Numerical Modeling of Electrospinning

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Application & Technology

Applications

Their very large surface-to-volume ratios make nano-sized fibers especially suitable for:

- Nano-biotechnology, tissue engineering, chemical catalysts, electronic devices
- Bio-active fibers: catalysis of tissue cells growth
- New composite materials
- Thin materials: solar and light sails, ...

Technologies

- Air-blast atomization
- Pulling from melts
- Electrospinning of polymers and melts

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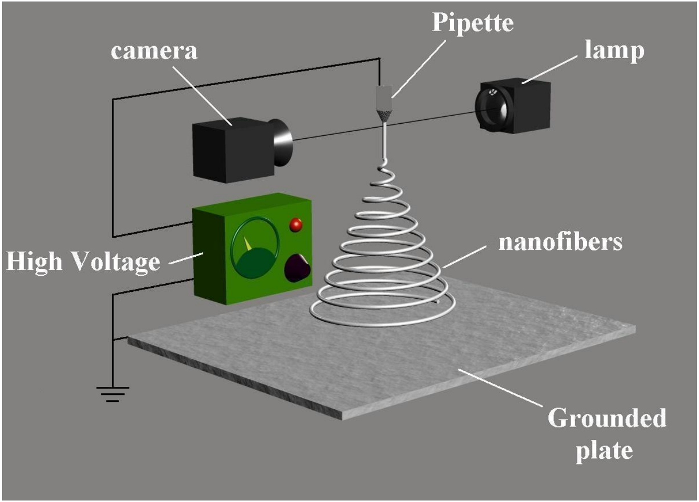
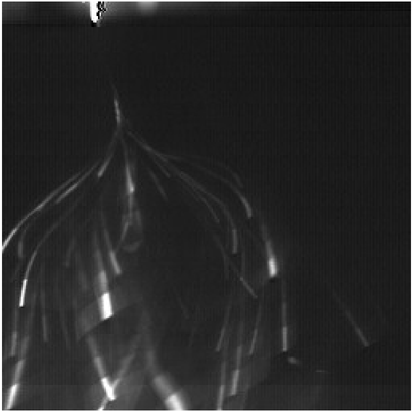
Electrospinning setup

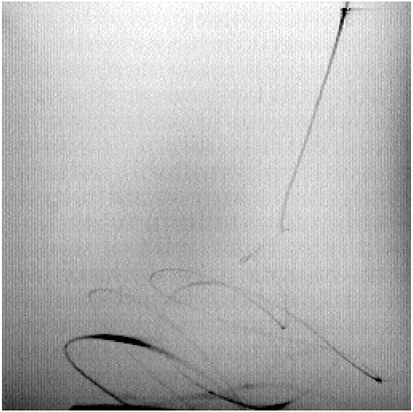


Electrospinning of PEO



Low frame rate video (30 fps)

Electrospinning of PEO

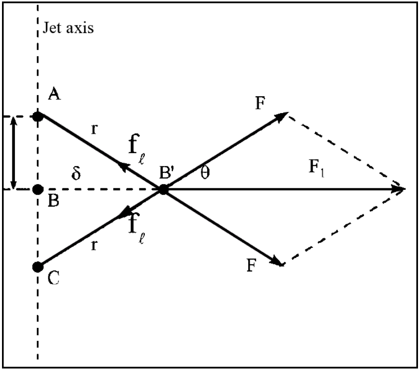


Fast frame rate video (4500 fps)

The electrostatic instability

Earnshaw's theorem

"A collection of point charges cannot be maintained in a stable stationary equilibrium configuration solely by the electrostatic interaction of the charges"

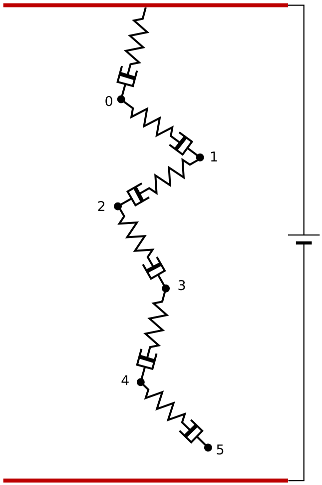


D. H. Reneker, A. Yarin *et al.* (2000)

Main assumptions

Main assumptions

- The background electric field created by the generator is considered static
- The fiber is a perfect insulator
- The polymer solution is a viscoelastic medium with constant elastic modulus, viscosity and surface tension



