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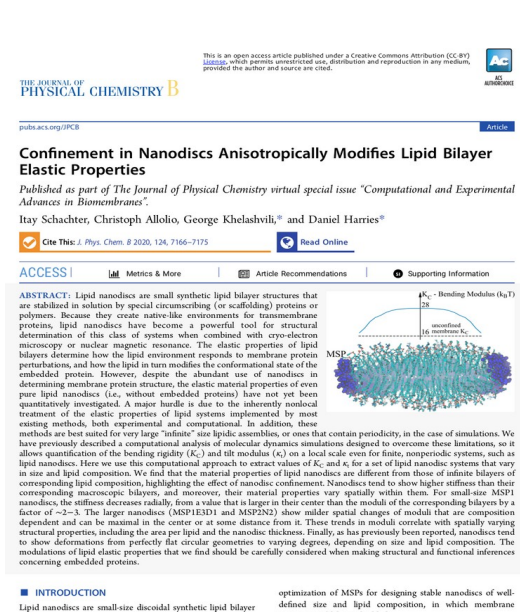
Interests:

- Contiuum theory of lipid membranes
- Endosomal escape
- Membrane proteins
- Mitochondrial membranes
- Semiconductors in membranes



THE JOURNAL OF PHYSICAL CHEMISTRY B

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Article

Confinement in Nanodiscs Anisotropically Modifies Lipid Bilayer Elastic Properties

Published as part of The Journal of Physical Chemistry virtual special issue "Computational and Experimental Advances in Biomembranes".

Itay Schachter, Christoph Allolio, George Khelashvili,* and Daniel Harries*

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ABSTRACT: Lipid nanodiscs are small synthetic lipid bilayer structures that are stabilized in solution by special circumscribing (or scaffolding) proteins or polymers. Because they create native-like environments for transmembrane proteins, lipid nanodiscs have become a powerful tool for structural determination of this class of systems when combined with cryo-electron microscopy or nuclear magnetic resonance. The elastic properties of lipid bilayers determine how the lipid environment responds to membrane protein perturbations, and how the lipid in turn modifies the conformational state of the embedded protein. However, despite the abundant use of nanodiscs in determining membrane protein structure, the elastic material properties of even pure lipid nanodiscs (i.e., without embedded proteins) have not yet been quantitatively investigated. A major hurdle is due to the inherently nonlocal treatment of the elastic properties of lipid systems implemented by most existing methods, both experimental and computational. In addition, these methods are best suited for very large "infinite" size lipidic assemblies, or ones that contain periodicity, in the case of simulations. We have previously described a computational analysis of molecular dynamics simulations designed to overcome these limitations, so it allows quantification of the bending rigidity (K_c) and tilt modulus (κ_t) on a local scale even for finite, nonperiodic systems, such as lipid nanodiscs. Here we use this computational approach to extract values of K_c and κ_t for a set of lipid nanodisc systems that vary in size and lipid composition. We find that the material properties of lipid nanodiscs are different from those of infinite bilayers of corresponding lipid composition, highlighting the effect of nanodisc confinement. Nanodiscs tend to show higher stiffness than their corresponding macroscopic bilayers, and moreover, their material properties vary spatially within them. For small-size MSP1 nanodiscs, the stiffness decreases radially, from a value that is larger in their center than the moduli of the corresponding bilayers by a factor of ∼2−3. The larger nanodiscs (MSP1E3D1 and MSP2N2) show milder spatial changes of moduli that are composition dependent and can be maximal in the center or at some distance from it. These trends in moduli correlate with spatially varying structural properties, including the area per lipid and the nanodisc thickness. Finally, as has previously been reported, nanodiscs tend to show deformations from perfectly flat circular geometries to varying degrees, depending on size and lipid composition. The modulations of lipid elastic properties that we find should be carefully considered when making structural and functional inferences concerning embedded proteins.

INTRODUCTION

Lipid nanodiscs are small-size discoidal synthetic lipid bilayer structures girdled by amphiphilic scaffolding structures. The first nanodiscs were created using membrane scaffolding proteins (MSPs). These MSPs were originally designed from the ApoA1 protein component of high-density lipoprotein particles.[1,2] Because of their amphipathic character, MSPs shield the hydrophobic core of the nanodisc membrane from unfavorable exposure to the aqueous solution, thus stabilizing the nanodiscs in solution.[3] Since their introduction, a variety of other synthetic proteins and polymers of similar amphipathic nature have been developed.[4,5] This has allowed the careful optimization of MSPs for designing stable nanodiscs of well-defined size and lipid composition, in which membrane proteins could be embedded.

Because the lipid nanodisc closely resembles the environment of membrane proteins under physiological conditions,

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PNAS

Arginine-rich cell-penetrating peptides induce membrane multilamellarity and subsequently enter via formation of a fusion pore

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Edited by Michael L. Klein, Temple University, Philadelphia, PA, and approved October 10, 2018 (received for review July 6, 2018)

Arginine-rich cell-penetrating peptides do not enter cells by directly passing through a lipid membrane; they instead passively enter vesicles and live cells by inducing membrane multilamellarity and fusion. The molecular picture of this penetration mode, which differs qualitatively from the previously proposed direct mechanism, is provided by molecular dynamics simulations. The kinetics of vesicle agglomeration and fusion by an iconic cell-penetrating peptide—nonaarginine—are documented via real-time fluorescence techniques, while the induction of multilamellar phases in vesicles and live cells is demonstrated by a combination of electron and fluorescence microscopies. This concert of experiments and simulations reveals that the identified passive cell penetration mechanism bears analogy to vesicle fusion induced by calcium ions, indicating that the two processes may share a common mechanistic origin.

cell-penetrating peptide | membrane fusion | fluorescence microscopy | electron microscopy | molecular dynamics

Cell-penetrating peptides have a unique potential for targeted drug delivery; therefore, mechanistic understanding of their membrane action has been sought since their discovery over 20 y ago (1). While ATP-driven endocytosis is known to play a major role in their internalization (2), there has been also ample evidence for the importance of passive translocation (3–5) for which the direct mechanism, where the peptide is thought to directly pass through the membrane via a temporary pore, has been widely advocated (4, 6–8). Here, we question this view and show that arginine-rich cell-penetrating peptides instead passively enter vesicles and live cells by inducing membrane multilamellarity and fusion.

