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honoring 80th birthday of Prof. J. Tinsley Oden

Fractional Cahn-Hilliard Equation(s)
Analysis, Properties and Approximation

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The classical Cahn-Hilliard equation [1] is a non-linear, fourth order in space, parabolic partial differential equation which is often used as a diffuse interface model for the phase separation of a binary alloy. Despite the widespread adoption of the model, there are good reasons for preferring models in which fractional spatial derivatives appear [2,3]. We consider two such Fractional Cahn-Hilliard equations (FCHE).

The first [4] corresponds to considering a gradient flow of the free energy functional in a negative order Sobolev space H^α, $\alpha \in [0, 1]$ where the choice $\alpha = 1$ corresponds to the classical Cahn-Hilliard equation whilst the choice $\alpha = 0$ recovers the Allen-Cahn equation. It is shown that the equation preserves mass for all positive values of fractional order and that it indeed reduces the free energy. The well-posedness of the problem is established in the sense that the H^1-norm of the solution remains uniformly bounded. We then turn to the delicate question of the L_∞ boundedness of the solution and establish an L_∞ bound for the FCHE in the case where the non-linearity is a quartic polynomial. As a consequence of the estimates, we are able to show that the Fourier-Galerkin method delivers a spectral rate of convergence for the FCHE in the case of a semi-discrete approximation scheme. Finally, we present results obtained using computational simulation of the FCHE for a variety of choices of fractional order α. We then consider an alternative FCHE [3,5] in which the free energy functional involves a fractional order derivative.

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A Multiscale Hybrid Model of Tumor Growth

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Cancer development results from a complex interplay of different phenomena that span a wide range of time and length scales. Computational modeling may help to unfold the role of multiple evolving factors that exist and interact in the tumor microenvironment. Understanding these complex multiscale interactions is a crucial step towards developing effective drug therapies.

We integrate here different modeling approaches in a hybrid multiscale avascular tumor growth model. At the tissue level, we consider the dispersion of nutrients and growth factors in the tumor microenvironment, which are modeled through reaction-diffusion equations. At the cell level, we use an agent based model to describe normal and tumor cell dynamics, with normal cells kept in homeostasis and cancer cells differentiate into quiescent, proliferative, apoptotic, hypoxic and necrotic states. Cell movement is driven by the balance of a variety of forces according to Newton's second law, including those related to growth-induced stresses. Phenotypic transitions are mainly deterministic, although the switches from quiescent to apoptotic and to proliferative states are stochastic. We integrate in each cell/agent a branch of the Epidermal Growth Factor Receptor (EGFR) pathway which is known to be hyperactivated in about 30% of all cancers. This intracellular mechanism regulates proliferative advantage in response to microenvironment stimuli. The EGFR pathway is modeled by a system of nonlinear differential equations involving the chemical kinetics of 20 molecules, and the rates of change in the concentration of key molecules trigger the regulatory response. The bridge between cell and tissue scales is built through the source/sink terms of the partial differential equations.

Our hybrid model is built in a modular way, enabling the investigation of the role of potential different mechanisms at multiple scales on the tumor progression. This strategy allows the representation of both the collective behavior due to cell assembly as well as microscopic intracellular phenomena described by signal transduction pathways. Here, we investigate cell-proliferation-decision-response impact on cancer progression. Computational simulations demonstrate that the model can adequately describe some complex mechanisms of tumor dynamics, including growth arrest in avascular tumors.

Bridging Multiple Structural Scales with a Generalized Finite Element Method

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Interactions among multiple spatial scales are pervasive in many engineering applications. Structural failure is often caused by the onset of localized damage like cracks or shear bands that are orders of magnitude smaller than the structural dimensions. In this talk, we present a Generalized Finite Element Method (GFEM) based on the solution of interdependent macro/global and fine/local scale problems. The local problems focus on the resolution of fine-scale features of the solution near regions with singularities or localized nonlinearities, while the global problem addresses the macro-scale behavior of the structure. Fine-scale solutions are accurately computed in parallel using the h-version of the GFEM and embedded into the global solution space using the partition of unity method. Thus, the proposed method does not rely on a-priori knowledge about the solution of the problem. This GFEM enables accurate modeling of problems involving nonlinear, multi-scale phenomena on macro-scale meshes that are orders of magnitude coarser than those required by the FEM. Numerical examples demonstrate applications to the simulation of propagating cohesive fractures, and to the analysis of structural connections (spot welds) in built-up panels for the next-generation hypersonic aircraft currently under investigation at U.S. Air Force Research Laboratories. They also show that the conditioning of the method is of the same order as in the FEM and that it is controlled by the mesh size of the *coarse* scale discretization. Extensions of the method to three-dimensional simulations of multi-stage hydraulic fracturing of gas and oil reservoirs are also discussed.

