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Abstract

Tribologists are confronted on a daily basis by the need to understand the causes and consequences of friction on the behavior of bodies in contact. Understanding contact behaviour is not only a scientific curiosity but the key to solving numerous industrial issues. Numerical tools have been developed to overcome the problems encountered in experiments due to limitations in the local dynamic analysis of multi-scale systems (mechanisms, bodies in contact, interfaces). More than an exhibition of numerical results, the present paper proposes reviewing the literature on the numerical tribology of dry contacts by analysing the different scales involved.

Keywords: triblogy, modeling, dry friction, multi-scale

1. Tribological context

Friction is part of our everyday lives, in common actions such as holding a pencil, walking, etc. From a pragmatic point of view, it is also the key issue of many industrial problems (mechanism lifetime [1, 2, 3], different types of wear [4, 5], brake squeal noise [6], vibration and noise reduction[7],etc.) and economic challenges (energetic expense, warming, etc.). These are just a few of the reasons, why, from the beginning of history (e.g. tribology on

Egyptian frescoes [8]), human beings have tried to minimise or maximise friction according to their needs.

Since the Renaissance, with the research of Leonardo Da Vinci (1453-1519), followed by that of Guillaume Amontons (1663-1705) and Charles Augustin de Coulomb (1736-1806), researchers have attempted to interpret friction by formulating basic equations. The first contact model was proposed in 1881 by Hertz [9] while the first wear laws were proposed by Archard, who developed pin on disk experiments in 1953 ([10, 11, 12]). These involved total wear volume, normal load, running distance and an additional physics-less parameter k. Since Archard's pioneering works and other directly related studies, more than one hundred wear models have emerged [13]. These models are based on the fact that the more parameters they contain, the easier it is to match them to experimental results. To overcome this generality, Lim et al [13] defined wear maps incorporating velocity and contact pressure, making it possible to characterize the nature of wear (soft, hard, delamination, etc.). Nevertheless, it was soon apparent that this kind of approach could not be transferred from one contact condition to another.

One of the main reasons for the difficulties encountered so far is that problems involving friction and wear are multiscale and multiphysical by nature, as well as being strongly coupled. From the mechanical viewpoint, constraints at contact level depend on the contact itself as well as on the whole mechanism. From the material standpoint, the materials forming the bodies in contact (first bodies) and the interface (third body [14]) respond to both temporal and local spatial distributions of stresses, by exhibiting complex behavior. In addition, friction and wear models are confronted by

the great complexity of mechanical, thermal and physicochemical phenomena occurring within contacts and affecting the different parameters used in the models. This complexity results from the large number of strongly correlated parameters.

This complexity, involving different scales and physics, has led to the appearance of several approaches to studying tribological problems that range from experimental validations to numerical simulations. The innovative concept of "tribological triplet", proposed in the 1980s by Godet and Berthier [4, 14], takes a different path from that of conventional schemes, as it underlines the importance of solving a tribological problem by simultaneously considering the bodies in contact, the mechanism (mechanical system) that contains them, and the interface that separates them; the latter is called the third body which refers to the so-called "first bodies" that it separates.

From an experimental viewpoint, at least four main difficulties can be identified when analysing a contact locally:

- the confinement of the contact makes it difficult (if not impossible) to perform measurements "in situ" without disturbing the contact itself;
- the three components of the tribological system (mechanism, first bodies and third body) act simultaneously, making it difficult to determine the pilot component and its degree of interaction, bringing to mind the image of the snake swallowing its own tail;
- the local response of the material (work-hardening, Superficial Tribological Transformation (STT) [5, 15, 16], etc.) to tribological stresses (quasi-hydrostatic pressure, shearing gradient, etc.);

- tribometric measurements are difficult to transpose to real mechanisms because they always correspond to specific mechanical loads and physicochemical contact conditions.

To overcome such experimental difficulties, tribologists were quick to recognise the potential of numerical tools for overcoming them; nowadays, simulations can be carried out at different scales, taking advantage of the fact that it is possible to vary one parameter at a time, somthing that is almost impossible experimentally. Following a guideline based on the concept of the tribological triplet, approaches at the scales of the mechanism, the bodies in contact and the interface are dealt with in the following sections. After presenting the first contact models in Section 2, Sections 3 and 4 present numerical tools used at the scale of the mechanism and the first bodies and at the scale of the interface, while Section 6 presents more recent advances in dry numerical tribology. For each section, the variety of numerical methods used in tribology at each scale is presented, the hypothesis retained to consider the other scales (above or below) is described, and a relevant example is given.

2. First contact models

For many decades, researchers in the field of contact mechanics have tried to use simple models to describe the behavior of the relative motion between two bodies. Hertz was undoubtedly the first to propose a contact model [9] that initially comprised contact between a cylinder and a flat surface and then between two spheres of different radii. The model offered a simplified

representation of the local deformation of the body, depending on the elasticity of the materials in contact, and provided the stress field in the contact area relating to the normal force, the radii of curvature of the two bodies and their elastic modulus in a static configuration. This model is valid for frictionless contacts, assuming that the contact area is small in comparison to the size of bodies in contact and that the stresses localised at the contact zone are less than the limit of elasticity. It also assumes a continuous and smooth distribution of the pressure in the contact area.

