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From multi-body to many-body dynamics

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Abstract: This article provides a brief historical review of multi-body dynamics analysis, initiated by the Newtonian axioms through constrained (*removed* degrees of freedom) Lagrangian dynamics or restrained (*resisted* degrees of freedom) Newton–Euler formulation. It provides a generic formulation method, based on system dynamics in a reduced configuration space, which encompasses both the aforementioned methods and is applicable to any cluster of material points. A detailed example is provided to show the integration of other physical phenomena such as flexibility and acoustic wave propagation into multi-body dynamics analysis.

It is shown that in the scale of minutiae, when the action potentials deviate from Newtonian laws, the forces are often described by empirical or stochastic functions of separation and the medium of interactions. These make for complex analyses and distinguish a host of many body problems from Newtonian laws of motion. A simple example is provided to demonstrate this. It is suggested that unification of many-body analysis with that of multi-body dynamics is incumbent on the fundamental understanding of interaction potentials at close separations.

Keywords: multi-body dynamics, many-body dynamics, boundary elements, component mode synthesis, elasto-acoustic coupling, molecular dynamics, gravitation, adhesion, meniscus action, hydration

1 INTRODUCTION

Humans have always been curious and at the same time intimidated by the plethora of events taking place in or about their environment, all of which by definition are dynamic (changing) in nature. The quest to understand these events can be regarded as a primal goal of survival. Initially, the understanding was instinctive, and thus often erroneous. Later, the evolved understanding was observation-based (kinematics). Geometers such as Euclid, Homer, and Pythagoras led the way in this growing quest in ancient times. The status afforded to geometry was fundamental as clearly noted by Plato: *let no man enter who knows no geometry*. By the middle ages geometry was at the heart of understanding of the known Universe, one which was centred on Earth, an Aristotelian view that was later firmly established in the

Al-Majest by Cladius Ptolemy. Tusi's elaborate correction for the apparent retrograding orbital motion of Jupiter when observed from Earth had put any doubt about the Earth-centred universe beyond question. Yet his own doubts in *Al-tadhika fi 'ilm al-hay'a* (*Memoir on astronomy*) was probably instrumental in Copernican objections, although it is suggested that Copernicus was not aware of Tusi's work. The key point is that observation of motion within a geometrical framework led to the heliocentric system, declared by Galileo [1]. The motions of planets around the sun were explained by Keplerian laws [2]. Then, kinematics attained the status that had hitherto been afforded to geometry. The underlying cause (force) was, however, not yet understood.

Dynamics is the natural extension of kinematics, as the observation-based model (the effect) is supplemented by the addition of kinetics (the cause, i.e. force laws). Like kinematics, the definition of force also has a long history. The first attempt for the definition of force was put forward by Empedocles as *love* brings things together, while *hate* pushes them apart (a rather electromagnetic interpretation). His contemporary, Anaxagoras, described the beginnings of the

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world and its evolution in *Nous* in terms of *the whirling motion, the surrounding fiery aether tore stones away from the earth and kindled them into stars* (Perhaps the centrifugal effect?). The definitions put forward for force did not improve significantly, even two millennia later, as Leonardo Da Vinci noted: (force is) *an immaterial power, an invisible potency which is created and infused by animated bodies in inanimate ones through acquired violence*. Although the idea of gravity is implicit in Galileo's law of inertia and Kepler's laws of motion, no fundamental understanding existed before Newton. The law of Universal Gravitation and the concept of a central force came as a 'bolt out of the blue' and caused much controversy (see for example reference [3]). Nevertheless, the discipline of dynamics, as is understood today, was born then [4].

The law of Universal Gravitation naturally leads to Newton's second and third axioms, with the first axiom being a special case of the second and a restatement of Galileo's law of inertia. It is clear that the axioms favour the principle of conservation of momentum, while Leibniz showed that this can only be conditionally upheld. Leibniz [5] favoured the law of conservation of *vis viva* (the living force), denoted at the time as mv^2 , which in modern times has become the principle of conservation of energy. In time, kinetic energy was properly defined and formed the basis of Lagrange's equation, with the body/restoring forces defined by Euler in terms of potential energy as [6] $F_q = -\partial U / \partial q$ for the generalized coordinates q . Thus, Lagrange's equation became [7]

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{q}} + \frac{\partial U}{\partial q} = 0$$

where $q = [x, y, z, \psi, \theta, \varphi]^T$ is the Euler's 3-1-3 frame of reference; the superscript T denotes transposed representation. Now substituting for the kinetic energy, the second Newtonian axiom is arrived at, underpinning it by a mathematical proof (for example, see reference [3]).

