SYMPOSIUM ON TRENDS IN APPLICATIONS OF MATHEMATICS TO MECHANICS

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BOOK OF ABSTRACTS

A DEGENERATE PARABOLIC PHASE FIELD MODEL – ANALYTIC PROPERTIES AND NUMERICAL SIMULATIONS

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The talk discusses a phase field model for the evolution of a phase interface in an elastic solid, which consists of the elasticity equations coupled to the equation

$$\partial_t S = -c\,(\partial_S \psi(\varepsilon, S) - \nu \Delta_x S)|\nabla_x S|.$$

We explain the motivation for the formulation of this model and compare the properties of this model to the well known alternative phase field model, which consists of the elasticity equations and the Allen-Cahn equation.

The properties of the new model are derived by construction of asymptotic solutions. Since an existence result is only available in one space dimension and since no rigorous convergence proof for the asymptotic solutions has been found yet, the justification of the asymptotic solutions relies on numerical simulations. At the end of the talk we present the results of these numerical simulation, which have been carried out in cooperation with Bernd Markert from the RWTH Aachen University.

INFLUENCE OF SOIL MOISTURE HYSTERESIS ON THE PROPAGATION OF SOUND WAVES

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If the voids of a porous medium are filled by two (or more) immiscible fluids, as for example, water and air, then they are called partially saturated. The pore fluids possess different partial pressures, i.e. there exists a discontinuity in the pressure across the interface separating them. This difference is called capillary pressure p_c. It depends on the geometry of the void space, on the nature of the solids and and on the degree of saturation S, i.e. the ratio of the volume occupied by one of the pore fluids over the entire void volume.

The capillary pressure exhibits different values depending on the initial state of saturation. If, initially, a sample is saturated by a wetting fluid (index w) which tends to adhere to the solid walls of the void space (in contrast to the non-wetting fluid which tends to stay away from the solid wall) then drainage takes place. In the case of a non-wetting fluid (index n) filling the void space initially, the wetting fluid which invades the void space will tend to spread on the solid wall by imbibition (wetting), gradually displacing the non-wetting fluid. The hysteresis, i.e. the occurrence of two different branches of the capillary pressure curve as function of the saturation, reflects the dependence of the curve upon the history of draining and wetting.

For simplicity, in most approaches of partially saturated porous media – including my own investigations – only one of the branches is taken into account. But also investigations including hysteresis exist, though at the beginning not the hysteresis in the capillary pressure-saturation relationship was addressed but general considerations, following from studies of magnetism or ferroelectrics. The outcome are several either empirical or mathematically derived models. However, none of them has been constructed to describe the propagation of sound waves and, as a consequence, these models are also not suitable for this purpose.

In this contribution two objectives are pursued: The first is the presentation of nonlinear mathematical hysteresis modeling by use of operators like the Preisach operator. The other is the application of a linear model to wave propagation. Also in the latter case hysteresis is accounted for: the analysis is performed for the two limit cases of main drying and main wetting. The application of drying and wetting data on the propagation of sound waves is studied theoretically by means of the continuum model introduced by Albers in 2010 and numerically exploited for the example of Del Monte sand filled by an air-water mixture.

Four waves appear: one transversal wave and three longitudinal waves. For the waves driven mainly by the skeleton, the fastest longitudinal wave and the shear wave, it could be expected that the influence of the hysteresis in the capillary pressure curve is negligible. This is different from the expectations for the waves driven by the pore fluids. The numerical results exhibit – at least for the present example – a smaller influence than expected.

Acknowledgment

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A LINEARIZED APPROACH TO WORST-CASE DESIGN IN SHAPE OPTIMIZATION

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The purpose of this work is to propose a deterministic method for optimizing a structure with respect to its worst possible behavior when a 'small' uncertainty exists over some of its features. The main idea of the method is to linearize the considered cost function with respect to the uncertain parameters, then to consider the supremum function of the obtained linear approximation, which can be rewritten as a more classical function of the design, owing to standard adjoint techniques from optimal control theory. The resulting "linearized worst-case" objective function turns out to be the sum of the initial cost function and of a norm of an adjoint state function, which is dual with respect to the considered norm over perturbations. This formal approach is very general, and can be justified in some special cases. In particular, it allows to address several problems of considerable importance in both parametric and shape optimization of elastic structures, in a unified framework.

ENERGY RELEASES AND ESCHELBY FORCES IN ELASTIC STRUCTURES

Davide BIGONI
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Eshelby forces, similar to those driving dislocations in solids, are analyzed on elastic structures designed to produce an energy release and therefore give evidence for configurational forces. These structures have been realized and they have shown unexpected behaviors, which opens new perspectives in the design of flexible mechanisms, like for instance, the realization of an elastic deformable scale.

NON-LINEAR DIFFUSION OF EXTENDED OBJECTS

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We are all familiar with linear equations when speaking of elementary diffusion processes, such as the heat equation for the brownian motion of particles. However, when adressing diffusion mechanisms for extended objects such as strings or loops, while preserving (at least formally) their topology, it is necessary to move to genuinely non-linear diffusion equations. We will discuss some examples related to Fluid Mechanics and Electromagnetism.

ATOMISTIC-TO-CONTINUUM VARIATIONAL ANALYSIS OF RANDOM LATTICE SYSTEMS

Marco CICALESE
Techinische Universität München

We give an overview of some recent results regarding the atomistic-to-continuum limit of random lattice models via Γ-convergence. Our investigation is motivated by toy models related to the study of hyperelasticity of rubbers and to the analysis of Weiss domains formation in polymeric composite magnetic materials. This is a joint project with R. Alicandro, A. Gloria and M. Ruf.

HYPERBOLIC SYSTEMS OF BALANCE LAWS WITH DISSIPATION

Constantine M. DAFERMOS
Brown University

The lecture will outline a research program which aims at exploring the behavior of solutions for hyperbolic systems of balance laws with partially dissipative source, manifesting relaxation, in the class of functions of bounded variation, allowing for the presence of shock waves.

QUASI-STATIC CRACK GROWTH IN HYDRAULIC FRACTURE

Gianni DAL MASO
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We present a variational model for the quasi-static crack growth in hydraulic fracture in the framework of the energy formulation of rate-independent processes. The cracks are assumed to lie on a prescribed plane and to satisfy a very weak regularity assumption.