Ions do not dissolve in oil. From this point of view the direct passive mechanism of cell penetration is intuitively problematic, as cationic peptides such as polyarginines or the transactivating transcriptional activator (TAT) are too highly charged to be able to pass through the "oily" interior of a lipid membrane. The concept of direct penetration was seen plausible due to the action of the related antimicrobial peptides, which are also charged, but in addition contain a large fraction of hydrophobic residues (9): These peptides are known to stabilize pores in membranes (10). At a close inspection, however, it becomes clear that their charged side chains do not interact directly with the aliphatic chains in the low dielectric interior of the phospholipid bilayer, but rather stabilize transient water channels or act as terminal residues anchoring the transmembrane helix (9). Taken together, the passive action of cell-penetrating peptides (CPPs) seems to be very different from direct translocation across an otherwise unperturbed cell membrane.

To make matters even more confusing, experimental facts and suggested mechanisms often seem contradictory to each other. For example, there are conflicting reports whether or not nonaarginine (R_9) is able to penetrate vesicles composed purely of 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) (5, 11, 12). Additionally, fluorescence microscopy suggests that R_9 is able to deform membranes (5, 13) and small-angle X-ray scattering (SAXS) experiments reveal phase transitions induced in lipid systems by polyarginines (4). An important factor in these observations appears to be the membrane composition with negatively charged lipids facilitating membrane translocation of cationic peptides (7, 14). Indeed, there is some evidence that a direct mechanism may be enabled by hydrophobic counterions, such as pyrene butyrate (12, 15) or presence of an unphysiological concentration of phosphatidic acids (7). The relevance to of these phenomena to actual cellular uptake is not clear, so that current discussions present direct mechanisms side by side with endocytosis-like membrane deformations induced by the CPPs (16).

Another fundamental cellular process involving membranes and charged species is fusion of vesicles with the cell membrane during calcium-triggered exocytosis. In neuronal cells,

Significance

The passive translocation mechanism of arginine-rich cell-penetrating peptides has puzzled the scientific community for more than 20 y. In this study we propose a hitherto unrecognized mechanism of passive cell entry involving fusion of multilamellar structures generated by the cell-penetrating peptides. The geometry of entry for this mechanism is completely different from previously suggested direct translocation mechanisms, leading to another paradigm for designing molecular carriers for drug delivery to the cell.

Author contributions: C.A., A.M., and P. Jungwirth designed research; C.A., A.M., P. Jurkiewicz, K.B., M.J., P.E.M., R.Š., M.C., D.H., V.H., R.R., C.M.Z., and A.S. performed research; P.E.M., M.H., V.H., R.R., and P. Jungwirth analyzed data; and C.A. and P. Jungwirth wrote the paper.

The authors declare no conflict of interest.

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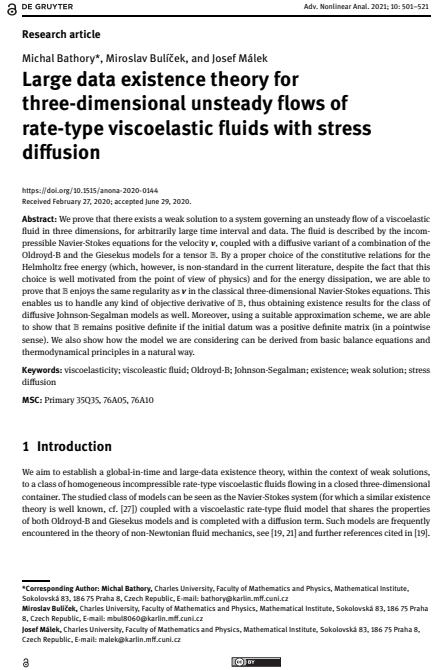
Interests:

- Analysis of partial differential equations of continuum thermodynamics
- Stability analysis
- Regularity theory



DE GRUYTER Adv. Nonlinear Anal. 2021; 10: 501–521

Research article

Michal Bathory*, Miroslav Bulíček, and Josef Málek

Large data existence theory for three-dimensional unsteady flows of rate-type viscoelastic fluids with stress diffusion

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Received February 27, 2020; accepted June 29, 2020.

Abstract: We prove that there exists a weak solution to a system governing an unsteady flow of a viscoelastic fluid in three dimensions, for arbitrarily large time interval and data. The fluid is described by the incompressible Navier-Stokes equations for the velocity $\boldsymbol{v}$, coupled with a diffusive variant of a combination of the Oldroyd-B and the Giesekus models for a tensor $\mathbb{B}$. By a proper choice of the constitutive relations for the Helmholtz free energy (which, however, is non-standard in the current literature, despite the fact that this choice is well motivated from the point of view of physics) and for the energy dissipation, we are able to prove that $\mathbb{B}$ enjoys the same regularity as $\boldsymbol{v}$ in the classical three-dimensional Navier-Stokes equations. This enables us to handle any kind of objective derivative of $\mathbb{B}$, thus obtaining existence results for the class of diffusive Johnson-Segalman models as well. Moreover, using a suitable approximation scheme, we are able to show that $\mathbb{B}$ remains positive definite if the initial datum was a positive definite matrix (in a pointwise sense). We also show how the model we are considering can be derived from basic balance equations and thermodynamical principles in a natural way.

Keywords: viscoelasticity; viscoelastic fluid; Oldroyd-B; Johnson-Segalman; existence; weak solution; stress diffusion

MSC: Primary 35Q35, 76A05, 76A10

1 Introduction

We aim to establish a global-in-time and large-data existence theory, within the context of weak solutions, to a class of homogeneous incompressible rate-type viscoelastic fluids flowing in a closed three-dimensional container. The studied class of models can be seen as the Navier-Stokes system (for which a similar existence theory is well known, cf. [27]) coupled with a viscoelastic rate-type fluid model that shares the properties of both Oldroyd-B and Giesekus models and is completed with a diffusion term. Such models are frequently encountered in the theory of non-Newtonian fluid mechanics, see [19, 21] and further references cited in [19].