2 MULTI-BODY DYNAMICS

Lagrange's equation mentioned above yields six equations of motion for an unconstrained *material point* (a body or a particle) in the Euler's frame of reference. System of a unitary entity cannot exist and thus a number of material points render a constrained system due to their interactions. This means that a reduced configuration space results (certain coordinates are removed), say l such coordinates. Therefore, the set of equations for n material points comprise $r = 3n - l$ differential equations of motion and l algebraic scalar functions, representing the constrained coordinates. If motions of material points are described in the global coordinates $\xi^j, j = 1, 6$ and q^k are local coordinates,

fixed to each body in a multi-body system or a cluster of objects, then

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{\xi}^j} \right) + \frac{\partial U}{\partial \xi^j} = F_{a_j} \quad (1)$$

$$q_{|k=1,3n}^k = f(\xi_{|j=1,6}^j, t)$$

and

$$\xi_{|j=i+1,3n}^j = f(q_{|k=1,3n}^k, t) = 0 \quad (2)$$

Equations (2) provide holonomic constraints as functions of time in a generalized form. When the constraints are functions other than those predefined by coordinate relations (as in equation (2)), non-holonomic constraint functions would result.

Noting that

$$\{q^k, k = 1, 3\}^T = [T]_k \{\xi^j, j = 1, 3\}^T$$

where the Euler transformation matrix between coordinates q^k and ξ^j is

$$[T] = \begin{bmatrix} C\psi C\varphi - S\psi C\theta S\varphi & & \\ S\psi C\psi + C\psi C\theta S\varphi & & \\ S\theta S\varphi & & \\ -C\psi S\varphi - S\psi C\theta C\varphi & S\psi S\theta & \\ -S\psi S\varphi + C\psi C\theta C\varphi & -C\psi S\theta & \\ S\theta C\varphi & C\theta & \end{bmatrix} \quad (3)$$

Note $S \equiv \sin, C \equiv \cos$. For detailed formulation of multi-body systems, refer to Rahnejat [8]. In the Euler's frame of reference, rotations of a local frame q^k relative to the global ξ^j , in terms of Euler angle derivatives, are given as $\{\xi^j, j = 4, 6\}^T = \{\dot{\psi}, \dot{\theta}, \dot{\varphi}\}^T$. Rotational kinetic energy is obtained in terms of derivatives of the local coordinates $\dot{q}^k, k = 4, 6$. These are transformed to the global frame of reference as $\{\dot{q}^k, k = 4, 6\}^T = [T^*] \{\dot{\psi}, \dot{\theta}, \dot{\varphi}\}^T$ where [8]

$$[T^*] = \begin{bmatrix} S\theta S\varphi & 0 & C\varphi \\ S\theta & 0 & -S\varphi \\ C\theta & 1 & 0 \end{bmatrix} \quad (4)$$

In mechanical systems the joints may be considered as a combination of primitive constraint functions [8–10]. These constraint functions, defined similar to equation (2), are time invariant holonomic functions (those of coordinates of joined components within a system) or non-holonomic functions of coordinate derivatives, such as specified motions or gearing pairs. Thus, in general Lagrange's equation becomes

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\xi}^j} \right) - \frac{\partial L}{\partial \xi^j} + \sum_{p=1}^m \lambda_p \frac{\partial C_p}{\partial \xi^j} = F_{a_j} \quad (5)$$

where the Lagrangian is $L = T - U$, C_p is the primitive scalar constraint function of coordinates of joined

components l and l' . The ultimate term on the left-hand side of equation (5) provides the reaction forces resulting from the constraint functions C_p which are in terms of coordinates such as those in equation (2). Lagrange multipliers λ_p are used to represent these reactions in correct units. Thus, changes $\delta\lambda_p$, coordinates $\delta\xi^j$, and derivatives $\delta\dot{\xi}^j$ constitute the unknowns to be determined. The term on the right-hand side of equation (5) provides the resistive force, representative of the reduced configuration space, described by

$$C_p = f(q_i^k, q_{i'}^{k'}) = 0 \quad \text{for any combination of } k, k'$$

For at least two centuries, Lagrange's equation for constrained systems was thought to adequately describe dynamics of all problems. This is true of almost 90 per cent of all dynamics even today. However, as Navier–Stoke's equations based on Euler's equation were applied to fluid flow in ever diminishing channels (e.g. lubrication problems), body and inertial forces were deemed as insignificant compared with the viscous shearing force. Reynolds ignored the effect of body and inertial forces to arrive at his hydrodynamic equation. Referring back to equation (5) (the essence of Newton's second axiom), one can note that the applied force is now equilibrated by the interaction of a cluster of particles of insignificant inertial and body forces that constitute the system. These interactions do not often follow the inverse distance squared force law of universal gravitation. This point was not dwelt upon in hydrodynamics, but in electromagnetics [11] around the turn of the 20th century. In fact, in the scale of minutiae, the interactions seem to follow force laws as powers of separation of material points exceeding 3 as shown by Israelachvili [12] and Teodorescu and Rahnejat [13]. Therefore, the interaction potential varies as a function of the ratio of size of the material point to the characteristic size of the system [3]. The lack of a fundamental understanding has resulted in the description of a plethora of force laws according to physical chemistry and prevailing thermodynamics.