Governing equations (1/3)

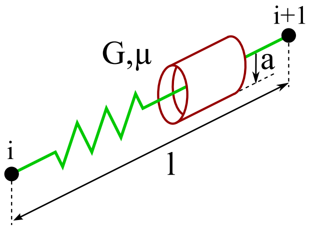
Governing equations for each bead

- Mass conservation:

$$\frac{d}{dt}\left(\pi a^2 l\right) = 0$$

- Stress balance:

$$\frac{d\sigma}{dt} = G\frac{1}{l}\frac{dl}{dt} - \frac{G}{\mu}\sigma$$



a: fiber radius

l: bead length

σ: longitudinal stress

G: Young modulus

μ: viscosity

Governing equations (2/3)

Momentum conservation for charges

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \sum_{j \neq i} q_j \kappa \frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^3}$$

v: velocity vector
m: mass
q: electric charge
κ: Coulomb constant
r: position vector
E: electric field
a: bead radius
σ: longitudinal stress

External forces

- Coulomb forces
- Electric force
- Mechanical forces

Governing equations (2/3)

Momentum conservation for charges

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \sum_{j \neq i} q_j \kappa \frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^3} + q_i \mathbf{E}$$

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m: mass
q: electric charge
κ: Coulomb constant
$\mathbf{r}$: position vector
$\mathbf{E}$: electric field
a: bead radius
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External forces

- Coulomb forces
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Governing equations (2/3)

Momentum conservation for charges

$$
\begin{aligned}
m_i \frac{d\mathbf{v}_i}{dt} &= q_i \sum_{j \neq i} q_j \kappa \frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^3} \\
&+ q_i \mathbf{E} \\
&+ \pi a_{i,i+1}^2 \, \sigma_{i,i+1} \frac{\mathbf{r}_{i+1} - \mathbf{r}_i}{\left|\mathbf{r}_{i+1} - \mathbf{r}_i\right|} \\
&- \pi a_{i-1,i}^2 \, \sigma_{i-1,i} \frac{\mathbf{r}_i - \mathbf{r}_{i-1}}{\left|\mathbf{r}_i - \mathbf{r}_{i-1}\right|}
\end{aligned}
$$

$\mathbf{v}$: velocity vector

m: mass

q: electric charge

κ: Coulomb constant

$\mathbf{r}$: position vector

$\mathbf{E}$: electric field

a: bead radius

σ: longitudinal stress

External forces

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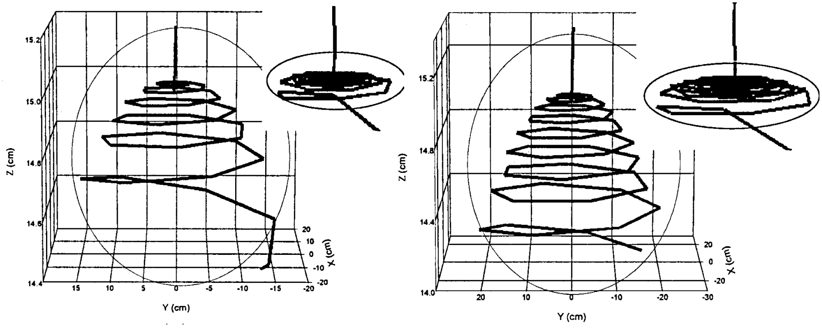
Governing equations (3/3)

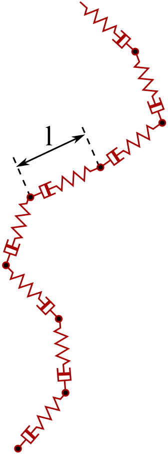
Boundary conditions

- A small initial perturbation is added to the position of the first bead (“rotating tip”)
- The background electric field is axial and uniform
- The first bead is described by a stationary equation

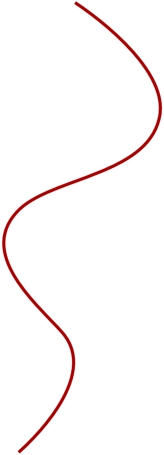
Typical results



But ...is the discretization consistent?