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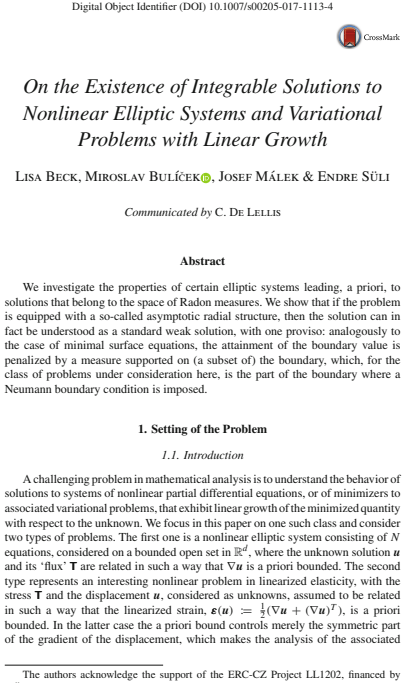

Arch. Rational Mech. Anal. 225 (2017) 717–769
Digital Object Identifier (DOI) 10.1007/s00205-017-1113-4

CrossMark

On the Existence of Integrable Solutions to Nonlinear Elliptic Systems and Variational Problems with Linear Growth

Lisa Beck, Miroslav Bulíček, Josef Málek & Endre Süli

Communicated by C. De Lellis

Abstract

We investigate the properties of certain elliptic systems leading, a priori, to solutions that belong to the space of Radon measures. We show that if the problem is equipped with a so-called asymptotic radial structure, then the solution can in fact be understood as a standard weak solution, with one proviso: analogously to the case of minimal surface equations, the attainment of the boundary value is penalized by a measure supported on (a subset of) the boundary, which, for the class of problems under consideration here, is the part of the boundary where a Neumann boundary condition is imposed.

1. Setting of the Problem

1.1. Introduction

A challenging problem in mathematical analysis is to understand the behavior of solutions to systems of nonlinear partial differential equations, or of minimizers to associated variational problems, that exhibit linear growth of the minimized quantity with respect to the unknown. We focus in this paper on one such class and consider two types of problems. The first one is a nonlinear elliptic system consisting of N equations, considered on a bounded open set in $\mathbb{R}^d$, where the unknown solution $\boldsymbol{u}$ and its 'flux' $\mathbf{T}$ are related in such a way that $\nabla \boldsymbol{u}$ is a priori bounded. The second type represents an interesting nonlinear problem in linearized elasticity, with the stress $\mathbf{T}$ and the displacement $\boldsymbol{u}$, considered as unknowns, assumed to be related in such a way that the linearized strain, $\boldsymbol{\varepsilon}(\boldsymbol{u}) := \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$, is a priori bounded. In the latter case the a priori bound controls merely the symmetric part of the gradient of the displacement, which makes the analysis of the associated

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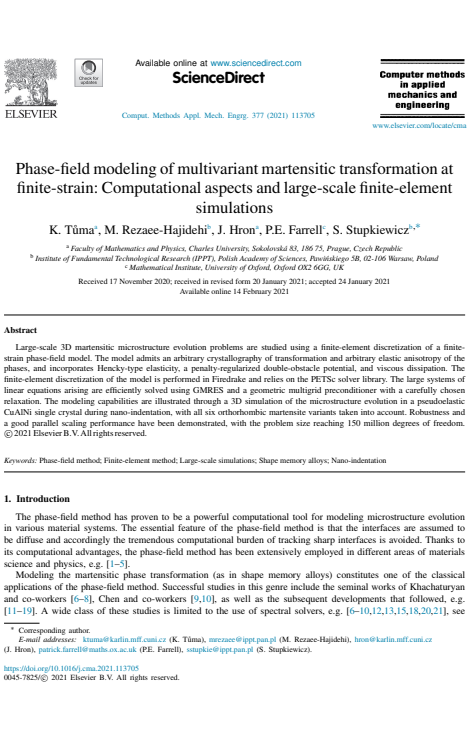
Interests:

- Fluid structure interaction.
- Biofluid dynamics.
- Finite element method.
- High performace computing.



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Comput. Methods Appl. Mech. Engrg. 377 (2021) 113705

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Phase-field modeling of multivariant martensitic transformation at finite-strain: Computational aspects and large-scale finite-element simulations

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Abstract

Large-scale 3D martensitic microstructure evolution problems are studied using a finite-element discretization of a finite-strain phase-field model. The model admits an arbitrary crystallography of transformation and arbitrary elastic anisotropy of the phases, and incorporates Hencky-type elasticity, a penalty-regularized double-obstacle potential, and viscous dissipation. The finite-element discretization of the model is performed in Firedrake and relies on the PETSc solver library. The large systems of linear equations arising are efficiently solved using GMRES and a geometric multigrid preconditioner with a carefully chosen relaxation. The modeling capabilities are illustrated through a 3D simulation of the microstructure evolution in a pseudoelastic CuAlNi single crystal during nano-indentation, with all six orthorhombic martensite variants taken into account. Robustness and a good parallel scaling performance have been demonstrated, with the problem size reaching 150 million degrees of freedom.

Keywords: Phase-field method; Finite-element method; Large-scale simulations; Shape memory alloys; Nano-indentation

1. Introduction

The phase-field method has proven to be a powerful computational tool for modeling microstructure evolution in various material systems. The essential feature of the phase-field method is that the interfaces are assumed to be diffuse and accordingly the tremendous computational burden of tracking sharp interfaces is avoided. Thanks to its computational advantages, the phase-field method has been extensively employed in different areas of materials science and physics, e.g. [1–5].

Modeling the martensitic phase transformation (as in shape memory alloys) constitutes one of the classical applications of the phase-field method. Successful studies in this genre include the seminal works of Khachaturyan and co-workers [6–8], Chen and co-workers [9,10], as well as the subsequent developments that followed, e.g. [11–19]. A wide class of these studies is limited to the use of spectral solvers, e.g. [6–10,12,13,15,18,20,21], see

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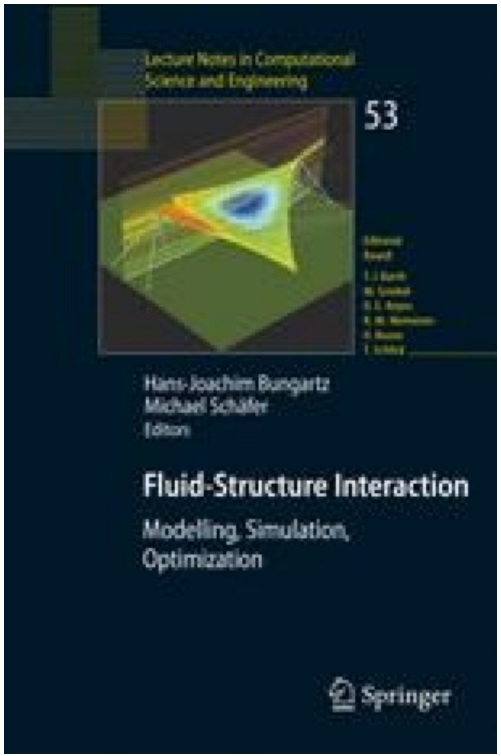
0045-7825/