This theory formed the basis of many models, some of which used the hypotheses of the original model. Extensions were proposed for other regular geometries [17, 18], more complex geometries and for accounting for the presence of friction and inelastic behaviour [19].

In his model, Hertz considered perfectly smooth contact surfaces. In the 60s, Greenwood proposed a static contact model for rough surfaces [20]. This generalisation was to be the basis of many other models proposed to describe contact surfaces by more or less complex functions developed by the combination of trigonometric functions [21], by the use of fractal model [22] or by numerical models involving finite element (FE) approaches [23, 24, 25, 26, 27, 28].

Hertz's theory was extended to models that took into account dynamic aspects. Carter [29] proposed a model of a line contact to describe the contact between wheel and rail, accounting for longitudinal slip only. He highlighted the coexistence of areas of sticking and sliding within the contact

zone. Carter's simplified model was then extended to circular contacts [18] and elliptic contacts [30], allowing the consideration of transverse sliding. Based on the work of Johnson, Kalker proposed a set of algorithms using more or less complex models [31, 32]. The contact area was no longer seen as a uniform sliding or sticking region but as an area divided into sliding/sticking sub-regions depending on the type of stress involved. These models have been used since the first simulations of railway dynamics and can be found in several multi-body software applications dedicated to wheel-rail contacts. Rolling contacts are still the subject of many works and the reader can consult specific works for more details [33, 34, 35, 36].

Due to the huge number and variety of contact and friction models available in the literature, it is not possible here to provide a complete review. Therefore, those readers who are interested can refer to the texts of Bowden and Tabor [37], Rabinowicz [38], Suh [39], Kragelskii [40], and Dowson [8] for further details and references.

3. Modelling Mechanism and First Bodies

3.1. Modelling reality

Although previous analytical models were meaningful tools that led to understanding of the phenomena involved in contact mechanics and tribology, their limits quickly became apparent when dealing with more realistic issues in which the role of the mechanism, together with the contact, has to be accounted for. For example, predicting the lifetime of a mechanical component like a bearing, blade disk or brake system must take into account

both the dynamic analysis of the mechanism up to its end-of-life and knowledge of the local transformations of the bodies in contact (local deformations [15, 41], surface degradation [42, 43], etc.).

Thus additional modelling of both the dynamics of the whole system (mechanism) and the local behaviour of the bodies in contact (first bodies) is necessary. Nevertheless, the difference between the spatial and temporal scales of the two aspects of the problem implies that developing a single model that includes both the global behaviour of the mechanism and the detailed description of the bodies in contact results in cumbersome operations that are often impossible to achieve.

Defining objectives as a function of the problem to be solved.

In the case where the model is designed to simulate the dynamic response of a mechanical system, the contact (either sliding or static contact joints) is accounted for by reduced parameters that are assumed to represent the effect of the contact on the system's dynamics. These parameters generally consist of global contact stiffness factors [44, 45], contact damping factors [46] and energy loss factors if the model includes energetics [47]. Moreover, to overcome the complexity and the non-deterministic effects of the nonlinearities of contact joints on the dynamics of a mechanism, statistical techniques dealing with uncertainties have been developed, such as Statistical Energy Analysis (SEA) [48]. In such models the contact between the subsystems (components) of a complex mechanical system are represented by energy loss factors accounting for the loss of energy at the joint, and energy coupling factors accounting for the energy transfer between the subsystems. An extensive review of these approaches and the huge amount of related literature is beyond

the scope of this work, although readers will find the articles mentioned in the references.

On the other hand, when dealing with the contact itself, two different approaches have been proposed over recent decades: analytical or semi-analytical models, and numerical models (finite element). These approaches may appear contradictory although they sometimes complement each other.

Table 3.3 shows a comparison between the different approaches, emphasizing their respective advantages, drawbacks and several typical applications. Readers new to the field can take advantage of this initial comparison for choosing the approach to be used for each specific problem.

3.2. Semi-analytical models

Semi-analytical (SA) models were the first tools to be used either for simplifying contact problems by trying to account for mechanism behaviour, or for understanding the behaviour of solids subjected to contact stresses over long periods of time. The latter approach is that most commonly adopted for modelling the behaviour of mechanical systems over several hours operation. In such cases computing-time becomes one of the main constraints, forcing researchers to develop simplified models of both the dynamic behaviour of system components and contact stresses. These approaches have become efficient tools for solving well-defined problems more than general tools for understanding contact problems [1, 49], because the phenomena and the scales of the mechanism and the contact are completely uncoupled. Consequently one of the main drawbacks of these models, as pointed out in table 3.3, is their specificity with respect to the problem to be solved. There is no general formulation capable of being used for several different problems.

The SA feature of the models described above can be used for time discretization in analytical models to simulate the evolution of a solution to a problem through time. Different simplified analytical models accounting for friction, plastic deformation or wear are often implemented; these models are then assembled together and dialog with each other them through their respective inputs and outputs.

