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Fully-Coupled Transient Modeling of a Highly Miniaturized Electrostatic Pull-In Driven Micropump

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Abstract
We present a problem-adapted finite element model for the simulation of an electrostatically actuated micro-membrane pump. The pumping principle heavily relies on the electrostatic pull-in. However, the combination of electrostatic pull-in and mechanical contact in a transient fluid-structure interaction FEM simulation poses a hard-to-solve problem. We developed adaptations, which overcome the numerical singularities, and drastically improve convergence.
Keywords: Electrostatic pull-in, mechanical contact, fluid-structure interaction, MEMS membrane pump

Introduction

We developed a new type of electrostatically actuated, monolithic MEMS membrane pump [1]. It is based on a radial design with an annular valve ring surrounding the pump chamber. The pump and valve membranes are actively steered and can be moved independently. The membranes are equipped with anti-sticking structures similar to those presented in [2] to prevent adhesion to the counter electrodes at pull-in.
The pump cycle consists of four consecutive actions (see Figure 1): sucking new fluid into the deflated pump chamber, closing the inlet, expelling the fluid, and closing the outlet. The valve specially designed for this purpose closes the inlet when the outlet is opened in one single action, and vice versa. First prototypes show promising results. However, further improvement necessitates deeper insights into the internal behavior of the system. Due to the monolithic nature and the small size of the micropumps, conventional methods of live monitoring, e.g. with sensors inside the pump chamber, are not possible. Therefore, a simulation model is to be developed.

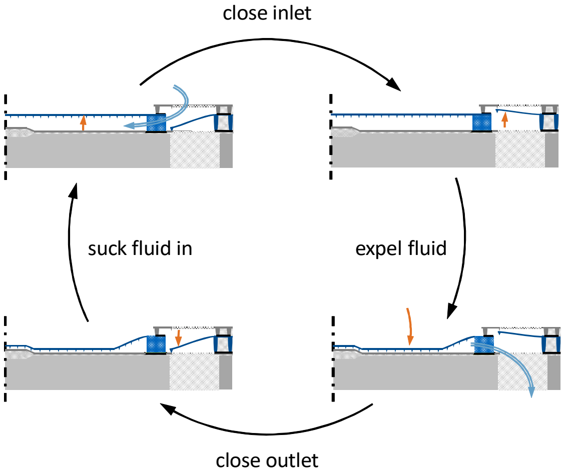

Figure 1. Pump cycle.

Governing Physical Models

As a first simplification, the pump can be very well approximated with a two-dimensional, axisymmetric model.
Simulating a pumping cycle incorporates coupling electrostatics, structural mechanics, and fluid dynamics. Additionally, the deforming fluid domain requires a moving mesh.
This section describes the physical models for the different domains. COMSOL provides interfaces for all these physical models. However the straightforward approach to combine the default interfaces led to either unacceptable small time steps, or no convergence at all. We identified the combination of mechanical contact and singularities in the electrostatic interaction as the main problem. The section after this describes how we solved these problems and achieved stable convergence.

Fluid Dynamics

The pump is designed to pump air at isothermal standard conditions. Due to the small velocities, the air can be considered incompressible. As is common in MEMS, the Reynold's number is very small. However, we cannot neglect the convective acceleration term $\rho(\vec{u} \cdot \nabla)\vec{u}$, because air flowing radially in- or outwards undergoes a large change in velocity due to the strongly changing cross-sectional area.
At standard conditions, the mean free path of air molecules is roughly 68 nm. For our pump, this leads to a Knudsen number in the order of 0.1, which is the start of the slip-flow regime. As a consequence, the no-slip condition at walls must be replaced with a slip-velocity condition [3].
This is a straightforward application of the *Laminar Flow interface*.

Structural Mechanics

The deformation of the membrane at pull-in is rather small compared to the overall geometrical extensions. At these deformations, Polysilicon can be described by an isotropic linear elastic material, which is fully characterized by Young's modulus, Poisson's ratio, and the density. Furthermore, we need the mechanical contact functionality to model the anti-sticking structures touching the counter electrodes at pull-in.

Fluid-Structure Interaction and Moving Mesh

We deal with a fully-coupled fluid-structure interaction problem, where the fluidic pressure acts as a boundary load on the structures, and the deforming structure acts as a moving wall. The deformation of the fluid domain is handled by the *Moving Mesh* functionality of COMSOL.

Electrostatics and Electromechanical Forces

The electrodes can be modelled as terminals with the *Electrostatics interface*. This leads to COMSOL solving for the electrostatic potential everywhere. The *Electromechanical Forces node* then results in a boundary load on the structure due to the sudden change in electric susceptibility.

