. This distinction suggests the introduction of the following definition: *we call global variable in time every variable which is not the rate of another physical variable.*



 Table 2. Distinction between rate and derivative.

Table 2 helps to grasp the notion of global variable in time. Hence the displacement, the impulse of a force, the radius vector and momentum are global variables in time,

while velocity and force are rates.

A distinction needs to be made regarding these four global variables: some of them refer to a time instant, like radius vector and momentum, while others refer to a time interval, like displacement and impulse.

2 Algebraic formulation of particle dynamics

The best way to show the role of a primal and a dual cell complex in time is to describe particle dynamics. This is also useful for introducing elastodynamics. In fact elastodynamics combines notions of elastostatics and of particle dynamics.

To perform a direct algebraic formulation we need to classify the physical variables of particle dynamics. This must be done to find the correct instant (primal or dual) at which we have to evaluate the variables.

2.1 Useful concepts for classification

It is not always immediate to find the right association with time elements as in the case of radius vector, and velocity, i.e. performing a time classification. Useful classification rules for this purpose are obtained by analyzing the notions of *reversal of motion* and *oddness condition*.

Reversal of motion. Reversal of motion means the inversion of the time order, hence the reversal of the orientation of time intervals, i.e. $\overline{T} \longrightarrow -\overline{T}$. This fact sometime implies that the sign of the variable changes into into its opposite. Hence, for ex. when the order of the time sequence is reversed, the displacement of the particle changes sign, i.e.

$$\mathscr{R}\vec{\eta} \stackrel{\text{def}}{=} \vec{r}(t_{n-1}) - \vec{r}(t_n) = -[\vec{r}(t_n) - \vec{r}(t_{n-1})] = -\vec{\eta} .$$
(13)

This fact is important for the present analysis because the behavior of a physical variable under reversal of motion gives the criterion for the association with primal or dual time elements.

Oddness condition. We make explicit a truth that is implicitly used in physics: *a global physical variable, associated with a space or time element, changes its sign if the element reverses its orientation.* This will be taken as a general principle. In algebraic topology this condition is known as *oddness condition* and we will use the same name in physics.

2.1.1 Classification rules

We want to highlight the logical path which allows us to identify the right time element with which a given physical variable is associated. Given a variable, we first identify whether it is associated with an instant or an interval by using the very definition of the variable.

To decide if the time element is primal or dual we must see how the variable behaves under *reversal of motion* and make use of the *oddness condition*. If the variable changes its sign by reversal of motion and it is associated with an interval, the interval is primal; if the variable is associated with an instant, the instant is dual. Conversely, if the variable does not change sign under reversal of motion and it is associated with an interval, then the interval cannot be primal, hence by exclusion it must be dual; if the variable is associated with an instant and does not change its sign under reversal of motion, the instant is primal.

Table 3 summarizes the above discussion.

Table 3.	Procedure to find the association.
----------	------------------------------------

	time elem.	<i>chang</i> yes	<i>ges sign?</i> no
a given variable is associated with	Ι	ĩ	Ī
	Т	T	$\widetilde{\mathbf{T}}$

2.2 Classification of variables of particle dynamics

The main variables of particle dynamics are: position vector \vec{r} , displacement $\vec{\eta}$, velocity \vec{v} , momentum \vec{p} , impulse \vec{J} , force \vec{F} . The first thing we have to do is divide these variables into *configuration* and *source* variables.

We will see that configuration variables will be associated with the primal time complex, while source variables will be associated with the dual time complex.

Radius vector. This is a configuration variable. With reference to Fig. (4) *left*, let us consider the motion of a particle. At every instant **I**, the position of the particle is described by the position vector, $\vec{r}[\mathbf{I}]$. Is it a primal or a dual instant? Since \vec{r} does not change sign under reversal of motion it is associated with the primal instants: hence $\vec{r}[\mathbf{I}]$.



Figure 4. *left*) Displacement in particle dynamics; *right*) displacement in continuum mechanics.

Displacement. This is a configuration variable. The time analysis of the displacement requires a clarification because the term "displacement" is used with different meanings in particle mechanics and in continuum mechanics.

a) PARTICLE DYNAMICS. Considering two instants t^- and t^+ , the displacement $\vec{\eta}$ is the difference between the position at the final and the initial instant of a time interval and can be properly called **incremental displacement**

$$\vec{\eta} (t^+, t^-) \stackrel{\text{def}}{=} \vec{r} (t^+) - \vec{r} (t^-) .$$
(14)

Since the radius vector is associated with a primal instant $\mathbf{\overline{I}}$, the displacement $\vec{\eta}$ is **associated** with a primal time interval $\mathbf{\overline{T}}$. Hence we can rewrite Eq.(14) as follows

$$\vec{\eta}\left[\mathbf{\overline{T}}\right] = \vec{r}\left(\mathbf{\overline{I}}^{+}\right) - \vec{r}\left(\mathbf{\overline{I}}^{-}\right). \tag{15}$$

This equation underlines something new with respect to the traditional notation, i.e. the time elements involved are those of the primal time complex. In fact, the traditional notation is unable to show whether the istant or the interval belongs to a primal or a dual time complex.

b) CONTINUUM MECHANICS. In the deformation of a continuum, the displacement \vec{u} of a point is measured from a *fixed* position, i.e. from its position in the reference configuration to its actual position at the instant $\bar{\mathbf{I}}$ (Fig. 4 *right*), hence \vec{u} is associated with a primal instant, i.e. $\vec{u}[\bar{\mathbf{I}}]$. The vector \vec{u} can be properly called **initial displacement**. We see that the initial displacement \vec{u} in continuum mechanics plays the same role as the position vector \vec{r} of particle dynamics and it is a *function of* an instant. The **incremental displacement** $\vec{\eta}$, defined by

$$\vec{\eta}(t,x,y,z) \stackrel{\text{def}}{=} \vec{u}(t^+,\mathbf{P}) - \vec{u}(t^-,\mathbf{P})$$
(16)

can be rewritten as follows

1 0

$$\vec{\eta} \left[\overline{\mathbf{T}}, \overline{\mathbf{P}} \right] \stackrel{\text{def}}{=} \vec{u} \left(\overline{\mathbf{I}}^+, \overline{\mathbf{P}} \right) - \vec{u} \left(\overline{\mathbf{I}}^-, \overline{\mathbf{P}} \right). \tag{17}$$

