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New and Advanced Numerical Strategies for the Simulation of Material Forming

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Abstract. In recent years new and advanced numerical strategies have opened new possibilities in the simulation of forming processes. Multiscale descriptions, meshless methods and enhanced finite element approaches are some techniques that have contributed to the enhancement of forming process simulations. These approaches will be revisited in this chapter.

1 Microscopic approaches

1.1 Solid mechanics framework

Materials can be described at different scales. The finest level of description consists of the atomic level and the coarsest one concerns the scale at which the conformed part is defined. Molecular dynamics simulation works at the atomic level and allows to account for complex physics in a simple and natural way. Thus, knowing at a certain time the position of the atoms, the resultant force applying at each atom can be easily computed from a semi-empirical atomic potential, and from it the atoms acceleration computed and the velocities and atomic positions updated. The main drawback of this approach lies in the extremely large computing time required to perform realistic simulations even when small domains and time periods are considered,as well as the semi-empirical interatomic potentials usually considered in such approaches.

The establishment of more accurate atomic potentials require the solution of the Schrodinger equation in the quantum mechanics framework, whose main difficulty lies in the curse of dimensionality that we consider later, and that constitutes today a real challenge. In recent years molecular dynamics approaches were considered in the framework of forming processes involving cutting [39] or contact with friction [12], both presented during the recent Esaform conferences.

The micro-macro approach when both descriptions coexist in the physical space as well as the definition of efficient bridges between both descriptions defined in contiguous regions are topics in active development nowadays [24] [43] [23].

In an intermediate scale other approach based on the discrete finite element was successfully applied for treating granular media, being [40] or [21] some examples of works presented during the Esaform conferences in recent years.

1.2 Fluid mechanics framework

This section concerns the liquid state of different materials involved in forming processes. In some cases, as in casting, the resulting constitutive equation of involved materials results simple, but the high Reynolds number involved in the forming processes induce numerous numerical difficulties. For other kind of materials, the ones involving microstructure, the main difficulty is coming from the inherent multiscale character of its mechanical behavior. This section focuses on this complex fluids (polymer melts or particle suspensions).

Many natural and synthetic fluids are viscoelastic materials, in the sense that the stress endured by a macroscopic fluid element depends upon the history of the deformation experienced by that element. Notable examples include polymer solutions and melts, liquid crystalline polymers and fibre suspensions. Rheologists thus face a challenging non-linear coupling between flow-induced evolution of molecular configurations, macroscopic rheological response, flow parameters (such as the geometry and boundary conditions) and final properties. Theoretical modelling and methods of computational rheology have an important role to play in elucidating this coupling.

Atomistic modelling is the most detailed level of description that can be applied today in rheological studies, using techniques of non equilibrium molecular dynamics. Such calculations require enormous computer resources, and then they are currently limited to flow geometries of molecular dimensions. Consideration of macroscopic flows found in processing applications calls for less detailed mesoscopic models, such as those of kinetic theory.

Kinetic theory models can be very complicated mathematical objects. It is usually not easy to compute their rheological response in rheometric flows, and their use in numerical simulations of complex flows has long been thought impossible. The traditional approach has been to derive from a particular kinetic theory model a macroscopic constitutive equation that relates the viscoelastic stress to the deformation history. The majority of constitutive equations used in continuum numerical simulations are indeed derived (or at least very much inspired) from kinetic theory. Indeed, derivation of a constitutive equation from a model of kinetic theory usually involves closure approximations of a purely mathematical nature such as decoupling or pre-averaging. It is now widely accepted that closure approximations have a significant impact on rheological predictions for dilute polymer, solutions, or fiber suspensions.