SOLID VS FLUID: WHERE'S THE DIFFERENCE?

Antonio DI CARLO
Università Roma Tre

In my protracted effort to develop a continuum theory of the acousto-optic effect in nematic liquid crystals, I found a major source of inspiration in a remarkable paper by Mullen, Lüthi and Steven, published on PRL in 1972. These experimentalists, while not attempting a theory, did hint at a plausible theoretical explanation:

> The experimental anisotropy in the sound velocity indicates that at finite frequencies a liquid crystal has an anisotropic compressibility. This anisotropy can be explained if at these frequencies a liquid crystal in some respects behaves like a solid [...]. However, the elastic constants must have an important frequency dependence [...]. If this were not the case, it would cost a finite energy to change the shape of a liquid crystal, the volume being kept constant. This is not consistent with our present ideas of the structure of a liquid crystal. The frequency dependence of the elastic constants could arise out of some structural relaxation process in the liquid crystal.

The ideas I have been working on—a first-gradient continuum theory characterised by a hyperelastic anisotropic response from an evolving relaxed configuration—are now ripe for publication: a paper, coauthored with Biscari and Turzi from Politecnico di Milano, is due to appear on Soft Matter, a former version of it having been available on arXiv:cond-mat since November 2013. My intention here is not to present our results, but to discuss the bigoted distinction between 'solid' and 'fluid' and the related fallacies that motivated rejection from another physical journal. Thus spoke the anonymous referee:

> The basic assumption of this manuscript is [...] that nematic liquid crystals are hyperelastic solids. However, nematics are fluids with a spontaneous broken rotational symmetry that makes them anisotropic, but not solid. In particular, nematics cannot sustain static strains (only static orientational deformations). In an infinite bulk system first sound is isotropic according to thermodynamics. In a finite nematic cell, where the orientation of the preferred direction is distorted due to some boundary conditions, first sound can show a small anisotropy. This has been successfully described by [...] and their subsequent works using standard nematohydrodynamics. Therefore, there is no need to postulate an elasticity [...] to describe those experiments.
>
> Of course, if true elasticity is postulated (rather than orientational elasticity) the anisotropy of first sound is trivial. The present manuscript might be a valuable exercise for continuum mechanics, but I cannot see any relevance for real physical nematic liquid crystal systems. The manuscript should be published in a mathematical journal.

In my view, the question in dispute has a bearing far beyond nematoacoustics. In fact, this discussion will bring me to argue against the viscoelastic paradigm, where non-equilibrium response is modelled by memory functionals, and in favour of the elastoplastic paradigm, whose basic tenet is an enlarged set of state variables—and, correspondingly, of evolution equations. The former paradigm has been dominant in the mathematical theory of materials since the appearance of the foundational papers by Noll and Coleman & Noll until recently, when the latter has been gaining prominence, as testified by the 2010 textbook by Gurtin, Fried & Anand.

DECAY PROPERTY OF REGULARITY-LOSS TYPE FOR SOLUTIONS IN ELASTIC SOLIDS WITH VOIDS

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In this paper, we consider the Cauchy problem for a system of elastic solids with voids. First, we show that a linear porous dissipation leads to decay rates of regularity-loss type of the solution. We show some decay estimates for initial data in $H^s(\mathbb{R}) \cap L^1(\mathbb{R})$. Furthermore, we prove that by restricting the initial data to be in $H^s(\mathbb{R}) \cap L^{1,\gamma}(\mathbb{R})$ and $\gamma \in [0,1]$, we can derive faster decay estimates of the solution. Second, we prove that by adding a viscoelstic damping term, then we gain some regularity of the solution and obtain the optimal decay rate.

THERMODYNAMICS OF FLUIDS: ANALYSIS AND/OR NUMERICS

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We discuss several issues related to the Navier-Stokes-Fourier system describing the time evolution of a general compressible, viscous, and heat conducting fluid. We introduce the concept of relative energy and its implications on the problems of weak strong uniqueness and conditional regularity of weak solutions. As a corollary, we show convergence of a FEDG numerical scheme that is unconditional as soon as the numerical approximation remains uniformly bounded.

BI-LIPSCHITZ SOLUTIONS TO THE PRESCRIBED JACOBIAN INEQUALITY IN THE PLANE AND APPLICATIONS TO FUNCTIONALS IN NONLINEAR ELASTICITY

Julian FISCHER
University of Zürich

We show that the prescribed Jacobian inequality in the plane admits – unlike the prescribed Jacobian equation – a bi-Lipschitz solution in case of L^∞ right-hand sides (with an identity boundary condition). Our construction relies on a refinement of a covering result due to Alberti, Csörnyei, and Preiss, which enables us to construct bi-Lipschitz maps stretching a given measurable subset of the plane by a chosen factor. We then apply our result to a model functional in nonlinear elasticity, the integrand of which blows up as the Jacobian determinant of the map in consideration

drops below a certain positive threshold. For such functionals, the derivation of the equilibrium equations for minimizers requires an additional regularization of test functions, which is provided by our newly constructed maps.

Joint work with Olivier Kneuss (University of Zürich)

LARGE DEFORMATIONS. MECHANICS AND MATHEMATICS.

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We study the motion of a solid with large deformations. The motion is described by a function Φ specifying the position $\mathbf{x}$ at time t of the material point of the solid which was at the position $\mathbf{a} \in \mathcal{D}_a$ at time 0, i.e.,

$$\mathbf{x} = \Phi(\mathbf{a}, t),$$

and $\mathbf{a} = \Phi(\mathbf{a}, 0)$.

The exterior loads may be applied to the solid by needles, wires, curved rods or beams, plates or shells. In case of a beam, the velocities of the beam are equal to the traces of the velocities of the body. It is known that the principle of virtual power written for beams requires the second gradient of the traces of the velocities of the body. Thus, it is wise to have a third gradient theory in the body.