Many-body systems as opposed to multi-body systems have emerged as a result of mechanical engineering science studies of smaller systems or clusters of material points, initially particles of insignificant inertia, such as colloids [14, 15]. In recent times, component miniaturization as the result of system downsizing, as well as the growing involvement of mechanical engineers in physio-chemical and biological systems have added impetus to the dynamics of systems, where the force laws deviate from those of Newtonian perspective. These applications include micro-electromechanical systems (MEMS) [16] and biomimetics such as microfibres [17, 18].

Therefore, the understanding of dynamics as a discipline has become a problem of scale. The initial

curiosity regarding the motion of heavenly bodies can be regarded as that of macro-scale as is the dynamics of almost 95 per cent of mechanical systems. In the latter case, recent years have witnessed the growing inclusion of component flexibility [19, 20] and the study of acoustic emission, particularly with regard to noise and vibration issues [21], a form of analysis that one may refer to as elasto-multi-body dynamics. This trend, which will continue apace into the future, includes rigid body inertial dynamics, small amplitude structural vibration, micro-scale tribology of load bearing conjunctions, and even nano-scale wavelength acoustic propagation (an example is provided below). The approach is referred to as *multi-physics* (indicating various physical phenomena) *multi-scale* approach. The other trend would be the interactions of many minute material points: many-body dynamics. This includes several distinct areas of study: molecular dynamics [14], many-body discrete particulate interactions and those of fluid molecules, and distributed features such as surface roughness on larger bodies [16–18]. An example of such a many-body system is also provided below.

3 ELASTO-MULTI-BODY DYNAMICS

Clearly, components of any multi-body system are compliant. When subjected to applied forces, system components deform even by an infinitesimal amount. As the applied forces alter in time, one concern regarding component compliance is structural integrity. Progressively, another significant concern is noise propagation from vibrating structures, termed as NVH (an acronym for noise, vibration, and harshness). Palliative refinements for NVH issues require an understanding of system deformation behaviour under transient conditions. Hitherto, for each body in a multi-body system the coordinates $\{\xi^j\}_{j=1 \rightarrow 6} = \{x, y, z, \psi, \theta, \phi\}^T$ are used, which relate to the local rigid coordinates q^k . However, for flexible parts, coordinates ξ are also functions of deformation behaviour of parts as functions of local elastic coordinates, thus $\{\xi^j\} = f(q^k | k \in 7, 6 + m')$, where the first six local coordinates q^k refer to the usual Euler frame of reference, describing the rigid body motions of a part. The m' remaining coordinates are those denoting the deformation behaviour of a body at any point of interest. Therefore, the global position vector of a point p is a function of coordinates and linear deformation of a number of nodal degrees of freedom by Bernoulli's principle of linear superposition, u_p^k . These can be represented as a smaller number of shape vectors $u_p^k = \sum_{k=1}^{m'} \phi_k q^k$. Using finite elements, this relationship can be written in a matrix form as

$$u^k = \Phi q^k \quad (6)$$

where the modes ϕ_k are included in the columns of the modal matrix, Φ [22]. This matrix is the transformation from the small set of modal coordinates, q , to the larger set of physical coordinates, u .

Depending on a component's compliance and magnitude of applied forces, a number of modal responses are excited. In many cases, there can be a large number of such modes, making the analysis computationally prohibitive. Often, one is only concerned with the inclusion of certain modal behaviour only, which contributes to certain NVH phenomenon (an example is outlined in section 4). This means that other unrelated deformation behaviour can be discarded. Hence, a mode reduction technique is required to determine the modal matrix Φ of a manageable size, such as the Craig–Bampton component mode synthesis technique [22]. The procedure to obtain such a matrix and integrate it into an elasto-multi-body dynamic analysis is described in reference [21].

Therefore, finite elements and a component mode synthesis technique can be used to represent the elastic behaviour of components with multi-body dynamics. *Mode shape ortho-normalization* determines the orthogonal modal matrix Φ' and permits the address of the six rigid body modes of a component. The association of the rest of the modes to natural frequencies helps in their physical classification, and thus allows simulation of non-linear systems with unknown spectral content. Once modal behaviour of elastic components is included in a multi-body dynamic model, elastic wave propagation of some modes may coincide with the acoustic modes of the same structure. This can lead to sound propagation, a phenomenon referred to as *elasto-acoustic coupling*.

A phenomenon referred to as driveline clonk is an NVH concern in automobiles, where a sudden impulsive torque results because of throttle tip-in or back-out actions or sudden release of the clutch. This results in structure-borne waves, inducing the modal response of hollow driveshaft tubes, with a large modal density. Some of these modes are efficient noise radiators (effective elasto-acoustic coupling) [21].

4 ELASTO-ACOUSTICS

Since the response of the system is usually determined for a period of interest, the surface velocities of the vibrating structures are computed for every time-step. These eventually become the initial conditions for an acoustic analysis, using the indirect boundary element method (BEM) to obtain the sound pressure fields around the structures of interest. The BEM presents certain advantages compared with other numerical methods for acoustic problems, such as finite-element method (FEM) and statistical energy analysis. The latter is a time-consuming method for high-frequency problems (such as clonk described

here), where resonant frequencies are densely packed. FEM is usually, but not necessarily, limited to low frequencies, because accurate modelling of a large structure for high-frequency studies requires a correspondingly large number of elements. Additionally, FEM requires the computation of the entire domain (not just the boundary: for example the surface of driveshaft tubes). Therefore, there are computational advantages in using BEM.