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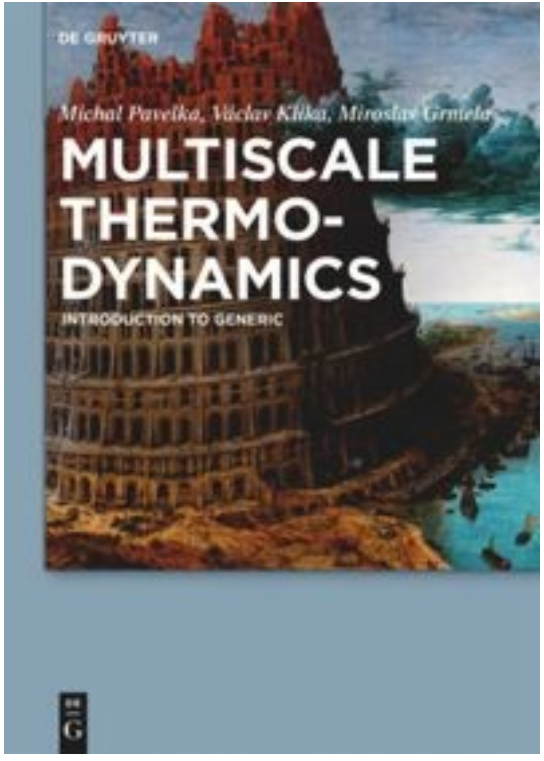
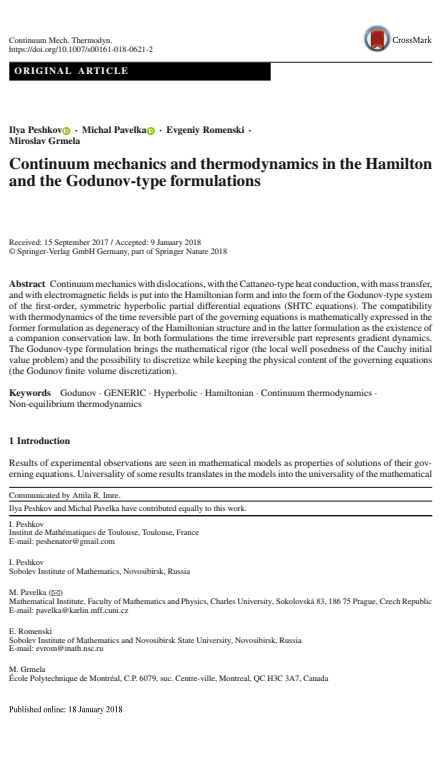
Interests:

- Hamiltonian mechanics
- Continuum thermodynamics
- GENERIC
- Hyperbolic equations
- Theoretical electrochemistry





Continuum Mech. Thermodyn.
https://doi.org/10.1007/s00161-018-0621-2

ORIGINAL ARTICLE

Ilya Peshkov · Michal Pavelka · Evgeniy Romenski · Miroslav Grmela

Continuum mechanics and thermodynamics in the Hamilton and the Godunov-type formulations

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Abstract Continuum mechanics with dislocations, with the Cattaneo-type heat conduction, with mass transfer, and with electromagnetic fields is put into the Hamiltonian form and into the form of the Godunov-type system of the first-order, symmetric hyperbolic partial differential equations (SHTC equations). The compatibility with thermodynamics of the time reversible part of the governing equations is mathematically expressed in the former formulation as degeneracy of the Hamiltonian structure and in the latter formulation as the existence of a companion conservation law. In both formulations the time irreversible part represents gradient dynamics. The Godunov-type formulation brings the mathematical rigor (the local well posedness of the Cauchy initial value problem) and the possibility to discretize while keeping the physical content of the governing equations (the Godunov finite volume discretization).

Keywords Godunov · GENERIC · Hyperbolic · Hamiltonian · Continuum thermodynamics · Non-equilibrium thermodynamics

1 Introduction

Results of experimental observations are seen in mathematical models as properties of solutions of their governing equations. Universality of some results translates in the models into the universality of the mathematical

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Ilya Peshkov and Michal Pavelka have contributed equally to this work.

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Published online: 18 January 2018

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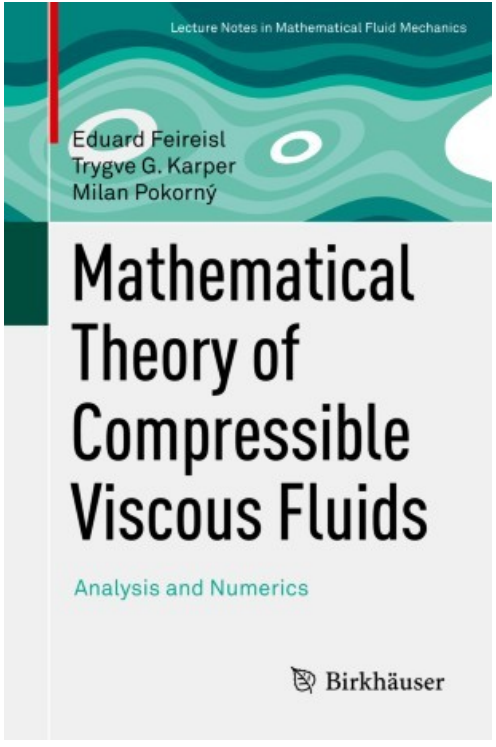
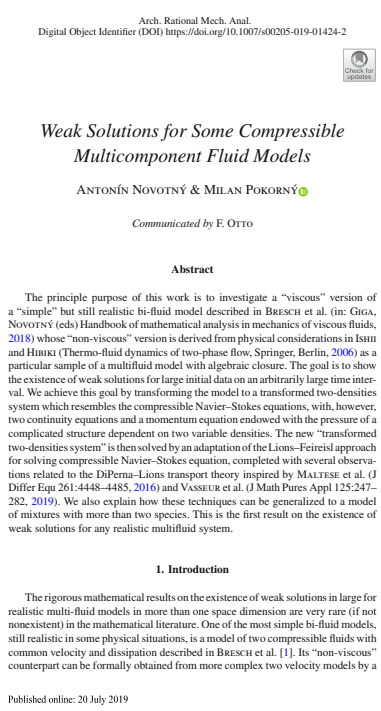
Interests:

- Mathematical analysis of partial differential equations
- Fluid mechanics
- Multicomponent fluids




Arch. Rational Mech. Anal.
Digital Object Identifier (DOI) https://doi.org/10.1007/s00205-019-01424-2