The elongation matrix $\mathbf{W}$ of the polar decomposition

$$\mathrm{grad}\Phi = \mathbf{RW}$$

has to be symmetric. This is an internal constraint which introduces a reaction stress, an antisymmetric matrix $\mathbf{A}(\mathbf{a}, t)$. This reaction stress contributes to the Piola-Kirchhoff-Boussinesq stress and intervenes in the angular and linear momentum equations of motion.

Constitutive laws for elasticity, viscosity, plasticity... are described.

In case of visco-elasticity, we prove that there exist a local in time motion, i.e., a position function $\Phi(a, t)$ and a reaction antisymmetric matrix $\mathbf{A}(\mathbf{a}, t)$, depending on initial position a and on time t, which satisfy the complete equations of mechanics. The position is smooth enough $\Phi \in L^\infty(0, T; H^3(\mathcal{D}_a))$, $d\Phi/dt \in L^2(0, T; H^1(\mathcal{D}_a)) \cap L^\infty(0, T; L^2(\mathcal{D}_a))$, $d^2\Phi_n/dt^2$ is in the dual space of the space of the velocities $\mathcal{V}$, where $T > 0$. The reaction stress $\mathbf{A}$ is an element of dual space of the angular velocities.

This motion is local in time, because it may be interrupted by crushing resulting in a discontinuity of velocity with respect to time, i.e., a collision within the solid. Crushing occurs when squeezing fresh pasta between two fingers.

We investigate discontinuities of the velocity with respect to time resulting from crushing, from collisions with obstacle together with self collisions. Existence theorem for the velocities after collisions are given.

Flattening of a 3D solid into 2D plate by a power hammer, of a 3D solid into a 2D wire by an extruder, even the flattening of a 3D solid into a point are also investigated.

EXISTENCE FOR FINITE-STRAIN GRADIENT PLASTICITY WITHIN A CAUCHY-GREEN STRAIN FORMULATION

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A finite-strain gradient plasticity model is investigated. Thanks to isotropy and frame indifference, the model model can be entirely formulated in terms of the (right) Cauchy-Green strain tensors $\mathbf{C}$ and $\mathbf{C}_p$ referring, respectively, to the overall and plastic deformations ($\mathbf{C}$-plasticity). A quasi-static setting is assumed for elastic response, while the plastic flow rule is expressed in a variational form in terms of free-energy and dissipation potentials, corresponding to a rate-independent process. An existence result in terms of an *energetic solution* is proven in analogy with the well-established results on finite plasticity in plastic strain formulation ($\mathbf{P}$-plasticity). The $\mathbf{P}$-plasticity and $\mathbf{C}$-plasticity models are equivalent except for the gradient regularizing terms, respectively $\nabla\mathbf{P}$ and $\nabla\mathbf{C}$, whose different meaning is emphasized.

THEORETICAL ASPECTS OF DIFFUSE INTERFACE MODELS FOR TWO-PHASE FLUIDS

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The diffuse interface approach is the natural extension of van Der Waals' theory of critical phenomena. In particular, it is also used to give a more tractable description of problems characterized by the presence of sharp interfaces (e.g. solid-liquid phase transitions, mixtures of fluids, liquid crystals, superconductive materials). The method essentially consists in replacing the sharp interface with the level set (the so-called diffused interface) of a smooth function called order parameter (or phase-field) whose evolution is governed by a suitable nonlinear PDE. Such an equation depends on the thickness of the diffuse interface. It is usually possible to show (formally, at least) that the sharp interface problem can be obtained by letting the thickness go to zero. The phase-field approach is very effective from the numerical viewpoint (e.g. no interface tracking) and it gives a satisfactory representation of the phenomenon. A typical example is the so-called Caginalp system, that is, a semilinear parabolic equation for the phase-field coupled with the temperature equation. This is a model for solid-liquid phase transitions whose sharp interface limit is the Stefan problem.

Another interesting class of phase-field models arises in multiphase flows. For instance, in the phase separation of mixtures of two incompressible and partially miscible viscous fluids. In this case the model is known as the Cahn-Hilliard-Navier-Stokes (CHNS) system, namely, the Navier-Stokes equations are nonlinearly coupled with a convective Cahn-Hilliard equation for the relative concentration of one fluid. This kind of model has recently been analyzed by several authors both from the numerical and theoretical viewpoints. Further related models are the Cahn-Hilliard-Brinkman system as well as the Cahn-Hilliard-Hele-Shaw system. Both are used to describe phase separation in viscous binary fluids in a porous medium. It is worth mentioning that the latter also finds applications in modeling tumor growth.

I intend first to recall briefly the state-of-the-art focusing on some basic theoretical aspects of CHNS systems (i.e., well-posedness, existence of attractors, convergence to equilibria). Then I will present a number of recent results devoted to CHNS systems characterized by a nonlocal Cahn-Hilliard equation. This means that the spatial interactions are not approximated by the square gradient of the order parameter like in the standard Cahn-Hilliard equation. Such results have been obtained with various collaborators, namely, P. Colli, S. Frigeri, C.G. Gal, P. Krejčí and E. Rocca.

LAGRANGIAN ANALYSIS OF VELOCITY FIELDS IN FLUID MECHANICS USING THE FINITE TIME LYAPUNOV EXPONENT: APPLICATION TO THE STUDY OF A TIDAL BORE

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With the development of technology, instantaneous flow fields measurements of computations are available now. It has been followed by a rise of interest for the lagrangian analysis of such data. One tool to analyze the flow fields is the Finite Time Lyapunov Exponent (FTLE). Lyapunov exponents are well known in the field of dynamical systems. They show the asymptotical growth of infinitesimal perturbations. As the transport of passive tracers in fluid flows can be viewed as a dynamical system problem, the phase space being the physical space, the temptation was huge to apply dynamical systems theory to real flows. The Lyapunov exponents are measuring the stability of the fluid particles trajectories. As the available data is always limited (in space and in time), Lyapunov exponents cannot be computed. Moreover, the flows are highly unsteady and then, it is interesting to consider short time unstabilities.
Let $\mathbf{\Phi}_t^{t+T}$ be a flow describing the trajectory of a fluid particle from the position $\mathbf{x}_0$ at time t to the position $\mathbf{x} = \mathbf{\Phi}_t^{t+T}(\mathbf{x}_0)$ at time $t + T$, T being the integration time. The classical definition of the FTLE σ_t^T is given in equation (0.1).

