

Microstructure simulation of early paper forming using immersed boundary methods

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ABSTRACT: Paper forming is the first step in the paper machine where a fiber suspension leaves the headbox and flows through a forming fabric. Complex physical phenomena occur as the paper forms, during which fibers, fillers, fines, and chemicals added to the suspension interact. Understanding this process is important for the development of improved paper products because the configuration of the fibers during this step greatly influences the final paper quality. Because the effective paper properties depend on the microstructure of the fiber web, a continuum model is inadequate to explain the process and the properties of each fiber need to be accounted for in simulations. This study describes a new framework for microstructure simulation of early paper forming. The simulation framework includes a Navier-Stokes solver and immersed boundary methods to resolve the flow around the fibers. The fibers were modeled with a finite element discretization of the Euler-Bernoulli beam equation in a co-rotational formulation. The contact model is based on a penalty method and includes friction and elastic and inelastic collisions. We validated the fiber model and the contact model against demanding test cases from the literature, with excellent results. The fluid-structure interaction in the model was examined by simulating an elastic beam oscillating in a cross flow. We also simulated early paper formation to demonstrate the potential of the proposed framework.

Application: This unique modeling approach for microstructure simulation of early paper forming can increase the fundamental understanding of paper forming and support process optimization.

Paper forming is the first step in the paper machine where a fiber suspension leaves the headbox and flows through a forming fabric. The water flows through the holes of the forming fabric and a fiber web is gradually built up. The water content decreases during this process from approximately 98% to roughly 80%. Complex physical phenomena occur during paper forming as a result of the interaction between fibers, fillers, fines, and chemicals added to the suspension. Furthermore, the forming fabric moves with high speed relative to the paper machine. Understanding paper forming is important for the development of improved paper products, because the orientation and distribution of fibers during this step have a large influence on the final paper quality. Because the effective paper properties depend on the microstructure of the fiber web, a continuum model is inadequate and the properties of each fiber need to be accounted for in the simulations.

Simulation of paper forming is particularly challenging because it involves transient fluid flow with many immersed solid objects subjected to large displacements. The fibers are buoyant, which results in strong coupling between the fluid and the fibers. Immersed boundary methods (IBMs) are well suited for this type of application because they allow the flow around the immersed objects to be resolved without the need of a body-fitted mesh. The original IBM developed by Peskin [1] is first order accurate in space and enforces the boundary condition explicitly with a force. Mohd-Yusof [2,3] devel-

oped a second order accurate, explicit momentum forcing method. Majumdar and coworkers [4] developed an implicit IBM. Because this method has potential problems with oscillations in the solution, Mark and coworkers [5] developed a second order accurate hybrid IBM.

Different methods for simulation of fiber suspensions are described in the literature. Yamamoto and Matsuoka [6] modeled a fiber as a chain of spheres connected with springs. Ross and Klingenberg [7] attempted to reduce computation times by modeling a fiber as a chain of prolate spheroids, thus allowing a fiber to be modeled with fewer elongated bodies. Lindström [8] developed a model in which a fiber is treated as a chain of rigid rods and used the model to study paper forming. This model includes contacts between fibers and two-way coupling between the fibers and the fluid. However, the flow around the fibers is not resolved. The model proposed by Lindström is not based on a beam theory; the derivation starts with Newton's second law and expressions for the bending moments in the joints are inserted.

Understanding the phenomena occurring on the length scale of a single fiber requires direct numerical simulations (DNS) that resolve the flow around every fiber. Furthermore, the fiber model should be based on a rigorous beam theory. Therefore, an implementation of more accurate methods is necessary. In our study, we used immersed boundary methods to resolve the flow around the fibers. The fibers are modeled

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as Euler-Bernoulli beams in a co-rotational formulation and discretized with the finite element method. We solve the non-linear system of equations with Newton's method and use Hilber's α -method for the temporal discretization. The fiber-fiber and fiber-fabric contacts are modeled with a penalty method and elastic/inelastic contacts, and friction also is taken into account.

We validated the fiber model and the contact model against demanding cases described in the structural mechanics literature. We investigated the interaction between a slender object and a fluid by simulating a flexible beam in a cross flow and conducted a paper forming simulation.

GOVERNING EQUATIONS

Fluid model

The motion of the fluid is governed by the Navier-Stokes equations:

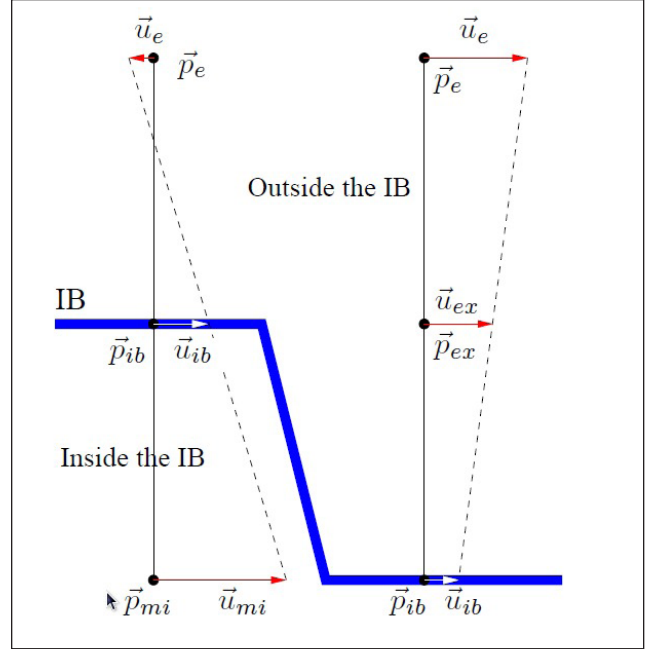
$$\begin{aligned} \nabla \cdot \vec{u} &= 0 \\ \rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \cdot \nabla \vec{u} &= -\nabla p + \mu \nabla^2 \vec{u} \end{aligned} \quad (1)$$

where $\vec{u}$ is the fluid velocity, ρ_f is the fluid density, p is the pressure, and μ is the dynamic viscosity. We used IBOFlow (immersed boundary octree flow solver) developed at FCC (Fraunhofer-Chalmers Centre; Gothenburg, Sweden) to solve the incompressible Navier-Stokes equations. A finite volume discretization was used and the immersed boundary method was used to model the presence of arbitrary moving objects in the flow. The solver uses a Cartesian octree grid that can be dynamically refined and coarsened, enabling adaptive grid refinements to follow moving bodies. The octree grid allows grid refinements to be created without deterioration of the mesh quality. The Navier-Stokes equations were solved in a segregated way and the velocity and pressure fields were coupled with the SIMPLEC [9] method. All variables were stored in a co-located arrangement and Rhie-Chow interpolation [10] was used to prevent pressure oscillations.

The forming fabrics we studied have complex geometries that cannot be described analytically. The geometries are described numerically by voxelizations generated with GeoDict software (Fraunhofer ITWM; Kaiserslautern, Germany). These voxelizations are used to set boundary conditions on the fluid and to detect collisions between the fibers and the forming fabric. The voxelizations are based on CAD geometries from Albany International (Halmstad, Sweden).

Fluid-structure coupling

IBM can be used to study the flow around arbitrary moving objects without the need of a body-fitted mesh. In our study, we used the hybrid IBM [5] to model the presence of fibers in the flow. This method extends the mirroring IBM [11,12] by adding extrapolation points at the immersed boundary. Application of the IBM requires that a cell type is assigned to each cell in the fluid domain. The cells are marked as fluid cells,



1. Two-dimensional visualization of an immersed boundary.

internal cells, mirroring cells, or extrapolation cells, depending on the position relative to the immersed boundary.

The velocity in the internal cells is set to the velocity of the immersed object with a Dirichlet boundary condition. For the mirroring cells, an exterior normal point $\vec{p}_e$ is defined as [5]:

$$\vec{p}_e = \vec{p}_{mi} + 2.0(\vec{p}_{ib} - \vec{p}_{mi}) \quad (2)$$

where $\vec{p}_{mi}$ is the center of the mirroring cell and $\vec{p}_{ib}$ is the closest point on the immersed boundary. For extrapolation cells, an exterior point is defined as:

$$\vec{p}_e = \vec{p}_{ib} + 2.0(\vec{p}_{ex} - \vec{p}_{ib}) \quad (3)$$

where $\vec{p}_{ex}$ is the cell center of the extrapolation cell. **Figure 1** illustrates the definition of these points.

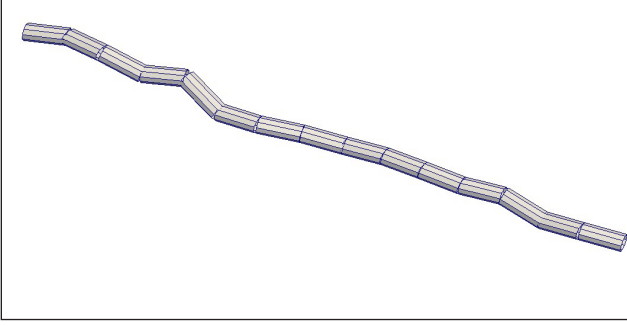
The boundary condition for a mirroring cell is:

$$\frac{\vec{u}_{mi} + \vec{u}_e}{2} = \vec{u}_{ib} \quad (4)$$

The boundary condition for an extrapolation cell takes the following form:

$$\frac{\vec{u}_{ib} + \vec{u}_e}{2} = \vec{u}_{ex} \quad (5)$$

The velocity in the point $\vec{p}_e$ is interpolated and inserted into the immersed boundary condition. As a result, Eqs. (4) and (5) become implicit boundary conditions which can be added to the operator for the momentum equations. This results in a fictitious fluid velocity field inside the immersed



2. A typical fiber divided into several elements.

object. Mass conservation is ensured by excluding the fictitious velocity field in the discretized continuity equation. The result is a robust method that is second order accurate in space [5,12].