In the case of driveshafts, the boundary discretization can be based on the desired maximum frequency to be captured. Therefore, the hollow thin-walled elastic shafts can be discretized with sufficiently refined meshes to capture the structural modes of interest, as well as the wavelength of the fluid in the acoustic medium.

The BEM is used to obtain the surface velocities of vibrating structures and the acoustic pressure at a given point away from it. This point is considered to be the location of noise monitoring (for example where a microphone may be placed to acquire sound level).

The propagation of small amplitude waves can be represented by the von Helmholtz equation in the frequency domain, as [23]

$$(\nabla^2 + k^2)p = 0 \quad (7)$$

where $\nabla^2 = (\partial^2/\partial^2x) + (\partial^2/\partial^2y) + (\partial^2/\partial^2z)$ is termed the Laplacian and $k = (\omega/c)$.

The solution to equation (7) can be in terms of the free-space Green's function (appropriate for the space around driveshaft tubes in the clonk problem described here)

$$G = \frac{e^{-jkr}}{4\pi r} \quad (8)$$

This is the fundamental solution to the von Helmholtz equation in the form

$$\nabla^2 G + k^2 G = -\delta(x, y) \quad (9)$$

where Kronecker function is

$$\delta(x, y) = \begin{cases} 0 & \text{if } x \neq y \\ 1 & \text{if } x = y \end{cases}$$

In order to evaluate the sound pressure field at a distance r_i from a surface Γ where r_Γ is a typical boundary point on the surface, then as shown originally by Waterman [24]

$$p(r_i) = \int_{\Gamma} \int \left[p(r_\Gamma) \frac{\partial G(r_i, r_\Gamma)}{\partial n_\Gamma} - G(r_i, r_\Gamma) \frac{\partial p(r_\Gamma)}{\partial n_\Gamma} \right] dS_\Gamma \quad (10)$$

where n_Γ represents the normal to the boundary surface Γ . The sound pressure at the distant point r_i is

found numerically by integration over all the scattering area Γ [25]. The distant point represents a virtual position, where in the physical world a free field microphone may be placed to measure the sound level.

5 DRIVELINE CLONK AS AN ELASTO-ACOUSTIC MULTI-BODY DYNAMICS PROBLEM

Figure 1 shows the multi-body driveline system, comprising all the components of the powertrain system, from the transmission input shaft up to and including the rear axle half-shafts. Parasolid CAD files are used to exactly represent the physical properties of system components.

The driveline model is described in detail in Gnanakumarr *et al.* [21]. It comprises a number of rigid body degrees of freedom, related to motions of transmission input and output shafts, the driveshaft tubes, the pinion and ring gear of the differential, the rear axle half-shafts and road wheels, as well as flexible body modal behaviour of driveshaft tubes, typical examples of which are shown in Fig. 1. These modal behaviours of driveshaft tubes are responsible for vibration of their surfaces, which can coincide with their acoustic modes. To capture these efficient noise radiating modes, four-noded shell elements are used for the finite-element models of the elastic driveshaft tubes. The number of elements and their size across the shaft length and along its perimeter are made sufficiently large so as to capture the higher modal responses. A sufficient number of structural modes have been kept during the creation of super-elements in order to obtain the specified frequency area of interest to study the clonk problem, which usually occurs in the frequency range 300–5000 Hz. Since the same mesh is also used in the boundary element models of the driveshaft tubes, particular attention is paid so that the number of elements per wavelength is adequate

for the noise radiation analysis, exterior to the tube boundaries (as described in section 4). The location of virtual microphones (data recovery nodes that measure the noise levels) with respect to the vibrating structure is calculated in such a way that the minimum frequency of interest can be captured.

Typical mode shapes for this three-piece driveline system are shown in the figure. The modal behaviour results when an impulsive torque of short duration is applied to the drivetrain system.

Figure 2 shows a few modal responses of a two-piece driveline system. The modal behaviour is exaggerated in the figure for ease of observation. The efficient noise radiators are higher-frequency responses, which are combinations of torsional and bending modes (flexural modes). These are usually referred to as *breathing modes*: (a) for the front driveshaft tube and (b) for the rear driveshaft tube in Fig. 2.