$$\sigma_t^T = \frac{1}{2T} \ln(\lambda_{\max}) \tag{0.1}$$

where $\lambda_{\max}$ is the largest eigenvalue of the Cauchy-Green tensor defined as ${}^t(\nabla_0 \mathbf{\Phi}_t^{t+T})(\nabla_0 \mathbf{\Phi}_t^{t+T})$. In the paper, a new definition of the FTLE is introduced, using a local linearization of the flow field. This new definition is known as the L-FTLE, and is closer to the original Lyapunov exponent. A comparison between the two definitions will be made.
The FTLE field is computed for experimental measurements of the velocity field of a tidal bore. The experiment was performed at the Pprime institute. In a channel flow, a gate closes brutally the channel, creating a gravity current propagating upstream. This flow is studied in the laboratory to understand its impact on river sediments. The measurement was performed using high speed PIV. The FTLE was computed with the idea to find a separation between the main flow and the flow going upstream, as a property of the FTLE is that ridges of FTLE, defined as LCS, are quasi transport bareers. An example of such FTLE field is given in figure 1.

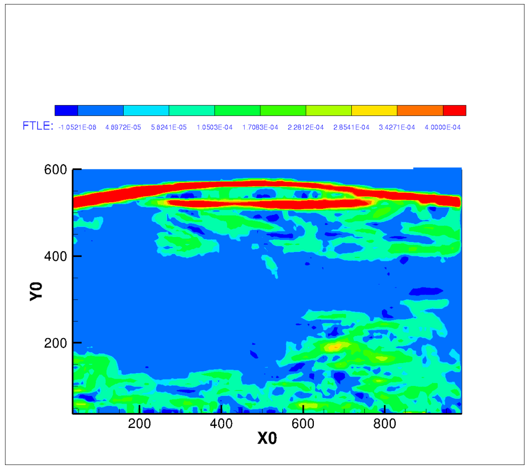

FIGURE 1. Example of a FTLE field computed for a tidal bore ($Fr = 1.29$), at one time.

A DAMAGE MODEL BASED ON MICROSTRUCTURE EVOLUTION

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Macroscopic damage and failure phenomena of solids typically are the result of the accumulation of small cracks or defects on a microscopic scale. In engineering literature, various multi-scale or homogenized models are proposed in order to describe time-dependent damage phenomena with microscopic origins like the growth of micro-cracks or micro-voids. In this lecture, we discuss these approaches in the framework of homogenization and evolutionary Γ-convergence, allowing for micro-defects that may grow individually with respect to the time-dependent loadings. The lecture relies on joint work with Hauke Hanke (WIAS Berlin).

THIN-FILM LIMITS OF FUNCTIONALS ON $\mathcal{A}$-FREE VECTOR FIELDS

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Weierstraß-Institut Berlin

Working with variational principles subject to linear PDE constraints conveyed by a constant-rank operator $\mathcal{A}$ allows us to treat a number of problems in continuum mechanics and electromagnetism in a unified way. The topic of this talk, which reports on a joint work with Filip Rindler (University of Warwick), is 3d-2d dimension reduction within this general $\mathcal{A}$-free framework. We study the effective behavior of integral functionals as the thickness ε of the domain tends to zero. Under certain conditions we show that the Γ-limit is an integral functional and give an explicit formula. The limit functional turns out to be constrained to $\mathcal{A}_0$-free vector fields, where the limit operator $\mathcal{A}_0$ is in general not of constant rank. While the lower bound follows from a Young measure approach together with a new decomposition lemma, the construction of a recovery sequence relies on algebraic considerations in Fourier space. This part of the argument requires a careful analysis of the limiting behavior of the rescaled operators $\mathcal{A}_\varepsilon$ by a suitable convergence of their symbols, as well as an explicit construction for plane waves. As applications, we characterize a thin-film Γ-limit in micromagnetics and recover the energy of a membrane model with bending moment in nonlinear elasticity.

HIGH-FIDELITY SIMULATION OF TURBULENCE USING HPC

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Thanks to the development of massively parallel supercomputers, high fidelity simulation has become a major tool for the investigation of turbulence. In this context, the two main approaches are Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). DNS is well known to be very demanding in computational resources while requiring the use of high-order numerical methods. The strength of DNS is its ability to provide the fully multiscale state of turbulent flows as converged solution of the Navier-Stokes equations free from any extra modelling. This feature leads to the development throughout the world of very useful databases to better understand the physical processes involved in the turbulent dynamics and to help in the various strategies for turbulence modelling.

For high-Reynolds number flows, LES can be a good compromise in terms of balance between computational cost and modelling uncertainty. LES is often successful but it should be recognized that its related subgrid-scale modelling suffers from significant drawbacks in terms of formalism and also in its strong sensitivity to numerical methods. The proliferation of very different and sometimes contradictory subgrid-scale models is a symptom of these two weaknesses.

In this presentation, an original DNS/LES strategy is presented. This strategy gives priority to the computational efficiency through the use of a Cartesian grid with a spatial differentiation based on high-order finite difference schemes. This very simple numerical configuration allows the simulation of turbulent problems at high-Reynolds number with a very large number of degrees of freedom. The corresponding highly resolved computational grid enables the treatment of complex geometry with the aid of a specific Immersed Boundary Method (IBM) based on an “alternating direction forcing”. This new IBM is compatible with the use of massively parallel supercomputers and with the requirement of high-order schemes in terms of accuracy and reduction of spurious numerical oscillations. When the code is used in LES mode, the subgrid-scale modelling is ensured via a spectral viscosity in harmony with the numerical methods. To show the benefits offered by this high-order LES modelling and also by the new IBM, several examples of DNS/LES are presented for a turbulent impinging jet on a heated wall and for the control of a turbulent jet using microjets.

The conclusion is that the present customized DNS/LES approach is an alternative to more sophisticated methods (e.g. high-order finite elements on unstructured grid) that enables us to tackle accurately turbulence problems with the maximum of degrees of freedom for a given generation of supercomputers.