SA models have been used for understanding wear phenomena like fretting [1, 50], in simplified elasto-plastic and wear models [49]. Other researchers have developed semi-analytical methods for modelling ball bearing behaviour [2, 51, 3], by simplifying the interaction between the bearing elements with visco-elastic contact laws. The literature on semi-analytical models is extremely rich and is growing rapidly every year, with specific branches that each deal with particular issues, thus it is not possible to give a complete overview of existing works and those readers interested should refer to more detailed reviews that deal with specific applications. Nevertheless, it is worth mentioning the works of Nélias [52, 1, 49] concerning dry contact problems and the works of Wensing [7, 3] dealing with lubrificated contact problems. A detailed review of friction models for friction compensation methods in mechanical systems with contact is provided by Armstrong-Héloury [53]. A bridge between semi-analytical and continuous models is given by the review presented by Oden and Martins [54].

An interesting improvement and analysis of SA models can be found in the works of Gallego et al. [49]. The authors propose an alternative method to the FE method to perform wear computations on dovetail joints. Although an FE model is used to solve the structural problem, the SA model focuses

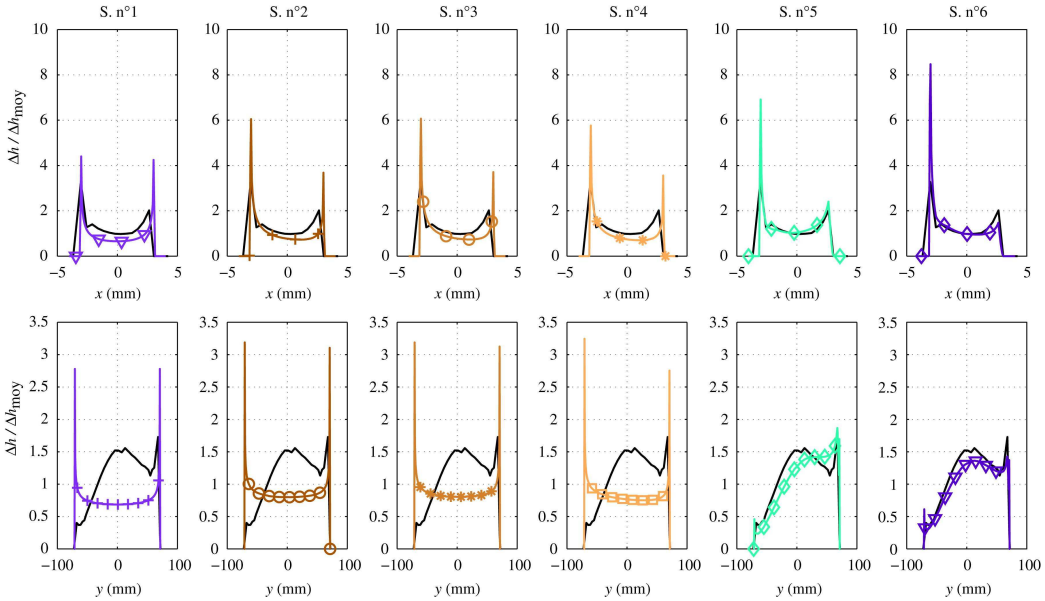

Figure 1: Wear depth profiles after one fretting cycle with unworn surfaces (i.e. after the first cycle). The solid line in black corresponds to the FE results while the lines with symbols correspond to the results provided by the SA model with various levels of complexity [49]

on each contact area and its speed allow computing cyclic wear easily. Figure 1 shows the wear depth profiles after one fretting cycle with unworn surfaces (i.e. after the first cycle). The solid line in black corresponds to the FE results used as a reference case while the lines with symbols correspond to the results provided by the SA model with different levels of complexity.

3.3. Numerical methods for continuous modelling

Finite element modelling is the most commonly used numerical method for solving contact problems with friction between deformable bodies [55]. Initially, researchers in tribology were not attracted by this numerical tool.

One of the main reasons was the extremely long computational time required in comparison to more efficient analytical or semi-analytical approaches (see table 3.3). Nevertheless, numerical approaches using finite element methods were given increasing attention by tribology journals by the end of the 80s [56]. Nowadays, they have become an essential method for solving contact problems where mechanism and first body behaviour is the main subject of analysis. Notwithstanding, it is important to pay attention to the different approaches and methods that can be adopted. Indeed, both the time integration method and the modelling of contact elements can considerably affect the results of finite element simulations.

Transient analysis by the finite element method is better adapted to the analysis of local phenomena over short periods (from a few milliseconds to several seconds, according to the application) rather than the simulation of the transient behaviour of a complex system over long periods (several hours). The computational effort, as opposed to semi-analytical methods, is no longer considered to be a constraint, despite the fact that it can be cumbersome. Despite this expense in terms of computational effort, these models have proved useful tools for understanding problems. Moreover, this limitation is being constantly reduced by numerical optimizations that use clusters and parallel calculation. Nevertheless, semi-analytical models continue to be more efficient concerning computational effort and are thus still preferred for prediction over longer periods of time.