The structural breathing modes couple effectively with the acoustic modes of the tubes. To demonstrate this, the pressure time histories obtained through boundary element analysis under transient conditions are subjected to an auto-regressive moving average (ARMA) spectral analysis. If a model y_k can be successfully fitted to a data stream x_k it can be transformed into the frequency domain instead of the data upon which it is based, producing a continuous and smooth spectrum. This is the basic premise of the spectra produced using ARMA. For a data series x_k of length N , the model is defined as the reverse prediction for the first p values and forward prediction for the remaining $N - p$ values as the output of a pole-zero filter excited by white noise, as [26]

$$u_k = 0 \quad k = 1 \dots N$$

$$u_k = x_k - \sum_{j=1}^p a_j x_{k+j} + \sum_{i=1}^q b_i u_{k+i}$$

Fig. 1 The multi-body model of the driveline system (1, 2, 3: refer to driveshaft tubes, uj: refers to universal joint)

Fig. 2 Magnified graphical scale of dominant breathing mode shapes: (a) 3368 Hz and (b) 3923 Hz

$$k = \min[N - p, \max(100, p + q)] \dots 1$$

$$u_k = x_k - \sum_{j=1}^p a_j x_{k-j} + \sum_{i=1}^q b_i u_{k-i} \quad k = p + 1 \dots N$$

$$y_k = x_k + u_k \quad k = 1 \dots N$$

(11)

where a is the auto-regressive parameter array of order p and b is the moving average parameter array of order q . Once the parameters of the ARMA model are identified, their spectral density function can be obtained as [26]

$$\rho_{\text{ARMA}}(f) = V \Delta t \left| \frac{1 + \sum_{k=1}^q b_k e^{-j2\pi f k \Delta t}}{1 + \sum_{k=1}^p a_k e^{-j2\pi f k \Delta t}} \right|^2 \quad (12)$$

where V is the driving white noise variance, f is the frequency, k is the harmonic number, and Δt is the sampling interval. This provides the active spectral content contained within a measured/acquired vibration signal.

Figure 3 shows the driveshaft tubes' active acoustic band of frequencies, acquired by a free field microphone and subjected to ARMA. These coincide with the breathing elastic mode shapes in Fig. 2.

The example of clonk phenomenon serves the purpose of illustrating the evolution of the field of dynamics from the Newtonian second axiom to constrained Lagrangian dynamics and through to its integration with elasticity and acoustics into a multi-physics multi-scale analysis. This trend is set to continue into the future with increased computing power and more efficient methods of solution, reducing the computation times.

As described in the Introduction and in section 2, Newton's second axiom is also applicable to a cluster of objects other than multi-body inertial systems. However, the forces acting at short range between material points of insignificant inertia are due to action potentials that deviate from that of gravitation. This is not only true of very small particles and colloids, but is also progressively the case for some very small micro-mechanical systems.

Fig. 3 ARMA spectra of the acoustic pressure time histories of (a) the front and (b) the rear driveshaft tubes corresponding to Fig. 2 (frequency is in Hz and amplitude is normalized)

6 MANY-BODY SYSTEMS

The multi-body dynamics approach expounded above requires an accurate description of uninterrupted constraint functions to render a reduced configuration space. As shown in section 2, these constraints are often functions of coordinates as state variables or their derivatives. The constraints, therefore, eliminate these coordinates from the analysis altogether. However, in many multi-body dynamics' problems the state variables or their derivatives are only restrained. In other words, the reduced configuration space is a function of some restraining conditions, rather than rigid constraints. A generic example of this is the elasto-multi-body systems described in section 3. Elasto-acoustic coupling, highlighted in section 4, can also be interpreted as another form of reduced configuration space, being conditional on the coincidence of elastic and acoustic waves. The difference, in this type of problem, is that the restraining function or constraining conditions are conditional and cannot be upheld at all times. Such problems cannot be solved by Lagrangian dynamics alone, this being the reason for inclusion of other methods such as boundary element analysis. Unfortunately, there are many such problems, particularly at the scale of minutiae, where a host of interaction potentials as functions of separation act between many-body systems. Since separation or gap between material points in an ensemble has traditionally been used to describe the various action potentials, the mechanism of *contact* is often used to trigger simple interactions for a large number of material points. Newton–Euler method lends itself well to representation of such systems, thus as presented in references [14], [27], and [28]

$$\mathbf{M}_q \frac{d\dot{q}}{dt} = \mathbf{F}_{q,\dot{q}} + \mathbf{f}_q \quad (13)$$

where $\mathbf{M}_q$ is the inertial matrix, $\mathbf{F}_{q,\dot{q}}$ is the vector of generalized forces such as coriolis, centripetal, and generalized smooth contact forces (e.g. viscous and Stribeck effects), and $\mathbf{f}_q$ is the sum of friction components of generalized contact forces.

Therefore, for this approach one needs a contact constraint function [29] or a gap function [27] of coordinates q . Thus, a switchable simple potential $\varphi(q)$ can be specified, which assumes almost a Boolean form with a positive value representing the separation of material points, a negative value for no contact, and a zero value for onset of contact. This rather simple approach has the advantage of including a large ensemble of material points, such as grains of sand, but has the drawback of being confined to Coulomb friction or other simplified force laws and discounts the stored potential energy due to penetration of material points.