Weak Solutions for Some Compressible Multicomponent Fluid Models

Antonín Novotný & Milan Pokorný

Communicated by F. Otto

Abstract

The principle purpose of this work is to investigate a "viscous" version of a "simple" but still realistic bi-fluid model described in Bresch et al. (in: Giga, Novotný (eds) Handbook of mathematical analysis in mechanics of viscous fluids, 2018) whose "non-viscous" version is derived from physical considerations in Ishii and Hibiki (Thermo-fluid dynamics of two-phase flow, Springer, Berlin, 2006) as a particular sample of a multifluid model with algebraic closure. The goal is to show the existence of weak solutions for large initial data on an arbitrarily large time interval. We achieve this goal by transforming the model to a transformed two-densities system which resembles the compressible Navier–Stokes equations, with, however, two continuity equations and a momentum equation endowed with the pressure of a complicated structure dependent on two variable densities. The new "transformed two-densities system" is then solved by an adaptation of the Lions–Feireisl approach for solving compressible Navier–Stokes equation, completed with several observations related to the DiPerna–Lions transport theory inspired by Maltese et al. (J Differ Equ 261:4448–4485, 2016) and Vasseur et al. (J Math Pures Appl 125:247–282, 2019). We also explain how these techniques can be generalized to a model of mixtures with more than two species. This is the first result on the existence of weak solutions for any realistic multifluid system.

1. Introduction

The rigorous mathematical results on the existence of weak solutions in large for realistic multi-fluid models in more than one space dimension are very rare (if not nonexistent) in the mathematical literature. One of the most simple bi-fluid models, still realistic in some physical situations, is a model of two compressible fluids with common velocity and dissipation described in Bresch et al. [1]. Its "non-viscous" counterpart can be formally obtained from more complex two velocity models by a

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Interests:

- Continuum thermodynamics
- Viscoelastic fluids – mathematical models
- Solids – mathematical models
- Stability analysis

Physics of Fluids

Thermodynamics of viscoelastic rate-type fluids with stress diffusion

Cite as: Phys. Fluids 30, 023101 (2018); https://doi.org/10.1063/1.5018172
Submitted: 04 December 2017 • Accepted: 08 January 2018 • Published Online: 02 February 2018

Josef Málek, Vít Průša, Tomáš Skřivan, et al.

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This paper was selected as an Editor's Pick

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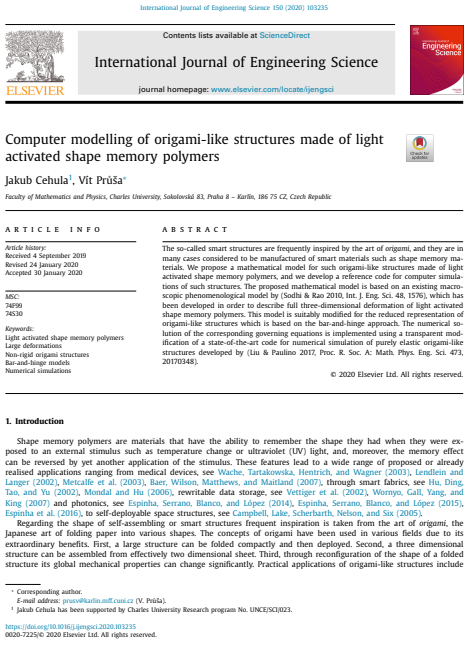

International Journal of Engineering Science 150 (2020) 103235

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Computer modelling of origami-like structures made of light activated shape memory polymers

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ABSTRACT

The so-called smart structures are frequently inspired by the art of *origami*, and they are in many cases considered to be manufactured of smart materials such as shape memory materials. We propose a mathematical model for such origami-like structures made of light activated shape memory polymers, and we develop a reference code for computer simulations of such structures. The proposed mathematical model is based on an existing macroscopic phenomenological model by (Sodhi & Rao 2010, Int. J. Eng. Sci. 48, 1576), which has been developed in order to describe full three-dimensional deformation of light activated shape memory polymers. This model is suitably modified for the reduced representation of origami-like structures which is based on the bar-and-hinge approach. The numerical solution of the corresponding governing equations is implemented using a transparent modification of a state-of-the-art code for numerical simulation of purely elastic origami-like structures developed by (Liu & Paulino 2017, Proc. R. Soc. A: Math. Phys. Eng. Sci. 473, 20170348).

1. Introduction

Shape memory polymers are materials that have the ability to remember the shape they had when they were exposed to an external stimulus such as temperature change or ultraviolet (UV) light, and, moreover, the memory effect can be reversed by yet another application of the stimulus. These features lead to a wide range of proposed or already realised applications ranging from medical devices, see Wache, Tartakowska, Hentrich, and Wagner (2003), Lendlein and Langer (2002), Metcalfe et al. (2003), Baer, Wilson, Matthews, and Maitland (2007), through smart fabrics, see Hu, Ding, Tao, and Yu (2002), Mondal and Hu (2006), rewritable data storage, see Vettiger et al. (2002), Wornyo, Gall, Yang, and King (2007) and photonics, see Espinha, Serrano, Blanco, and López (2014), Espinha, Serrano, Blanco, and López (2015), Espinha et al. (2016), to self-deployable space structures, see Campbell, Lake, Scherbarth, Nelson, and Six (2005).

Regarding the shape of self-assembling or smart structures frequent inspiration is taken from the art of *origami*, the Japanese art of folding paper into various shapes. The concepts of origami have been used in various fields due to its extraordinary benefits. First, a large structure can be folded compactly and then deployed. Second, a three dimensional structure can be assembled from effectively two dimensional sheet. Third, through reconfiguration of the shape of a folded structure its global mechanical properties can change significantly. Practical applications of origami-like structures include

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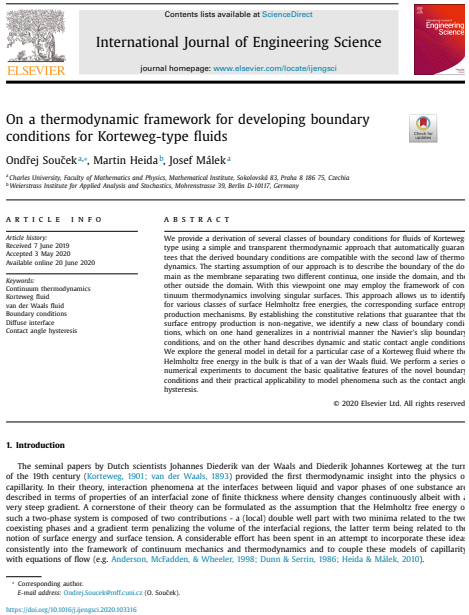
Interests:

- Continuum thermodynamics
- Mixture theory
- Computational geophysics



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On a thermodynamic framework for developing boundary conditions for Korteweg-type fluids

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ABSTRACT

We provide a derivation of several classes of boundary conditions for fluids of Korteweg type using a simple and transparent thermodynamic approach that automatically guarantees that the derived boundary conditions are compatible with the second law of thermodynamics. The starting assumption of our approach is to describe the boundary of the domain as the membrane separating two different continua, one inside the domain, and the other outside the domain. With this viewpoint one may employ the framework of continuum thermodynamics involving singular surfaces. This approach allows us to identify for various classes of surface Helmholtz free energies, the corresponding surface entropy production mechanisms. By establishing the constitutive relations that guarantee that the surface entropy production is non-negative, we identify a new class of boundary conditions, which on one hand generalizes in a nontrivial manner the Navier's slip boundary conditions, and on the other hand describes dynamic and static contact angle conditions. We explore the general model in detail for a particular case of a Korteweg fluid where the Helmholtz free energy in the bulk is that of a van der Waals fluid. We perform a series of numerical experiments to document the basic qualitative features of the novel boundary conditions and their practical applicability to model phenomena such as the contact angle hysteresis.