Since the early 1990's the field has developed considerably following the introduction of the CONNFFESSIT method by Ottinger and Laso [37]. Kinetic theory provides two basic building blocks: the diffusion or Fokker-Planck equation that governs the evolution of the distribution function (giving the probability distribution of configurations) and an expression relating the viscoelastic

stress to the distribution function. The Fokker-Planck equation has the general form:

$$\frac{d\psi}{dt} + \frac{\partial}{\partial \mathbf{X}} (\mathbf{A}\psi) = \frac{\partial}{\partial \mathbf{X}} \left(\mathbf{D} \frac{\partial \psi}{\partial \mathbf{x}} \right) \tag{1}$$

where $\frac{d\psi}{dt}$ is the material derivative, vector $\mathbf{X}$ defines the coarse-grained configuration and has dimensions N. Factor $\mathbf{A}$ is a N-dimensional vector that defines the drift or deterministic component of the molecular model. Finally $\mathbf{D}$ is a symmetric, positive definite $N \times N$ matrix that embodies the diffusive or stochastic component of molecular model. In general both $\mathbf{A}$ and $\mathbf{D}$ (and in consequence the distribution function ψ) depend on the physical coordinates $\mathbf{x}$, on the configuration coordinates $\mathbf{X}$ and on the time t.

The second building block of a kinetic theory model is an expression relating the distribution function and the stress. It takes the form:

$$\tau_p = \int_C \mathbf{g}(\mathbf{X}) \psi d\mathbf{X} \tag{2}$$

where C represents the configuration space and $\mathbf{g}()$ is a model-dependent tensorial function of configuration. In a complex flow, the velocity field is a priori unknown and stress fields are coupled through the conservation laws. In the isothermal and incompressible case the conservation of mass and momentum balance are then expressed (neglecting the body forces) by:

$$\begin{cases} \nabla \cdot \mathbf{v} = 0 \\ \rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (-p\mathbf{I} + \tau_p + \eta_s \mathbf{d}) \end{cases} \tag{3}$$

where ρ is the fluid density, p the pressure and $\eta_s \mathbf{d}$ a purely viscous component. The set of coupled equations (1)-(3), supplemented with suitable initial and boundary conditions in both physical and configuration spaces, is the generic multiscale formulation. Three basic approaches have been adopted for exploiting the generic multiscale model:

1. *The continuum approach* wherein a constitutive equation of continuum mechanics that relates the viscoelastic stress to the deformation history is derived from, and replaces altogether, the kinetic theory model (1) and (2). The derivation process usually involves closure approximations. The resulting constitutive model takes the form of a differential, integral or integro-differential equation.
2. *The Fokker-Planck approach* wherein one solves the generic problem (1) to (3) as such, in both configuration and physical spaces. The distribution function is thus computed explicitly as a solution of the Fokker-Planck equation (1). The viscoelastic stress is computed from (2).
3. *The Stochastic approach* which draws on the mathematical equivalence between the Fokker-Planck equation (1) and the following Ito stochastic differential equation:

$$\mathbf{dX} = \mathbf{A}\ dt + \mathbf{B}\ \mathbf{dW} \tag{4}$$

where $\mathbf{D} = \mathbf{B}\,\mathbf{B}^T$ and $\mathbf{W}$ is a Wiener stochastic process of dimension N. In a complex flow, the stochastic differential equation (4) applies along individual flow trajectories, the time derivative is thus a material derivation. Instead of solving the deterministic Fokker-Planck equation (1), one solves the associated stochastic differential equation (4) for a large ensemble of realizations of the stochastic process $\mathbf{X}$ by means of a suitable numerical technique. The distribution function is not computed explicitly, and the viscoelastic stress (2) is readily obtained as an ensemble average.

The control of the statistical noise is a major issue in stochastic micro-macro simulations based on the stochastic approach (for more details concerning the micro-macro approach reader can refers to the excellent review paper [28] and the references therein). Some stochastic simulations of muti-bead-spring (MBS) models have been successfully carried out, see for example [44]. These problems do not arise at all in the Fokker-Planck approach. The difficulty, however, is that the Fokker-Planck equation (1) must be solved for the distribution function in both physical and configuration spaces. This necessitates a suitable discretization procedure for all relevant variables, namely position $\mathbf{x}$, configuration $\mathbf{X}$ and time t. Until now, the dimensionality of the problem could be daunting and consideration of molecular models with many configurational degrees of freedom did not appear feasible. This probably explains why relatively few studies based of the Fokker-Planck approach have appeared in the literature until very recently at least. In [14] [30] the resolution of the Fokker-Planck equation involving a moderate number of dimensions is considered. Another deterministic particle approach, very close to that proposed in [13], was analyzed in [3] using the SPH meshless approach.