Many-body systems are not only characterized by a high number of material points, usually of insignificant inertia, but also of multiple interactions, often with many force laws. There are various more detailed methods employed to tackle the dynamics of such systems, including Brownian dynamics [15] or molecular dynamics [14]. In Brownian dynamics trajectories of particles are defined by a set of probability distributions, based on a Markov process. In contrast, molecular dynamics represents a cluster of material points with a system of equations of motion, based on the Newtonian second axiom. Therefore, Verlet [14] declared molecular dynamics as an exact solution, implying that the use of probability functions in Brownian dynamics renders it as rather empirical. However, as the number of material points increases, exact solutions become computationally arduous and hybrid Brownian-molecular dynamics approaches have become more common [15], the threshold moving from one form of analysis to another is debated in reference [30]. In Verlet's approach, for a particular particle i within a system of particles, using Newton's second axiom

$$m_i \mathbf{a}^i = \sum_{j \neq i} \mathbf{F}^{ij} \quad \text{where } \mathbf{a}^i = \frac{d^2 \mathbf{r}^i}{dt^2}, \quad \mathbf{F}^{ij} = f(\mathbf{r}_{ij}) \quad (14)$$

where $\mathbf{F}^{ij}$ is the force between material points i and j at a distance $\mathbf{r}_{ij}$. Because the material points are considered to be of very small size, the force law as a function of distance becomes $|\mathbf{F}^{ij}| \propto C'/|\mathbf{r}_{ij}|^n$, $n > 3$ [12, 13] and depends on the nature of interactions (e.g. van der Waals, electrostatic, etc.) and C' is usually a constant dependent on the nature of the material point and the environment/medium in which it resides, unlike the force of gravity which is universal, with $C' = G_u m$, m being the mass of a heavy body (source).

In molecular dynamics interactions between material points at separations of r_{ij} are considered in terms of a potential, usually of the Leonard–Jones type [12, 14], where van der Waals attraction as inverse sixth power of the interparticle distance and electrostatic repulsion at the closer distance (a 12th inverse power of their separation)

$$\varphi = C' \left[\left(\frac{\varepsilon}{r} \right)^{12} - \left(\frac{\varepsilon}{r} \right)^6 \right] \quad (15)$$

Now for a cluster of n material points, integration of equation (13) is needed. Verlet's solution made use of a difference equation, requiring $n(n-1)/2$ computations for each integration time step. When the separation between the material points exceeds a certain distance, usually referred to as a *cut-off separation*, the corresponding interactions are ignored. Of course this approach has many applications and can be applied to any cluster of material points of

different physical characteristics, with other interaction potentials. In fact, the definition of many-body dynamics may not be confined to fluid molecules or colloids, but also to grains of sand and other small particles.

Many-body systems have been interpreted as discrete individual material points. However, many engineering problems in micro and nano-scales can also be regarded as many-body systems, where definition of a material point may be extended to features residing on larger bodies such as roughness on engineering surfaces. Their interactions are also described by various force laws, mainly of empirical or of a stochastic nature. These include their adhesion, which becomes progressively more significant with their decreasing size [31–34]. Also of significance is the interactions caused between these features and any other material points that ingress between them, usually molecules of a fluid, often moisture [13, 34]. The interactions at the scale of minutiae often determine the outcome of multi-body dynamics at the larger scale, such as in micro-gears and motion of insects and geckos [13, 16]. In such small scale the forces can include van der Waals and electrostatics (resulting from Leonard–Jones potential), asperity adhesion, meniscus action, hydration, or solvation [12, 35–38]. The same approach in references [13], [16], and [34] can also be used in detailed study of interactions of discrete individual material points. Here grains of sand can again be used as an example, though the level of detail necessitates a reduction in the size of the system (only few grains of sand).

More detail can be included in the interactions of material points if their number is reduced, producing a computationally manageable problem. This depends on the available computer power. Here, a simple example is used, where interactions between seven grains of sand in free fall are investigated (see Fig. 4). The simulation is carried out in normal atmosphere, implying the presence of moisture. The example is a one-dimensional analysis, where h_i is the height of the i th grain of sand and $\bar{h}_i$ the cumulative distance between all the grains below it. This excludes the size of the grain size itself and it is defined as $\bar{h}_i = \sum_i \delta_{i-1}$.

Fig. 4 Schematic representation of falling and rebounding spherical sand grains

In practice, the interactions will be in three dimensions and that of an ensemble of grains, also subject to some form of gust. Therefore, a much more complex analysis would normally be required. The grains of sand are assumed to be rough spheres, meaning that their direct interactions can result in adhesion of their asperity pairs due to contact/impact loads [31–34]. The presence of moisture also means that direct interactions between asperity pairs for a sufficient period of time can lead to the formation of nano-menisci. This is a function of condensation activation time, which depends on the prevailing atmospheric and condensation saturation pressures [39]. The activation time for a mono-layer of water condensate is taken to be 25 μ s in this example. When the gap between grains' opposing asperities reduces further, a monotonic repulsive hydration potential can also operate against their adhesion [13, 34].

These complex interactions cannot be represented by the simple Leonard–Jones potential alone nor by the simple switchable contact models employed in references [27] to [29]. The interaction between a pair of spherical sand grains is considered to be that of a sphere of equivalent radius R against a semi-infinite surface of equivalent elastic modulus E^* . In the case of impact with the assumed rigid plane in Fig. 4, this equivalent radius is that of a spherical sand grain itself.

