# Book of abstracts

## New Challenges in Computational Mechanics

### A Conference Celebrating the 70th Birthday of Pierre Ladevèze

École Normale Supérieure de Cachan
France - May 23-25, 2016

nccm2016.sciencesconf.org

LMT Cachan

ENS CACHAN — université PARIS-SACLAY — cnrs

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LMT (ENS Cachan / CNRS / Université Paris-Saclay)


# New Challenges in Computational Mechanics
## A Conference Celebrating the 70th Birthday of Pierre Ladevèze

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## Motivation

The New Challenges in Computational Mechanics - NCCM 2016 conference is unusual in that it has a dual overarching objective.

On the one hand, it is a celebratory conference, on the occasion of Pierre Ladevèze's 70th anniversary in which the participants will honor Pierre Ladevèze and recognize his numerous, important, and sustained contributions to the field of computational mechanics.

On the other hand, NCCM 2016 will provide a venue for the exchange of ideas and latest research results in Computational Mechanics. Organizers would like to promote Pierre's favorites:

- Verification
- Validation
- Damage and fracture, composites
- Multiscale computational methods
- Inverse problems, identification
- Stochastic modeling and uncertainties
- Dynamic from low to high frequencies
- Virtual testing
- Robust design

The workshop is of course also open to new ideas in all other exciting topics of Computational Mechanics.

It will bring together scientists and engineers belonging to the Computational Mechanics community in order to discuss the main recent advances in the field.

Discussion sessions will give the opportunity to debate the future of Computational Mechanics with respect to science and industry.

## Local organizing and scientific committee

P.A. Boucard, E. Baranger, F. Daghia, P.A. Guidault, F. Louf , L. Matijevic

## Supporting organizations

## Location

The conference will take place at the Ecole Normale Supérieure de Cachan, 61 avenue du président Wilson, 94230 Cachan, France. It can be easily reached by metro (RER line B, stop at Bagneux) followed by 15 minutes walk. RER B serves both Orly airport and Roissy-Charles de Gaulle airport.

The conference room is Espace Condorcet, on the first floor of the main building of ENS Cachan.

# Program

## Day 1 - Monday, May 23

| | |
|---|---|
| 09:30<br>10:15 | **Welcome and registration** |

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|---|---|
| 10:15<br>10:30 | **Opening**<br>Olivier Allix, Francisco Chinesta |

| | **REDUCTION I** Chair: Charbel Farhat |
|---|---|
| 10:30<br>11:05 | **Nicolas Cagniart, Yvon Maday, Andrea Manzoni, Alfio Quarteroni, Benjamin Stamm**<br>Recent advances the reduced basis simulation for advection-dominated problems |
| 11:05<br>11:40 | **Alberto Corigliano, Martino Dossi, Stefano Mariani**<br>Coupled domain decomposition – Proper Orthogonal Decomposition methods for the simulation of non-linear and multi-physics problems |
| 11:40<br>12:15 | **David Néron**<br>Recent advances of the PGD in the context of the LATIN method for solving nonlinear structural problems |
| 12:15<br>12:50 | **Sergio Zlotnik, Pedro Díez, Antonio Huerta**<br>Generalized parametric solutions for Stokes flow |
| 12:50<br>14:00 | **Lunch** |