1. Introduction

The seminal papers by Dutch scientists Johannes Diederik van der Waals and Diederik Johannes Korteweg at the turn of the 19th century (Korteweg, 1901; van der Waals, 1893) provided the first thermodynamic insight into the physics of capillarity. In their theory, interaction phenomena at the interfaces between liquid and vapor phases of one substance are described in terms of properties of an interfacial zone of finite thickness where density changes continuously albeit with a very steep gradient. A cornerstone of their theory can be formulated as the assumption that the Helmholtz free energy of such a two-phase system is composed of two contributions - a (local) double well part with two minima related to the two coexisting phases and a gradient term penalizing the volume of the interfacial regions, the latter term being related to the notion of surface energy and surface tension. A considerable effort has been spent in an attempt to incorporate these ideas consistently into the framework of continuum mechanics and thermodynamics and to couple these models of capillarity with equations of flow (e.g. Anderson, McFadden, & Wheeler, 1998; Dunn & Serrin, 1986; Heida & Málek, 2010).

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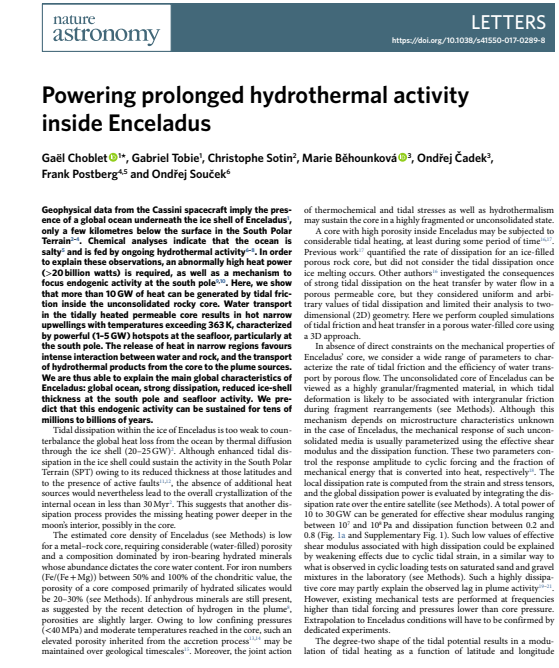

nature astronomy

LETTERS

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Powering prolonged hydrothermal activity inside Enceladus

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Geophysical data from the Cassini spacecraft imply the presence of a global ocean underneath the ice shell of Enceladus', only a few kilometres below the surface in the South Polar Terrain [1–3]. Chemical analyses indicate that the ocean is salty [2] and is fed by ongoing hydrothermal activity [4–8]. In order to explain these observations, an abnormally high heat power (>20 billion watts) is required, as well as a mechanism to focus endogenic activity at the south pole [9,10]. Here, we show that more than 10 GW of heat can be generated by tidal friction inside the unconsolidated rocky core. Water transport in the tidally heated permeable core results in hot narrow upwellings with temperatures exceeding 363 K, characterized by powerful (1–5 GW) hotspots at the seafloor, particularly at the south pole. The release of heat in narrow regions favours intense interaction between water and rock, and the transport of hydrothermal products from the core to the plume sources. We are thus able to explain the main global characteristics of Enceladus: global ocean, strong dissipation, reduced ice-shell thickness at the south pole and seafloor activity. We predict that this endogenic activity can be sustained for tens of millions to billions of years.

Tidal dissipation within the ice of Enceladus is too weak to counterbalance the global heat loss from the ocean by thermal diffusion through the ice shell (20–25 GW)[11]. Although enhanced tidal dissipation in the ice shell could sustain the activity in the South Polar Terrain (SPT) owing to its reduced thickness at those latitudes and to the presence of active faults[12,13], the absence of additional heat sources would nevertheless lead to the overall crystallization of the internal ocean in less than 30 Myr[2]. This suggests that another dissipation process provides the missing heating power deeper in the moon's interior, possibly in the core.

The estimated core density of Enceladus (see Methods) is low for a metal–rock core, requiring considerable (water-filled) porosity and a composition dominated by iron-bearing hydrated minerals whose abundance dictates the core water content. For iron numbers (Fe/(Fe+Mg)) between 50% and 100% of the chondritic value, the porosity of a core composed primarily of hydrated silicates would be 20–30% (see Methods). If anhydrous minerals are still present, as suggested by the recent detection of hydrogen in the plume[7], porosities are slightly larger. Owing to low confining pressures (<40 MPa) and moderate temperatures reached in the core, such an elevated porosity inherited from the accretion process[14,15] may be maintained over geological timescales[11]. Moreover, the joint action of thermochemical and tidal stresses as well as hydrothermalism may sustain the core in a highly fragmented or unconsolidated state.

A core with high porosity inside Enceladus may be subjected to considerable tidal heating, at least during some period of time[16,17]. Previous work[11] quantified the rate of dissipation for an ice-filled porous rock core, but did not consider the tidal dissipation once ice melting occurs. Other authors[18] investigated the consequences of strong tidal dissipation on the heat transfer by water flow in a porous permeable core, but they considered uniform and arbitrary values of tidal dissipation and limited their analysis to two-dimensional (2D) geometry. Here we perform coupled simulations of tidal friction and heat transfer in a porous water-filled core using a 3D approach.