Convergence Difficulties

This combination of COMSOL interfaces, however, did not lead to satisfactory results. Due to the nature of electrostatic interaction, the force pulling on the membrane increases with the inverse square of the distance:

$$F_{\mathrm{es}} \propto r^{-2}.$$

This leads to a quadratic singularity during pull-in that has to be balanced by the mechanical contact forces. However, the mechanical contact forces pose already a strongly non-linear problem themselves. They arise suddenly once contact is established and are solved for to be large enough to counterbalance the electrostatic interaction.
In addition, during transient simulations, the sudden spike in the boundary loads causes vibrations within the structural mechanics part, which in turn leads to very small time steps for the solver.
Finally, we do not need the detailed spatial distribution of the electrostatic potential.
Thus we abandoned the modelling approach with mechanical contact and the electrostatics interface, in favor of a numerical more stable approximation.

Numerical Stabilization Measures

This section first explains our solution to the singularity within the electrostatic interaction, and after that the smoothing of the mechanical contact.

Regularized Electrostatic Interaction

Due to the geometric extensions, the electric field between the electrodes can be adequately described by a plate capacitor. In this case, the boundary load can be written as

$$\vec{b}_{\mathrm{es}} = \frac{\varepsilon_0 \varepsilon_r}{2} \cdot \left(\frac{V}{z}\right)^2 \cdot \vec{n},$$

with z as the distance between the two plates. To overcome the quadratic singularity, we replaced the function z^{-2} with a non-singular approximation, which behaves like z^{-2} within the range of interest, while staying regular otherwise.
This process is called regularization. In our case we took inspiration from the work in [4], where the authors describe a way to solve for incompressible

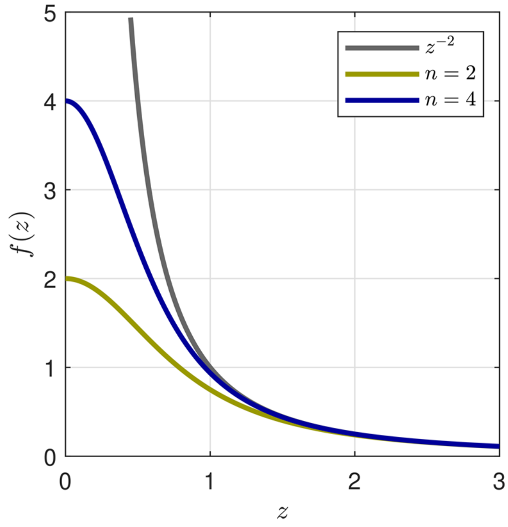

Figure 2. Comparison of z^{-2} and $f_n(z)$ for $n \in \{2,4\}$.

fluid flow by reducing it to a mesh-free N-body problem, where vortices are described by particles. Combining these particles results in equations similar to the law of Biot-Savart, which becomes singular for small distances. The solution is to smear out the particles over a finite distance while altering the force computation accordingly.
However, the regularization functions listed in [4] are developed with vortex particles in mind.
For our problem, we discovered the function family

$$f_n(z) = \sum_{k=1}^{n} \frac{1}{(z^2+1)^k}$$

to be a very good candidate for a regularized version of z^{-2}, given a suitable value of n. It behaves as $f_n(z) \in \mathcal{O}(z^{-2})$ for large z, and is smooth everywhere.
Figure 2 shows a comparison for different values of n. The relative error can be computed as

$$\frac{z^{-2} - f_n(z)}{z^{-2}} = \frac{1}{(z^2+1)^n}.$$

We decided to use $n = 4$, resulting in

$$f_4(z) = \frac{z^6 + 4z^4 + 6z^2 + 4}{(z^2+1)^4}.$$

Given some characteristic distance z_0, the boundary load can be approximated as

$$\vec{b}_{\mathrm{es}} = \frac{\varepsilon_0 \varepsilon_r}{2} \cdot \left(\frac{V}{z_0}\right)^2 \cdot f_n\left(\frac{z}{z_0}\right) \cdot \vec{n}.$$

The minimum distance between the electrodes is given by the height h_0 of the anti-sticking structures. With $z_0 = {}^{h_0}/_{2}$, the argument for f_n is always larger than 2, thus the maximum relative error is about 0.2%. This is by far accurate enough, as neither material parameters, nor the temperature, or the humidity conditions are known to such precision.
This allows to replace the entire *Electrostatic interface* and the *Electromechanical Forces multiphysics node* with an equivalent boundary load for the *Structural Mechanics interface*.

