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BACHELOR THESIS

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Numerical simulation of ferrofluids

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Dedication.

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Contents

Introduction

Free surface fluid flows and processes involved in a fluid behavior fascinated scientists since the very beginning of the scientific history. Problems as a breakup of a liquid jet, droplet formation and merging, rising bubbles etc. still lacks deeper understanding because of a complex and nonlinear equations governing such phenomena. In addition, they play a role in many industrial processes: *fuel injection, fibre spinning, ink-jet printing etc.* EGGERS

The equations for the motion of a fluid formulated in the 19th century came to relevance as computers started to provide number of numerical methods for finding their approximate solutions. However, majority of the methods are well suited for problems involving one-phase flows or fluid-wall interactions, multiphase flows, fluid-fluid interactions, surface forces and similar issues still remain debated and incomplete.

Imagine some usual situation, where a water droplet hanging on a tap is being pulled down by the gravity. From a physical point of view, the behavior and evolution is well described. *Navier-Stokes* equations govern the fluid motion in each phase, water and air separately, while discrete surface forces(surface tension) are balanced with the gravitational, volume force. Mathematically, not only an existence and uniqueness of a solution of the equations was proven, but multiple domains coupled with complex boundary conditions must be taken into account.

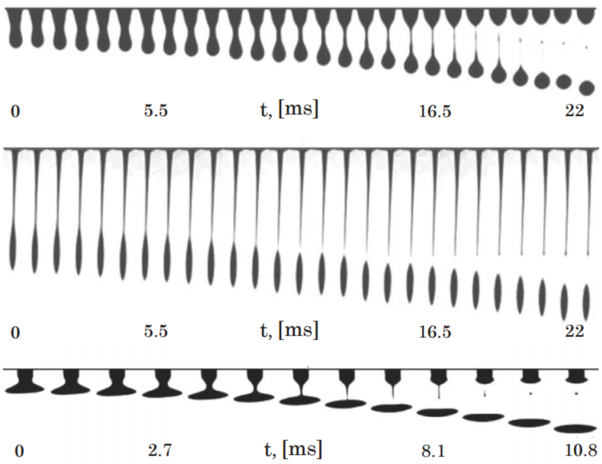

Figure 1: High-speed image sequence of ferrofluid droplet dripping out of a container. Influence of a magnetic field parallel(middle) and perpendicular(bottom) to the direction of the flow is clearly visible. Taken from [HABERA]

All these phenomena become even more attractive in terms of *ferrohydrodynamics*. Ferrofluid reacts to magnetic field and changes its shape due to an additional surface force. This entirely changes dynamics of the droplet formation process and it will be the object for our studies.

In the first part of the thesis a brief summary of the physical and mathematical model and numerical methods are given. Navier-Stokes equations are solved using the *projection methods* and spatially approximated in sense of weak derivates and *finite element method*. Interface is represented with the *level-set* function, while the conservation of its volume is assured with the reinitialization step.

In the second part we discuss the results of the implemented methods and give a direct comparison of our results with experimental data obtained in HABERA.

1. Ferrofluids /

1.1 Introduction

A **ferrofluid** is a colloidial suspension composed of small (3-15 nm) solid, single-domain, magnetic particles coated with a molecular layer of a dispersant and suspended in a liquid carrier(Fig. !!). Thermal agitation keeps the particles suspended(under sufficient stability conditions) because of the Brownian motion and the coatings prevents the particles from sticking to each other.

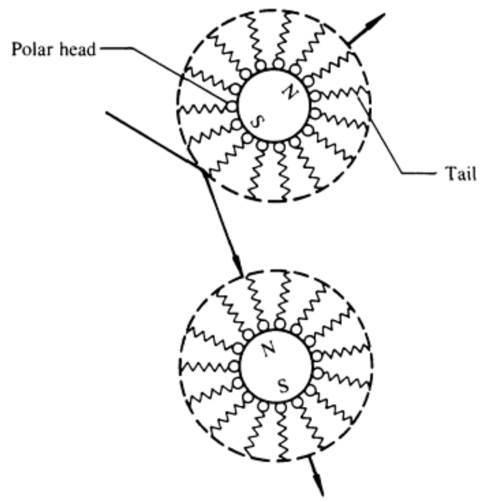

Figure 1.1: Coated magnetic particles in ferrofluid. Taken from [RW]

The magnetic ferrofluids of the type in general use today are an outgrowth of discoveries made in the early 1960s.