$$\lim_{l \to 0} = ?$$



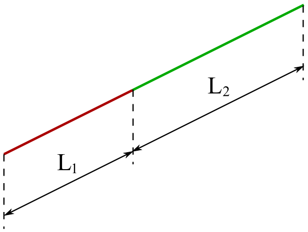
The 1D discretized model is not consistent

...because the limit continuous model is itself inconsistent

Electrostatic force exerted by a fiber portion of length L_1 on a contiguous fiber portion of length L_2, assuming a constant linear charge density q_l:

$$F_{1\to 2} = \int_{-L_1}^{0} dz_1 \int_{0}^{L_2} dz_2 \frac{\kappa q_l^2}{(z_2 - z_1)^2}$$

$$= \infty \, !!!$$

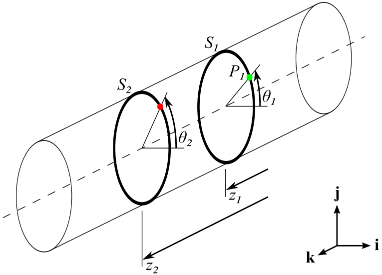


Effect of surface charges (1/2)

Introduction of "ring-charges"

The 1D discrete model assumes point-charges. In reality, charges migrate to the surface of the fiber.

$\Longrightarrow$ Coulomb forces on neighboring “ring-charges” are weaker than for point-charges.



$$dF_{S_2 \to S_1} = -\kappa \frac{dQ_1 dQ_2}{(z_2 - z_1)^2} \times \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \frac{d\psi}{\left[1 + \left(\frac{2a}{z_2 - z_1}\right)^2 \sin^2 \psi\right]^{3/2}},$$

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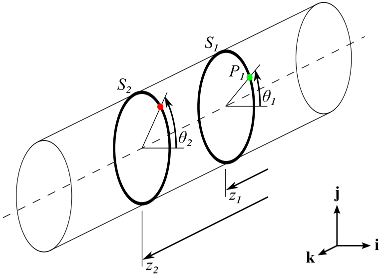

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Effect of surface charges (2/2)

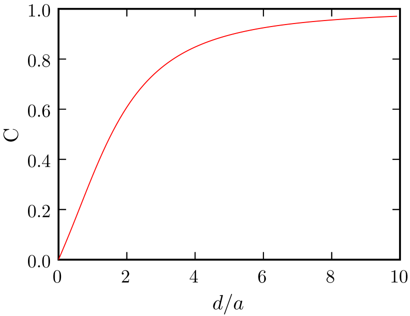
Behavior of short-range cutoff

The former result can be generalized to a weakly curved fiber ($R \gg a$), replacing $z_2 - z_1$ by the distance d between ring centers:

$$C = \frac{2}{\pi}\int_0^{\frac{\pi}{2}} \frac{d\psi}{\left[1+\left(\frac{2a}{d}\right)^2 \sin^2\psi\right]^{3/2}}$$

$$= \overset{d\to 0}{\sim} \frac{d}{\pi a}$$

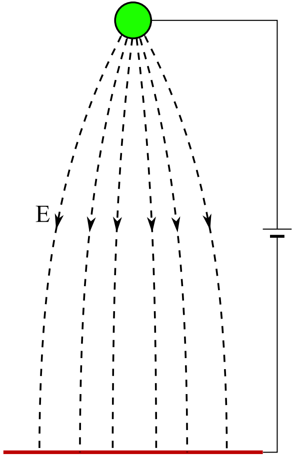
$\Longrightarrow$ the longitudinal stress due to Coulomb forces becomes finite



Governing equations and BCs

Differences with D. H. Reneker's model

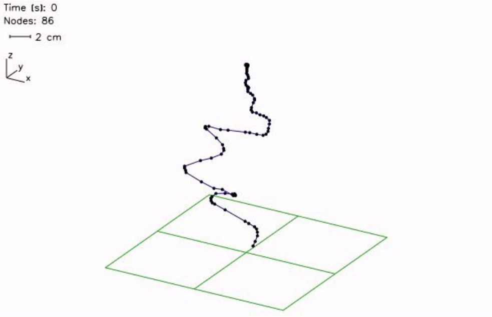
- Random perturbation of the initial position
- 3D surface tension effects
- Sphere-plate capacitor configuration for the background field $\Longrightarrow$
- No evaporation