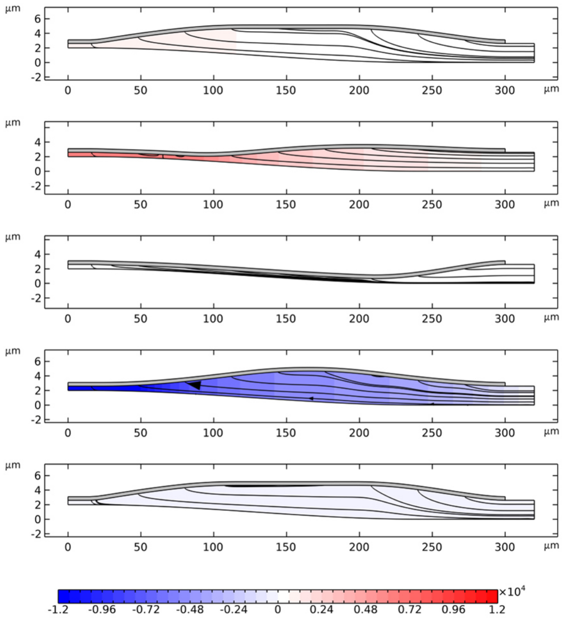

Figure 3. Pumping cycle at selected points in time. Simulation results of the model with adapted bottom counter-electrode shape.

Smooth Mechanical Contact

COMSOL allows to simulate mechanical contact by introducing the contact pressure as Lagrange multipliers, together with a no-penetration-constraint. This leads to a highly non-linear problem.

However, during pull-in, the contact boils down to a load on the boundaries, that counterbalances the electrostatic load. Then the anti-sticking structures will undergo a small deformation. We analyzed this behavior with separate COMSOL simulations. Given the typical electrostatic load at distance h_0, we determined the deformation Δz. This allows to model the contact force as a spring-like boundary load

$$\vec{b}_{\text{contact}}(z) = -k \cdot \Delta z \cdot \vec{n},$$

with a spring constant k, extracted from the separate simulation runs.

This spring load is smoothly ramped up within the vicinity of the anti-sticking bumps and behaves as a normal linear spring load around the distance, where contact is expected.

Combination and Final Model

These two regularization approaches still result in an overall non-linear form for the electrostatic and the contact force. However, the interactions are free of singularities and all loads vary smoothly now. As a result, the non-linear system of equations became easier to solve, and the convergence behavior improved dramatically. This also prevented the time-dependent solver from using unreasonable small time steps.

Simulation Results

All those solutions combined result in a stable and fast calculating simulation model. This model has already been used to carry out optimization cycles for the micropumps [5].

Within the scope of these optimization cycles, an error condition could also be identified, which was verified by tests on prototypes. At high drive frequencies, a phenomenon occurs in micropumps with pump chamber diameters above 300 µm that has a detrimental effect on pumping performance: During the ejection process, fluid is trapped in the center of the pump chamber because the diaphragm can lay down on the pump chamber floor faster in the surrounding areas than in the center [5].

However, the simulation model could not only be used to identify the problem and trace the causes. It was also possible to test different solutions to the problem through this kind of digital prototyping. A working solution resulted from an adapted geometry of the bottom counter-electrode. The bottom counter-electrode now forms a hill in the center of the pump chamber, touching the pump membrane. During the ejection process, the pump membrane can come into contact with the bottom counter electrode along the flanks of this hill, starting at its top. Thus, the fluid is now ejected completely from the center to the edge of the pump chamber (see Figure 3).

Subsequently, a parameter study using this new pump chamber geometry could be carried out, which allows the selection of optimal combinations of geometry parameters for different applications. An exemplary result of this parameter study can be seen in Figure 4.

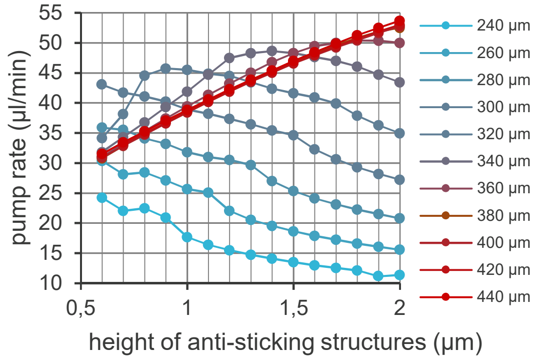

Figure 4. Results of parametric studies and selected combinations (pressure in Pa) [4].

Conclusions

We developed a problem-adapted finite element model to support the design and optimization of a novel, electrostatically actuated MEMS pump. However, the required combination of electrostatic pull-in and mechanical contact in a time-dependent FSI-FEM simulation is a problem that could not be solved by simply combining COMSOL's default interfaces. Thus, adaptations were made to overcome the numerical singularities. This has also drastically improved convergence.

The simulation model has since proven its usefulness and validity during optimization cycles for the micropumps. In addition, it was even

possible to identify a previously unknown, potential fault case, which was later confirmed by tests with prototypes.
As a next step, new prototypes with this adapted geometry have to be produced and tested. The simulation model must then be validated and calibrated again using the new measurement data.

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