An appealing strategy that allows alleviating the computational effort is based on the use of reduced approximation bases obtained by applying the Karhunen-Loève decomposition, succesfully applied in complex fluid simulation in [41] and [2], however high dimensional models are out of its applicability, because in this case the definition of a mesh results simply prohibitory.

Some attempts exist concerning the treatment of multidimensional problems. The interested reader can refer to [11] for a review on sparse grids methods involving sparse tensor product spaces, but despite of its optimality, the interpolation is defined in the whole multidimensional domain, and consequently only problems defined in spaces of dimension of the order of tens can be treated [1]. In [10] multidimensional problems are revisited and deeply analyzed, and for this purpose new mathematical entities are introduced. In [4] we considered the steady state solution of some classes of multidimensional partial differential equations by using a separated representation. In [5] this technique was extended for solving accurately and efficiently multidimensional transient kinetic theory models.

Some works focussing in the solution of the multidimensional Fokker-Planck equation defining the micro-macro description were presented during the recent Esaform conferences (see for example [6]) however these models only concerned simple rheological flows. The real challenge for the next 10 years will be the exten-

sion of these procedures for treating the complex flows encountered in polymer forming processes.

2 Meshless methods: the possibility for Lagrangian simulations and much more

2.1 Introduction

It is not easy to explain what a meshless method is in few words. Since the meshless irruption after the pioneer work by Touzot and Villon [36], many different meshless methods have arisen, with many different characteristics and names. Just to cite a few, the Element-Free Galerkin [9], the Reproducing Kernel Particle Method [29], the Natural Element Method [46] [20], or the Generalized Finite Element Method [45], are examples of these different methods. They are based either in Galerkin or collocation approaches, employ different kinds of approximation for the essential variables (moving least squares, natural neighbour approximants, wavelets, etc.) and also employ —when talking about Galerkin strategies— different numerical integration procedures.

What is essential then in a numerical method to be considered as *meshless* is its ability to maintain the accuracy despite the distortion of the mesh (or, more properly, the cloud of points). It is well-known that the Finite Element method suffers from lack of accuracy if the mesh becomes distorted [7]. Meshless methods, however, adapt the connectivity of the "elements" as the cloud of points evolves, in a process transparent to the user. Many meshless methods use radially-supported shape functions (or employ tensor-product shape functions, thus giving a rectangular support), see Fig. 1. Thus, the connectivity of each element (defined as the list of nodes influencing the portion of the space in which numerical integration is to be performed) changes as the cloud evolves.

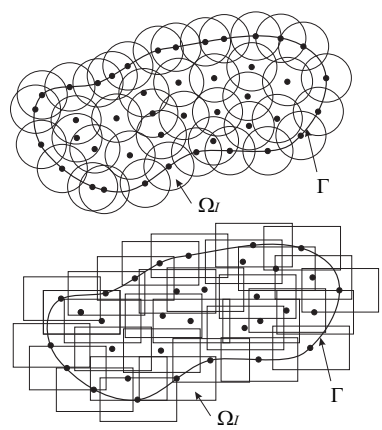


Fig. 1. Covering of a two-dimensional domain Ω by the shape functions' support, Ω_I.

Element-Free Galerkin methods (EFGM) fall within the class of meshless methods that employ cobertures of the domain such as that in Fig. 1. In this case, EFGM employ a Galerkin perspective and Moving Least Squares interpolation to construct shape functions with arbitrary degree of reproducibility. Reproducing Kernel Particle Methods, although originally developed from Smooth Particle Hydrodynamics approaches, are entirely equivalent to EFGM.