An example of more phenomenological approaches is the effort employed by researchers in modeling brake systems by FE methods, in order to investigate the brake squeal phenomenon. A review of recent literature [57] dealing

with the numerical analysis of brake squeal shows how FE transient analysis has been employed for reproducing and investigating squeal vibrations (Figure 2) and local contact stresses, while FE complex eigenvalue analysis has been developed for predicting brake dynamic instabilities (Figure 3). While FE models have been of fundamental importance for understanding the mechanism at the origin of the self-excited friction vibrations that cause squeal noise, their limits have been highlighted as they cannot be used to develop a predictive FE tool. The lack of information at the scales of the third body and of the global mechanical system, together with limitations on model size and the huge computational efforts demanded for transient analysis, prohibit the development of a quantitative FE model of such systems without updating the parameters through experimental comparison. Therefore, despite several efforts, FE models remain more useful as tools for understanding than for predicting.

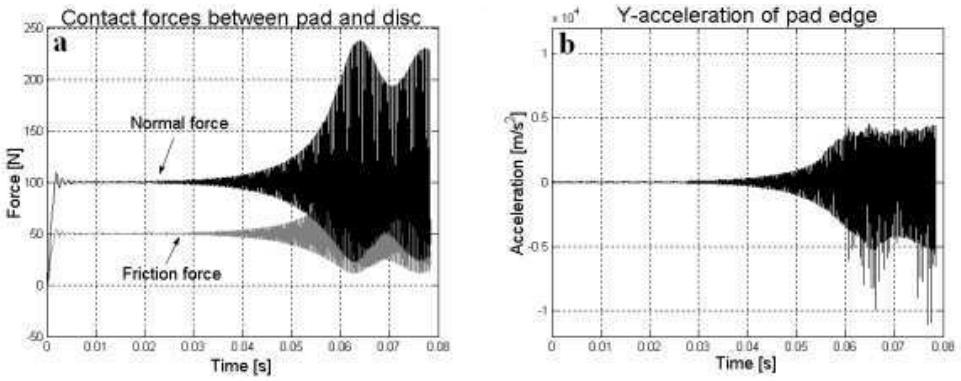

Figure 2: Transient FE analysis of brake squeal: a)Normal and tangential forces between brake pad and disc; b) Tangential acceleration calculated at the brake pad. FE simulation makes it possible to reproduce the vibrations triggered in the contact [58].

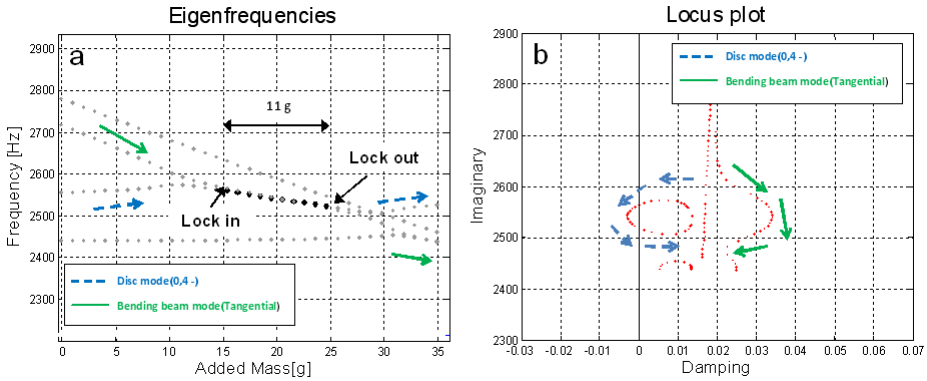

Figure 3: Complex eigenvalue FE analysis of brake squeal: a)Natural frequencies of the brake system cross each other and can become unstable; b) Locus plot of system eigenvalues: the real part of one eigenvalue become positive, i.e. the system is unstable.

Several methods have been developed over recent decades for solving contact problems between two deformable bodies. They are generally classified as a function of the contact algorithm and the time integration scheme used. The contact algorithms most commonly used employ either Lagrange multiplicators [59, 60, 61], the regularization parameters [62], or LCP (Linear Complementary Problems) [63]. Time integration schemes can be either explicit or implicit for describing the motion of a structure and for dealing with a contact [61, 64, 65, 62].

As asserted for the semi-analytical models, it would be difficult and, in any case, beyond the scope of this review to cite all the works dealing with contact problems and finite element methods. The combination of these issues covers theoretical works dealing with convergence and the unicity of numerical solutions [66], works dedicated to developing efficient algorithms [67, 63, 68, 69], and an extremely wide range of different applications (e.g.

[70, 34]). With resepct to tribological issues, i.e. understanding the causes and effects of friction in bodies in contact, the works of Ham [56] and Baillet [59, 60] deserve metnion. Others works have aimed at understanding specific contact phenomena, for example the behaviour of composite materials subjected to tribological stresses [71], the development of contact instabilities [72], wear laws in biomechanics [73], the occurrence of rail defects [34], dynamic instabilities leading to squeal noise [58, 74], contact rupture [75, 76], contact wave generation and propagation [77, 78, 79]. The reader will find a more complete bibliography concerning each specific domain in the works cited .