Delayed Feedback Control Method for Calculating Space-Time Periodic Solutions of 3D Viscoelastic Problems

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In industrial applications, in order to avoid the inversion of very large matrices, time periodic states are often computed as the asymptotic limit solution of an initial value boundary value problem with arbitrarily chosen initial data. This kind of problems can be faced, for instance, in the cardiac contractions modeling [1]. Another example concerns the steady rolling of a viscoelastic tyre [2] with a periodic sculpture. In this case, the stable state satisfies a "rolling" periodicity condition, including shifts both in time and space: the state $\underline{u}(x,t)$ at any point $\underline{x}$ is the same that at the corresponding point observed at the next sculpture one time period T ago

$$\underline{u}(t,\underline{x}) = R_{\omega T}^{-1}\,\underline{u}(t-T, R_{\omega T}\underline{x}).$$

Above, R_θ denotes the rotation of angle θ and ω the rotation speed. Calculating such initial value problems until the asymptotic limit may take a lot of time for "viscous" problems, when memory effects are very large. In such cases nonetheless, one is not interested in the evolution history, but only in a fast access to the asymptotic limit cycle. Thus developing methods accelerating convergence to this limit is of high interest.

Here, even if the asymptotic limit is periodic, the solution of the initial value evolution problem is not. The lack of periodicity of the calculated solution is then an extra information (observation) on which one can apply control techniques. In other words, we can modify the original evolution problem through a feedback control term based on this observation error. In this framework, the present work is dedicated to the development and validation of an optimal feedback control minimizing the convergence time to the limit cycle.

First, we present an analytical analysis of an abstract linear evolution problem, and find the solution to the modified (controlled) problem, based on the theory of delayed differential equations [3] and using the Lambert W function [4]. Having studied the influence of the control on the convergence rate, we propose then the optimal control, by optimizing the spectrum of the problem and minimizing thus the convergence time. The resulting method is similar to the feedback control methods, stabilizing unstable steady states [5,6]. It turns out that it can also be mechanically interpreted as a correction of the present solution in proportion of the periodicity errors which would be observed in the next periods in the absence of control.

We have also proved that the acceleration increases with the memory of the problem. So the developed method might not be efficient for fast converging problems (which is not really of interest) but becomes more and more efficient for the slowly converging problems. Unfortunately, the optimal control term involves the exponential of the underlying operator, whose numerical calculation induces a loss of sparsity and a high numerical cost. So a modified control term has been proposed, where the matrix exponential is replaced by a scalar while preserving the acceleration rate, control which can then be applied to a nonlinear problem as well.

The developed method has been applied to two problems. In the first one, we consider a 2D disk heated with a source periodically moving along a circular path, which may be a simple model problem for additive manufacturing. This problem corresponds exactly to the theoretical framework. The second problem considers the steady rolling of a viscoelastic 3D tyre with periodic sculpture. This problem is three dimensional and non-linear. Both problems have been solved numerically with the finite element method, while comparing the controlled and non-controlled solutions. The simulation results confirm the theoretical statements. Even when using the scalar construction of the exponential, the method accelerates convergence to the limit cycle at the rate predicted by the theory, and its efficiency increases with the size of the memory effects.

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Journey through Mechanics Research and Education: A Personal Retrospective

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This is a personal retrospective of the author's journey through mechanics research and education in the United States of America that began while the author was a Ph.D. student of Professor J.T. Oden in 1970. The publication of a seminal paper on 14 primal and dual variational principles of mechanics [1] and two books on mathematical theory of finite elements and variational principles in theoretical mechanics with Professor Oden provided the inspiration and paved the way for the author's professional journey through composite materials and structures, penalty and least-squares finite elements models of fluid flow, higher-order shell finite elements, and non-local continuum theories.