However, many meshless methods with radially-supported shape functions lack of an appropriate interpolation along the boundaries (which is readily seen

from Fig. 1 if we note that interior nodes influence on the boundary values). This is a particularly important problem in the simulation of forming processes, where issues related to friction, for instance, are frequently noteworthy. The Natural Element Method (NEM) [46] [20] solves this problem in a very elegant way, by utilizing natural neighbour interpolation, instead of Moving Least Squares, in a Galerkin framework. Natural neighbour interpolation functions do not have circular support (instead, they cover the union of circumcircles of each Delaunay triangle containing the node) and this fact makes possible the exact imposition of essential boundary conditions, up to the degree of consistency of the method.

Other, similar, methods, that also employ natural neighbour-based interpolants have been developed in recent years and applied to the simulation of forming processes, see, for instance, [25] [26].

Many other meshless methods exist, based on collocation as well as Galerkin approaches, but probably the EFGM and the NEM have been the most popular ones within the forming processes community.

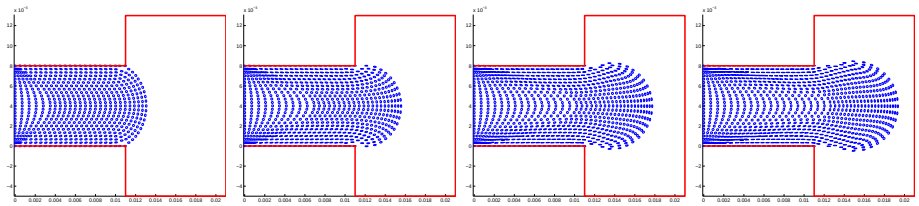
2.2 Application of meshless methods to the simulation of forming processes.

The fact that meshless methods do not lack accuracy as mesh distorts opens the possibility to perform Lagrangian simulations instead of Eulerian or Arbitrary Lagrangian-Eulerian ones, which had been the most employed ones. This is especially challenging in fields where traditional Finite Element procedures fail or present difficulties. Some examples developed by the authors follow. They are only included intending show how, qualitatively, meshless methods can help in the simulation of very complex forming processes.

Simulation of injection moulding of short fiber reinforced thermoplastics. Free-surface flows is a typical example of this kind of problems. The location of the free surface had been traditionally done by means of Volume of Fluid (VoF) or similar techniques, in which a variable representing the portion of an Eulerian element which is filled by a liquid must be advected with the material velocities.

Mechanical modelling of short fibers suspensions flows is usually achieved in the framework of dilute or semi-dilute suspensions of non-spherical particles in a Newtonian fluid. The resulting system of equations involves the coupling of an elliptic problem with an advection problem related to the fluid history. The elliptic problem is associated with the equations of motion whereas the advection equation describes the time evolution of the anisotropic viscosity tensor (fiber orientation) or more generally the microstructural state. The second problem presents two difficulties: it is non-linear and hyperbolic.

Coupled models take into account both the dependence of the kinematics with the fiber orientation and the orientation induced by the flow kinematics. Usually the coupled models are solved by means of a fixed point strategy. In this case, at each iteration the flow kinematics results from the solution of motion and



(a) (b) (c) (d)

Fig. 2. Evolution of the orientation field in the simulation of an injection moulding.

mass conservation equations, using the fiber orientation field from the previous iteration. From the kinematics just computed, the fiber orientation is updated solving the advection equation governing its evolution. In Fig. 2 four snapshots of the evolution of the orientation field are shown. The orientation is represented by elipses indicating the probability of finding a fiber oriented in each direction.

In [31] a deeper insight on the constitutive modelling of such flows can be found. The accuracy in the numerical treatment of the free surface flow is also noteworthy [32].

Simulation of orthogonal cutting. One of the very first applications of the NEM to the field of forming processes was made towards the simulation of cutting [17]. The extremely large deformations appearing in such a process make meshless methods an interesting approach to be considered.