Because the colloidial ferrofluid is not found in the nature is must be synthetized. Methods called *size reduction* and *chemical precipitation* are used. Details of both methods can be found in [RW].

Very important property of ferrofluid is its stability. It ensures the investigator of well-defined material for scientific studies and also fluid applications. We mean

- *stability in a magnetic field gradient*,
- *stability against settling in a gravitational field*,
- *stability against magnetic agglomeration* and
- *neccesity to guard against the van der Waals attractive force.*

To derive the physicochemical stability dimensionless analysis can be used introducing various energy terms:

- *thermal energy* kT,
- *magnetic energy* $\mu_0 MHV$ and

- *gravitational energy* $\Delta\rho V g L$,

where k is Boltzmann's constant, T the absolute temperature in degrees Kelvin, μ_0 is the permeability of free space, V volume of a sperical particle, L the elevation in gravitational field, $\Delta\rho$ difference in fluid carrier and ferromagnetic particles densities and M, H magnetization and magnetic field intensity.

Such stability analysis leads to inequalities for the particle diameter, for instance, for the magnetite(Fe_3O_4) particles at the room temperature stability against magnetic agglomeration requires diameter $d \leq 7.8$ nm [RW].

1.2 Ferrohydrodynamics

The term **ferrohydrodynamics** (FHD) was first introduced by **Ronald E. Rosensweig**. Development of FHD in early to mid- 1960s was motivated by engineering task of converting heat to work with no mechanical parts.

"*Ferrohydrodynamics is an interdisciplinary topic having inherent interest of a physical and mathematical nature with applications in tribology, separations science, instrumentation, information display, printing, medicine, and other areas*" R.E.Rosensweig.

In the begining of this chapter we would like to emphasize the differences between various studies of fluid–field interactions:

1. *electrohydrodynamics* (EHD) deals with the influence of the electric field on a fluid motion,

2. *magnetohydrodynamics* (MHD) is the study of the interaction between magnetic field and fluid conductors of electricity,

3. *ferrohydrodynamics* (FHD) deals with the mechanics of fluid motion influenced by forces of magnetic polarization.

This work is mainly concerned with ferrohydrodynamics, because ferrofluids are non–conducting therefore there is zero Lorentz force acting as body force(in contrast with MHD). The body force in FHD is due to *polarization force* which requires material magnetization in presence of magnetic field gradients or discontinuities.

1.2.1 Magnetic stress tensor

As we have mentioned above, understanding the differences between several fluid–field interactions play important role in a development of a physical model for the flow of a ferrofluid.

The only body force acting from the outside in hydrodynamics is gravitational. In electrohydrodynamics electrically charged particles are affected with electrical forces while in magnetohydrodynamics conductive fluid is subject to the Lorentz body force.

The derivation of the *magnetic stress tensor* with respect to the thermodynamic background and conservation of energy leads to [RW]

$$\mathbf{T}'_m = -\left[p(\rho,T) + \int_0^H \mu_0 \left(\frac{\partial(\nu M)}{\partial \nu}\right)_{H,T} \mathrm{d}H + \frac{1}{2}\mu_0 H^2\right]\mathbf{I} + \mathbf{B}\otimes\mathbf{H}, \tag{1.1}$$

where notation from [RW] is adopted so $\mathbf{B}\otimes\mathbf{H} = B_i H_j$ represents dyadic product, p is thermodynamics pressure, ρ the density, T thermodynamic pressure, H, M associated norm of the magentic field intensity and magnetization respectively, $\mathbf{H}, \mathbf{M}$, μ_0 permeability of free space, $\nu = \rho^{-1}$ the specific volume, $\mathbf{I}$ the identity tensor and $\mathbf{B}$ magnetic field induction.

Note, that the *tensor is symmetric*, because $\mathbf{B}\otimes\mathbf{H} = \mathbf{H}\otimes\mathbf{B}$ follows from $\mathbf{B} = \mu\mathbf{H}$ and $\mathbf{I} = \mathbf{I}^{\mathrm{T}}$. This result is obtained including nonlinear effects, i.e. nonlinear magnetization of the ferrofluid. In this work a linearly magnetizable ferrofluid is assumed, so the corresponding simplification will be given in the following section.

