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Dynamic mesh refinement for discrete models of jet electro-hydrodynamics

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ABSTRACT

Nowadays, several models of unidimensional fluid jets exploit discrete element methods. In some cases, as for models aiming at describing the electrospinning nanofabrication process of polymer fibers, discrete element methods suffer a non-constant resolution of the jet representation. We develop a dynamic mesh-refinement method for the numerical study of the electro-hydrodynamic behavior of charged jets using discrete element methods. To this purpose, we import ideas and techniques from the string method originally developed in the framework of free-energy landscape simulations. The mesh-refined discrete element method is demonstrated for the case of electrospinning applications.

1. Introduction

Discrete element methods are widely employed to model fluid flows in air channels, pipes and several other applications, such as modeling ink-jet printing processes, electrospinning, spray jets, micro-fluid dynamics in nozzles, etc. [1–5]. In particular, unidimensional jets can be easily modeled as a sequence of discrete elements by defining a mesh of points, which is used to discretize a continuous object (e.g. a liquid body) as a finite sequence of discrete elements. The aim of such model is to provide a relatively simple computational framework based on particle-like ordinary differential equations, rather than on the discretization of the partial differential equations of continuum fluids. Electro-hydrodynamic flows, however, are often subject to strong interactions leading to major deformation of the jet, hence to significant heterogeneities in the spatial distribution of the discrete particle. The latter, in turn, imply a loss of accuracy of the numerical method, since the most stretched portions of the jet become highly under-resolved. One of these cases is the electrospinning process, where a polymeric liquid jet is ejected from a nozzle and accelerated toward a conductive collector by a strong electric field. In this framework, the jet is stretched so that its diameter decreases below the micrometer-scale, providing a one-dimensional structure with very high surface area to volume ratio. This intriguing feature of the resulting polymer nanofibers spawned several papers [6–11] and books [12–14] focussing on the electrospinning process.

In this framework, pioneering works by the Reneker and Yarin groups were focused on developing *ad-hoc* discrete element methods for electrospinning, which describe nanofibers as a series of beads obeying the equations of Newtonian mechanics [1,15]. This modeling approach has gained an important role in predicting the outcome of electrospinning experiments. In addition, such models might support experimental researchers with a likely starting point for calibrating processes in order to save time before subsequent optimization work.

In these models, the excess charge is distributed to each element composing the jet representation, and it is static in the frame of reference of the extruded fluid jet. Once the solution surface tension is overcome by electrical forces at the spinneret, the jet serves as fluid medium to push away the mutually repulsing electric charges from the droplet pending at the nozzle of the apparatus. The main forces affecting the jet dynamics, which are accounted for in such models, include viscoelasticity, surface tension and electrostatic interactions with the external field and among excess charges in the liquid. In particular, the Coulomb repulsion between electric charges triggers bending instabilities in electrically charged jets, as demonstrated by Reneker et al. [15]. Despite being often neglected, air drag and aerodynamic effects, which may also lead to bending instabilities, have been recently modeled by discrete element methods [16–18]. Further, several complex viscoelastic

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models were included in order to simulate viscoelastic Boger fluid solutions [19,20]. Systematic investigations were carried out on several simulations parameters: polymer concentration, solution density, electric potential, and perturbation frequency [21,22].

Notwithstanding a satisfactory, though generally qualitative, agreement with experimental results has been shown [23,24,15], all these methods suffer the non-constant resolution of the jet representation, which usually decreases downstream. Indeed, given a uniform discretization of the initial polymeric drop pending at the nozzle, the initial step of the jet dynamics is characterized by the prevalent viscoelastic force, and it leads to a second regime, when the longitudinal stress changes under the effect of the applied electric voltage, accelerating the jet toward the collector [15]. Hence, a free-fall regime describes the later jet dynamics. Since the longitudinal viscoelastic stress along the fiber is usually larger close to the nozzle, the distance between each discrete element increases as a result of the uniformly accelerated motion, which drives the farthest elements from the spinneret. As a consequence, the jet discretization close the collector becomes rather coarse to model efficiently the filament, and the information (position, velocity, radius, stress, etc.) describing the jet is lost downstream.

A refined description of jet is necessary in every instance where a high-resolution description of physical quantities is requested, such as for bending instabilities, varicose instabilities of diameter, etc. Further, a dense mesh provides a more strict assessment of the Coulomb repulsion term, which is important to properly account the transverse force acting on the jet. Recently, refinement procedures were proposed in few works in order to avoid low resolution problems downstream [25,26]. Nonetheless, these procedures exploit only linear interpolations, and are not able to impose a uniform mesh of jet representation, which is likely the simplest choice to model properly the entire jet, from the nozzle to the collector.

Here, we present an algorithm specifically developed to address the issue. The aim of the algorithm is to recover a finer jet representation at constant time interval, before the information describing the jet is scattered downstream, so as to preserve the jet modeling representation and make the simulation more realistic. Further, the algorithm can be used to enforce several types of mesh depending on the physical quantities under investigation, providing an adaptive description of the process.

The article is organized as follows. In Section 2, we summarize the 3D model for electrospinning, with the set of equations of motion (EOM) which govern the dynamics of system. In Section 3, we present the algorithm, with the relative step for its implementation. In Section 4 we report a numerical example of its application within a discrete element method for electrospinning modeling. Finally, conclusions are outlined in Section 5.