The lecture will begin with an overview of the author's highly-cited shear deformation and layerwise theories for composite laminates [2,3], the least-squares finite element models of the flows of viscous incompressible fluids [4], and a robust shell finite element [5]. Then overview of the authors recent research on nonlocal elasticity and couple stress theories in formulating the governing equations of functionally graded material beams and plates will be presented. Two different nonlinear gradient elasticity theories that account for (a) geometric nonlinearity and (b) microstructure-dependent size effects are revisited to establish the connection between them. The first theory is based on modified couple stress theory and the second one is based on Srinivasa-Reddy gradient elasticity theory [6]. These two theories are used to derive the governing equations of beams and plates. In addition, the graph-based finite element framework (GraFEA) suitable for the study of damage in brittle materials will be discussed (see Khodabakhshi, Reddy, and Srinivasa [7]). GraFEA stems from conventional finite element method by transforming it to a network representation based on the study by Reddy and Srinivasa [8]. Figure 1(b-h) display the evolution of cracks for a rectangular plate with an elliptic hole ($a = 0.8$, $b = 0.2$, $W = 4$, $L = 6$, $E = 3 \times 10^6$, $\nu = 0.25$, and $\varepsilon_{critical} = 0.005$). The figures show that as the crack reaches ends of the plate, some form of crack branching initiates near the ends.

Dedication. This lecture is dedicated to his teacher and mentor, Professor J.T. Oden, with sincere gratitude, high respect, and love.

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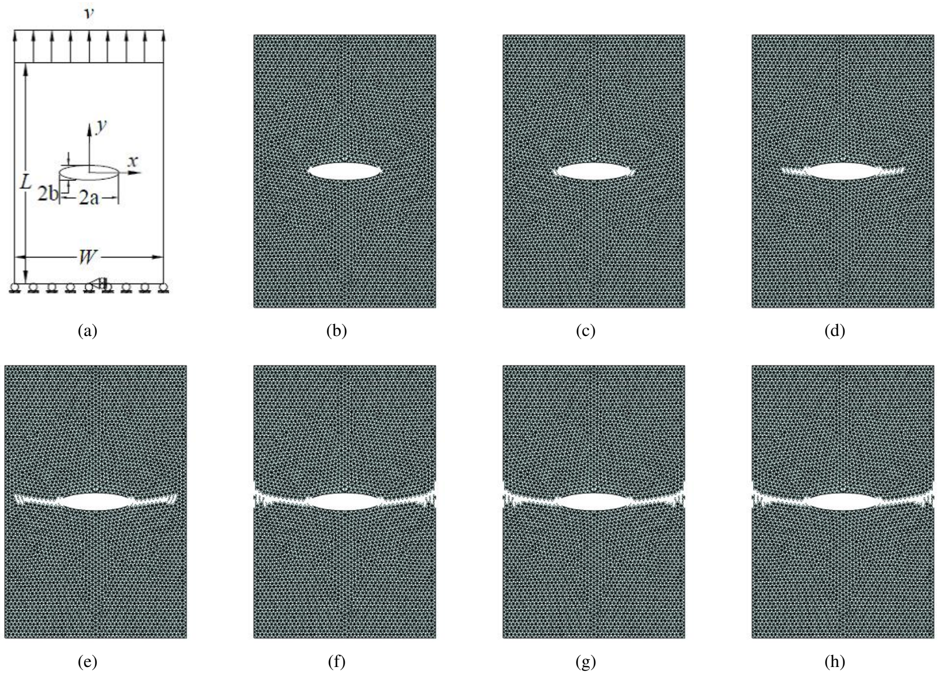

Figure 1: Evolution of the broken edges for a rectangular plate with an elliptic hole. (a) Rectangular plate with an elliptic hole under the application of displacement boundary conditions. (b) $I = 1$ (c) $I = 25$ (d) $I = 30$ (e) $I = 35$ (f) $I = 40$ (g) $I = 45$ (h) $I = 50$, where I denotes the number of links broken

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The Inequality Level Set Approach (ILS) to Handle Variational Inequalities: Application to Contact and Visco-plastic Fluids

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The key idea of the Inequality Level Set approach (ILS) for variational inequalities is to locate with a level set the domain over which the inequality reaches an equality. For contact problem, it means that the main unknown is the contact zone. This is an important departure from classical contact algorithm since at any iteration an explicit contact contour is known as a level set. A true Newton-Raphson may thus be built with respect to the contact location. The derivative of the energy with respect to the contact zone location has the meaning of a configurational force. For frictionless contact it must be driven to zero to reach the exact contact zone, whereas in case of adhesion the force must correspond to the adhesion level.

The main advantages of the ILS are :

- possibility to enrich with the the extended finite element approach (X-FEM) the contact zone boundary to capture non-smoothness of the displacement field (higher order convergence rate with respect to the mesh size is thus at hand)
- robustness in the iterative process since it is based on a full Newton-Raphson.
- achieve stability analysis of a given contact zone
- design reduced order modeling for contact

Examples of simulation of contact of membranes or deformable bodies on a rigid obstacle will show the capabilities of the ILS. Also, we will discuss the capabilities of the ILS for visco-plastic fluids.