In continuum mechanics there is also the **relative displacement** of two points, $\overline{\mathbf{P}}$ and $\overline{\mathbf{Q}}$, defined as the difference of the displacement \vec{u} at two points at a same instant, i.e.

$$\vec{h}[\bar{\mathbf{I}},\bar{\mathbf{L}}] \stackrel{\text{def}}{=} \vec{u}\,[\bar{\mathbf{I}},\bar{\mathbf{Q}}] - \vec{u}\,[\bar{\mathbf{I}},\bar{\mathbf{P}}]. \tag{18}$$

Hence \vec{h} is associated with a primal instant and with a line endowed with inner orientation.

Velocity. This is a configuration variable. Let us pose the question: Which time element is velocity associated with? To answer this question let us consider the mean velocity $\langle \vec{v} \rangle$ of a particle, given by the ratio between the displacement and the duration of a primal time interval. Since velocity requires a time interval for its definition, we will say that the velocity **inherits** from the displacement an association with a primal time interval \overline{T} : we write $\vec{v}[\overline{T}]$. But which is the time instant at which we have to evaluate velocity? To answer this question, we have to consider the *instantaneous* velocity. In a small time interval in which the motion is regular, i.e. continuous and with continuous variation (no rebounds), we can approximate particle motion with uniformly accelerated motion. The mean velocity is given by

$$\langle \vec{v} \rangle = \frac{\vec{\eta}}{T} = \frac{\vec{r}(t^+) - \vec{r}(t^-)}{t^+ - t^-} = \vec{v}_0 + \vec{a} \frac{t^- + t^+}{2} = \vec{v} \left(\frac{t^- + t^+}{2}\right)$$
(19)

therefore, it coincides with the instantaneous velocity in the middle instant of the interval which is a dual instant. It becomes natural to say that velocity is a **function** of the dual instants, i.e. $\vec{v}(\mathbf{\widetilde{I}})$.

Hence, velocity has two features: it is a *function* of dual instants and it is *associated* with a primal intervals; these two features are described by the notations $\vec{v}(\widetilde{\mathbf{I}})$ and $\vec{v}[\overline{\mathbf{T}}]$ respectively. It is somewhat similar to the name (round brackets) and surname (square brackets) of a person.

REMARK. By stating that a physical variable is *associated with* a time interval or a time instant we want to emphasize that a time interval or a time instant enters in the definition of the physical variable and therefore in its measurement, when the variable is measurable.

Let us remark that velocity in particle mechanics is the *rate* of the incremental *displacement* $\vec{\eta}$ and, consequently, it is the *time derivative* of the *position vector* \vec{r} ; in continuum mechanics velocity is the *rate* of the *incremental displacement* $\vec{\eta}$

and, consequently, it is the *time derivative* of the *initial displacement* \vec{u} .

particle mechanics continuum mechanics

$$\vec{v} = \lim \frac{\vec{\eta}}{\tau} = \frac{d\vec{r}}{dt}$$
 $\vec{v} = \lim \frac{\vec{\eta}}{\tau} = \frac{d\vec{u}}{dt}$
(20)

Impulse. It is a source variable. The impulse communicated to a particle during a time interval is the *definite* time integral of force

$$\vec{J}(t_1, t_2) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \vec{F}(t) \, \mathrm{d}t \,.$$

$$\tag{21}$$

Hence \vec{J} is associated with intervals, i.e. $\vec{J}[\mathbf{T}]$. We want to explore if the impulse is associated with a primal or a dual interval. In agreement with the oddness condition, if the impulse changes sign under reversal of motion, it will be associated with the primal interval. Otherwise, by exclusion, it will be associated with the dual interval.

Impulse *does not* change sign under reversal of motion: in fact let us consider the rebound of a ball on a wall (Fig. 5). In forward motion or in backward motion the ball always gives the same impulse to the wall. This implies that, to respect the oddness condition, the impulse *is not* associated with primal intervals, hence $\vec{J}[\tilde{T}]$.



Figure 5. *a*) forward motion; *b*) backward motion.

Force. This is a source variable. In dynamics force is not a global variable because it is the rate of the impulse. Hence, force *inherits* from impulse the association with dual time intervals, i.e. $\vec{F}[\tilde{T}]$. A further reason which confirms that force is associated with dual intervals is that force does not change sign under reversal of motion. For example, the force of gravity acting on a stone is the same when the motion is upwards or downwards, while in the two cases its velocity is reversed.

Momentum. This is a source variable. The algebraic formulation of particle dynamics, as well as all other physical theories, is based on an *operative definition* of its variables. We define momentum as the *indefinite* time integral of force

$$\vec{p}(t) \stackrel{\text{def}}{=} \int_0^t \vec{F}(t') \, \mathrm{d}t' \text{ (with the condition that for } t = 0 \text{ is } \vec{v} = 0\text{)}.$$
(22)

This agrees with [Weyl (1962)]; [Van Dantzig (1954)]; [Williams (1996), p. 138].

Force and momentum are measurable physical variables: the devices for doing so are the dynamometer and the ballistic pendulum, respectively.

The momentum of a particle in motion is the physical quantity measured with a ballistic pendulum when the particle has stopped.

Momentum is a function of time instants and since it is not the rate of another variable, it is a global variable in time, hence it is *associated* with time instants **I**. Is it a primal or a dual instant?

When a ball impacts on a wall, the momentum of the ball is directed towards the wall. In a reversal of motion the momentum of the ball is reversed, hence it cannot be associated with primal time instants but, by exclusion, it is associated with dual time instants: \vec{p} [$\tilde{\mathbf{I}}$].