Fiber model

The fibers are modeled as slender beams with hollow elliptical cross section. The strong form of the equations of motion for a beam are given in [13]:

$$\begin{aligned}\frac{\partial \vec{k}}{\partial t} &= \vec{f}_{ext} + \frac{\partial}{\partial x} \left(\underline{\underline{E}} \cdot \vec{f}_{int} \right) \\ \frac{\partial \vec{\pi}}{\partial t} &= \vec{m}_{ext} + \frac{\partial \vec{r}}{\partial x} \times \left(\underline{\underline{E}} \cdot \vec{f}_{int} \right) + \frac{\partial}{\partial x} \left(\underline{\underline{E}} \cdot \vec{m}_{int} \right)\end{aligned}\quad (6)$$

Following the notation in [13], $\vec{k}$ is the linear momentum and $\vec{\pi}$ is the angular momentum, $\vec{f}_{ext}$ is the externally applied body force, $\vec{m}_{ext}$ is the externally applied body moment, $\underline{\underline{E}}$ is the transformation from local to global coordinates, $\vec{f}_{int}$ is the internal force in a point, and $\vec{m}_{int}$ is the internal moment in a point.

The equations governing the motion of the fibers are discretized with the finite element method. A fiber is discretized by dividing it into several elements (**Fig. 2**) and each element is associated with two nodes, a node at the start point and a node at the end point. Every node has six degrees of freedom: translation in three directions and rotation about three axes. Hence, a beam element has 12 degrees of freedom. A local coordinate system is fixed to each element, and this coordinate system is defined in such a way that the local $\vec{e}_x$ axis is always aligned with the centerline of the element. The $\vec{e}_y$ and $\vec{e}_z$ axes are perpendicular to the centerline. The effect of large rotations is included with the method of co-rotational frames as described by Nour-Omid and Rankin [14,15].

The essence of this method is that the linear finite element model is formulated in a coordinate system that moves with the element. In this way, geometric nonlinearities are included through the motion of the coordinate system. The inertia terms are computed as described by Crisfield et al. [13] and the bending terms are computed according to the Euler-Bernoulli beam theory. The nonlinear system of equations is solved with Newton's method and Hilber's α -method is used

for the temporal discretization.

The contacts are modeled with a penalty method. Elastic and inelastic collisions are modeled by introducing the coefficient of restitution directly into the expression for the normal force as suggested by Harmon [16]. Friction is modeled with a square root regularization of Coulomb's law as described by Wriggers [17].

NUMERICAL RESULTS

To validate the implementation of the beam model, large amplitude oscillations of an L-shaped cantilever beam are studied. The contact model is validated by simulation of a tumbling rod impacting a table. Comparisons are made with results from the literature. The fluid-structure coupling is examined by simulation of a flexible beam oscillating in a cross flow. A comparison is made with a simplified one-way coupling simulation and a Fourier series expansion of the Euler-Bernoulli beam equation.

The physics of paper forming is very complex; therefore, we could not validate all important phenomena with a single test case. The purpose of the first three test cases is to validate the fundamental physical phenomena separately rather than trying to validate the whole process at the same time. Finally, a paper forming test case is simulated.

Oscillation of an L-shaped beam

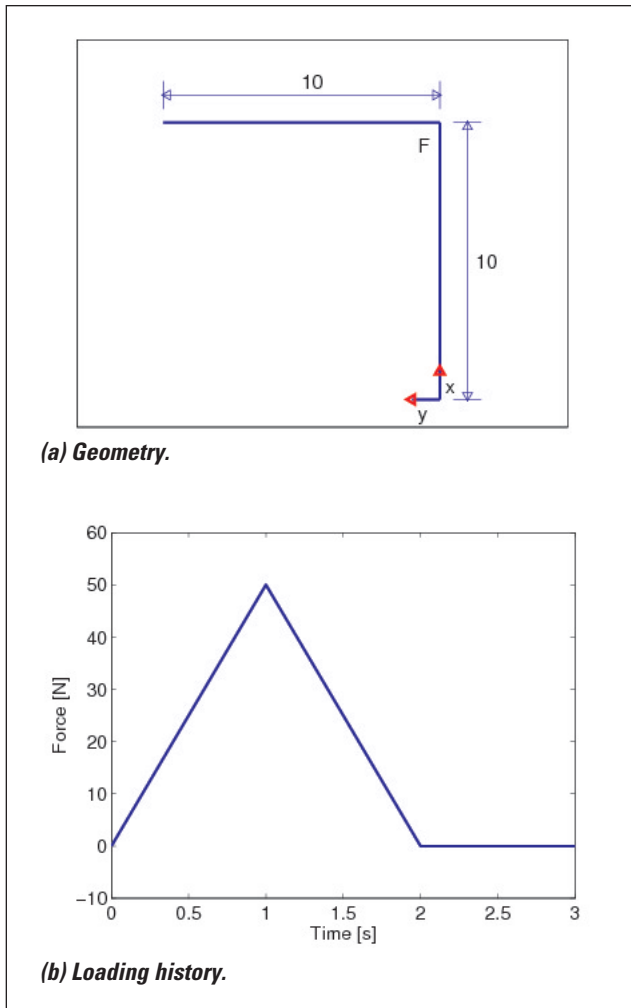
The first test case investigates the dynamic response of an elastic beam and has been studied by several authors. Simo and Vu-Quoc [18] analyzed the case with a fully nonlinear, geometrically exact finite strain beam model. It was later studied by Ibrahimbegović and Mikdad [19], who used a geometrically exact beam model based on the Reissner beam theory. In this case, the L-shaped cantilever beam shown in **Fig. 3** was studied. A point force is applied in the out-of-plane direction at the elbow. Figure 3 also shows the time history of the force, which has a maximum value of 50 N and is applied for 2 s. The cross section of the beam has the following properties:

- $GA_y = GA_z = EA = 10^6$ N
- $EI_y = EI_z = GJ = 10^3$ Nm²
- $A\rho = 1$ kg/m
- $I\rho_x = 20$ kg/m
- $I\rho_y = I\rho_z = 10$ kg/m

The beam is discretized with 20 elements and a time step size of $\Delta t = 0.25$ s is used.

The beam is initially at rest and starts to deflect when the external force is applied. After the force has been removed, the structure performs free vibrations with large magnitude. The amplitude of the vibration is of the same order of magnitude as the length of the structure [18,19]. Therefore, this case is a good test of the model's capability of handling transient problems involving large rotations and displacements.

Figure 4 shows the z-displacement of the elbow and the tip as a function of time. Values predicted by Ibrahimbegović and Mikdad [19] and by Simo and Vu-Quoc [18] are shown for

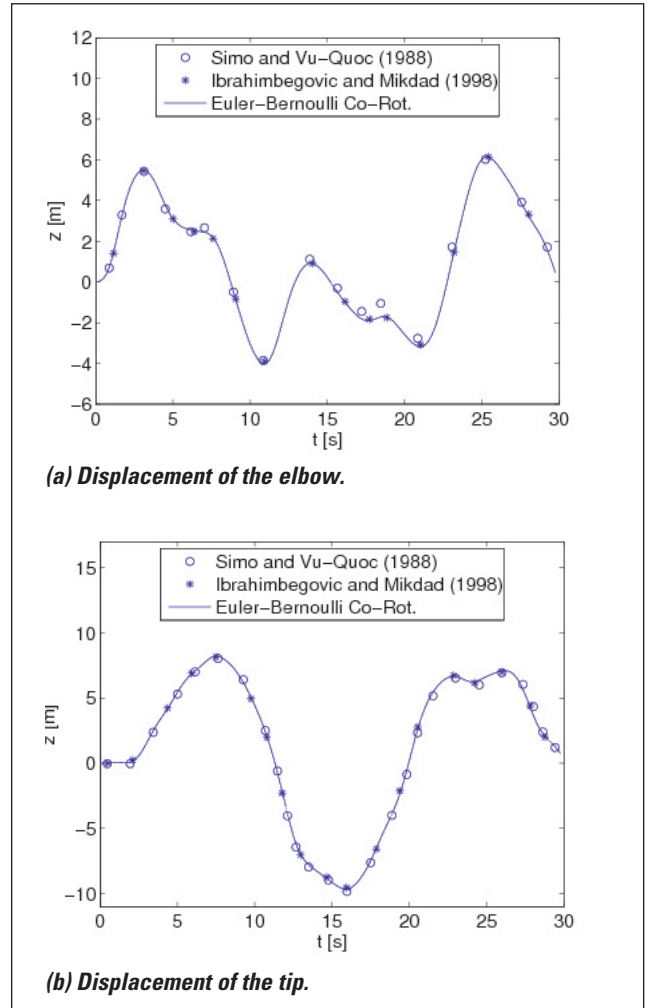


3. The L-shaped beam considered in the first test case.

comparison. The agreement is very good even though different beam models were used in our study and the reference solutions [18,19]. The results shown in Fig. 4 were obtained with the same time step size as used by Simo and Vu-Quoc: $\Delta t = 0.25$ s, but 20 elements were used for the spatial resolution. The solution presented by Simo and Vu-Quoc was obtained with 10 elements with quadratic base functions; however, those authors did not investigate whether the solution obtained was grid-independent or not. This lack of grid-independency is probably the reason for the discrepancy observed for the deflection of the elbow at $t = 17$ s. The results from our study agree well with the results predicted by Ibrahimbegović and Mikdad, although slightly different results are given by Simo and Vu-Quoc.