Fig. 5 Contact of a pair of rough spherical sand grains

Figure 5 shows the instantaneous gap H and any deformation caused Δ by the impact of a rigid sphere against the elastic half-space. The rough surfaces of the grains are assumed to follow a Gaussian distribution of hemispherical asperities with an equivalent asperity pair radius of R_e as shown in the figure. These asperities are very small with force interactions due to various phenomena.

Teodorescu and Rahnejat [34] proposed a model that predicts the contact load and distributed pressure arising from a number of participating phenomena. This model is used here to predict the contact between grains of sand. Briefly, the interactions considered are:

1. Adhesion [31–34]

$$w_a = \frac{4E^*A^3}{3R_e} - \sqrt{8\pi A^3 \Delta \gamma E^*} \quad (16)$$

2. Meniscus action [12, 13, 34, 38]

$$w_m = -2\pi R_e \gamma (\cos \theta_1 + \cos \theta_2) \quad (17)$$

3. Hydration [12, 13, 17, 18]

$$w_h = \frac{2A_m \gamma e^{-(h-z)/\lambda_0}}{\lambda_0} \quad (18)$$

Now the generated contact pressure can be obtained in any of the conjunctions when a distribution of asperity heights is assumed to be $\varphi(z) = 1/\sqrt{2\pi}\sigma e^{-z^2/2\sigma^2}$, $\delta = f(H + \Delta, z)$, thus

$$p = \int_{-L}^{\delta_i} (w_a + w_m + w_h) dz \quad (19)$$

Now the contact force between any pair of sand grains can be obtained by determining the number of asperities interacting with any of the forces described

above. This procedure is described in references [13] and [34]. Thus $F = \int_A p dA$. Figure 6 shows the typical variation of contact force between a pair of sand grains as a function of δ/σ . It can be seen that the force required to separate the grains in their rebound is lower than that in impact, indicating a loss of energy due to the contributing mechanisms in their adhesion.

When the whole cluster of sand grains are considered, their vertical displacements during repetitive impacts and rebounds are shown in Fig. 7. This shows a gradual loss of their free fall kinetic energies due to combined deformation energy and losses in asperity pairs' adhesion and work done against the formed nano-menisci.

Figure 8 shows the total force acting on each grain of sand during the simulation. For clarity forces between pairs of sand grains are plotted separately, but the order of the grains is the same as those in Fig. 7.

The lower sand grains transfer their net stored rebound energy to those residing directly above them.

Fig. 6 Impact and rebound force variation between a pair of sand grains

Fig. 7 Many-body dynamics of a cluster of sand grains in free fall: (a) the first millisecond of simulation and (b) detail of the first set of impacts

Fig. 8 Contact forces of a cluster of sand grains in free fall (numbers 0–6 denote sand grains in ascending height): (a) the first millisecond of simulation and (b) detail of the first set of impacts

As a result, they settle more quickly (similar to the conventional Newton trolley). The net energy of the ensemble eventually reduces as a combination of their stored energies and those dissipated to overcome their work of adhesion. This lost energy would be in terms of heat changing the thermodynamic balance, thus affecting the surface energy effects. This indicates that the interactions of such a small many-body system are even more complicated than that presented here. This complexity and the plethora of action potentials at close range (as partially indicated in the tackled example) are perceived to run contrary to the underlying simplicity of Nature itself.

Equation (15) suggests that interaction potential depends on the size of the material points and their separation and as already noted, there is a limit to this for any particular power law of separation to hold true.

In Gohar and Rahnejat [38], chapter 14, Dowson suggests that an equilibrium of various interaction potentials result in a given separation. Thus, for idealized smooth surfaces, for example, their separation would be at atomic scale. However, rough surfaces would interact at their asperity levels, a form of many-body interactions, which also includes those of the solid surfaces' asperities and molecules of any intervening fluid. This would usually be the case in normal atmosphere, where molecules of water condense on the surfaces.

The distinction made between many-body dynamics of very small material points and multi-body dynamics of larger ones arises from the seemingly irreconcilable nature of the interaction potentials as a problem of scale. At close range, the potential is of an electromagnetic nature, while at long range it

is gravitational. This explains the formidable task of unifying gravitational and electromagnetic potentials. However, Rahnejat [3] suggests that a generic interaction potential may be assumed to unify these. This generic potential proposes that interactions between any pair of material points are summation of the form $w = C' \sum_{i=1}^n \varepsilon^{n-1}/r^n$ instead of many rather empirical potentials such as those in equations (16) to (18). Thus, for a material point subject to a host of interaction potentials of varying power indices with its neighbours within a system of characteristic size $\ell = r - \varepsilon$, its net acceleration becomes

$$a = -\frac{\partial w}{\partial r} = -\frac{C'}{\varepsilon^2} \left\{ \left(\frac{\varepsilon}{r} \right)^2 + \sum_2^\infty n \left[\left(\frac{\varepsilon}{r} \right)^{n+1} - \left(\frac{n-1}{n} \right)^{n+1} \right] \right\} \quad (20)$$