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Some a Posteriori Error Estimators for PDEs with Random Coefficients

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We consider Partial Differential Equations (PDEs) with uncertain parameters described as random variables.

In the case of small uncertainties, we advocate a perturbation approach in which only the deterministic solution corresponding to the nominal value of the parameters is computed by the finite element method, eventually complemented by a correction term linear in the parameters. We derive residual based a-posteriori error estimates, which quantify both the finite element error and the error due to the perturbation method, in the case of an elliptic equation with random parameters as well as the steady state Navier-Stokes equations on a randomly perturbed domain.

In the case of large uncertainties, we consider instead a sparse grids stochastic collocation finite element method. We derive a residual-based a posteriori error estimate that provides upper bounds on the two sources of error (finite element and stochastic collocation), in the special case of an elliptic diffusion equation with a random coefficient that depends affinely on a finite number of random variables. The error estimator on the stochastic component is then used to drive an adaptive sparse grid algorithm which aims at circumventing the "curse of dimensionality" inherent to tensor grids approximations. Several numerical examples are given to illustrate the performance of the adaptive procedure.

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The Inequality Level Set Approach (ILS) Computing, Data, Models, Mathematics – Gumbo or Salad?

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In honor of my dear teacher and Professor for life J. T. Oden

Modeling and reliable accurate predictions based on models is at the heart of much human endeavor and in particular hazard risk analysis from extreme events that threaten life and property. In this talk, I will review the development of predictive tools for analysis of hazard risks that integrate developments in modeling, computing and numerical methodologies. The complex physics, need to quantify uncertainties in models and parameters, and produce tools that are scaleable, robust and reliable while being computationally efficient drive the need for integrated development of mathematical and computational procedures. New methods for reliable and accurate computation from adaptivity to parallel computing and uncertainty quantification must all be developed and used. The availability of unprecedented levels of data from observation and simulations and invention of tools to make inferences from such large data sets adds another very promising line of attack to this challenge. The key to a successful strategy is the art of harnessing all of these methodologies in a consistent and comprehensive manner. Haphazard juxtaposition of disparate elements is rarely. I will present an integrated vision that harnesses all of these methodologies and over the last decade has resulted in a consistent set of integrated tools for volcanological applications.

On a Goal-oriented Finite Element Formulation for the Estimation of Quantities of Interest

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We will present in this talk a finite element formulation of boundary-value problems that aims at constructing approximations tailored towards the estimation of quantities of interest. The main idea is to reformulate a boundary-value problem as a minimization problem that involves inequality constraints on the error in the goal functionals so that the resulting model is capable of delivering quantities of interest within some prescribed tolerance. Chaudhry et al. have proposed in [1] a similar method in which constraints are enforced via a penalization approach. However, an issue with that approach is concerned with the selection of suitable penalization parameters. Our goal in this work aims at circumventing this difficulty by imposing the inequality constraints through Lagrange multipliers using the Karush-Kuhn-Tucker (KKT) conditions. We will also show how to design an adaptive strategy to construct adapted meshes based on a posteriori error estimates. Such a paradigm represents a departure from classical goal-oriented approaches in which one computes first the finite element solution and then adapts the mesh by controlling the error with respect to quantities of interest using dual-based error estimates [2]. Numerical examples will be presented in order to demonstrate the efficiency of the proposed approach. We will also show how such a formulation can be applied to the construction of reduced models using the so-called proper generalized decomposition (or low-rank approximation) method [3]. Preliminary work related to that topic has been presented in [4].

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The Nonlinear Petrov-Galerkin Method: Quasi-optimal Discretization in Banach Spaces

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Is it possible to obtain near-best approximations to solutions of linear operator equations in a general Banach-space setting? Can this be done with guaranteed stability? We address these questions by introducing nonstandard, nonlinear Petrov–Galerkin (NPG) discretizations [1]. These methods are imperative for PDEs with rough data or nonsmooth solutions having discontinuities.

The NPG method builds on recent developments in Petrov–Galerkin and residual minimization methods: It extends the seminal optimal Petrov–Galerkin methodology of Demkowicz and Gopalakrishnan [2] to Banach spaces; it provides for a (monotone) nonlinear extension of the corresponding mixed formulation, cf. Dahmen et al [3]; and it extends the L^p residual-minimization method of Guermond [4] to arbitrary dual Banach spaces.

The essential component in the NPG method is the (nonlinear) duality map, which is the natural extension of the Riesz map (a Hilbert-space construct) to Banach spaces. Whenever the residual is measured in a negative (Banach) Sobolev norm, a inexact version of NPG is needed to discretely invert the duality map. We demonstrate the stability of the resulting inexact method and prove a priori error estimates by extending a projection identity going back to Kato, cf. [5].