Simulations

Reference case

$$\rho = 1000\,\mathrm{kg \cdot m^{-3}}$$
$$a_0 = 150\,\mu\mathrm{m}$$
$$h = 20\,\mathrm{cm}$$
$$d_0 = 1\,\mu\mathrm{m}$$
$$q_e = 200\,\mathrm{C \cdot m^{-3}}$$
$$Q_v = 3.6\,\mathrm{cm \cdot h^{-1}}$$
$$\Phi = 5000\,\mathrm{V}$$
$$\mu = 10\,\mathrm{Pa \cdot s}$$
$$G = 0.1\,\mathrm{MPa}$$
$$\alpha = 0.07\,\mathrm{N \cdot m^{-1}}$$



$\alpha \times 3$

$\alpha/3$

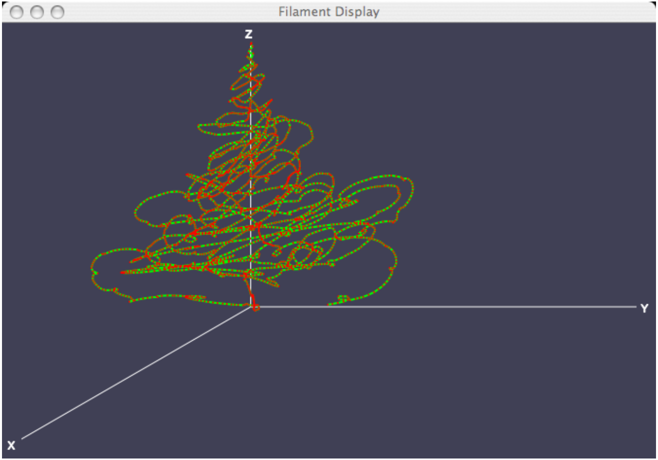
$\Phi/2$

$\mu \times 5$

$G \times 2$

$G/2$

Simulations results from ORNL



Courtesy of Srdjan Simunovic

Open issues

Issues with the physical model

- Very idealized rheological model
- No electrical conduction
- No evaporation
- ...

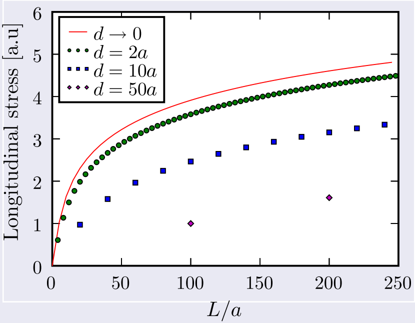
Issues with the numerics

- Coulomb forces are computed pairwise
  $\Longrightarrow N^2$ problem
- Inefficient mathematical discretization for coarse meshes
- Accuracy worsens as beads elongate
- ...

Mathematical discretization

Discretization error

Computed Coulomb stress in the middle section of a fiber of length L, using beads of length d.



Possible solutions

- For close Coulomb interactions, use the exact solution for weakly bent fibers with constant radius
- Dynamic mesh refinement by dichtotomic splitting of long beads

Fast Coulomb interaction computation

Main idea

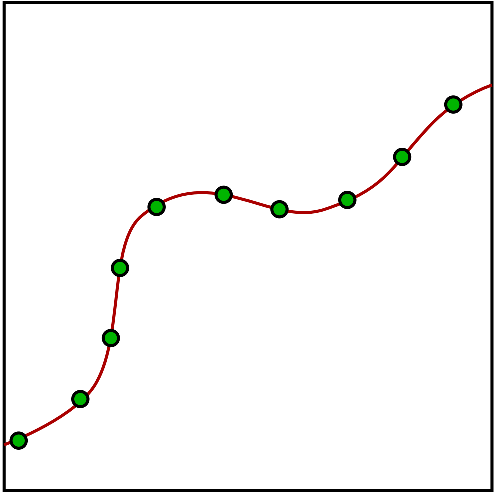
Solve a N-body force problem in less than $\mathcal{O}\left(N^2\right)$ by clustering the N bodies into a smaller number of "super"-bodies of various sizes.

The acceptable error defines the largest cluster to be used in computations.