RATE-INDEPENDENT DAMAGE IN THERMO-VISCO-ELASTIC MATERIALS WITH INERTIA

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We present a model for rate-independent, unidirectional, partial damage in visco-elastic materials with thermal effects and inertia. The damage process is modeled by means of an internal variable, governed by a rate-independent flow rule. The heat equation and the momentum balance for the displacements are coupled in a nonlinear way giving a thermodynamically consistent system. We discuss a suitable weak formulation and prove an existence theorem obtained with the aid of a decoupled time-discrete scheme and variational convergence methods. Our results apply e.g. to the study of the dynamics of the Ambrosio-Tortorelli phase-field model.

This is joint work with Riccarda Rossi (University of Brescia), Marita Thomas (WIAS Berlin), and Rodica Toader (University of Udine).

UNIQUE CONTINUATION PROPERTY OF SOLUTIONS OF THE KADOMTSEV-PETVIASHVILI EQUATIONS

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The propagation of small amplitude long waves in shallow water moving mainly in the x-direction is described by the Kadomtsev-Petviashvili equations

$$(u_t + u_x + su_{xxx} + uu_x)_x + u_{yy} = 0,$$

or its regularized version

$$(u_t + u_x - u_{xxt} + uu_x)_x + u_{yy} = 0.$$

We focus on a unique continuation propertry of the solutions. More precisely, we prove that the only solution of the Kadomtsev-Petviashvili equations with compact support for all time is identically zero. This result is first established using a result of Bourgain, then via a Carleman estimate. We conclude with a very simple proof in the regularized case.

BOUNDARY INTEGRAL EQUATION TECHNIQUE FOR ANALYSIS OF PLASMON RESONANCES IN NANOPARTICLES AND ITS RELATION TO THE RIEMANN HYPOTHESIS

Isaak D. MAYERGOYZ
University of Maryland

It will be discussed in the talk that the analysis of plasmon resonances in nanoparticles can be stated as an eigenvalue problem for specific boundary integral equations of potential theory. In the 2D case, these integral equations have, for any boundary, real spectra with "mirror symmetry," and their Fredholm determinants have the properties that have been proved or conjectured for the

Riemann xi-function. This naturally suggests the idea to find such a boundary that the Fredholm determinant of the corresponding integral operator coincides with the xi-function. This approach can be regarded as one of the realizations of the spectral Hilbert-Pólya conjecture originally stated for self-adjoint operators. Another related approach based on the J. Grommer theorem which reduces the Riemann hypothesis to polynomial analysis will be discussed as well.

ON THE MICROSCOPIC ORIGIN OF GENERALIZED GRADIENT STRUCTURES FOR REACTION-DIFFUSION SYSTEMS

Alexander MIELKE
WIAS Berlin

We discuss joint work with Mark Peletier, Giuseppe Savaré, Michiel Renger, and Matthias Liero concerning the derivation of generalized gradient structures for reaction-diffusion systems. The energy is the relative entropy while the dual dissipation functional is the sum of a quadratic diffusion term with a Onsager operator of JKO type and exponential terms for the reactions. Because of the non-quadratic nature of the dissipation potential we speak of a *generalized* gradient system.

We show that this generalized gradient structure arises from three different cases:

(1) via the large-deviation principle for the Markov processes with containing Brownian motion and discrete jumps;
(2) for a simple reaction arising as evolutionary Γ-limit from a Fokker-Planck equation with a high potential barrier
(3) for transmission conditions arising as evolutionary Γ-limit for an entropic gradient flow with a thin layer with very low mobility.

It is interesting that in the cases (2) and (3) we obtain a generalized gradient flow (i.e. the dissipation potential is non-quadratic) as an evolutionary Γ-limit from classical gradient flows (i.e. the dissipation potential is quadratic).

EXISTENCE OF SOLUTIONS IN PERIDYNAMICS AND CONVERGENCE TO CLASSICAL ELASTICITY

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José C. BELLIDO and Pablo PEDREGAL
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Peridynamics is a model in Solid Mechanics formulated by S. Silling in 2000. Its main difference with the usual Cauchy-Green elasticity relies in its non-locality, which reflects the fact that particles at a positive distance exert an interaction force upon each other. Mathematically, the deformations are not assumed to have weak derivatives, in contrast with hyperelasticity, where they are assumed to be Sobolev. In this talk we study the variational theory of time-independent problems in peridynamics. In this formulation, the energy of a deformation u is expressed as the double integral

$$I(u) := \int_\Omega \int_\Omega w(u(x') - u(x), x' - x) \, dx' \, dx,$$

where Ω is the body in the reference configuration and w is the nonlocal pairwise potential. One could take, for example, the nonlocal singular p-Laplacian

$$\int_\Omega \int_\Omega \frac{|u(x') - u(x)|^p}{|x' - x|^\alpha} \, dx' \, dx.$$

We will explain optimal conditions on w guaranteeing that the energy admits a minimum, and, hence, that the problem has an equilibrium solution.

Then, we introduce a length scale $\delta > 0$, called *horizon*, that measures the maximum interaction distance between two particles. Hence, the functional I becomes

$$I_\delta(u) := \int_\Omega \int_{\Omega \cap B(x,\delta)} w(u(x') - u(x), x' - x) \, dx' \, dx,$$

so that a particle x only interacts with those particles x' in the ball $B(x, \delta)$. We will see how the Cauchy-Green elasticity theory can be recovered from this nonlocal theory. To be precise, we prove that the functional I_δ converges, in the sense of Γ-limit, to the local functional

$$\int_\Omega W(\nabla u) \, dx$$

as $\delta \to 0$, for a suitable stored-energy function W.

MIXED SHARP-DIFFUSE APPROACH FOR SEAWATER MODELING

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Groundwater is a major source of water supply. In coastal zones there exist hydraulic exchanges between fresh groundwater and seawater. And intensive extraction of freshwater may lead to local water table depression causing problems of saltwater intrusion in the aquifer. We thus need efficient and accurate models to simulate the displacement of fresh and salt water fronts in coastal aquifer for the optimal exploitation of groundwater.