As highlighted in Table 3.3, recent advances in sub-structuring methods make it possible to consider a new approach halfway between semi-analytical and FE models [80, 81]. Sub-structured FE modelling allows accounting for contact distribution, the connections between substructures, and it drastically reduces the number of degrees of freedom of the global FE model. First, single substructures are modelled and the matrix reduction technique is used to reduce the system matrices to a smaller set of degrees of freedoms. Then the reduced matrices of the single substructures are assembled together to account for the general boundary conditions and the contact stresses at the contact interfaces between single substructures. This approach dramatically reduces computational effort at the expense of simplifying (reducing) modelling of the first bodies (sub-structure) response.

model	typical application	advantages	drawbacks	scales
semi-analytical	- transmission systems - full bearing systems - vehicle dynamics	- low computational cost - full system modelling - long time simulation	- lost of local contact information - simplified first body modelling - application depending modelling	- mechanical system scale - large time and space scale
Energetical formulation	- vibration analysis of jointed structures - fluid-structure coupling	low computational cost - interaction between different - behaviour of first bodies	- no local contact information - simplified first body modelling need of pre-modelling	- first body scale or simple system scale - only stationary states
Standard F.E.	- transient model analysis of simple systems - contact instabilities - first body contact analysis	- local contact information - full first body modelling - availability of robust general formulations	- large computational cost result precision depending on the contact modelling no third-body effects	- first body scale or simple system scale - contact space scale - short time scale
sub-structured F.E.	transient model analysis of simple systems - contact instabilities - first body contact analysis	- local contact information - reasonable computational cost - robust formulation availability	reduced first body modelling result precision depending on the contact modelling - no third-body effects	- first body scale or simple system scale - contact space scale - relative short time scale

Table 1: Comparison between methods for modelling mechanism and first bodies

4. Within the tribological interface

4.1. From reality to modeling

When focusing on the interface that separates two bodies in contact, flows of the latter can be observed under certain conditions (high pressures and shear rates). This is easily understandable in the case of a fluid lubricant, and the same idea can be generalised to solid interfaces. Indeed, Godet [14] and Berthier [4] showed that this more or less heterogeneous and discontinuous interface called "third body" can have different thicknesses (ranging from several nanometers [82] to several tens of micrometers [83]) and flow with an as yet unknown rheology. This discontinuous interface is present in an artificial way in lubrication powder (e.g. MoS2 for space lubrication, etc.) and, in this case, the properties of the media are assumed to be known. Nevertheless, the evolution of such media and their behavior in response to strong pressures and shear rates could change, making the interpretation of results complex. Therefore having a continuous view of this kind of interface does not always ensure that the reality of the contact is apparent, especially when the wear rate is accounted for, or when the third body flows are not in steady state (which is rarely the case).

Two kinds of approaches are commonly used to model the third body flow: continuous and discrete approaches. Continuous approaches offer extensions of models derived from continuum mechanics and are essentially used in applications involving lubrication powder, i.e. using an artificial third-body. In the case of a natural third body (resulting for the most part from the bodies in contact), continuity hypotheses cannot be retained and, under such conditions, it is necessary to verify whether this approach is still valid and what

its limits are. This is the main reason for using discrete element approaches to describe the evolution of a discontinuous medium and to infer rheological behavior.

4.2. Continuous approaches

There is no universal method for describing lubrication powder or, more generally, granular flows. Therefore many approaches attempt to describe such flows that are often reduced to specific geometries. In the granular tribology community, the most widely used equations are those proposed by Haff [84] or Lun [85]. They are used in many applications involving bearings [51], Couette geometries (annular) [86], parallel plates [87, 88] and converging plates [89].

The equations of conservation (mass and momentum) are used to describe the continuous behaviour of the medium [90]. These equations are similar to the energetic equations used for fluids in which variations of granular temperature are a balance between the energy injected into the system and the energy dissipated by friction and collisions. In this set of equations, the system is closed by a constitutive equation that connects the stress tensor to the strain tensor. Regarding the available models satisfying such a condition, the reader can refer to the work of Heshmat [91, 92], Tichy [93, 94, 89] or those of Khonsari [88] involving different geometries.

4.3. Discrete approaches

Discrete element approaches allow representing the interface as a collection of more or less heterogeneous particles independent of each other. This

type of method emerged in the early 70s to model the evolution of rockfalls [95, 96]. It was quickly adapted to modelling numerous problems involving media with divided features (geophysical structures [97], ballast [98], masonry [99], etc.).

The equations of continuum mechanics are no longer used to describe the evolution of systems, instead the equations of motion and laws managing the interactions between particles are implemented. They play the role of conservation and constitutive equations respectively. Although there are many variations of the discrete element method (DEM) used in tribology, they all rely on three key ingredients:

- the time integration of the equation of mechanics;
- contact detection between particles;
- computation of interaction forces between particles.