The impulse, defined by Eq. (21), can be expressed in terms of momentum as follows

$$\vec{J}[\widetilde{\mathbf{T}}] \stackrel{\text{def}}{=} \vec{p}(\widetilde{\mathbf{I}}^+) - \vec{p}(\widetilde{\mathbf{I}}^-) .$$
(23)

This equation shows that impulse plays the same role with respect to momentum that the incremental displacement plays with respect to the position vector, Eq. (14).

REMARK. In the differential formulation, the limit process removes the distinction between primal and dual instants or between primal and dual intervals: this is a great loss for a numerical formulation. So, the integrals

$$\vec{\eta} = \int_{t_0}^{t_1} \vec{v}(t) dt \qquad \vec{J} = \int_{t_0}^{t_1} \vec{F}(t) dt$$
(24)

are considered the same process applied to two different vector valued functions, i.e. velocity and force. The different behavior under reversal of motion is not taken into consideration. In contrast, the algebraic setting mantains information about the association with time (and space) elements. Dividing a time interval $\overline{\mathbf{T}}$ into small intervals $\overline{\mathbf{T}}_n$ and, in an analogous way, a time interval $\widetilde{\mathbf{T}}$ into small intervals $\widetilde{\mathbf{T}}_n$, Eqs. (24) can be rewritten in the form

$$\vec{\eta}\left[\overline{\mathbf{T}}\right] = \sum_{n} \vec{v}\left(\widetilde{\mathbf{I}}_{n}\right) \overline{T}_{n} \qquad \vec{J}\left[\widetilde{\mathbf{T}}\right] = \sum_{n} \vec{F}\left(\overline{\mathbf{I}}_{n}\right) \widetilde{T}_{n}$$
(25)

which takes into consideration that velocity is a function of dual instants $\mathbf{\tilde{I}}$, while force is function of primal instants $\mathbf{\bar{I}}$. Note that the time intervals are not in bold because they mean a duration.

Fig. 6 shows the association between physical variables of particle dynamics and time elements of the primal and dual complexes.



Figure 6. The association of variables of particle dynamics with time elements. Global variables are in bold.

2.3 Constitutive laws

Now we can explore the constitutive laws of particle dynamics.

Momentum-velocity. Since we gave an operative definition of momentum and velocity, we can explore the nature of their link. To this end, let us consider the ballistic pendulum, the calibration of which has been obtained by firing bullets of a same mass with the *same* velocity. We can fire the same bullet with various velocities and measure the corresponding momenta. The data thus obtained can be mapped in a diagram (p, v). Measurements show that momentum is proportional to velocity and has the same direction: i.e. $\vec{p} \propto \vec{v}$. This leads us to introduce a parameter *m* and to write

$$\vec{p} \stackrel{\text{law}}{=} m\vec{v} \,. \tag{26}$$

The parameter *m* is a proportionality constant between two variables previously and independently defined and is called *inertial mass*.

REMARK. The interpretation of the relation (26) as a constitutive equation was given by Van Dantzig [Van Dantzig (1954)]. He stated: "*The relation between momentum and velocity* $\vec{p} = m\vec{v}$ is a linking equation and implies metrics."¹ Relation (26) can be written in an algebraic setting as

$$\vec{p}(\widetilde{\mathbf{I}}) \stackrel{\text{law}}{=} m \vec{v}(\widetilde{\mathbf{I}}) \qquad commonly \qquad \vec{p}(t) \stackrel{\text{law}}{=} m \vec{v}(t).$$
 (27)



Table 4. Classification diagram of particle dynamics.

Force-displacement. Force can depend on the position of the particle, on its velocity and on other field variables. In the simple case of an elastic restoring force we have the constitutive relation

$$\vec{F}(\bar{\mathbf{I}}) \stackrel{\text{law}}{=} -k\vec{r}(\bar{\mathbf{I}}) \qquad commonly \qquad \vec{F}(t) \stackrel{\text{law}}{=} -k\vec{r}(t)$$
(28)

where k is the *stiffness*. Every possible link between force and position, like Coulomb force, is a different constitutive relation.

¹ Here the word *metric* means measure of lengths, areas, angles, that are indispensable notions in all constitutive equations.

Force-velocity. Let us consider a force-velocity relation, like the one of viscous force

$$\vec{F}(\vec{\mathbf{I}}) \stackrel{\text{law}}{=} -h\vec{v}(\widetilde{\mathbf{I}}) \qquad commonly \qquad \vec{F}(t) \stackrel{\text{law}}{=} -h\vec{v}(t).$$
(29)

The fact that velocity changes sign under reversal of motion, while force does not change sign, is a spy that this relation describes an irreversible link.

After we have performed the classification of physical variables and equations, we can put them into a classification diagram as shown in Table 4.

2.4 Numerical formulation of particle dynamics

For a numerical formulation it is useful to number the primal and the dual instants respectively with *n* and \tilde{n} and abandon the notation $\overline{\mathbf{I}}$ and $\widetilde{\mathbf{I}}$ used until now. With the preceeding analysis we found the correct association between physical variables of particle mechanics and time elements of the primal and dual time cell complexes. We know that position vector, which is associated with primal instants, must be evaluated at *n*, i.e. $\vec{r}(n)$, while velocity must be evaluated at \tilde{n} , i.e. $\vec{r}(n)$. Momentum must be evaluated at \tilde{n} , i.e. $\vec{p}(\tilde{n})$; force must be evaluated at *n*, i.e. $\vec{F}(n)$. In this way the *algebraic formulation leads to the leapfrog algorithm as a natural consequence of physical considerations* and not as a simple mathematical expedient to increase accuracy. In this formulation the leap-frog algorithm stems from the discovery that some variables are function of the primal instants, while others are function of dual instants.