Impact of tumbling rod

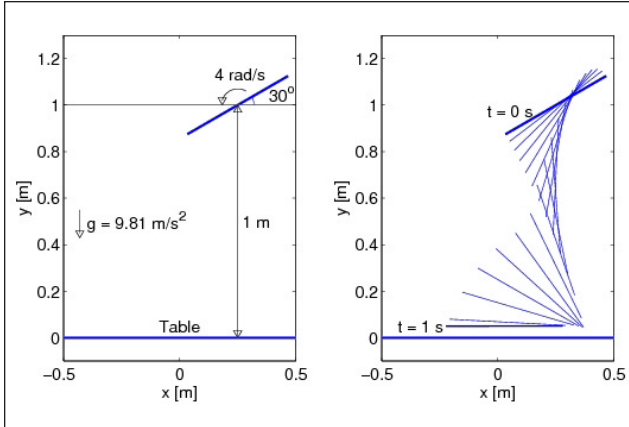
The second test case is a tumbling rod falling onto a table. This case, which involves friction and inelastic contact, was previously studied by Stewart and Trinkle [20]. The rod shown to the left in **Fig. 5** is released from a height of 1 m with an angle of 30° to the horizontal. Initially, the center of



4. Out-of-plane displacement of an oscillating beam.

mass of the rod has no translational velocity, but the initial angular velocity is 4 rad/s about the center of mass. Gravity causes the rod to fall downwards and impact the rigid table located at $y = 0$. The purpose of this simulation example is to make a comparison with the results presented by Stewart and Trinkle [20]. The coefficient of friction for the contact between the rod and the table is therefore set to $\mu_{fr} = 0.6$, which is the same value as used by Stewart and Trinkle [20]. The impacts are considered to be inelastic with $e_{cor} = 0$. The length of the rod, excluding the rounded ends, is $l = 0.5$ m and it has a radius of $r = 0.05$ m. The mass of the rod is 1 kg and its moment of inertia with respect to the center of gravity is $J = 0.002$ kgm². Stewart and Trinkle studied a rigid rod. The code developed in our study deals with elastic applications and cannot simulate perfectly rigid objects. Instead, the rod was meshed with one element and the material parameters of steel were used ($E = 210$ GPa, $\nu = 0.3$). In this way, the rod will behave as almost rigid in the simulations.

The initial angular velocity causes the rod to rotate as it falls toward the table. The rod impacts the table with one of its ends and continues to rotate towards the table with its



5. Geometry of a rod impacting a table (left) and the location of the rod at different instants in time (right).

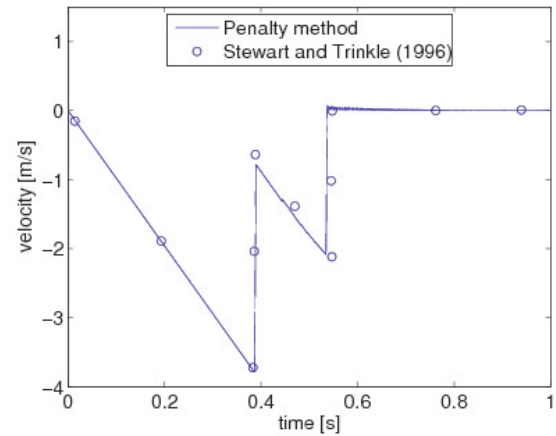
other end. Eventually the other end hits the table and the rod comes to rest. Figure 5 (right) shows the centerline of the rod at different instants in time as it falls towards the table. Note that the rod has a radius of $r = 0.05$ m and, therefore, the centerline of the rod stops at a distance of 0.05m from the table.

Figure 6 shows a comparison with the results given by Stewart and Trinkle [20]. The agreement between the penalty method used in the present work and the reference solution is good. Note that this good agreement was achieved even though a regularization of Coulomb's law was used in this simulation.

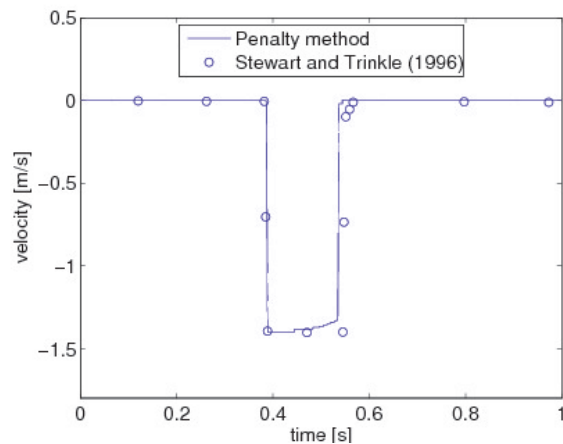
Oscillating beam in cross flow

The first fluid-structure interaction test case investigates the interaction between a fluid flow and a slender structure. An elastic beam is clamped at the wall in a domain filled with a Newtonian, incompressible fluid. The beam is initially at rest, but the forces from the fluid cause the beam to deflect and start oscillating. These oscillations are gradually damped out by the fluid and a wake develops as a result of the presence of the beam. The case has been studied with three methods: a DNS with two-way coupling, a simulation with one-way coupling, and a Fourier series expansion.