Time integration must not modify the mechanical balance of the system. Indeed, if a given energy is injected into the system, it is not dissipated numerically by the numerical scheme used (Euler [100], Newmark [101], theta-method [64], Verlet [102], etc.). Contact detection must be accurate to properly describe the connections between the particles of the system. Although this appears easy for spherical particles, it is more difficult when bodies with complex geometries are used. Finally, computation of interaction forces between particles must satisfy the mechanical equilibrium of the system and use local laws with a physical sense involving the fewest possible calibration parameters.

Ten years after the first discrete element simulations in fluid lubrication [103, 104], discrete element methods were used for the first time to simulate lubrication by bearing powder [105]. The third body is represented by a collection of rigid spheres moving between two rough inclined planes. This work paved the way for many succeeding studies. The first were very exploratory and concerned the influence of different numerical [100, 106] and geometric parameters (size of samples and particles) [107] on the mechanical response of the medium. Then more representative laws involving phenomena within an interface were used (JKR contact model [108]) [109] and the influence of particle size and the cohesion between particles on the flow behaviour were studied.

These methods were then extended to the study of wear mechanisms with simple shear [110, 111], offering wear laws based on discrete approaches. Other works concerned third body flows in fretting-like simulations [112].

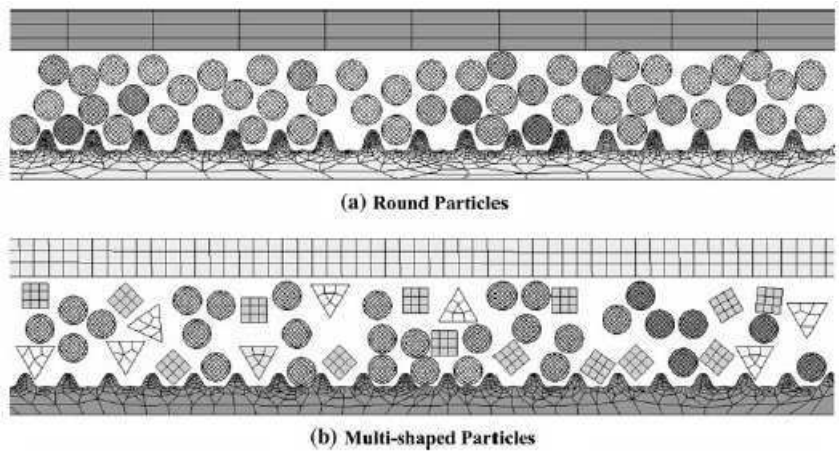

Figure 4: Two-dimensional 52 particle granular flow shear cell finite element model [101]

More recently some authors have accounted for the deformation of particles in simple shear simulations [101, 113]. The models are not representative of dense granular flows observed experimentally, but they propose a new approach in the simulation of interfaces that accounts for particle deformation. Figure 4 presents the sample used in the works of Kabir et al [101] using an explicit dynamic finite element model of parallel shear cells, containing 52 particles and consisting of round and multishaped granules (diamond, triangle, and rectangle). From a different perspective this kind of approach is used to revisit the theory of Hertz in a medium with inclusions [114].

Although several improvements have been performed in the last decade, three questions remain unanswered relating to modelling the third body by using the discrete element method.

The first question is that of how to choose the size of a single particle, since numerical particles do not represent real particles. The shapes used in models remain geometrically simple (disks or spheres according to the dimension) and and exhibit bulk behaviour (essentially rigid even if recent improvements take into account elastic deformation). Consequently, numerical particles play the role of (representative?) elementary volume when used with homogenisation techniques, while the law that governs their interaction represents the integration of local phenomena.

The determination of such laws is the second main open question. How can local elasticity, plasticity, viscosity, damage, etc. be accounted for? Models use phenomenological laws based on basic assumptions. This is due to the lack of experimental results concerning real interactions of third body particles. Therefore current models offer only phenomenological results and

should not be considered as generic.

The last open question is related to spatial and temporal scales. Simulating third body flows takes into account only a small part of the contact interface within a short time. How can these local results be extended to the evolution of a whole contact? At present mean local values are used by the upper scale. The subsection 6.1 will propose a few alternatives.

5. Nanometric characterization of interfaces

One of the major problems for discrete simulations of third body flows at the mesoscale (because of the complexity of matter) is the quantitative definition of the interaction forces between particles. Nevertheless, at the scale of the atoms and molecules composing this medium, it is possible to define reliable interatomic laws from quantum calculations [115]. Thus two main kinds of method are used to describe the motion of atoms: The Monte Carlo (MC) approach and Molecular Dynamics (MD) [116].

MC approach solves the Boltzman equation where the motions of atoms are simulated by statistical laws. This method proves to be very efficient for finding equilibrium positions but is unable to obtain an explicit evolution for atoms through time. On the contrary, MD simulation sums up inter-atomic forces, and then solves the classical Newton equation of motion over each atom, providing a deterministic way of simulating their displacement through time. Nevertheless they are very computationally costly and simulate only several nanometers. A variety of adaptations of Molecular Dynamics can be found in the literature to increase the size of the system, ranging from nanoscale to higher scales. Atoms can be grouped together, represented in

only one point of space and their interaction potentiels merged together in order to define an equivalent interaction site (United Atoms, Coarse Grain methods). However, when going up in scale, as soon as geometry and potentiels are simplified in the models (as matter becomes increasingly complex) the latter looses its precision.