Two applications are presented: First we consider a non-Hilbert setting for the Laplace operator allowing for rough solutions $\notin H^1$, where discrete stability will hinge on the $W^{1,p}$-stability of the H_0^1-projector. Then we focus on the advection-reaction PDE in a weak setting leading to quasi-best approximations in L^p ($1<p<\infty$). It is furthermore demonstrated that in the approximation of discontinuities, the notorious Gibbs phenomena, inherently present in the Hilbert case ($p = 2$), is eliminated as $p \searrow 1$.

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Modeling and Simulation of Advanced Manufacturing Processes

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Within the last decade, several industrialized countries have stressed the importance of advanced manufacturing to their economies. Many of these plans have highlighted the development of additive manufacturing techniques, such as 3D printing, which are still in their infancy. The objective is to develop superior products, produced at lower overall operational costs. For these goals to be realized, a deep understanding of the essential ingredients comprising the materials involved in additive manufacturing is needed. The combination of rigorous material modeling theories, coupled with the dramatic increase of computational power can potentially play a significant role in the analysis, control, and design of many emerging additive manufacturing processes. Specialized materials and the precise design of their properties are key factors in the processes. Specifically, particle-functionalized materials play a central role in this field, in three main ways: (1) to endow filament-based materials by adding particles to a heated binder (2) to "functionalize" inks by adding particles to freely flowing solvents and (3) to directly deposit particles, as dry powders, onto surfaces and then to heat them with a laser, e-beam or other external source, in order to fuse them into place. The goal of these processes is primarily to build surface structures, coatings, etc., which are extremely difficult to construct using classical manufacturing methods. The objective of this presentation is to introduce the audience to basic modeling and simulation techniques which can allow them to rapidly develop and analyze particulate-based materials needed in new additive manufacturing processes, for example:

1. Modeling dynamics deposition of new inks, sprays and powders
2. Modeling multiphysical properties of depositions
3. Modeling laser processing
4. Revoxelization modeling of curing and residual stresses
5. Material performance evaluation-electromagnetics

The industrial goal is the development of additive-subtractive machines. This presentation employs two main methodologies: continuum and discrete element approaches. The materials associated with particles embedded in a continuous binder and are treated using continuum approaches. The materials associated with dry powders, which are of a discrete particulate character, are analyzed using discrete element methods.

Background Context: Additive Manufacturing (AM) is usually defined as the process of joining materials to make objects from 3D model data, typically layer upon layer, as opposed to subtractive manufacturing methodologies, which remove material (American Society for Testing and Materials, ASTM). One subclass of AM, so-called 3D Printing (3DP), has received a great

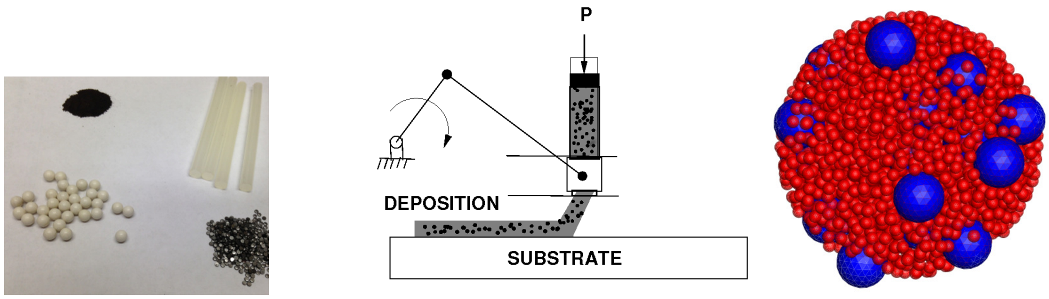

Figure 2: LEFT: Typical printing ingredients: (a) Finely ground metallic powder (iron). (b) Extruded PLA. BOTTOM (c) ABS pellets and (d) Coarsely ground steel flakes. MIDDLE: A linkage schematic of a 3D printer. RIGHT: A multiphase droplet representation using the Discrete Element Method.

deal of attention over the last few years. Typically such a process takes CAD drawings and slices them into layers, printing layer by layer. 3DP was a 2.2 billion dollar industry in 2014, with applications ranging from motor vehicles, consumer products, medical devices, military hardware and the arts. In order for *emerging additive approaches to succeed, such as the ones mentioned, one must draw upon rigorous theory and computation to guide and simultaneously develop design rules for the proper selection of particle, binder and solvent combinations for upscaling to industrial manufacturing levels.*

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