The beam is surrounded by water with viscosity $\mu_f = 10^{-3}$ Pas and density $\rho_f = 1000$ kg/m³. The fluid domain is bounded by its lower corner $\vec{p}_{lc} = (0,0,0)$ and its upper corner $\vec{p}_{uc} = (0.5, 3.0, 1.0)$ mm. The beam is made of a linear elastic material with Young's modulus $E = 10^7$ Pa and Poisson's ratio $\nu_s = 0.3$. The density of the beam material is $\rho_s = 5000$ kg/m³. The beam has a circular cross section and its geometry is defined by the start point $\vec{p}_s = (0,1.0, 0.5)$ mm, the end point $\vec{p}_e = (0.15, 1.0, 0.5)$ mm and the radius $r = 0.010$ mm. Fifteen elements are used for the discretization of the beam. The time step length was set to $\Delta t = 0.3125$ μ s, resulting in a Courant-Friedrichs-Lewy (CFL) number of roughly 0.5 on the finest grid. The end time of the simulation was set to $t_{end} = 2$ ms and the inlet velocity was set to $v_{in} = (0,1,0)$ m/s. **Figure 7** shows the fluid boundary



(a) Vertical velocity.



(b) Horizontal velocity.

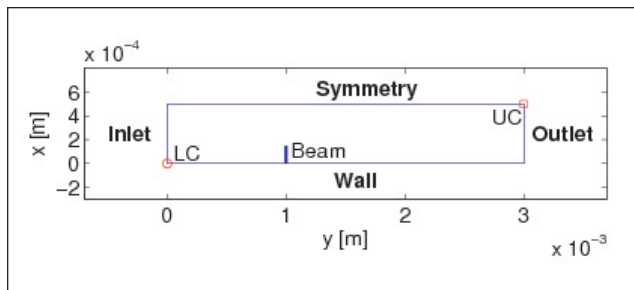
6. Velocity of a rod impacting a table, sampled at the center of mass of the rod.

conditions and the location of the beam. Symmetry boundary conditions are used on the z^- and z^+ surfaces.

We performed simulations with several different grids and monitored the deflection of the beam tip. The beam was kept fixed for the first 10^{-4} s in all the simulations to allow the boundary layer around the beam to develop. Five different grids were used, ranging from three refinements and $2.8 \cdot 10^4$ cells to six grid refinements and $2 \cdot 10^5$ cells. The first order upwind scheme was used for the convective terms and the implicit Euler scheme was used for the temporal discretization in the fluid simulation. DNS were performed; hence, no turbulence model was used. Hilber's α -method with $\alpha = -0.05$ was used for the temporal discretization of the finite element equations describing the motion of the beam.

We also studied the oscillation of a beam in a fluid with modal analysis. We computed a Fourier series expansion of the Euler-Bernoulli beam equation and included the influence of the surrounding fluid as a distributed load under the assumption of one-way coupling. The flow field was assumed

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7. Fluid domain seen in z^+ direction. LC = lower corner, UC = upper corner.

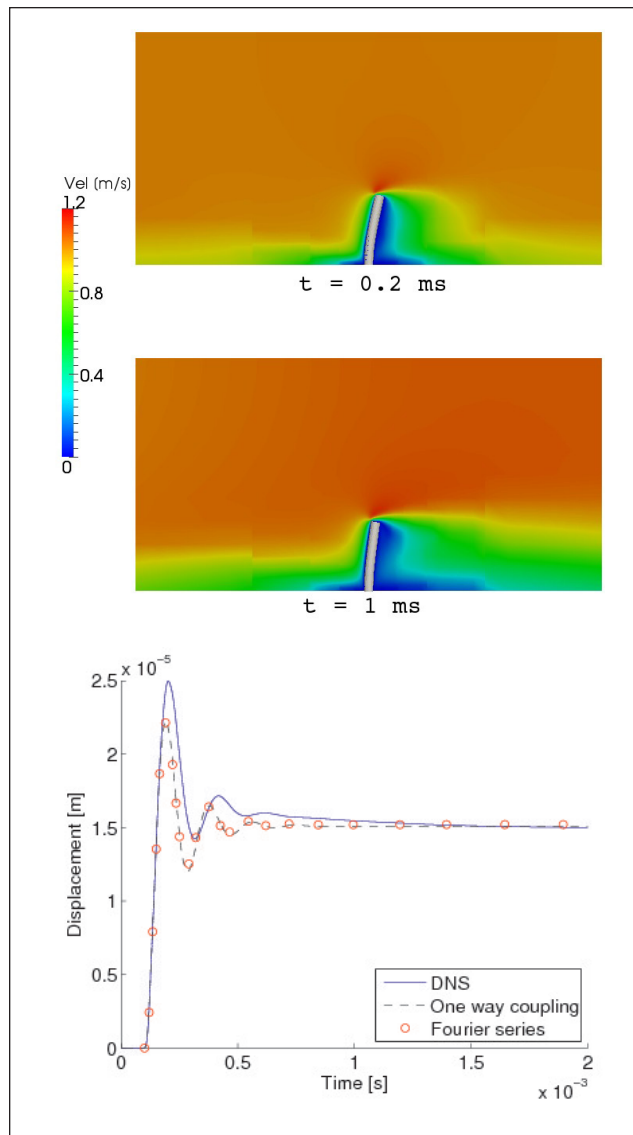
to be uniform, and a drag correlation for long cylinders was used to estimate the fluid force.