In the literature there are three categories of models for seawater intrusion:
Hidden diffuse interfaces : This is the physically correct approach. Fresh and salt water are two miscible fluids. Due to density contrast they tend to separate into two layers with a transition zone characterized by the variations of the salt concentration. Moreover the aquifer has to be considered as a partially saturated porous medium. There is another transition zone between the completely saturated part and the dry part of the reservoir, the definition of the area of desaturation being difficult. Two “diffusive interfaces” are thus hidden in this kind of model. The approach is very heavy from theoretical and numerical points of view
Hidden sharp interfaces : A first simplification consists in assuming that fresh and salt water are two immiscible fluids. Points where the salty phase disappears may be viewed as a sharp

interface. Nevertheless the explicit tracking of the interfaces remains unworkable to implement without further assumptions.
Abrupt interfaces : This approach is also based on the hypothesis that the two fluids are immiscible. Moreover the domains occupied by each fluid are assumed to be separated by a smooth interface, no mass transfert occurs between the fresh and the salt area and capillary pressure's type effects are neglected.
Of course, this type of model does not describe the behavior of the real transition zone but give informations concerning the movement of the saltwater front. The other price to pay for this simplified approach is the mathematical handling of free interfaces.

In this work we propose a mixed approach combining the (numerical) simplicity of sharp interfaces with the realism of diffuse interfaces. The derivation of the model is based on the coupling of Darcy's law and mass conservation principle written for freshwater and saltwater. The difficulty induced by the mathematical handling of free interfaces is compensated by an upscaling procedure reducing the problem to a two-dimensional setting. Mass transfers around the fronts are included through a phase-field model in fluid-fluid context.

The resulting model consists in a system of strongly and nonlinearly coupled pdes of parabolic type. We state an existence result of variational solutions for this model completed by initial and boundary conditions using a Schauder fixed point strategy. We introduce a weight based on the velocity of the salt front in the equation of the upper free interface. A subsequent difficulty is that the mapping used for the fixed point approach has to be continuous in $L^2(H^1)$. We then prove that we have sufficient control on the salt front to ignore the latter weight.

An important point is we can demonstrate a natural maximum principle from the point of view of physics, which is not possible in the case of sharp interface approximation.

MODELING OF INSTALLATION THE GLASS TAKING INTO ACCOUNT THE PROCESS OF FORMING GLUE SEAM

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The research focuses on the analysis of the typical technology of glass installation taking into account irregularity of forming a gap around the perimeter of the glass and rheological processes in case of glue polymerization. Also it contains the information on evaluation of residual stresses in glass occurring due to the difference of internal forces in glue seam after assembling.

Keywords: Body car; Glass; Glue bead; Glue seam; Deviation; Dimensions data; Elasto-plastic material; Polymerization of glue; Residual stresses; Rheological characteristic of glue; Technological pads

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DERIVATION OF A NONLINEAR PLATE MODEL VIA DIMENSION REDUCTION AND HOMOGENIZATION

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In 2002 Friesecke, James and Müller rigorously derived Kirchhoff's nonlinear plate model from 3d nonlinear elasticity. We combine their derivation with periodic homogenization and consider an energy functional that depends on two small parameters: h – the thickness of the plate, and ε – the size of the composite's microstructure. We derive effective models by passing to the Γ-limit as $h, \varepsilon \to 0$. Although the original and the limiting model are geometrically nonlinear, we prove that the effective elastic moduli are characterized by a simple single-cell problem. It turns out that the precise form of the cell problem (and thus the effective properties) depends on the relative scaling between h and ε.

The lecture is based joint works with Peter Hornung, Igor Velcic and Heiner Olbermann.

CRYSTALLINE AND ISOPERIMETRIC CONFIGURATIONS

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In this talk the fundamental crystallization problem of analytically explaining why particles at low temperature arrange in periodic lattices will be considered. At low temperatures particle interactions are expected to be essentially determined by particle positions. The two-dimensional problem in the square lattice will be the main reference setting.

It will be first shown that the ground states of a suitable configurational energy $E : \mathbb{R}^{2n} \to \mathbb{R} \cup \{+\infty\}$ accounting for two- and three-body short-ranged interactions are connected subsets of the reference lattice, and that ground-state energy can be exactly quantified in terms of the number of particles.

Furthermore, as the energy E favors particle bonding and 'boundary' particles have in general less bonds, ground states are intuitively expected to have minimal 'perimeter' and maximal 'area'. This intuition will be verified by characterizing the ground states as those configurations which realize equality in a discrete isoperimetric inequality.

Finally, the emergence of a macroscopic Wulff shape as the number of particles grows will be established. Precisely, ground states will be shown to deviate from the asymptotic Wulff shape at most by $O(n^{3/4})$ particles. This result nicely reflects the inherent multiscale nature of the crystallization phenomenon.

NANOMECHANICS

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The rapid development of synthesis and characterization of nanostructured materials as well as unprecedented computational power have brought forth a new era of materials research in which experiments, simulation and modeling are performed side by side to probe the unique mechanical properties of nanoscale materials. This talk aims to present an overview of our recent studies of the mechanics of graphene and related composites, including fracture strength [1], nanoscrolls [2] and flexible electronics [3], mainly via quasi continuum mechanics modeling. Theoretical analyses are performed e.g. to probe equilibrium and dynamic properties of carbon nanoscrolls – made of a continuous basal graphene sheet rolled up in a spiral form – such as their equilibrium core size as well as their oscillatory and translational motion with and without an external controlling field, and compared with results from molecular dynamics simulations; by analyzing the elastic bending and surface interaction energies in the system, we have developed equations of motion in terms of the surface energy, the bending stiffness, the interlayer spacing, the length and width of the basal graphene sheet and the core radius of the nanoscroll. The results suggest that the graphene hold great promises for applications such as high strength fibers and composites, nano-oscillators, nanoactuators, nanomotors, tunable water and ion channels, nanofluidic devices, nanofilters, flexible electronics, as well as tunable gene and drug delivery systems.

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DIRECTIONAL OSCILLATIONS VIA MICROLOCAL COMPACTNESS FORMS

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The new tool of microlocal compactness forms (MCFs) allows one to study oscillations and concentrations in sequences of functions (e.g. deformation gradients). Decisively, MCFs retain information about the location, value distribution, and direction of oscillations and concentrations, thus extending at the same time the theories of (generalized) Young measures and H-measures. In L^p-spaces oscillations and concentrations precisely discriminate between weak and strong compactness, and thus MCFs allow to quantify the difference in compactness. The definition of MCFs involves a Fourier variable, whereby also differential constraints on the functions in the sequence can be investigated. After presenting several aspects of the abstract theory, I will present applications to situations relevant for theoretical continuum mechanics.