| | COMPOSITES Chair: Roger Ohayon |
|---|---|
| 14:00<br>14:35 | **Didier Guedra-Degeorges**<br>Aerospace Challenge & subsequent critical simulation needs for Virtual Vehicle Testing & Integration |
| 14:35<br>15:10 | **Pedro P. Camanho, Rodrigo P. Tavares, Albert Turon**<br>The role of analysis models in the development of new generations of composite materials |
| 15:10<br>15:45 | **Gilles Lubineau, Fei Han, Yan Azdoud**<br>Adaptive coupling between damage mechanics and peridynamics:<br>a route for objective simulation of material degradation up to complete failure |
| 15:45<br>16:10 | **Coffee break** |
| | **COMPUTATION Chair: Alain Combescure** |
| 16:10<br>16:45 | **Eugenio Oñate**<br>Finite increment calculus (FIC). A framework for deriving enhanced computational methods in mechanics |
| 16:45<br>17:20 | **Federica Confalonieri, Aldo Ghisi, Jamil Mirzapour, Umberto Perego**<br>Explicit dynamics simulation of blade cutting of layered shells |
| 17:20<br>17:55 | **David Dureisseix**<br>How complex is origami design? |
| 17:55<br>18:25 | **Practical work** 😀 |
| | **SPECIAL EVENT** |
| 18:30<br>21:00 | **Special event organized by ENS Cachan**<br>**Pierre-Paul Zalio, President of ENS Cachan** |

# Day 2 - Tuesday, May 24

| | ADAPTIVITY Chair: Umberto Perego |
|---|---|
| 08:30<br>09:05 | **Carsten Carstensen, Leszek Demkowicz, Jay Gopalakrishnan**<br>Adaptivity in DPG methods for electromagnetics |
| 09:05<br>09:40 | **Olivier Allix, Pierre Gosselet**<br>Non-intrusive coupling technique: from theory to practice |
| 09:40<br>10:15 | **Pedro Diez, Régis Cottereau**<br>Adaptive mesh re-location for randomly fluctuating material fields |

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|---|---|
| 10:15<br>10:45 | **Coffee break** |

| | MODELLING Chair: Jay Gopalakrishnan |
|---|---|
| 10:45<br>11:20 | **Alain Combescure, Paul Profizi, Kahuziro Ogawa**<br>On the limits of standard continuum mechanics models for very small objects |
| 11:20<br>11:55 | **Djordje Perić, Zlatko Vidrih, Teja Vodlak, Deniz D. Somer, Eric Vezzoli, Betty Lemarie-Semail**<br>A computational framework for multiphysics and multiscale modelling of touch |
| 11:55<br>12:30 | **Nicolas Moës**<br>The Thick Level Set (TLS) damage model for quasi-brittle fracture: an overview |

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|---|---|
| 12:45<br>13:45 | **Lunch** |

| | REDUCTION 2 Chair: Yvon Maday |
|---|---|
| 13:45<br>14:20 | **David Gonzalez, Jose V. Aguado, Elias Cueto, Francisco Chinesta**<br>From Data to Knowledge: Combining Model Order Reduction and Machine Learning Techniques |
| 14:20<br>14:55 | **Charbel Farhat, Kyle Washabaugh, Todd Chapman, Christian Soize**<br>Recent advances in nonlinear model reduction for design and associated uncertainty quantification |
| 14:55<br>15:30 | **Alex Ferrer, Xavier Oliver, Juan Carlos Cante**<br>Multi-scale topological design: a Vademecum- based approach |
| 15:30<br>16:05 | **Ludovic Chamoin, Pierre-Éric Allier, Basile Marchand**<br>Synergies between the Constitutive Relation Error concept and PGD model reduction for simplified V&V procedures |

| | SOCIAL EVENT |
|---|---|
| 17:00<br>19:00 | **Visit of Quai Branly museum** |
| 19:30<br>23:00 | **Workshop Dinner** |