1.2.2 Classification of “pressures” in ferrofluid

In the expression for the magnetic stress tensor, thermodynamic pressure $p = p(\rho, T)$ appeared naturally as a result of the derivation. In order to emphasize the magnetic aspect of the result we define a new tensor $\mathbf{T}_m$ such that

$$\mathbf{T}_m := \mathbf{T}'_m + p(\rho,T)\mathbf{I}$$

so we separated thermodynamic pressure present also in non–polar fluid. The new tensor is

$$\mathbf{T}_m = -\left[\int_0^H \mu_0 \left(\frac{\partial(\nu M)}{\partial \nu}\right)_{H,T} \mathrm{d}H + \frac{1}{2}\mu_0 H^2\right]\mathbf{I} + \mathbf{B}\otimes\mathbf{H}, \tag{1.2}$$

and the *magnetic force per unit volume* corresponding to a magnetic stress tensor $\mathbf{T}_m$ is

$$\mathbf{f}_m = \nabla\cdot\mathbf{T}_m. \tag{1.3}$$

Assuming few vector identities, Maxwell's equation $\nabla\cdot\mathbf{B} = 0$ (non–existence of magnetic monopoles), current–free magnetostatic Ampere's law $\nabla\times\mathbf{H} = 0$ and with use of $B = \mu_0(M + H)$ one arrives at

$$\mathbf{f}_m = -\nabla\left[\mu_0 \int_0^H \left(\frac{\partial(\nu M)}{\partial \nu}\right)_{H,T} \mathrm{d}H\right] + \mu_0 M\nabla H. \tag{1.4}$$

There is an arbitrariness in grouping of magnetic terms in (1.4) that has led to some confusion in the literature. Here, we follow the classification introduced in [RW].

Applying the partial derivative in the term $\frac{\partial(\nu M)}{\partial \nu}$ and with use of the identity

$$\nabla\int_0^H M\mathrm{d}H = M\nabla H + \int_0^H \nabla M\mathrm{d}H$$

we finally have the expression for the magnetic force per unit volume

$$\mathbf{f}_m = -\nabla \left[\mu_0 \int_0^H \nu \left(\frac{\partial M}{\partial \nu} \right)_{H,T} \mathrm{d}H \right] - \mu_0 \int_0^H \nabla M \mathrm{d}H. \tag{1.5}$$

In the sense of the equation $\mathbf{f} = \nabla p$ some pressure–like terms in (1.5) are identified.

The **magnetostrictive pressure**

$$p_s := \mu_0 \int_0^H \nu \left(\frac{\partial M}{\partial \nu} \right)_{H,T} \mathrm{d}H \tag{1.6}$$

and the **fluid-magnetic pressure**

$$p_m := \mu_0 \int_0^H M \mathrm{d}H. \tag{1.7}$$

Applying definitions (1.6) and (1.7) expression for the magnetic stress tensor yelds

$$\mathbf{T}_m = -(p_s + p_m + \frac{1}{2}\mu_0 H^2)\mathbf{I} + \mu \mathbf{H} \otimes \mathbf{H}.$$

1.2.3 Magnetic force density reduced form

It could be shown due to *Korteweg and Helmholtz* that for *linearly magnetizable media* magnetic force density reduces to

$$\mathbf{f}_m = \nabla \left[\frac{H^2}{2} \rho \left(\frac{\partial \mu}{\partial \rho} \right)_T \right] - \frac{H^2}{2} \nabla \mu.$$

In this work, **incompressible linearly magnetizable ferrofluid with magnetization constant within ferrofluid domain** is assumed, therefore it is evident from the Korteweg–Helmholtz expression for the magnetic force that this force vanishes everywhere except for the phase interfaces, where non–zero jump in the permeability is present.

1.2.4 Equation of motion for a ferrofluid

Very important part of ferrohydrodynamics is devoted to the formulation and study of equation of motion for a ferrofluid. A momentum equation was first proposed by Neuringer and Rosensweig (1964) [NRW]. In order to satisfy the continuum mechanics assumptions, it is assumed, that the dynamic equilibrium holds for and "infinitesimal element" which is large enough to contain a large number of colloidial magnetic particles comparing to the dimensions of the flow field.