where $n = 1$ corresponds to the gravitational potential, yielding

$$a = -\frac{C'}{r^2}$$

independent of the size of material points. However, with $n > 1$, a summation of additional attractive potential (given by the first term in the summation) and repulsion (the second term) results. This means with smaller separations the higher inverse distance law dominates and repulsion inhibits attraction by lower power indices. This means that material points interact with a potential of continuous form and the acceleration of one depends on the summation of its interactions with all other surrounding matter in a system of size $\ell = r - \varepsilon$. This approach unifies dynamics problems of all scale from many to multi-body dynamics, making the latter a subset of the former and all within a Newtonian perspective. For large scale, the constant C' is the product $G_u m$, which differs from those defined for the scale of minutiae. This problem needs to be addressed. In the positivist perspective of the Cartesian School, such as that of D'Alembert the differences underlying C' , being mass, permittivity, charge, etc., are all regarded as imponderables. There should also be a definition of what is regarded as the size of a material point ε . Descartes would have suggested the ratio ε/ℓ to be his declared *geometric extension*. It would be an irony if the convergence of many and multi-body dynamics in the future vindicate his proposition. The proposition has a strong appeal as it is also in accord with Mach principle as expounded by Einstein that acceleration of a matter is as the result of all other matter residing within a *system* [3, 40–42]. In Mach's perspective, the underlying interaction potential would be a closed-field, one based on matter–space relationship, rather than the open-loop weak gravitational field of general relativity or atomistic pair-wise interactions such

as Newton's law of universal gravitation. A field of this form is proposed in reference [42], where the interaction potentials must be governed according to material point size as well as that of the system, as in equation (20) [3]. In such an interpretation interactions should not be a function of inertial properties, or charge or other physical properties, which create varying definitions for the constant C' in reference (18). What generic form the constant C' would eventually take will be the key to unified dynamics across the physics of scale. There is a long way to go before this issue would be resolved.

7 CONCLUDING REMARKS

This article has provided a brief historical review of multi-body dynamics as an evolution of Newtonian axioms through constrained Lagrangian dynamics or restrained Newton–Euler method. A generalized perspective is provided in which both the aforementioned methods may be regarded as dynamics within a reduced configuration space. It is also shown that as a better understanding has emerged, with refined numerical methods and greater computational power, salient features in system dynamics have been incorporated in the analyses, such as elasticity, tribology, noise propagation, and thermodynamics. A whole new area of what is termed as multi-physics, multi-scale analysis has dawned, which constitutes a growing area of applied research.

This article demonstrates another growing research trend from multi- to many-body dynamics, arising with a greater application of Newtonian laws to clusters of material points. This trend commenced with molecular dynamics and has been given an impetus with ever increasing computing power. However, in the scale of minutiae, where material points of insignificant inertia are subject to largely non-Newtonian action potentials, the analyses are hampered by largely empirical or stochastic force laws. Yet with growing multi-disciplinary work into micro-mechanical, biological, and physio-chemical systems, extensive research is required to fundamentally understand the nature of various interactions. In particular, the very basic and underlying disunity between electromagnetic and gravitational potentials should ultimately be resolved. In this respect, multi- and many-body dynamics would merge together as mere problems of scale not that of underlying physics.

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APPENDIX

Notation

$\mathbf{a}^i$	vector of acceleration
A	Hertzian contact radius of a pair of hemispherical asperities
A_m	cross-sectional area of a meniscus bridge
c	wave speed
C_p	algebraic constraint functions
E^*	effective elastic modulus of contact
f	frequency
$\mathbf{F}_a$	vector of applied forces
$\mathbf{F}_q$	vector of generalized forces
G_u	universal gravitational constant
h	height
$\bar{h}$	cumulative distance between an ensemble of particles
H	undeformed gap
l	number of constrained coordinates
ℓ	characteristic size of a cluster or an ensemble
L	Lagrangian
m	mass
$\mathbf{M}_q$	mass matrix
n	number of material points or order of action potential as specified
p	pressure

q^k	generalized Eulerian body-fixed 3-1-3 coordinates
r	number of coordinates in the reduced configuration space or distance or a position vector as specified
R	radius
R_e	equivalent radius
t	time
T	kinetic energy
$[\mathbf{T}]$	Euler's transformation matrix
$[\mathbf{T}^*]$	Euler's transformation matrix rotational dynamics
$\mathbf{u}_p^k$	local shape vector
U	potential energy
v	velocity
V	white noise variance
w_a	adhesive force per asperity pair
w_h	hydration repulsion per bridge
w_m	meniscus force per bridge
γ	surface tension
Γ	boundary variable
δ	distance between adjacent material points in a many-body ensemble
Δ	contact deformation
Δt	time step
ε	size of the material point
θ	contact angle (to bodies, designated by 1 and 2) in many-body dynamics
λ_0	limit of hydration potential
λ_p	Lagrange multipliers
ξ^j	fixed global frame of reference
σ	RMS surface roughness
ϕ^k	mode shape
Φ	modal matrix
φ	potential
ψ, θ, φ	Euler angles in multi-body dynamics
ω	radiancy