# Day 3 - Wednesday, May 25

| | FLUID Chair: Eugenio Oñate |
|---|---|
| 09:00<br>09:35 | **Roger Ohayon**<br>Modal Analysis of Vibrations of Internal Liquids Coupled with Structures. Computational and Reduced Order Models. |
| 09:35<br>10:10 | **Sergio Idelsohn, Norberto Nigro, Pablo Becker, Julio Marti, Juan Marcelo Gimenez**<br>Large time-step and coarse-mesh strategies suitable for problems with moving interfaces |
| 10:10<br>10:45 | **Wolgang Wall, Benedikt Schott, Christoph Ager, Benjamin Krank**<br>Enrichment in computational fluid-structure interaction |
| 10:45<br>11:15 | **Coffee break** |
| | **IDENTIFICATION Chair: Xavier Oliver** |
| 11:15<br>11:50 | **Hermann Mathhies, Elmar Zander, Bojana V. Rosić, Alexander Litvinenko**<br>Parameter Estimation via Conditional Expectation — A Bayesian Inversion |
| 11:50<br>12:25 | **François Hild, Amine Bouterf, Ludovic Chamoin, Hugo Leclerc, Florent Mathieu, Jan Neggers, Florent Pled, Zvonimir Tomičević, Stéphane Roux**<br>Putting Mechanical Content in DVC: Toward 4D Mechanical Correlation |
| 12:25<br>13:00 | **Marc G.D. Geers, Tom W.J. de Geus, Ron H.J. Peerlings**<br>From damage to fracture in dual-phase microstructures: a statistical analysis using a FFT-based microscale solver |
| 13:00<br>14:15 | **Lunch** |

# Day 1

# Monday, May 23

# Recent advances the reduced basis simulation for advection-dominated problems

**N. Cagniart[1], Y. Maday[1,2⋆], A. Manzoni[3], A. Quarteroni[3], B. Stamm[4]**

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Advection dominated equations is an important class of problems governed by time dependent Partial differential equations. Their numerical simulations is an important challenge for the community in numerical analysis and the class of reduced basis approximations has some difficulties to tackle these problems properly.

There are at least two reasons : the first one is due to the fact that the set of solutions (when time varies) is not with small Kolmogorov $n$-width — or at least does not seems so at first sight — the second is a stability issue one.

We propose here two new contributions that adresses the two issues and are explained independently in two publications [1], [2].

## References

[1] Y. Maday, A. Manzoni, A. Quarteroni An online intrinsic stabilization strategy for the reduced basis approximation of parametrized advection-dominated problems, Submitted, 2016.

[2] N. Cagniart, Y. Maday, B. Stamm. in preparation, 2016.

# Coupled domain decomposition – Proper Orthogonal Decomposition methods for the simulation of non-linear and multi-physics problems

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A computational strategy for the simulation of multi-physics and non-linear, irreversible problems, based on a combined use of Domain Decomposition (DD) and Proper Orthogonal Decomposition (POD) Model Order Reduction (MOR) techniques, is presented and discussed. The strategy was recently proposed by the Authors in [1]-[4] and exploits the potentialities of the coupled use of DD [5] and POD methods [6]. Applications have been done for the solution of the coupled electro-mechanical problem in microsystems, the simulation of dynamic elasto-plastic structural problems, the study of fracture propagation in quasi-brittle polycrystalline materials. More recently, the approach was extended to the simulation of the fully coupled thermo-elastic problem.
The presented numerical examples concern applications to electrostatically driven micro-resonators, polycrystalline silicon, elasto-plastic frames.

## References

[1] F. Confalonieri, A. Corigliano, M. Dossi, M. Gornati, A domain decomposition technique applied to the solution of the coupled electro-mechanical problem. *Int. J. Numer. Meth. Engng.* Vol. 93 (2), pp. 137-159, 2013.

[2] Corigliano, M. Dossi, S. Mariani. Domain decomposition and model order reduction methods applied to the simulation of multiphysics problems in MEMS. *Computers & Structures*, Vol. 122, pp.113-127, 2013.

[3] F. Confalonieri, A. Ghisi, G. Cocchetti, A. Corigliano. A domain decomposition approach for the simulation of fracture phenomena in polycrystalline microsystems. *Comp. Meth. Appl. Mech. Engng*, 277, 180, 218 (2014).

[4] A. Corigliano, M. Dossi, S. Mariani. Model order reduction and domain decomposition strategies for the solution of the dynamic elasto-plastic structural problem. *Comp. Meth. Appl. Mech. Engng*, 290, 127-155 (2015).