"ENTROPIC" SOLUTIONS TO A THERMODYNAMICALLY CONSISTENT PDE SYSTEM FOR PHASE TRANSITIONS AND DAMAGE

Elisabetta ROCCA
WIAS - Berlin

Riccarda ROSSI
University of Brescia

In this talk we present a PDE system modelling (non-isothermal) phase transitions and damage phenomena in thermoviscoelastic materials. The model is thermodynamically consistent: in particular, no *small perturbation assumption* is adopted, which results in the presence of quadratic terms on the right-hand side of the temperature equation, only estimated in L^1. The whole system has a highly nonlinear character.

We address the existence of a weak notion of solution, referred to as "entropic", where the temperature equation is formulated with the aid of an entropy inequality, and of a total energy inequality. This solvability concept reflects the basic principles of thermomechanics as well as the thermodynamical consistency of the model. It allows us to obtain *global-in-time* existence theorems without imposing any restriction on the size of the initial data.

We prove our results by passing to the limit in a time discretization scheme, carefully tailored to the nonlinear features of the PDE system (with its "entropic" formulation), and of the a priori estimates performed on it. Our time-discrete analysis could be useful towards the numerical study of this model.

VARIOUS CONCEPTS OF SOLUTIONS TO RATE-INDEPENDENT SYSTEMS ILLUSTRATED ON A DELAMINATION CONTACT PROBLEM

Tomáš ROUBÍČEK
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Evolution of mechanical systems are often governed by nonconvex stored energies and by dissipated energies. The latter can be considered homogeneous of degree-1 if the outer loading is on much slower time scale than internal processes in the system. The weak (or here also called the local) solutions represent typically very wide class within which solutions of a very different kind can be sought.

Some solutions, called energetic, conserve energy during evolution, being based on the usual global-minimum concept for incremental problems. In spite of this physically relevant energy-conservation attribute, they may often be less physical than some force-driven local solutions. Various time-discretisations will be discussed, together with the role of the maximum-dissipation principle in the relation to the force-driven solution concept.

Abstract considerations will be illustrated on a delamination problem (= an adhesive contact problem), together with some of its variant as a brittle or a mode-sensitive delamination, illustrated by several 2-dimensional numerical experiments, performed mainly by Christos G. Panagiotopoulos (U. of Seville/U. of Heraklion) and Roman Vodička (T. U. Košice, Slovakia) by using the boundary-element method. In particular, energetic solutions, maximally-dissipative local solutions, and vanishing-viscosity solutions will be compared.

CONSERVATION OF BULK MASS IN CAHN-HILLIARD AND RELATED EQUATIONS

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The Cahn-Hilliard model describes.phase separation for a bi- nary mixture. The description of mass conservation in a region with nonper- meable walls leads to consideration of a dierent boundary condition for the chemical potential rather than the usual Neumann condition. Dynamic bound- ary conditions for the relative concentration are considered. The notion of bulk mass conservation can also be considered in more general models, such as Cahn-Hilliard-Gurtin equation and others. The derivation of the appropriate boundary conditions in some of these more general models as well as results further analytic results will be presented.

ON THE MATHEMATICAL AND GEOMETRICAL STRUCTURE OF THE DETERMINING EQUATIONS FOR SHEAR WAVES IN NONLINEAR ISOTROPIC INCOMPRESSIBLE ELASTODYNAMICS

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Using the theory of $1+1$ hyperbolic systems we put in perspective the mathematical and geometrical structure of the celebrated circularly polarized waves solutions for isotropic hyperelastic materials determined by Carroll in Acta Mechanica 3 (1967) 167–181. We show that a natural generalization of this class of solutions yields an infinite family of *linear* solutions for the equations of isotropic elastodynamics. Moreover, we determine a huge class of hyperbolic partial differential equations having the same property of the shear wave system. Restricting the attention to the usual first order asymptotic approximation of the equations determining transverse waves we provide the complete integration of this system using generalized symmetries.

ABOUT SOME DISCRETE MODELS FOR DISLOCATIONS IN NANOWIRE HETEROSTRUCTURES AND THEIR CONTINUUM LIMIT

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We discuss discrete models for heterogeneous nanowires, allowing for dislocations at the interface. We study the limit as the atomic distance converges to zero, considering simultaneously a dimension reduction and the passage from discrete to continuum. Employing the notion of Gamma-convergence, we establish the minimal energies associated to defect-free configurations and configurations with dislocations at the interface, respectively. It turns out that dislocations are favoured if the thickness of the wire is sufficiently large.

This is joint work with G. Lazzaroni (SISSA, Trieste) and M. Palombaro (University of Sussex).

POROUS CONVECTION WITH LOCAL THERMAL NON-EQUILIBRIUM TEMPERATURES AND WITH CATTANEO EFFECTS IN THE SOLID

Brian STRAUGHAN
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There is increasing interest in convection in local thermal non - equilibrium (LTNE) porous media. This is where the solid skeleton and the fluid may have different temperatures. There is also increasing interest in thermal wave motion, especially at micro- nano-scales, and particularly in solids. Much of this work has been based on the famous model proposed in 1948 by Carlo Cattaneo. In this paper we develop a model for thermal convection in a fluid saturated Darcy porous medium allowing the solid and fluid parts to be at different temperatures. However, we base our thermodynamics for the fluid on Fourier's law of heat conduction, whereas we allow the solid skeleton to transfer heat by means of the Cattaneo heat flux theory. This leads to a novel system of partial differential equations involving Darcy's law, a parabolic fluid temperature equation and effectively a hyperbolic solid skeleton temperature equation. This system leads to novel physics and oscillatory convection is found whereas for the standard LTNE Darcy model this does not exist. We are also able to derive a rigorous nonlinear global stability theory unlike work in thermal convection in other second sound systems in porous media.