2. Model

In this work, we apply our algorithm to the electrospinning model implemented in JETSPIN, an open-source code specifically developed for electrospinning simulation [23], which is briefly summarized in the following text. The model is an extension of the discrete model originally introduced by Reneker et al. [15]. The main assumption of such model is that the filament can be reasonable represented by a series of n discrete elements (jet beads). Each one of this elements is a particle-like labeled by an index ith. A Cartesian coordinate system is taken so that the origin is located at the nozzle, and x-axis is pointing perpendicularly toward a collector where the nanofiber is deposited. The nozzle is also represented as a particle like (nozzle bead) which can moves on the plane y–z (further details in the following text). Given a fluid jet starting at the nozzle and labeling $i = 0$ the nozzle bead, we obtain the set of beads indexed $i = 0, 1, \ldots, n$, where n denotes the bead of the other extremity of the filament. Thus, given $\vec{r}_i$ the position vector of a generic ith bead, we define the mutual distance between i and $i + 1$ elements

$$l_i = \left|\vec{\mathbf{r}}_{i+1} - \vec{\mathbf{r}}_i\right|. \tag{1}$$

Here, l_i stands for the length step used for discretizing the filament. Note that the length l is typically larger than the filament radius, but smaller than the characteristic lengths of other observables of interest (e.g. jet curvature radius). Denoted m_i the mass, t the time, and $\vec{\boldsymbol{\upsilon}}_i$ the velocity vector of ith bead, its acceleration is given by Newton's law

$$\frac{d\vec{\boldsymbol{\upsilon}}_i}{dt} = \frac{\vec{\mathbf{f}}_{tot,i}}{m_i}, \tag{2}$$

where $\vec{\mathbf{f}}_{tot,i}$ is the total force acting on ith bead, given as a sum of several terms

$$\vec{\mathbf{f}}_{tot,i} = \vec{\mathbf{f}}_{el,i} + \vec{\mathbf{f}}_{c,i} + \vec{\mathbf{f}}_{\upsilon e,i} + \vec{\mathbf{f}}_{st,i}. \tag{3}$$

In last equation, $\vec{\mathbf{f}}_{el,i}$ stands for the electric force due to the external electrical potential Φ_0 imposed between the nozzle and the collector located at distance h along versor $\vec{\mathbf{x}}$, and given as

$$\vec{\mathbf{f}}_{el,i} = q_i \frac{\Phi_0}{h} \cdot \vec{\mathbf{x}}. \tag{4}$$

Denoted q_i the charge of ith bead, the net Coulomb force $\vec{\mathbf{f}}_c$ is

$$\vec{\mathbf{f}}_{c,i} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{q_i q_j}{\left|\vec{\mathbf{r}}_j - \vec{\mathbf{r}}_i\right|^2} \cdot \vec{\mathbf{u}}_{ij} \tag{5}$$

acting on the ith bead and originated from all the other jth beads. Further, we denote $\vec{\mathbf{f}}_{st}$ the surface tension force

$$\vec{\mathbf{f}}_{st,i} = k_i \cdot \pi \left(\frac{a_i + a_{i-1}}{2}\right)^2 \alpha \cdot \vec{\mathbf{c}}_i, \tag{6}$$

acting on ith bead toward the center of the local curvature (according to $\vec{\mathbf{c}}_i$ versor) to restore the rectilinear shape of the jet, given α the surface tension coefficient, a_i the jet radius, and k_i the local curvature (measured at ith bead). Finally, $\vec{\mathbf{f}}_{\upsilon e}$ stands for the viscoelastic force

$$\vec{\mathbf{f}}_{\upsilon e,i} = -\pi a_i^2 \sigma_i \cdot \vec{\mathbf{t}}_i + \pi a_{i+1}^2 \sigma_{i+1} \cdot \vec{\mathbf{t}}_{i+1}, \tag{7}$$

pulling bead i back to $i - 1$ and toward $i + 1$, with σ the stress and $\vec{\mathbf{t}}_i$ the unit vector pointing bead i from bead $i - 1$. The polymeric jet is assumed as a viscoelastic Maxwellian liquid so that σ evolves in time following the constitutive equation:

$$\frac{d\sigma_i}{dt} = \frac{G}{l_i}\frac{dl_i}{dt} - \frac{G}{\mu}\sigma_i, \tag{8}$$

where G is the elastic modulus, and μ is the viscosity of the fluid jet.

Finally, the velocity $\vec{\boldsymbol{\upsilon}}_i$ satisfies the kinematic relation:

$$\frac{d\vec{\mathbf{r}}_i}{dt} = \vec{\boldsymbol{\upsilon}}_i. \tag{9}$$

The set of three Eqs. (2), (8) and (9) governs the time evolution of system.

The nozzle bead with charge $\bar{q}_0$ and $x_0 = 0$ is experiencing uniform circular motion in order to model fast mechanical oscillations of the spinneret [21], where we denote A the amplitude of the perturbation and ω its frequency.

The initial simulation conditions as well as the jet insertion at the nozzle are briefly described in the following. We assume that all the electrospinning simulations start with a single jet bead, which

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