Now we can write the *fundamental equation* of particle dynamics in algebraic form. With reference to Fig. 7, by combining Eq. (17), Eq. (27), Eq. (23) and being $\overline{\tau}^n$ and $\tilde{\tau}^n$ the duration of the *n*-th primal and dual interval respectively, we obtain the equations

$$\vec{v}(\tilde{n}) \stackrel{\text{def}}{=} \frac{\vec{r}(n) - \vec{r}(n-1)}{\overline{\tau}^n} \quad \vec{p}(\tilde{n}) \stackrel{\text{law}}{=} m \vec{v}(\tilde{n}) \quad \vec{F}(n) \stackrel{\text{def}}{=} \frac{\vec{p}(\tilde{n}+1) - \vec{p}(\tilde{n})}{\widetilde{\tau}^n} \tag{30}$$

which are the algebraic equivalent of the differential equations

$$\vec{v} \stackrel{\text{def}}{=} \frac{d\vec{r}}{dt} \qquad \vec{p} \stackrel{\text{law}}{=} m\vec{v} \qquad \vec{F} \stackrel{\text{def}}{=} \frac{d\vec{p}}{dt} .$$
 (31)



Figure 7. The time sequence of the position vector and momentum.

The fact that the force \vec{F} is, by definition, the derivative of momentum is a consequence of Eq. (22). This is in contrast with the traditional interpretation of this equation as Newton's law as a consequence of an incorrect *definition* of momentum as mass time velocity.

We see from Eq. (30) that displacement is the *backward* difference of the position vector in the primal time complex, while impulse is the *forward* difference of momentum in the dual time complex. We will choose a time complex with equally spaced intervals: $\bar{\tau} = \tilde{\tau} = \tau$.

Eqs. (30) can be combined in the following system of two equations

$$\begin{cases} \vec{r}(n) = \vec{r}(n-1) + \tau \frac{1}{m} \vec{p}(\tilde{n}) \\ \vec{p}(\tilde{n}+1) = \vec{p}(\tilde{n}) + \tau \vec{F}(n) . \end{cases}$$
(32)

With reference to Fig. 7, we see that we need to know momentum at the dual instant $\tilde{n} = 1$. We suppose that at the initial instant n = 0 the position vector and the velocity are assigned. This is obtained with the application of the second formula of system (32) using the interval $\tau/2$.

The leap-frog algoritm is commonly written by using velocities instead of momenta and acceleration instead of force. By dividing the second equation by the mass m and eliminating velocity we obtain

$$\vec{r}(n+1) = 2\vec{r}(n) - \vec{r}(n-1) + \tau^2 \vec{a}(n)$$
(33)

which is the traditional form of the leap-frog algorithm [Vesely (1994), p.115].

For a *damped* harmonic motion in one dimension, while in the differential formulation the force is given by $\vec{F} = -c\vec{v} - k\vec{r}$, in the algebraic formulation we must write

$$\vec{F}(n) = -c \vec{v}(n) - k \vec{r}(n)$$
 (34)

This implies that velocity must be known at primal instants, while we evaluate it at the dual instants. This is accomplished with the formula

$$\vec{v}(n) = \frac{\vec{v}(\tilde{n}+1) + \vec{v}(\tilde{n})}{2} .$$
(35)

Substituting Eq. (34) and Eq. (35) in system (32) and putting $s = c \tau/2m$ we obtain

$$\begin{cases} \vec{r}(n) = \vec{r}(n-1) + \frac{\tau}{m} \vec{p}(\tilde{n}) \\ \vec{p}(\tilde{n}+1) = \left(\frac{1-s}{1+s}\right) \vec{p}(\tilde{n}) + \left(\frac{\tau}{1+s}\right) \left[-k\vec{r}(n)\right]. \end{cases}$$
(36)

Since this system makes use of the leap-frog algorithm, its solution gives an accuracy of second order in time.

2.5 Implementation

The dual complex in time gives rise to a staggered grid, as in the *Finite-Difference Time-Domain method* [Taflove (2005)]. In order to avoid the use of the cumbersome notation like $t^{n+1/2}$, with reference to Fig. (8), we show the pseudocode of the leap-frog algorithm for one-dimensional motion using only integers.

dual complex	p(1)		p(2)		
0	•	-0	•	O	$\longrightarrow t$
x(0)		<i>x</i> (1)		x(2)	primal complex
<i>t</i> (0)		<i>t</i> (1)		t(2)	

Figure 8. A convenient arrangement of indices for the leap-frog algorithm.

```
% damped harmonic motion
% xe(t) = A*exp(-D*t)*sin(w*t); exact solution
m = 1 , k = 400 , c =0.1 , A = 10 % assigned parameters
D = c/(2*m) , w = sqrt(k/m-D*D) % derived parameters
tau = 0.005 , N = 2000 , s = c*tau /(2*m)
t(0) = 0 , x(0) = 0 , p0 = m*A*w
p(1) = p0*(1-s)/(1+s) - h/2*k*x(0)/(1+s)
FOR n = 1 TO N-1
t(n) = t(n-1)+ tau
x(n) = x(n-1) + tau*p(n)/m
p(n+1)= p(n)*(1-s)/(1+s) - tau*k*x(n)/(1+s)
ENDFOR
```

3 Algebraic formulation of elastodynamics

The direct algebraic formulation of elastodynamics is obtained by combining the results of elastostatics, see the paper [Tonti, Zarantonello (2009)], with the results just exposed here for particle dynamics.

The space and time global variables of elastodynamics and their densities are listed in the following. The corresponding association with the elements of the primal and dual complexes in space and in time is highlighted.

Configuration variables

- *ū*[Ī, P]: the initial displacement is associated with primal instants Ī and primal nodes P;
- $\vec{h}[\bar{\mathbf{I}},\bar{\mathbf{L}}]$: the relative displacement is associated with primal instants $\bar{\mathbf{I}}$ and primal edges $\bar{\mathbf{L}}$;
- $\vec{\eta}$ [$\overline{\mathbf{T}}$, $\overline{\mathbf{P}}$]: the incremental displacement is associated with primal intervals $\overline{\mathbf{T}}$ and primal nodes $\overline{\mathbf{P}}$;
- *v*[*T*, *P*]: the velocity inherits the association with *T* and *P* from the displacement *u*.
- $H[\overline{I},\overline{L}]$: the displacement gradient matrix inherits the association with \overline{I} and \overline{L} from the relative displacement \vec{h} ;
- $\mathcal{E}[\overline{I}, \overline{L}]$: the symmetric strain matrix inherits the association with \overline{I} and \overline{L} from the relative displacement \vec{h} .