[5] A. Combescure and A. Gravouil, Multi-time-step explicit-implicit method for non-linear structural dynamics. *Int. J. Numer. Methods Eng.*, Vol. 50, pp. 199-225, 2001.

[6] G. Kerschen, J.C. Golinval, A. Vakaris, L.A. Bergman, The method of proper orthogonal decomposition for dynamical characterization and order reduction of mechanical system: an overview. *Nonlinear dynamic*s, Vol.41, pp. 147-169, 2005.

# Recent advances of the PGD in the context of the LATIN method for solving nonlinear structural problems

**D. Néron**

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The numerical simulation of very large models is becoming increasingly important because of the need to describe more realistic scenarios and facilitate the virtual design of new structures. In that context, model reduction has a huge potential to develop innovative tools for intensive computations and allows a "real time" interaction between the user and the simulations, which gives the opportunity to explore a large number of scenarios.

The LArge Time INcrement (LATIN [1]) method was proposed by P. Ladevèze in the early 80's to solve nonlinear time-dependent problems (e.g. (visco)plasticity, damage ...) encountered in computational mechanics. Initially called "Radial Approximation" in the context of the LATIN method and recently renamed as "Proper Generalized Decomposition", the PGD model reduction technique allows to decrease drastically computational costs. Within the framework of the LATIN method, the PGD has given rise to a large number of works since its introduction, such as multiscale or multiphysics problems [2, 3] or multiparametric problems [4].

This talk proposes a short review of recent advances in the use the LATIN-PGD to solve nonlinear problems arising from some industrial collaborations.

## References

[1] P. Ladevèze. *Nonlinear Computational Structural Mechanics—New Approaches and Non-Incremental Methods of Calculation*. Springer Verlag, 1999.

[2] D. Néron and P. Ladevèze. Proper Generalized Decomposition for multiscale and multiphysics problems. *Archives of Computational Methods in Engineering*, 17(4):351–372, 2010.

[3] M. Cremonesi, D. Néron, P.-A. Guidault, and P. Ladevèze. A PGD-based homogenization technique for the resolution of nonlinear multiscale problems. *Computer Methods in Applied Mechanics and Engineering*, 267:275–292, 2013.

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# Generalized parametric solutions for Stokes flow

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Reduced order models are nowadays a standard approach to represent a solution with a few degrees of freedom. The large majority of available approaches require first, an *offline* calculation and then, solving a problem in the *online* phase. Whereas the Proper Generalized Decomposition (PGD) gives a generalized parametric solution: *computational vademecum* [1]. More precisely, the PGD computes an explicit function whose variables are the standard spatial coordinates (and time), but also other user-prescribed parameters: material constants, external loads, geometry, etc. Thus, the online phase consists merely in a functional evaluation and therefore is very efficient from a computational viewpoint. Moreover, the generalized parametric solution can be further exploited by making use of the explicit form of the parametric dependence (viz. Fourier transform, gradients for sensibilities, …).

In incompressible flows, PGD with spatial separation was considered for reducing the computational complexity [2,3]. Here, the influence of the incompressibility condition on the separated representation of velocity and pressure is studied for *parameterized* Stokes flow. Parameters characterizing the geometry of the computational domain are taken as new coordinates of the generalized parametric expression for velocity and pressure, see [4,5].

## References

[1] F. Chinesta, A. Leygue, F. Bordeu, J.V. Aguado, E. Cueto, D. González, I. Alfaro, A. Ammar, A. Huerta. PGD-Based Computational Vademecum for efficient design, optimization and control. *Arch. Comput. Method Eng.* 20:31–59, 2013.

[2] C. Leblond, C. Allery. A priori space–time separated representation for the reduced order modeling of low Reynolds number flows. *Comput. Methods Appl. Mech. Eng.*, 274:264–288, 2014.