EXTENDED THERMODYNAMICS OF POLYATOMIC GASES AND ITS APPLICATION TO SHOCK WAVES

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Recently extended thermodynamics (ET) of dense gases was proposed, where a rarefied polyatomic gas is regarded as a special case of a dense gas. The most typical one is the hyperbolic theory of 14 fields (ET14) of the mass density, the velocity, the temperature, the viscous stress, the dynamic (nonequilibrium) pressure, and the heat flux with two parallel hierarchical series of field equations of balance type, that is, the momentum series and the energy series. This is a natural extension of the well-known Navier-Stokes Fourier theory for viscous and heat-conducting fluids. By applying the constitutive theory of ET, the constitutive equations can be determined explicitly by the thermal and caloric equations of state together with the experimental data on the shear viscosity, the bulk viscosity and the heat conductivity.

The other typical one is the hyperbolic theory with 6 fields (ET6), which is a subsystem of the ET14 theory: the mass density, the velocity, the temperature and the dynamic pressure. This is the theory just next to the Euler theory for perfect fluids with 5 fields. This theory is useful in such a case where the relaxation time for the dynamic pressure is much larger than the relaxation times for the shear stress and the heat flux.

In the case of rarefied polyatomic gases, these theories are shown to be fully consistent with the moment equations derived from the kinetic theory of polyatomic gases. The ET theories with many moments have also been derived recently.

By using the theories of dense gases, the class of gases and the conditions for gases to which ET is applicable have been enlarged enormously. As an example of many possible applications of the theories, we show that the shock wave structure in a rarefied polyatomic gas is explained consistently by the ET theories, i.e., ET14 and ET6 theories. Three types of the shock wave structure observed in experiments, that is, the nearly symmetric shock wave structure (Type A, small Mach number), the asymmetric structure (Type B, moderate Mach number), and the structure composed of thin and thick layers (Type C, large Mach number), are explained by the theories in a unified way. The theoretical prediction of the profile of the mass density agrees well with the experimental data. The well-known Bethe-Teller theory of the shock wave structure in a rarefied polyatomic gas is reexamined in the light of the present theories.

The purpose of the present talk is to make a review of the recent developments in the ET theory of dense gases mentioned above and also to show its application to the shock wave structure in a polyatomic gas. The organization of the present talk is planned as follows:

1. INTRODUCTION: Brief survey of ET of rarefied monatomic gases.
2. THEORY of ET14: The basic system of equations is explained and discussed.
3. THEORY of ET6 : The basic system of equations and the relationship with ET14 are explained.
4. APPLICATION of the ET14 and ET6 theories to shock waves. The shock wave structure in rarefied polyatomic gases is explained.
5. DISCUSSIONS and CONCLUDING REMARKS: Problems to be studied are summarized.

The present speaker deeply thanks his co-workers: Takashi ARIMA (Kanagawa University, Japan), Tommaso RUGGERI (University of Bologna, Italy) and Shigeru TANIGUCHI (Kitakyushu National College of Technology, Japan).

FEEDBACK STABILIZATION OF AN OSCILLATING VERTICAL CYLINDER BY POD REDUCED-ORDER MODEL

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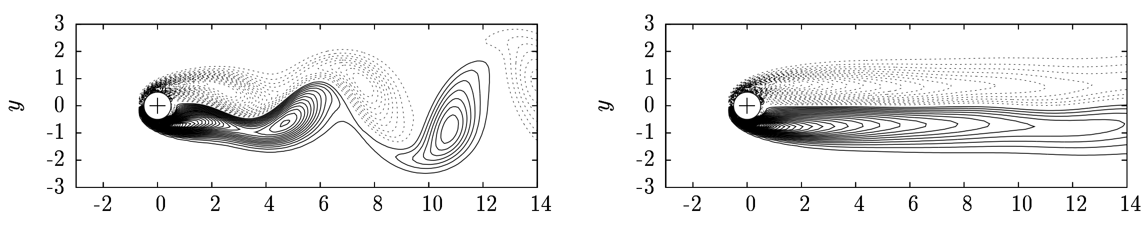
The objective of this paper is to demonstrate the use of Reduced-Order Models (ROM) based on Proper Orthogonal Decomposition (POD) to stabilize by vertical oscillations the flow over a circular cylinder for a Reynolds number equal to 60. The 2D Navier-Stokes equations are first solved by a finite element method with COMSOL Multiphysics in which the moving mesh is introduced via ALE. Since in Fluid-Structure Interaction, the POD algorithm cannot be applied directly, we then implement the fictitious domain method of Glowinski et al. (1999) where the solid domain is treated as a fluid undergoing an additional constraint. The POD-ROM is then classically obtained by projecting the Navier-Stokes equations on a small number of POD modes. At this level, the cylinder movement is enforced in the POD-ROM through the introduction of Lagrange multipliers. A Linear Quadratic Regulator framework is used to determine the optimal control law, in our case the vertical velocity of the cylinder, such that the flow is stabilized. After linearization of the POD-ROM around the steady flow state, the optimal linear feedback gain is obtained as solution of a Generalized Algebraic Riccati Equation. Finally, when the optimal feedback control is applied, it is shown that the flow converge rapidly to the steady state. In addition, a vanishing control is obtained proving the efficiency of the control approach.



(a) Natural flow

(b) Controlled flow by vertical oscillation of the cylinder.

Figure 2. Linear feedback stabilization of the wake behind a circular cylinder at $Re = 60$. Contour lines of vorticity.

COMPLETENESS OF A SYSTEM OF ROOT FUNCTIONS OF BOUNDARY VALUE PROBLEMS FROM PHYSICS AND MECHANICS

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The talk is devoted to boundary value problems for elliptic differential-operator equations of the second order with operator-boundary conditions and with the spectral parameter in both the equation and the boundary conditions. Unique solvability and the corresponding estimate of a solution (with respect to the space variable and the parameter) will be shown. The corresponding discreteness of the spectrum and completeness of a system of root functions of the homogeneous problem are also true. Then, applications of the abstract results to boundary value problems for elliptic differential equations with a parameter in non-smooth domains or to ordinary differential equations with a parameter on an interval are illustrated. Such problems may arise in Physics and Mechanics.