Figure 8 (top) shows the velocity field around the beam during the first oscillation and when the beam has settled in its steady state configuration. Figure 8 (bottom) also presents a comparison between the results obtained with the Fourier series analysis, the DNS, and the simulation with one-way coupling. The solution obtained from the Fourier series expansion is nearly identical to the simulation using one-way coupling. This is expected because both of these computations use the same assumption for the fluid force: one way coupling is used and it is assumed that the drag force is the only important force. The DNS predicts oscillations with larger amplitude than the simplified methods, especially during the first period. The reason for this most likely is that the DNS accounts for the history force and the added mass force, which were neglected in the simplified analysis. Furthermore, the DNS predicts a slightly larger period resulting from the strong coupling with the fluid. All three methods approach the same steady state value. This also was expected, because the simplified analysis included the stationary force but neglected some transient forces.

SIMULATION OF EARLY PAPER FORMING

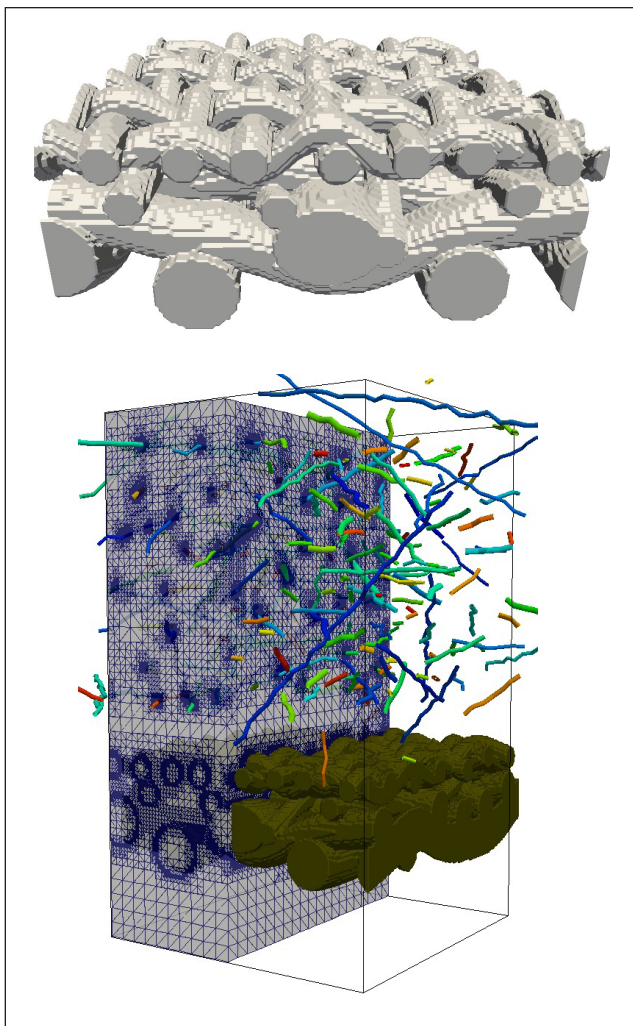
The last numerical example investigates the possibilities of simulating paper forming with the modeling framework developed in the Innovative Simulation of Paper (ISOP) project [21]. The simulation starts with a cloud of fibers randomly distributed in the fluid domain, as **Fig. 9** shows. Adaptive grid refinements are added around the fibers and the forming fabric. The forming fabric PRINTEX 5000 PB574 is a sheet-support binder fabric produced by Albany International. This is a 2/5 shed triple-layer fabric with cross direction paired binders. Figure 9 shows the geometry of a piece of the forming fabric.

The fluid flows from the inlet in the top of the domain through the forming fabric to the outlet in the bottom of the domain. Symmetry boundary conditions are used on the remaining faces. The fluid is water with a density of 1000 kg/m^3 and a viscosity of 0.001 Pas . The inlet velocity is 1 m/s downwards and 250 fibers are randomly injected into the domain. The fiber density is set to 1000 kg/m^3 (buoyant fibers) and Young's modulus is set to 0.1 GPa . Fiber lengths



8. An oscillating beam in a fluid. Flow field around during the first oscillation (top) and at steady state (bottom). Tip deflection in y -direction: Comparison of results obtained with DNS, simulation with one way coupling and Fourier series analysis.

and radii are sampled from a virtual paper sheet generated from tomography images. The size of the domain is $2 \cdot 2.2 \cdot 3.5 \text{ mm}^3$ and the grid consists of approximately $2 \cdot 10^6$ cells. The simulation is advanced in time until the fibers have come to rest on the forming fabric. The fibers follow the fluid and therefore gradually fall down onto the forming fabric, where they start to form a fiber web. **Figure 10** depicts this process. The forming fabric and the fiber web give rise to a complex flow field through the domain. The holes in the forming fabric, which are relatively thin, are gradually blocked by the paper fibers as the fiber web is built up. This results in a maximum velocity of approximately 11 m/s through the channels. This is much higher than the free-stream velocity of 1 m/s .