Concerning "nano-tribology", early models for atomic friction such as the Tomlinson model [117] or Frenkel-Kontorova model [118] involve two crystalline surfaces in direct contact, assuming that each surface atom is linked only to the center of the mass of the rubbing body [117] or that the surface atoms are linked only to their nearest neighbour by springs [118]. With the development of computers and the use of both MC and MD methods, these friction models have been developed over the years to represent a crystalline layer of adsorbed atoms, including rearrangements of atoms due to the equilibrium condition (i.e. temperature) or sliding.

To investigate atomic scale asperities and finite contact areas, many authors (such as [119], see figure 1) have modelled AFM-like tips-on-substrate contacts. Since the shearing velocity in classical MD simulations is very high compared to real AFM experiments, Large Scale Molecular Dynamics simulations are still under development, involving massive parallel programming [120].

Many tip-substrate simulations focusing on indentation were performed in the 90's [121, 122]. They showed that when approaching the two surfaces (usually metallic surfaces) to each other, the normal force remains almost null, after which it suddenly becomes extremely attractive with a jump to contact. This phenomenon was not so clear when approaching two diamond

model	typical application	advantages	drawbacks	scales
continuous	- powder lubrication	- low computational cost - rheological model	- unknown a priori interface behaviour - no wear modelling - no localisation phenomena	- interface scale
D.E.	- powder lubrication - wheel-rail contact - machining	- no a priori behaviour - wear modelling - localisation phenomena	- large computational cost - unknown a priori interaction laws	- part of the interface
C.G.	- polymer modelling	- Large number of atoms represented by an equivalent entity	- difficult to find equivalent interaction potential	systems with very long molecules
U.A.	- alkane modeling - biological molecules	- few atoms grouped in equivalent energy sites	- simplified molecule shape and interaction potentials	- Nanometer scale
M.D.	- nano-indentation	- deterministic simulation of atom motion	- very high computational cost	- nanometer scale
M.C.	- solids at rest	- fast to find equilibrium positions	no explicit time evolution	- nanometer scale
Ab Initio	- Atomic interactions determination	- includes electron modelling	- long computation for only a few atoms	- atomic / subatomic scales

Table 2: Comparison between continuous, Discrete Element (D.E.), Coarse Grain (CG), United Atom (UA), Molecular Dynamics (MD), Monte Carlo (MC) and Ab Initio approaches for modelling the third body and smaller system.

surfaces in the case where at least one was hydrogen-terminated [123].

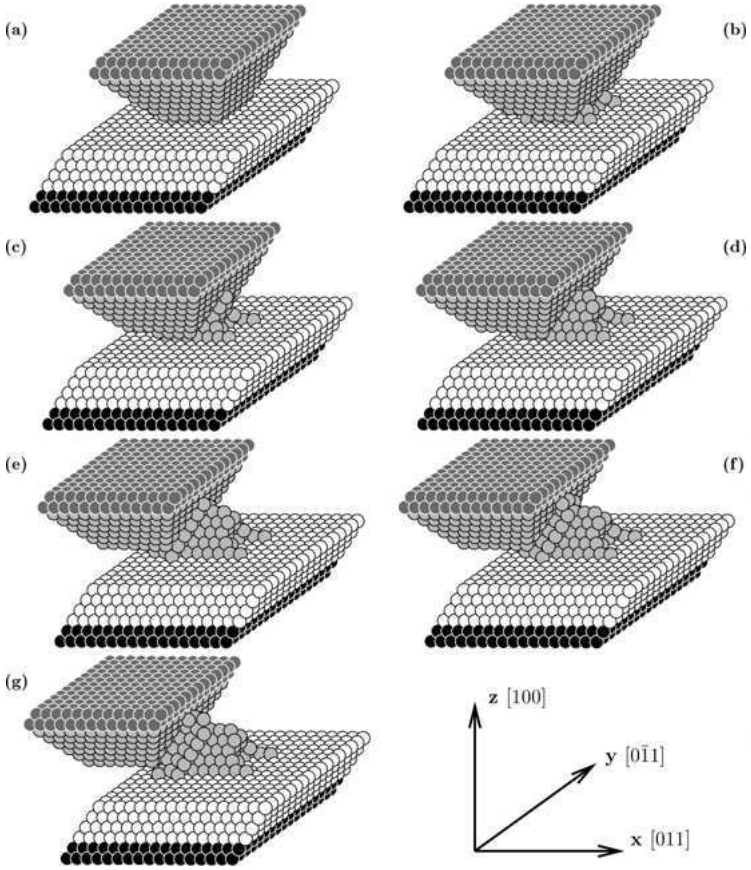

Figure 5: Snapshots showing the evolution of a Cu(100) tip on a Cu(100) substrate during sliding to the left [119].