In absence of direct constraints on the mechanical properties of Enceladus' core, we consider a wide range of parameters to characterize the rate of tidal friction and the efficiency of water transport by porous flow. The unconsolidated core of Enceladus can be viewed as a highly granular/fragmented material, in which tidal deformation is likely to be associated with intergranular friction during fragment rearrangements (see Methods). Although this mechanism depends on microstructure characteristics unknown in the case of Enceladus, the mechanical response of such unconsolidated media is usually parameterized using the effective shear modulus and the dissipation function. These two parameters control the response amplitude to cyclic forcing and the fraction of mechanical energy that is converted into heat, respectively[19]. The local dissipation rate is computed from the strain and stress tensors, and the global dissipation power is evaluated by integrating the dissipation rate over the entire satellite (see Methods). A total power of 10 to 30 GW can be generated for effective shear modulus ranging between 10^7 and 10^9 Pa and dissipation function between 0.2 and 0.8 (Fig. 1a and Supplementary Fig. 1). Such low values of effective shear modulus associated with high dissipation could be explained by weakening effects due to cyclic tidal strain, in a similar way to what is observed in cyclic loading tests on saturated sand and gravel mixtures in the laboratory (see Methods). Such a highly dissipative core may partly explain the observed lag in plume activity[20,21]. However, existing mechanical tests are performed at frequencies higher than tidal forcing and pressures lower than core pressure. Extrapolation to Enceladus conditions will have to be confirmed by dedicated experiments.

The degree-two shape of the tidal potential results in a modulation of tidal heating as a function of latitude and longitude

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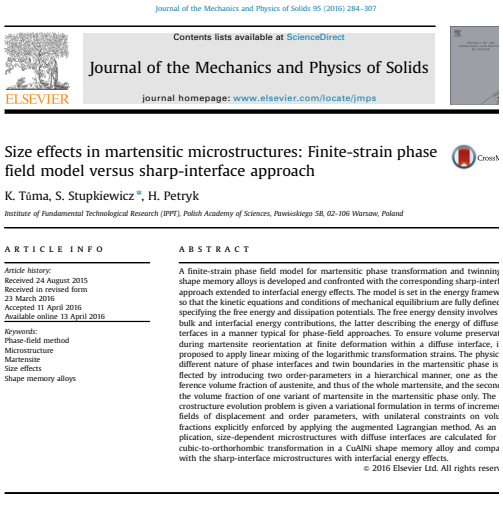
Interests:

- Continuum thermodynamics
- Viscoelastic fluids
- Complex solids
- Fluid structure interaction
- Finite element method
- Numerical simulation



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Size effects in martensitic microstructures: Finite-strain phase field model versus sharp-interface approach

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ABSTRACT

A finite-strain phase field model for martensitic phase transformation and twinning shape memory alloys is developed and confronted with the corresponding sharp-interf approach extended to interfacial energy effects. The model is set in the energy framew so that the kinetic equations and conditions of mechanical equilibrium are fully defines specifying the free energy and dissipation potentials. The free energy density involves bulk and interfacial energy contributions, the latter describing the energy of diffuse terfaces in a manner typical for phase-field approaches. To ensure volume preserva during martensite reorientation at finite deformation within a diffuse interface, i proposed to apply linear mixing of the logarithmic transformation strains. The physic different nature of phase interfaces and twin boundaries in the martensitic phase is flected by introducing two order-parameters in a hierarchical manner, one as the ference volume fraction of austenite, and thus of the whole martensite, and the secon the volume fraction of one variant of martensite in the martensitic phase only. The crostructure evolution problem is given a variational formulation in terms of increme fields of displacement and order parameters, with unilateral constraints on volu fractions explicitly enforced by applying the augmented Lagrangian method. As an plication, size-dependent microstructures with diffuse interfaces are calculated for cubic-to-orthorhombic transformation in a CuAlNi shape memory alloy and compa with the sharp-interface microstructures with interfacial energy effects.

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1. Introduction

Martensitic phase transformation plays an essential role in many material systems. Shape memory alloys (SMA) present a well-known example of the class of materials in which the martensitic transformation is crucial for their unus and spectacular behavior associated with shape recovery, pseudoelasticity, and related effects (Otsuka and Wayman, 19 Bhattacharya, 2003).

The martensitic transformation frequently proceeds by formation and evolution of complex microstructures involv several martensite variants. Commonly observed martensitic microstructures can be predicted by the classical crys lographic theory of martensite (Ball and James, 1987), which is essentially based on the thermodynamic argument of t energy minimization. In practice, the use of the crystallographic theory reduces to purely geometric relationships express compatibility of stress-free phases, as in the earlier theory of Wechsler et al. (1953). Those compatibility conditions im

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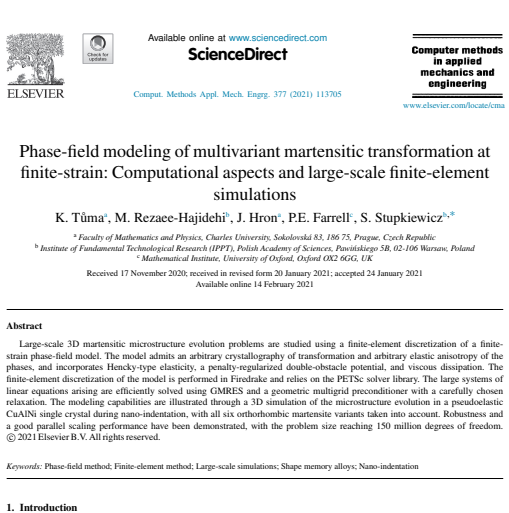

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Phase-field modeling of multivariant martensitic transformation at finite-strain: Computational aspects and large-scale finite-element simulations

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Abstract

Large-scale 3D martensitic microstructure evolution problems are studied using a finite-element discretization of a finite-strain phase-field model. The model admits an arbitrary crystallography of transformation and arbitrary elastic anisotropy of the phases, and incorporates Hencky-type elasticity, a penalty-regularized double-obstacle potential, and viscous dissipation. The finite-element discretization of the model is performed in Firedrake and relies on the PETSc solver library. The large systems of linear equations arising are efficiently solved using GMRES and a geometric multigrid preconditioner with a carefully chosen relaxation. The modeling capabilities are illustrated through a 3D simulation of the microstructure evolution in a pseudoelastic CuAlNi single crystal during nano-indentation, with all six orthorhombic martensite variants taken into account. Robustness and a good parallel scaling performance have been demonstrated, with the problem size reaching 150 million degrees of freedom.

Keywords: Phase-field method; Finite-element method; Large-scale simulations; Shape memory alloys; Nano-indentation

1. Introduction

The phase-field method has proven to be a powerful computational tool for modeling microstructure evolution in various material systems. The essential feature of the phase-field method is that the interfaces are assumed to be diffuse and accordingly the tremendous computational burden of tracking sharp interfaces is avoided. Thanks to its computational advantages, the phase-field method has been extensively employed in different areas of materials science and physics, e.g. [1–5].