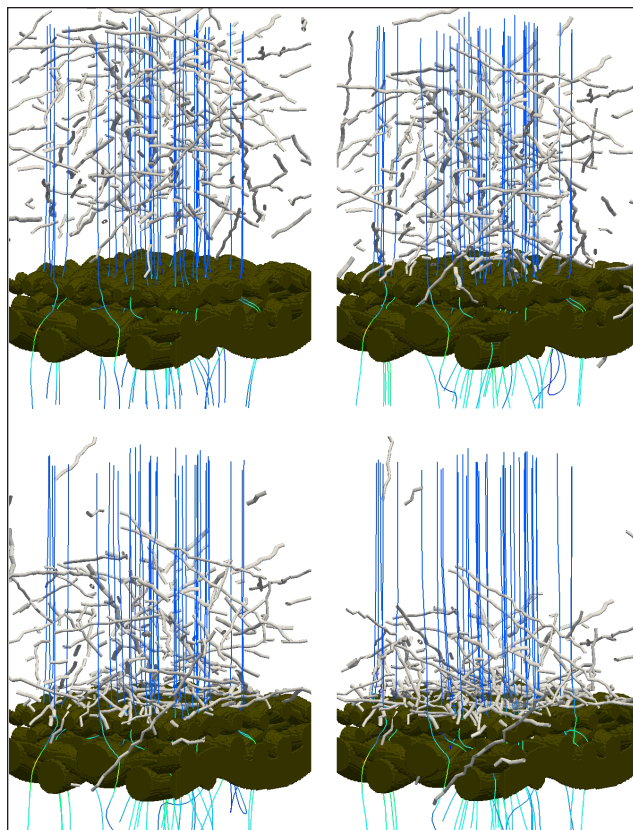


9. The forming fabric (top) and the simulation domain (bottom).

SUMMARY

The framework for microstructure simulation of early paper forming that we developed includes a Navier-Stokes solver and a fiber model based on a finite element discretization of the Euler-Bernoulli beam equation in a co-rotational formulation. The fluid-structure interaction is handled with the immersed boundary method, which allows the flow around every fiber to be resolved. Fiber-fiber and fiber-fabric contacts are modeled with a penalty method. Elastic and inelastic collisions and friction are taken into account. The fiber model has been validated against test cases described in the literature, with excellent results. Because the IBM allows the flow around each individual fiber to be resolved, it might be possible to use the results obtained with the resolved simulations to derive better macroscale models for the phenomena governing paper forming.

This paper has focused on model development. In a follow-up paper, we will validate the simulations of the paper forming process with measurements of surface density and fiber orientations. Future work also includes more advanced inter-



10. Simulation of 250 fibers falling down on a forming fabric. The streamlines are colored by the fluid velocity.

action models that take chemicals and surface charges into account. So far only fibers have been simulated, but fillers and fines also will be included. In addition, models will be developed for how the chemicals affect the retention of fillers and fines in the sheet formed on the fabric. **TJ**

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ABOUT THE AUTHORS

We developed a unique modeling approach that allows resolved microstructure simulations of the paper forming process. Understanding the paper forming process is important because the configuration of fibers during this step has a large influence on the final paper quality.

The paper forming process is a very complex fluid structure interaction problem, which is very challenging to simulate. We used novel immersed boundary methods to couple the fibers and the fluid suspension.

Among our discoveries was the fact that it is indeed possible to simulate in detail the laydown of hundreds of fibers on a standard laptop computer.

The results from this project can be used to increase the understanding of the interaction between the forming fabrics and the fiber suspension. From a

longer-term perspective, this means that the application of the fabrics in the mills can be optimized to reduce fibers, additives, and energy usage.

Our next step is validation of the simulations of the paper forming process with measurements of surface density and fiber orientations.

Mark, Svenning, and Rundqvist are applied researchers and Edelvik is department head with Fraunhofer-Chalmers Centre, Gothenburg, Sweden. Glatt and Rief are senior scientists and Wiegmann is deputy department head with Fraunhofer ITWM, Kaiserslautern, Germany. Fredlund is senior specialist with Stora Enso, Karlstad, Sweden. Lai is senior specialist with Eka Chemicals, Bohus, Sweden. Martinsson is technology leader with Albany International, Halmstad, Sweden. Nyman is development engineer with Tetra Pak Packaging Solutions, Lund, Sweden. Email Mark at andreas.mark@fcc.chalmers.se.



Mark



Svenning



Rundqvist



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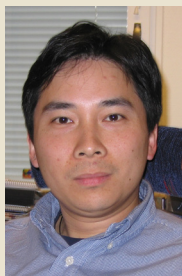
Rief



Wiegmann



Fredlund



Lai



Martinsson



Nyman