The Newton's law for such "infinitesimal" element yelds

$$\rho \left(\partial_t \mathbf{u} + \left(\mathbf{u} \cdot \nabla \right) \mathbf{u} \right) = \underset{\text{Pressure force}}{\mathbf{f}_p} + \underset{\text{Viscous force}}{\mathbf{f}_v} + \underset{\text{Gravity force}}{\mathbf{f}_g} + \underset{\text{Magnetic force}}{\mathbf{f}_m} \tag{1.8}$$

The equation (1.8) with the magnetic force density expression (1.5) simply unfolds the effect of a magnetic field on a ferrofluid, but more formal and rigorous problem definition with appropriate simplyfications is given in the form of the *Navier-Stokes equations* in the chapter 4.

2. The Finite element method /

In the following sections we give a very brief introduction into the finite element method. We also refer more advanced reader who seeks more detail to [3 in LINDBO].

2.1 Problem definition

We are interested in a solution of a partial differential equations of the type

$$\mathcal{L}(u(\mathbf{x})) = f(\mathbf{x}),\ \forall \mathbf{x} \in \Omega$$

on a given domain Ω, where $\mathcal{L}$ is a linear differential operator, $u = u(x_1, \ldots, x_n) =: u(\mathbf{x})$ and $f = f(x_1, \ldots, x_n) =: f(\mathbf{x})$ is some known right hand side.

It is necessary to impose boundary conditions on the boundary $\partial\Omega$ of the domain. These conditions are usually of type *Dirichlet*, so that

$$u = b_D(\mathbf{x}),\ \forall \mathbf{x} \in \partial\Omega$$

where b_D is a prescribed function. Another type of the boundary condition is so called *Neumann*, where

$$\nabla u \cdot \mathbf{n}(\mathbf{x}) = b_N(\mathbf{x}),\ \forall \mathbf{x} \in \partial\Omega$$

where $\mathbf{n}$ is unit normal to the boundary.

2.2 Weak solution and basis, variational formulation

Yet, we didn't define function spaces for the functions in the problems like (PDE DEF). This is very important part and plays significant role in the finite element method.

Let us find such solutions to our problem, that the desired function u is in some space $\mathcal{S}$. It is reasonable, to suppose, that the space is rich enough, to contain all the solutions, but the choice of this space is still up to us.

We define the inner product of two functions on Ω

$$(f(\mathbf{x}), g(\mathbf{x})) := \int_\Omega fg \ \mathrm{d}\mathbf{x}$$

and norm induced by the inner product

$$||f|| := \sqrt{(f, f)}.$$

We say, that u is a **weak solution** to the problem (PDE), if

$$(\mathcal{L}(u) - f, s(\mathbf{x})) = 0,\ \forall s \in \mathcal{S}.$$

Function s is often refered as a *test function*. It is clear, that the space $\mathcal{S}$ is not of finite dimension. This is a very restrictive condition. One might try to find an approximation of a solution, $\tilde{u}(\mathbf{x})$ in a finite dimensional subspace, say $\mathcal{S}_n$, where $n \in \mathbb{N}_1$ is a dimension of this space. Let then $\{s_i(\mathbf{x})\}, i = 1, \ldots, n$ be the *basis* of this space, so each function from our subspace $\mathcal{S}_n$ can be expressed as a linear combination of the basis functions

$$\tilde{u} = c_i s_i,$$

where summation convention is used.

The equation (PDE VAR) could be written in terms of the variational formulation. If we let

$$L(s) := \int_\Omega s f \mathrm{d}\mathbf{x}$$

and

$$a(\tilde{u}, s) := \int_\Omega \mathcal{L}(\tilde{u}) s \mathrm{d}\mathbf{x},$$

the problem (PDE) becomes an equality of the (uni)linear and bilinear form. The linearity of the forms is clear from the linearity of the Lebesgue integral.