Source variables

- $\vec{P}[\widetilde{\mathbf{I}}, \widetilde{\mathbf{V}}]$: the momentum is associated with dual instants $\widetilde{\mathbf{I}}$ and dual volumes $\widetilde{\mathbf{V}}$;
- *J*^v[T̃, Ṽ]: the impulse of the body forces, acting on the matter contained in the dual cell, is associated with dual intervals T̃ and dual volumes Ṽ;
- *J*^s[T̃, S̃]: the impulse of the surface forces, acting on the faces of the dual cells, is associated with dual intervals T̃ and dual volumes Ṽ;
- $\vec{F}[\widetilde{\mathbf{T}}, \widetilde{\mathbf{V}}]$: the resultant of the body forces, acting on the dual cell, inherits the association with $\widetilde{\mathbf{T}}$ and $\widetilde{\mathbf{V}}$ from the impulse of body forces;

- \vec{T} [$\widetilde{\mathbf{T}}$, $\widetilde{\mathbf{S}}$]: the resultant of the internal surface forces, acting on the boundary of dual cells, inherits the association with $\widetilde{\mathbf{T}}$ and $\widetilde{\mathbf{S}}$ from the impulse of surface forces;
- $\vec{B}[\widetilde{T}, \widetilde{S}]$: the resultant of the external surface forces, acting on the boundary of the broken dual cells, inherits the association with \widetilde{T} and \widetilde{S} from the impulse of surface forces;
- $\tau[\widetilde{T}, \widetilde{S}]$: the stress matrix inherits the association with \widetilde{T} and \widetilde{S} from the impulse of surface forces;
- $\sigma[\widetilde{T}, \widetilde{S}]$: the symmetric stress matrix inherits the association with \widetilde{T} and \widetilde{S} from the impulse of surface forces.

These variables are collected in Table 5: the global variables are in the first row, while the corresponding rates and densities are in the second row.

Table 5. The space and time global variables of elastodynamics and their densities and rates.

configuration variables			source variables		
(geometric and kinematic variables)			(static and dynamic variables)		
$\vec{u}[\overline{\mathbf{I}},\overline{\mathbf{P}}]$	$ar{\eta}[\overline{\mathbf{T}},\overline{\mathbf{P}}]$	$ec{h} [\overline{{f I}}, \overline{{f L}}]$	$ec{P}[\widetilde{\mathbf{I}},\widetilde{\mathbf{V}}]$	$ec{J}^{v}[\widetilde{\mathbf{T}},\widetilde{\mathbf{V}}]$	$ec{J}^{s}[\widetilde{\mathbf{T}},\widetilde{\mathbf{S}}]$
	\downarrow	\downarrow		\downarrow	\downarrow
	rate	density		rate	dens.rate
	$\vec{v}[\overline{\mathbf{T}},\overline{\mathbf{P}}]$	$H[\overline{I},\overline{L}]$		$ec{F}\left[\widetilde{\mathbf{T}},\widetilde{\mathbf{V}} ight]$	$\pmb{\tau}[\widetilde{\mathbf{T}},\widetilde{\mathbf{S}}]$

With reference to Fig. (11), let us consider a space region which can be constituted by one or more different materials. Let us subdivide this region into triangles forming the primal cell complex and consider the barycentric subdivision to form the dual cell complex. We apply the equation of motion to each dual cell. If we denote by N the number of primal nodes, we obtain a system of 2N equations in 2N unknowns.

Note that the dual cells are the core of the direct algebraic formulation because all forces and, as a consequence the equations of motion, make reference to these cells.

3.1 Center of mass of the dual cell

We will make the approximation of considering the center of mass of every dual cell h coincident with the node h. The stars in Fig. (9) show some of the positions of the

center of mass of the dual cell, in the worst cases: the center of mass lies near the common vertex of the triangles. We will see that on account of this approximation one obtains a diagonal mass matrix.



Figure 9. The center of mass, denoted by a star, of the dual cell, in the worst cases.

Let us express this approximation in mathematical terms. With reference to Fig. (10), the center of mass *C* of the dual cell is contained in one of the triangles with a common vertex *h*. By denoting the vertices of this triangle with the labels *h*, *i*, *j*, and the local affine coordinates with the origin in the vertex *h* with the labels ξ and η and with reference to the *x* coordinate alone, we can write

$$\begin{aligned} x(C) &= x(h) + \xi \left[x(i) - x(h) \right] + \eta \left[x(j) - x(h) \right] \\ &= \left[1 - \xi - \eta \right] x(h) + \xi x(i) + \eta x(j). \end{aligned}$$
 (37)

After a displacement, the new x coordinate of C is

$$x'(C) = [1 - \xi - \eta] x'(h) + \xi x'(i) + \eta x'(j).$$
(38)



Figure 10. The center of mass *C* and the affine coordinates.

The horizontal and vertical components of the displacement of the center of mass are

$$\begin{cases} u_x(C) = [1 - \xi - \eta] u_x(h) + \xi u_x(i) + \eta u_x(j) \\ u_y(C) = [1 - \xi - \eta] u_y(h) + \xi u_y(i) + \eta u_y(j) \end{cases}$$
(39)

The fact that the center of mass *C* is very near to the *h* node implies that ξ and η are very small with respect to unit. This suggests making the approximation $u_x(C) \approx u_x(h)$ and $u_y(C) \approx u_y(h)$.

3.2 Numerical formulation

Let us go into more detail and consider a generic dual cell h, see Fig. (11), the one with the same label as a primal node h and let us apply the formulae of Eq. (30) of particle dynamics to the dual cell.



Figure 11. A generic domain subdivided into primal and dual cells. Bottom: a) nodal displacements; b) body forces; c) surface forces; d) momenta; e) boundary forces.