Essentially, in this first applications a very simple visco-plasticity model based on a Norton-Hoff law and very simple contact detection algorithms, that considered rigid tool surfaces, was employed. The main purpose was, however, to demonstrate that such a method can easily suffer these high levels of strain without lack of accuracy, see Fig. 3.

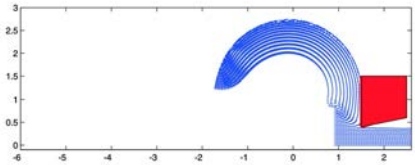
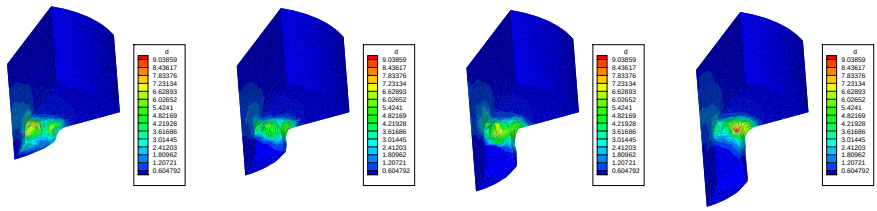


Fig. 3. Simulation of the orthogonal cutting process.

Three-dimensional simulation of the extrusion of a cross-shaped profile. In order to show the capabilities of the technique presented before, we analyze now the simulation of a cross-shaped aluminium profile.

Nodes located on the upper side of the billet were forced to move with a speed of $2\frac{mm}{s}$, in order to obtain an exit velocity of $1\frac{m}{min}$ approximately. Initially, slipping boundary conditions were considered between the billet and the die and the container. The initial temperature was set to $723K$. The whole model was

considered adiabatic, including the profile surface in contact with air. In this case a rigid-plastic Sellars-Tegart material model was used. The simulation ran over 42 time steps of $0.025s$. The obtained evolution for the equivalent strain rate is depicted in Fig. 4.



(a) 10th time step. (b) 20th time step. (c) 30th time step. (d) 40th time step.

Fig. 4. Equivalent strain rate (s^{-1}) for the extrusion simulation.

2.3 Meshless methods in the ESAFORM conferences: past, present and future

These examples are intended for suggesting only the wide range of potential application that meshless methods can have in the field of forming processes. But the applications are by no means limited to the before presented. Other examples include the simulation of expanding foams [16], Stefan problems, etc.

In all these cases, meshless methods opened the possibility for a Lagrangian procedure, which is in some cases a very convenient way of overcoming the before-mentioned problems of numerical diffusion in the results due to extensive remeshing.

Concerning the ESAFORM life, meshless methods have been present, up to our knowledge, since the conference held in Liege in 2001 [33] and their contribution extends up to the ninth ESAFORM conference's scientific prize plenary lecture [19]. In between, many papers have been presented in ESAFORM conferences employing meshless method to simulate forming processes. For instance, there is a very active group in Portugal applying these methods to the simulation of various forming proceses [51]. Applications include forging, sheet metal forming, etc. Other contributions include applications of the so-called eXtended Finite Element Method (X-FEM) [22] [35], or the excellent keynote given by N. Sukumar at Salerno in 2003 [47]. Concerning RKP methods, Joyot has made some interesting contributions along the years, see for instance [27] and references therein. Of course, Prof. Villon has been one of the most active researchers in this field and has presented many works on the topic along the years, see for instance [48].

There remain some interesting challenges concerning meshless methods (both within and out of ESAFORM life). There is a more or less unanimous opinion

that the issue of numerical integration is crucial in this field, and many groups are now focusing their efforts towards this end. Within ESAFORM life, there remains some problems where meshless methods have much to say. In general, these problems involve very large strains, as mentioned before. Friction stir welding is an example of candidate processes. The extremely large speed of rotation, the coupled thermo-mechanical problem and the extremely large deformations appearing make this process an ideal candidate to benchmark the behaviour of meshless methods.

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