Available methods

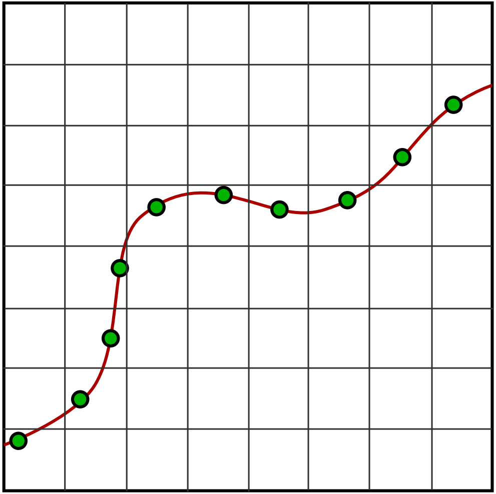
- Barnes-Hut Algorithm
  $\mathcal{O}\left(N \ln N\right)$
  Simple implementation
- Fast Multipole Method
  $\mathcal{O}\left(N\right)$
  Implementation is intricate, not very efficient for naturally clusterized bodies

Barnes-Hut Algorithm



- Discretize at particle level
- Discretize at level 2
- Discretize at level 3
- Discretize at top level
- Determine interacting clusters

Barnes-Hut Algorithm



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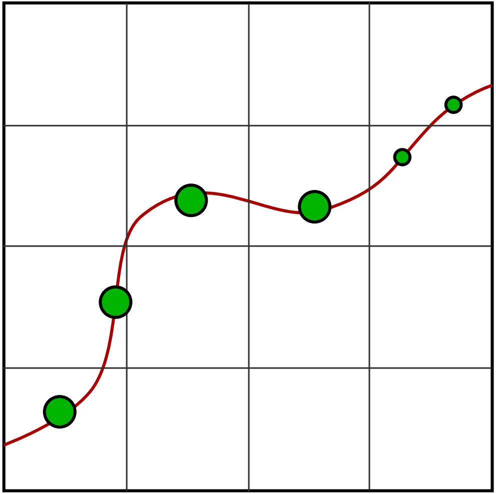

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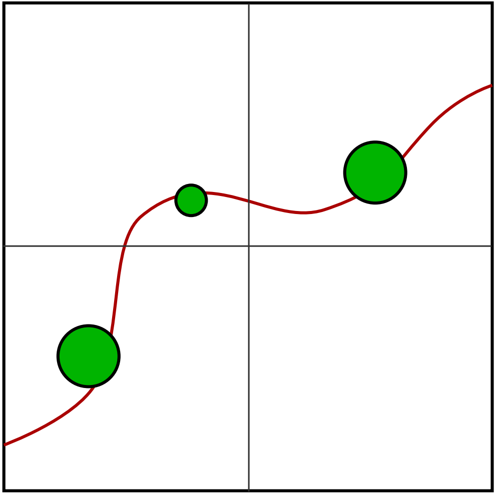

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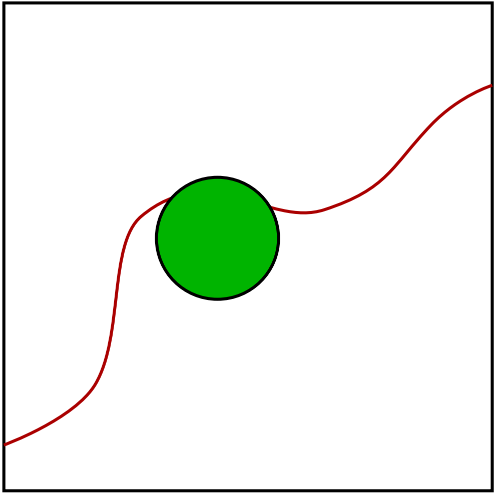

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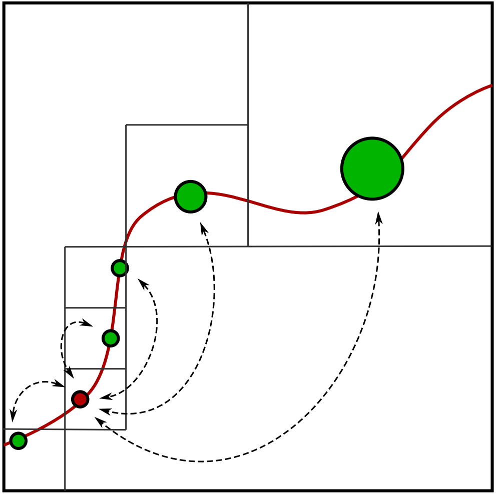

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