Let us consider the momentum \vec{P} of the dual cell *h*. It is expressed as the product of the mass of the dual cell for the velocity of its center of mass C: $\vec{P}(h) = m(h)\vec{v}(C) = m(h)\vec{u}(C)/\tau$. As previously stated, we can express the displacement of the center of mass as a linear combination of the displacements of the three nodes h, i, j of the triangle within which the mass center is located, see Eq. (39). Therefore we can express the momentum in the form

$$\vec{P}(h) = \frac{m(h)}{\tau} \left[(1 - \xi - \eta) \, \vec{u}(h) + \xi \, \vec{u}(i) + \eta \, \vec{u}(j) \right]. \tag{40}$$

So the momentum of the dual cell h does not depend only on the velocity of node h, but also on the velocities of the two nodes i and j. Thereby we obtain a system characterized by a sparse matrix with a diagonal dominance. Since the center of

mass is very close to the node h, see Fig. (9), the affine coordinates ξ and η are small compared to unity and can be neglected. By doing this approximation, the momentum of the node h is dependent only on the displacement of node h and therefore the mass matrix thus obtained is diagonal.

We will use two sets of equations, as in Eq. (32): one to increment the initial displacement \vec{u} , the other to increment the momentum \vec{P} . The notation $\vec{u}(n,h)$ means that the displacement \vec{u} is a function of the primal instant *n* and of the node number *h*. In a two-dimensional problem Eqs. (32) become

$$\begin{cases} u_{x}(n,h) = u_{x}(n-1,h) + \frac{\tau}{m(h)} P_{x}(\tilde{n},h) \\ u_{y}(n,h) = u_{y}(n-1,h) + \frac{\tau}{m(h)} P_{y}(\tilde{n},h) \\ P_{x}(\tilde{n}+1,h) = P_{x}(\tilde{n},h) + \tau \begin{bmatrix} T_{x}(n,h) + F_{x}(n,h) + B_{x}(n,h) \\ T_{y}(n,h) + F_{y}(n,h) + B_{y}(n,h) \end{bmatrix}.$$
(41)

This requires transporting the initial condition on momenta to the midpoint of the first interval, as shown in Fig. 7. This is accomplished with the equations

$$\begin{cases} P_x(2,h) = m(h)v_{0x}(h) + \frac{\tau}{2} \left[T_x(1,h) + F_x(1,h) + B_x(1,h) \right] \\ P_y(2,h) = m(h)v_{0y}(h) + \frac{\tau}{2} \left[T_y(1,h) + F_y(1,h) + B_y(1,h) \right]. \end{cases}$$
(42)

By eliminating the momenta, we can write the fundamental equation of elastodynamics in the form

$$\begin{cases} \frac{m(h)}{\tau^2} \left[u_x(n+1,h) - 2 u_x(n,h) + u_x(n-1,h) \right] = T_x(n,h) + F_x(n,h) + B_x(n,h) \\ \frac{m(h)}{\tau^2} \left[u_y(n+1,h) - 2 u_y(n,h) + u_y(n-1,h) \right] = T_y(n,h) + F_y(n,h) + B_y(n,h) \end{cases}$$
(43)

If we introduce the global vectors

$$\mathbf{U}(n) \stackrel{\text{def}}{=} \begin{bmatrix} u_x(n,1) \\ u_y(n,1) \\ \cdots \\ u_x(n,N) \\ u_y(n,N) \end{bmatrix} \quad \mathbf{F}(n) \stackrel{\text{def}}{=} \begin{bmatrix} F_x(n,1) \\ F_y(n,1) \\ \cdots \\ F_x(n,N) \\ F_y(n,N) \end{bmatrix} \quad \mathbf{T}(n) \stackrel{\text{def}}{=} \begin{bmatrix} T_x(n,1) \\ T_y(n,1) \\ \cdots \\ \cdots \\ T_x(n,N) \\ T_y(n,N) \end{bmatrix}$$
(44)

64 Copyright © 2010 Tech Science Press

$$\mathbf{B}(n) \stackrel{\text{def}}{=} \begin{bmatrix} B_x(n,1) \\ B_y(n,1) \\ \cdots \\ B_x(n,N) \\ B_y(n,N) \end{bmatrix} \qquad \mathbf{P}(\tilde{n}) \stackrel{\text{def}}{=} \begin{bmatrix} P_x(\tilde{n},1) \\ P_y(\tilde{n},1) \\ \cdots \\ \dots \\ P_x(\tilde{n},N) \\ P_y(\tilde{n},N) \end{bmatrix}$$
(45)

and the diagonal matrix \mathbf{Q} of the inverses of masses

$$\mathbf{Q} \stackrel{\text{def}}{=} \begin{bmatrix} 1/m(1) & 0 & \cdots & 0 & 0 \\ 0 & 1/m(1) & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1/m(N) & 0 \\ 0 & 0 & \cdots & 0 & 1/m(N) \end{bmatrix}$$
(46)

remembering that the vector of surface forces T is linked to the vector of displacements U by the stiffness matrix K, the two sets of equations, i.e. Eq. (41), can be written as

$$\begin{cases} \mathbf{U}(n) = \mathbf{U}(n-1) + \tau \mathbf{Q} \mathbf{P}(\tilde{n}) \\ \mathbf{P}(\tilde{n}+1) = \mathbf{P}(\tilde{n}) + \tau \left[-\mathbf{K} \mathbf{U}(n) + \mathbf{F}(n) + \mathbf{B}(n) \right]. \end{cases}$$
(47)

Note that the matrix \mathbf{Q} is *diagonal* and its elements are the inverse of the masses, hence with this method we obtain a diagonal mass matrix. By eliminating the momentum and denoting with $\mathbf{M} = \mathbf{Q}^{-1}$ the diagonal mass matrix, we can write the fundamental equation of elastodynamics in the form

$$\frac{1}{\tau^2} \mathsf{M}\left[\mathbf{U}(n+1) - 2\mathbf{U}(n) + \mathbf{U}(n-1)\right] = -\mathsf{K}\mathbf{U}(n) + \mathbf{F}(n) + \mathbf{B}(n) .$$
(48)

Note that in Eq. (48) all variables are evaluated at the instants of the primal time complex. This algebraic equation, compared with the **Navier differential equation**

$$\rho \,\partial_{tt} \vec{u} = (\lambda + \mu) \nabla (\nabla \cdot \vec{u}) + \mu \,\nabla^2 \vec{u} + \vec{f} \tag{49}$$

has the advantage of including the boundary conditions on forces, i.e. the natural boundary conditions of the variational formulation.