Regarding sliding, nanoscale simulations often highlighted intermittent motion, with the system alternatively sticking and slipping forward, as described by Rabinowicz [38] and Bowden and Tabor [124]. The stiffness of the contacting bodies and the commensurability of the surface, i.e. the way atoms are arranged regularly (or not) depending on the crystalline lattice orientation [125, 126, 127], play an important role in the dynamic friction

process.

The first tribochemical reactions in molecular dynamics simulations were observed by Harrison and Brenner in 1994 [128], who used reactive potentials that allow for the breaking and formation of chemical bounds. This brought to light the origin of the formation of molecular wear debris.

An impressive compilation has been proposed in [129], where the reader will find many complementary aspects related to this section.

6. Numerical tribology today

During the last decade, numerical tribology has evolved considerably. It has taken advantage of the numerous numerical developments achieved in the domain of contact mechanics and adapted them to its own needs. Numerical tribology has now become an indispensable tool for studying contact problems.

Nevertheless, the need for in-depth understanding of the phenomena involved is leading to the development of models that must be as accurate as possible. They are no longer purely mechanical, nor are they based on only one scale, as they incorporate different physics and consider several scales.

6.1. Towards multi-scale models

In the past, most numerical work in tribology was performed at a single scale, accounting for the other scales by boundary conditions or local conditions. Although the idea of coupling the different scales is not a new one [5, 130], it is only recently, in tribology, that different approaches have tried to account for the different scales of the tribological triplet within a single simulation, either directly or indirectly.

For example, certain works couple the mechanism and bodies in contact to analyse bearings [51, 131]. In the first case, a nodal reduction is performed on the whole system and coupled with condensation techniques. In the second case, the mechanism results from a multi-body model and injected as boundary conditions into the finite element simulation of the contact.

Other works couple smaller scales (the scale of the bodies in contact and the interface) to account for the effect of local damage on the behavior of bodies in contact [132, 133].

At the scale of the interface, models offer richer descriptions by mixing discrete and continuous approaches in a single simulation [134, 133]. The influence of the deformation of the bodies in contact is directly accounted for by the rheology of the interfaces. Other models provide a dialogue between different scales by applying an iterative method [134, 135]. The friction at the scale of the bodies in contact is the result of a simulation performed at the scale of the interface (third body), while the boundary conditions of the simulations at the interface scale are provided by the local dynamics at the scale of the first bodies.

Some models couple the finite element method and molecular dynamics to account for a richer description of the interface and the surface condition [136, 137], while other methods couple discrete models at the scale of the material's structure to reflect local degradation in gear dynamics [138].

6.2. Towards multi-physics models

Multi-physics models are commonly used at the scale of the first bodies. Indeed, thermo-mechanical models based on robust formalism have been implemented [139].

Concerning solid interfaces, multi-physics models have been developed only recently. Models coupling mechanical and electrical aspects have been developed to understand phenomena such as shunting in the wheel rail contact [140]; thermo-mechanical models have been developed to describe energy dissipation within the contact interfaces [141, 142, 143]. This work allowed a new approach to the concept of friction by incorporating thermal discontinuous aspects and updating the Blok theory [144].

More recent models are capable of coupling mechanical, thermal and physical chemistry within the interface. This kind of approach allows linking every physical feature within a single simulation [145, 146]. The limits of these approaches depend on the experimental data used feed the models.

7. Discussion and conclusion

The numerical tools used at the scales of the mechanism, the bodies in contact and the interface have been presented following a guideline based on the concept of the tribological triplet. The semi-analytical model, finite element method, discrete element method and molecular dynamics approach appear to be the most commonly used tools.

At the scale of the mechanism and the first bodies, Semi-Analytical models and Finite Element Methods appear to be the most appropriate tools for describing the behaviour of an entire system and that of each component. SA models can be used to simulate the long-term evolution of full systems at low computational cost. Nevertheless, they entail a loss of local contact information, the use of simplified first body modelling, and models dedicated to only one application. The Finite Element Method made full first body modelling

and the measurement of local contact characteristics possible. Moreover, robust general formulations are available. On the other hand, the approach is computationally costly when the results depend on contact modelling and it is not possible to simulate the long term evolution of a contact, even when using sub-structured approaches.

At the scale of the interface, rheological models are computationally inexpensive, enabling description through wear modelling and reproducing localisation phenomena. Finally, they can be used to postulate an a priori unknown interface behaviour. On the contrary, the Discrete Element Method can be used to consider wear and localisation processes but suffers from high computational costs and is based on a priori unknown interaction laws (in most cases).

At the nano-scale, Molecular Dynamic Approaches provide good descriptions of matter and are well-suited to nano-applications, but in the case of more microscopic problems, mapping information becomes complex.

Although many studies at different scales have led to clarifying the concept of friction, there is still some way to go before reliable predictive models of friction and wear can be obtaiend. Until we are able to model a full system, friction will remain a scientific smokescreen. A great deal of research work is currently taking this direction and integrating different physics, with dialogue between different scales. In conclusion, it is possible to assert that, thanks to numerical tribology and its interactions with experimental tribology, tribologists are wearing friction down.

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