[3] A. Dumon, C. Allery, A. Ammar, Proper general decomposition (PGD) for the resolution of Navier–Stokes equations, *J. Comput. Phys.*, 230:1387– 1407, 2011.

[4] A. Ammar, A. Huerta, F. Chinesta, E. Cueto, A. Leygue. Parametric solutions involving geometry: a step towards efficient shape optimization. *Comput. Methods Appl. Mech. Eng.*, 268:178–193, 2014.

[5] S. Zlotnik, P. Díez, D. Modesto, A. Huerta. Proper generalized decomposition of a geometrically parametrized heat problem with geophysical applications. *Int. J. Numer. Methods Eng.*, 103(10):737–758, 2015.

# Aerospace Challenge & subsequent critical simulation needs for Virtual Vehicle Testing & Integration

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Technical challenges for 2020 & beyond in the field of aerospace industry will be the development of new high performance, affordable, energy efficient & eco-friendly Aircraft configurations.

In order to achieve properly those innovations, the mastering of simulation capabilities will be a key driver. This paper will illustrate some typical engineering problems to be solved during the next decade regarding:

- Computed Aided Sizing to support Vehicle Engineering (eg: advanced damage mechanics of composites, Multi-physics Virtual behavior in aggressive environments…)
- Complex subcomponent parametric analysis (eg: crash, high velocity impact, assessment of uncertainties on performance…)

The technology readiness level of enabling methods for Virtual Structural Testing on the way for Industrial Implementation will be also addressed.

Finally, new paradigm such real time Interaction with a behavioral Digital Mock Up for Systems Integration will be described.

# The role of analysis models in the development of new generations of composite materials

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The need to understand the failure mechanisms in composite materials at the micro level has gained additional importance due to the pressing need to develop high performance materials for more demanding applications. This understanding makes it possible to develop *in-silico* a new generation of polymer composite materials by recurring to e.g. hybridization, either fibre hybridization [1] or ply hybridization [2].

In this work a micromechanical model that takes into account the statistical nature of fibre strength and the fibre waviness present in composite materials, as well as the proper constitutive response of the resin and fibre-matrix interface, is developed and used to determine the failure behaviour of hybrid and non-hybrid composite materials. The model is able to capture failure mechanisms in the three main components of a composite material: fibres, matrix and fibre-matrix interface. This study is performed for multiple load scenarios, with focus on the longitudinal tensile and compressive failure of these materials. The effect of transverse stresses in these types of failure is also assessed to better understand its effects on the failure mechanisms. Finally, the benefits of new types of composite materials in terms of enhanced mechanical performance are discussed.

## References

[1] Tavares, Rodrigo P., et al. Mechanics of hybrid polymer composites: analytical and computational study. *Computational Mechanics* (2016): 1–17.

[2] Furtado, C., et al. Selective ply-level hybridisation for improved notched response of composite laminates. *Composite Structures* 145 (2016): 1-14.

# Adaptive coupling between damage mechanics and peridynamics: a route for objective simulation of material degradation up to complete failure

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The objective (mesh-independent) simulation of evolving discontinuities, such as cracks, remains a challenge. Current techniques are highly complex or involve intractable computational costs, making simulations up to complete failure difficult. We propose a framework as a new route toward solving this problem that adaptively couples local-continuum damage mechanics with peridynamics to objectively simulate all the steps that lead to material failure: damage nucleation, crack formation and propagation. Local-continuum damage mechanics successfully describes the degradation related to dispersed microdefects before the formation of a macrocrack. However, when damage localizes, it suffers spurious mesh dependency, making the simulation of macrocracks challenging. On the other hand, the peridynamic theory is promising for the simulation of fractures, as it naturally allows discontinuities in the displacement field. Here, we present a hybrid local-continuum damage/peridynamic model. Local-continuum damage mechanics is used to describe “volume" damage before localization. Once localization is detected at a point, the remaining part of the energy is dissipated through an adaptive peridynamic model capable of the transition to a “surface" degradation, typically a crack. We believe that this framework, which actually mimics the real physical process of crack formation, is the first bridge between continuum damage theories and peridynamics. Two-dimensional numerical examples are used to illustrate that an objective simulation of material failure can be achieved by this method.