The Navier differential equation has lost the visual immediacy of the physical phenomenon while the algebraic formula Eq. (48) remains adherent to the physical fact, see Fig. (11). For a comparison with FEM see [Cosmi(2005)].

In the case of damping, denoting by *c* the damping coefficient of the dual cell *h*, we must add to the body force \vec{F} a damping force \vec{F}^d which can be written as follows

$$\vec{F}^{d}(n,h) = -c \,\vec{v}(n,h) = -\frac{c}{m(h)} \,\vec{P}(n,h) = -\frac{c}{2m(h)} \left[\vec{P}(\tilde{n}+1,h) + \vec{P}(\tilde{n},h) \right].$$
(50)

Putting $s(h) = [\tau c] / [2m(h)]$ the second set of Eq. (41) becomes

$$\vec{P}(\tilde{n}+1,h) = \vec{P}(\tilde{n},h) + \tau \left[\vec{T}(n,h) + \vec{F}(n,h) - s(h)\left(\vec{P}(\tilde{n}+1,h) - \vec{P}(\tilde{n},h)\right) + \vec{B}(n,h)\right].$$
(51)

Rearranging the terms, we obtain

$$\vec{P}(\tilde{n}+1,h) = \left[\frac{1-s(h)}{1+s(h)}\right]\vec{P}(\tilde{n},h) + \left[\frac{\tau}{1+s(h)}\right]\left(\vec{T}(n,h) + \vec{F}(n,h) + \vec{B}(n,h)\right)$$
(52)

which can be compared with Eq. (36) of damped motion of particle dynamics. For a damping model see [Cosmi(2008)].

All the formulae from Eq. (41) to Eq. (46) can be immediately extended to three dimensional elastodynamics referring them to a tridimensional simplicial complex and to its dual, as shown in Fig. (12).



Figure 12. A simplicial cell in 3D and its dual.

3.3 Normal modes in elastodynamics

Since the left side of Eq. (48) is the acceleration, putting

$$\mathbf{U} = \mathbf{b}\,\sin\omega(t) \tag{53}$$

and ignoring the volume and boundary forces, we obtain

$$-\boldsymbol{\omega}^2 \mathbf{M} \mathbf{b} \sin \boldsymbol{\omega}(t) = -\mathbf{K} \mathbf{b} \sin \boldsymbol{\omega}(t).$$
(54)

Dividing by $\sin \omega(t)$ and multipliving for the inverse mass matrix **Q**, putting $\lambda = \omega^2$, we have

$$\mathbf{Q}\mathbf{K}\mathbf{b} = \lambda \,\mathbf{b}.\tag{55}$$

It follows that the values λ , which allow the eigen-frequencies to be obtained, are the eigenvalues of the matrix QK.

3.4 Compressional waves

A possible application of elastodynamics is the study of compressional waves (Pwaves). These waves are usually obtained by considering the divergence of the displacement vector or applying the Helmholtz decomposition.

In the direct algebraic formulation P-waves, which are characterized by the bulk dilatation Θ , are obtained without resorting to divergence but by means of simple geometric considerations based on the physical meaning of Θ . Note that both variables are obtained from the displacement vector and as such must be associated with primal cells.

Let us show how to evaluate in discrete terms the bulk dilatation Θ_c for a generic primal cell c for a plane problem function of a simplicial complex. We focus our attention on a simplex (triangle) of this complex. The triangle must be conceived as the face of area A_c of a triangular prism of uniform thickness t, Fig. 13.

The bulk dilatation is the ratio of the linear part of the volume variation ΔV_c and the volume V_c . Let us consider the triangle h, i, j which represents the upper face of the prism. Let us indicate the area vectors related to the lateral sides of the prism with the label of the opposite vertex.



Figure 13. Deformation of a primal cell h, i, j.

As shown in Fig. 13, after a plane deformation the prism has changed its volume and the vertices of the triangle have moved to h', i', j'. Then, for each lateral face of the prism we evaluate the volume variation. We calculate the linear part of this increase because we consider only small displacements.



Figure 14. The shaded area multiplied by the thickness t represents the linear portion of the volume variation of the side hi.

Let us consider the side hi of the triangle in Fig. 14. We propose to evaluate the area of the quadrilateral hii'h'h. The volume variation for the side hi is evaluated by calculating the area \mathscr{A} of the quadrilateral times the thickness t of the cell. Assuming small displacements, the linear part of the volume variation is

$$t\mathscr{A} = \frac{g+g'}{2}bt \approx \vec{u}_M \cdot \hat{n}at = \frac{\vec{u}_h + \vec{u}_i}{2} \cdot \vec{A}_k .$$
(56)

Hence the change in volume of the triangular prism is given by

$$\Delta V_{c} = t \,\Delta A_{c} = \frac{\vec{u}_{h} + \vec{u}_{i}}{2} \cdot \vec{A}_{j} + \frac{\vec{u}_{i} + \vec{u}_{j}}{2} \cdot \vec{A}_{h} + \frac{\vec{u}_{j} + \vec{u}_{h}}{2} \cdot \vec{A}_{i}$$

$$= \frac{1}{2} [\vec{u}_{h} \cdot (\vec{A}_{j} + \vec{A}_{i}) + \vec{u}_{i} \cdot (\vec{A}_{j} + \vec{A}_{h}) + \vec{u}_{j} \cdot (\vec{A}_{h} + \vec{A}_{i})] .$$
(57)

Since the sum of the three oriented sides $\sum_k \vec{L}_k$ vanishes and the area vectors \vec{A}_k are obtained by rotating the vectors \vec{L}_k of 90° multiplied by the thickness *t*, it follows that also the sum of the three area vectors $\sum_k \vec{A}_k$ vanishes. Thus from Eq. (57) we obtain

$$\Theta_c = \frac{\Delta V_c}{V_c} = -\frac{1}{2tA_c} \left[\vec{u}_h \cdot \vec{A}_h + \vec{u}_i \cdot \vec{A}_i + \vec{u}_j \cdot \vec{A}_j \right]$$
(58)

which is the expression sought for Θ_c .