Modeling the martensitic phase transformation (as in shape memory alloys) constitutes one of the classical applications of the phase-field method. Successful studies in this genre include the seminal works of Khachaturyan and co-workers [6–8], Chen and co-workers [9,10], as well as the subsequent developments that followed, e.g. [11–19]. A wide class of these studies is limited to the use of spectral solvers, e.g. [6–10,12,13,15,18,20,21], see

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Interests:

- Analysis of partial differential equations of non-Newtonian fluid mechanics
- Constitutive theory
- Flows in arteries

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ON THE CLASSIFICATION OF INCOMPRESSIBLE FLUIDS AND A MATHEMATICAL ANALYSIS OF THE EQUATIONS THAT GOVERN THEIR MOTION*

JAN BLECHTA†, JOSEF MÁLEK‡, AND K. R. RAJAGOPAL§

Abstract. In the first part of the paper we provide a new classification of incompressible fluids characterized by a continuous monotone relation between the velocity gradient and the Cauchy stress. The considered class includes Euler fluids, Navier–Stokes fluids, classical power-law fluids as well as stress power-law fluids, and their various generalizations including the fluids that we refer to as activated fluids, namely, fluids that behave as an Euler fluid prior activation and behave as a viscous fluid once activation takes place. We also present a classification concerning boundary conditions that are viewed as the constitutive relations on the boundary. In the second part of the paper, we develop a robust mathematical theory for activated Euler fluids associated with different types of the boundary conditions ranging from no-slip to free-slip and include Navier's slip as well as stick-slip. Both steady and unsteady flows of such fluids in three-dimensional domains are analyzed.

Key words. implicit constitutive theory, generalized viscosity, generalized fluidity, stress power-law fluid, shear thinning/shear thickening fluids, activated fluids, activation criterion, boundary conditions, slip, activated boundary conditions, long-time and large-data existence theory, weak solution

AMS subject classifications. 76A02, 76A05, 76D03, 35Q35

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1. Introduction. The concept of a fluid defies precise definition as one can always come up with a counterexample to that definition that seems to fit in with our understanding of what constitutes a fluid. As Goodstein [36] appropriately remarks "Precisely what do we mean by the term liquid? Asking what is a liquid is like asking what is life; we usually know when we see it, but the existence of some doubtful cases make it hard to define precisely." The concept of a fluid is treated as a primitive concept in mechanics, but unfortunately it does not meet the fundamental requirement of a primitive, that of being amenable to intuitive understanding. This makes the study under consideration that much more difficult as it is our intent to classify fluid bodies. In this study we shall consider a subclass of the idealization of a fluid, namely, that of incompressible fluid bodies. While no material is truly incompressible, in many bodies the change of volume is sufficiently small to be ignorable. Our ambit will include at one extreme materials that could be viewed as incompressible Euler fluids and at the other extreme materials that offer so much resistance to flow that they are "rigid-like" in their response, with a whole host of "fluid-like" behavior exhibited

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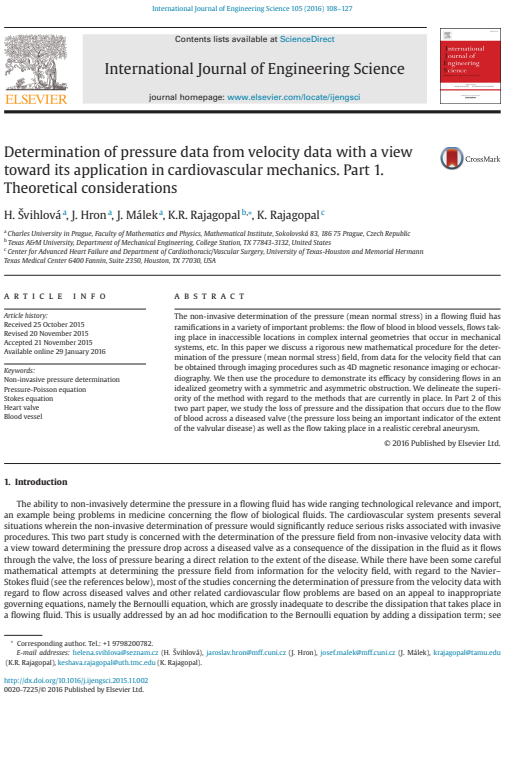

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Determination of pressure data from velocity data with a view toward its application in cardiovascular mechanics. Part 1. Theoretical considerations

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ABSTRACT

The non-invasive determination of the pressure (mean normal stress) in a flowing fluid has ramifications in a variety of important problems: the flow of blood in blood vessels, flows taking place in inaccessible locations in complex internal geometries that occur in mechanical systems, etc. In this paper we discuss a rigorous new mathematical procedure for the determination of the pressure (mean normal stress) field, from data for the velocity field that can be obtained through imaging procedures such as 4D magnetic resonance imaging or echocardiography. We then use the procedure to demonstrate its efficacy by considering flows in an idealized geometry with a symmetric and asymmetric obstruction. We delineate the superiority of the method with regard to the methods that are currently in place. In Part 2 of this two part paper, we study the loss of pressure and the dissipation that occurs due to the flow of blood across a diseased valve (the pressure loss being an important indicator of the extent of the valvular disease) as well as the flow taking place in a realistic cerebral aneurysm.

1. Introduction

The ability to non-invasively determine the pressure in a flowing fluid has wide ranging technological relevance and import, an example being problems in medicine concerning the flow of biological fluids. The cardiovascular system presents several situations wherein the non-invasive determination of pressure would significantly reduce serious risks associated with invasive procedures. This two part study is concerned with the determination of the pressure field from non-invasive velocity data with a view toward determining the pressure drop across a diseased valve as a consequence of the dissipation in the fluid as it flows through the valve, the loss of pressure bearing a direct relation to the extent of the disease. While there have been some careful mathematical attempts at determining the pressure field from information for the velocity field, with regard to the Navier-Stokes fluid (see the references below), most of the studies concerning the determination of pressure from the velocity data with regard to flow across diseased valves and other related cardiovascular flow problems are based on an appeal to inappropriate governing equations, namely the Bernoulli equation, which are grossly inadequate to describe the dissipation that takes place in a flowing fluid. This is usually addressed by an ad hoc modification to the Bernoulli equation by adding a dissipation term; see

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Charles University – Mathematical modelling group

If you – both students and researchers – are interested in any of these topics, please write directly to the individual members of the group.

Alternatively, ask me (Vít Průša, prusv@karlin.mff.cuni.cz) and I will put you in touch.