2.3 Principles and algorithm

We are thus interested in seeking a solutions of (PDE VAR). This can be rewritten taking $s_j(\mathbf{x})$ as the test function

$$(\mathcal{L}(\tilde{u}), s_j) = (f, s_j)$$

and decomposing approximate solution into our basis

$$\begin{aligned}(\mathcal{L}(c_i s_i), s_j) &= (f, s_j),\\ c_i(\mathcal{L}(s_i), s_j) &=\end{aligned}$$

We let

$$\begin{aligned}\mathbb{A} := A_{ij} &:= (\mathcal{L}(s_i), s_j),\\ \mathbf{b} &:= (f, s_j)\end{aligned}$$

and

$$\mathbf{c} := \{c_i\}$$

set of the coefficients we are interested in. This is clearly a system of the equations known from linear algebra, $\mathbb{A}\mathbf{c} = \mathbf{b}$.

We have derived the set of the equations that solves our problem in sense of a weak solution given by the condition (GALERKIN).

Let suppose, for the sake of simplicity, that $\Omega \subset \mathbb{R}^2$. Integral over Ω induced by the inner product is decomposed into the sum of integrals over subdomains of Ω. In sense of FEM, such decomposition is done into triangles, e.g. a **triangulation** in $\mathbb{R}^2$ into M cells.

We write

$$\Omega =: \bigcup_{k=1}^{M} T_k,$$

so the matrix elements become

$$A_{ij} = \int_\Omega \mathcal{L}(s_i) s_j \mathrm{d}\mathbf{x} = \sum_{k=1}^{M} \int_{T_k} \mathcal{L}(s_i) s_j \mathrm{d}\mathbf{x}.$$

2.4 Finite element spaces

The basis functions s_i were not yet specified. Since the only restriction on these functions is, that $\{s_i\},\ i = 0, \dots, n$ is the basis of our finite dimensional subspace $\mathcal{S}_n$, we choose them wisely.

Because the system $\mathbb{A}\mathbf{c} = \mathbf{b}$ will be solved, we would like them to vanish almost everywhere, i.e. to have non-zero value only on some element(triangle) with its neighbours. This implies, that the inner product $A_{ij} = (\mathcal{L}(s_i), s_j)$ forms a sparse matrix.

In the following, we refer to the **type** of the element. A type is simply a class of basis functions. Most common choice of this class is so called *Lagrange* polynomials.

The **order** is roughly the order of the interpolation polynomial.

The **shape** of the finite element is the geometry that defines the decomposition of Ω.

For instance the finite element of type Lagrange, third order and triangular shape means triangulation of the Ω and the choice of basis functions that are on each triangle Lagrange cubic polynomials.

3. The Level-Set method /

Our main goal is the simulation of two-phase flow. It is therefore evident, that some method for interface tracking must be implemented. The level-set method (LSM) is simple and straightforward mathematical construction that represents the surface. Recent studies [LSM] improved the level-set method and reduced several drawbacks of original formulation by []. The level-set method presented in our work conserves volume of fluid. This improvement is important if we would like to analyse the volume of droplets, jets, etc.

3.1 Mathematical formulation

Let say, $\Omega \subset \mathbb{R}^n$. We choose a domain $\Omega_1 \subset \Omega$ that represents one fluid phase. Let then $\Omega_2 = \Omega - \Omega_1$. We define the interface between two phases as

$$\Gamma = \mathbf{x} :: \ \mathbf{x} \in \partial\Omega.$$

General idea of LSM is to introduce function $\phi : \ \Omega \mapsto \mathbb{R}$ so that the interface is being the implicit hypersurface

$$\Gamma = \mathbf{x} :: \ \phi(\mathbf{x}) = 0.$$

The name level-set is derived from the fact, that surface is represented with the zero-level plane cross section of some hypersurface.

Standart level-set function, often refered as *distance level-set* function is defined such that

$$\phi(\mathbf{x}) = \mathrm{Ind}(\mathbf{x}) \min()$$

3.2 Level-set advection

3.3 Conservation of mass, reinitialization

4. The Navier-Stokes equations /

The goal of this chapter is the formulation of the equations governing physical problems we are interested in. In the beginning we introduce the postulates and simplifications. With the help of these we derive the dimensionless form of the Navier-Stokes equations and add forces present in a magnetic field.

At the end we formulate the equations in terms of the finite element method, i.e. a weak formulation of our problem is proposed.

4.1 Dimensionless form

Let us consider

4.2 Numerical solution and projection methods

4.3 Finite element formulation

5. Rising bubble benchmark /

5.1 Problem definition

5.2 Results

Conclusion

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