With reference to Fig. (12) in three dimensions we have

$$\Delta V_c = \frac{\vec{u}_i + \vec{u}_j + \vec{u}_k}{3} \cdot \vec{A}_h + \frac{\vec{u}_h + \vec{u}_j + \vec{u}_k}{3} \cdot \vec{A}_i + \frac{\vec{u}_h + \vec{u}_i + \vec{u}_k}{3} \cdot \vec{A}_j + \frac{\vec{u}_h + \vec{u}_i + \vec{u}_j}{3} \cdot \vec{A}_k$$

from which

$$\Theta_c = -\frac{1}{3V_c} \left[\vec{u}_h \cdot \vec{A}_h + \vec{u}_i \cdot \vec{A}_i + \vec{u}_j \cdot \vec{A}_j + \vec{u}_k \cdot \vec{A}_k \right].$$
(60)

For the application of the Cell Method to acoustics in fluids see [Tonti (2001c)].

4 Conclusion

Let us summarize the features of the direct algebraic formulation, briefly called *Cell Method*.

- It works on unstuctured grids;
- it is free of singularities because even concentrated loads are added to other forces acting on the dual cell and are not assigned to nodes according to the level rule;
- it works even in presence of different materials.
- it gives rise to a diagonal mass matrix, hence it produces an explicit timestepping scheme;
- it avoids the integration on lines, surfaces and volumes because it makes use directly of global variables;
- it uses two cell complexes in space and in time, one dual of the other. Some variables are evaluated at the primal instants, while other at the dual instants: this choice is not arbitrary but stems from the physical meaning of the variable. This avoids loss of accuracy, instability and the violation of energy conservation;
- physical equations are directly written in algebraic form, without the intermediation of the differential formulation and can be directly implemented;
- the direct algebraic formulation is based on two approximations: one is that the displacement field within each primal cell is considered as affine and higher degree interpolations are possible; the other is that the velocity of the center of mass of the dual cell is approximated to the velocity of the corresponding primal node;
- the core of the direct algebraic formulation are the dual cells;

- the boundary conditions involving forces are included the fundamental equation;
- is valid also for a non linear constitutive equation;
- the direct algebraic formulation remains adherent to the physical content until the end of the treatment: in fact, it uses intuitive physical concepts without passing through purely mathematical expedients such as the weak formulation, the introduction of the residual of a differential equation and its orthogonality to the shape functions;
- the direct algebraic formulation is automatically consistent. In fact, it performs the same steps that lead to the differential formulation, but operating on a finite portion (dual cell) rather than an infinitesimal portion of the continuum.

Acknowledgement: We are in debt to professor Massimo Fragiacomo and to engineer Christian Trampuz for their thorough review of the manuscript.

References

Bochev, P.B.; Hyman, J.M. (2006): Principles of Mimetic Discretizations of Differential Operators. *Compatible spatial discretization*, The IMA Volumes in Mathematics and its Applications. Springer, Vol.142.

Cosmi, F. (2005): Elastodynamics with the Cell Method. *CMES: Computer Modeling in Engineering & Sciences*. Vol. 8, No. 3, pp. 191-200.

Cosmi, F. (2008): Dynamical Analysis of Mechanical Components: A Discrete Model for Damping. *CMES Computer Modeling in Engineering & Sciences*. Vol. 27, No. 3, pp. 187-195.

Ferziger, J.H.; Peric, M. (1997): Computational Methods for Fluid Dynamics. Springer.

Harlow, F.H.; Welch, J.E. (1965): Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. *Phys. Fluids*. Vol. 8, p. 2182.

Isaacson, E.; Keller, H.B. (1966): Analysis of Numerical Methods. Wiley & Sons.

Jiang, B.N.; Wu, J.; Povinelli, L.A. (1996): The Origin of Spurious Solutions in Computational Electromagnetics. *Journal of Computational Physics*. 125, pp. 104-123.

Taflove, A. (2005): Computational Electrodynamics, The Finite-Difference Time-Domain Method. Artech House. **Tonti, E.** (2001a): A Direct Discrete Formulation of Field Laws: The Cell Method. *CMES Computer Modeling in Engineering & Sciences*. Vol. 2, No. 2, pp. 237-258.

Tonti, E. (2001b): Finite Formulation of the Electromagnetic Field. *PIER Progress in Electromagnetic Research 32*. EMW Publishing, pp. 1-42.

Tonti, E. (2001c): A Finite Formulation for the Wave Equation. *Journal of Computational Acoustics*. Vol. 9, No. 4, pp. 1355-1382.

Tonti, E.; Zarantonello, F. (2009): Algebraic Formulation of Elastostatics: the Cell Method. *Computational Modeling in Engineering and Science (CMES)*. Vol. 39, No. 3, pp. 201-136.

Van Dantzig, D. (1954): On the Geometrical Representations of Elementary Physical Objects and the Relations between Geometry and Physics. *Nieuw Archief vor Wiskunde*. 3, 2, pp. 73-89.

Vesely, F.J. (1994): Computational Physics, An Introduction. Plenum Press.

Weyl, H. (2009): *Philosophy of Mathematics and Natural Science*. Princeton University Press.

Williams, J.H. Jr. (1996): Fundamentals of Applied Dynamics. Wiley & Sons.

Yee, K.S. (1966): Numerical Solution of Initial Boundary Value Problems Involving MaxwellÕs Equations in Isotropic Media. *IEEE Trans. A.P.*. Vol. 14, No. 3.