## References

[1] G. Lubineau, Y. Azdoud, F. Han, Ch. Rey and A. Askari. A morphing strategy to couple non-local to local continuum mechanics. *Journal of the Mechanics and Physics of Solids*, 60(6):1088–1102, 2012.

[2] F. Han, G. Lubineau and Y. Azdoud, Adaptive coupling between damage mechanics and peridynamics: a route for objective simulation of material degradation up to complete failure. *Submitted for publication*, 2016.

# Finite increment calculus (FIC). A framework for deriving enhanced computational methods in mechanics

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The Finite Increment Calculus (FIC) (sometimes termed "finite calculus") was proposed by Oñate [1] as a conceptual framework for deriving stabilized numerical methods (mainly the finite element method (FEM)) for solving advective-diffusive transport and fluid compressible flow problems for situations where numerical methods typically fail (i.e. high Peclet/Reynolds numbers and incompressible situations).

The essence of the FIC approach lays in solving the governing differential equations in mechanics *written in a modified form*, using any discretization method. The FIC modified governing equations are obtained by *writing the equations for balance of heat, momentum and mass in a space-time domain of finite incremental size*, and not in a domain of infinitesimal size, as it is usually done.

The FIC approach naturally introduces additional terms in the classical differential equations of continuum mechanics, which how become a function of the balance domain dimensions. The merit of the modified governing equations derived via FIC is that *they are a natural starting point for deriving stabilized numerical schemes*. Moreover, the different stabilized FEM typically used in practice can be *recovered* using FIC [1-4]..

In the paper the main concepts of the FIC method are introduced. Details of the FIC/FEM approach for advection-diffusion-reaction problems are presented. The possibilities of FIC in fluid and solid mechanics and FSI problems solved with the Particle Finite Element Method are explained. Finally, the possibilities of the FIC/FEM approach for error estimation and mesh adaptivity are outlined. Examples of applications are given.

## References

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# Explicit dynamics simulation of blade cutting of layered shells

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The numerical simulation of blade cutting of thin layered shell is a challenging task, involving complex phenomena, such as large deformations, nonlinear material behaviour, contact, crack propagation, delamination. In particular, three small geometrical scales need be resolved: the scale of layer thicknesses, the scale of blade radius of curvature, the scale of fracture and delamination process zones.

In view of the problem nonlinearity, an explicit dynamics formulation with solid-shell elements is adopted to avoid convergence problems. A selective mass scaling approach [1,2] is used to enlarge the critical time step size, dictated by the layers thickness.

Crack propagation is modelled by inserting cohesive interfaces between adjacent elements placed along the prescribed blade trajectory. The problem of the interaction between the sharp blade and the cohesive process zone is addressed by using the so called “directional cohesive elements” proposed in [3].

Depending on the type of material and on the layer thickness, the problem may be characterized by very small process zone sizes. Techniques for the reduction of spurious oscillations in the presence of coarse discretization and for the improvement of overall accuracy are investigated.

Numerical applications to engineering problems are used to assess the effectiveness of the proposed simulation approach.

## References

[1] G. Cocchetti, M. Pagani, and U. Perego. Selective mass scaling for distorted solid-shell elements in explicit dynamics: optimal scaling factor and stable time step estimate. *International Journal for Numerical Methods in Engineering*, 101(9):700–731, 2015.

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# How complex is origami design?

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The latest decade saw the emergence of a new approach to the ancient paperfolding art: the computational origami. Indeed, the mechanical behavior of the paper sheet is usually idealized: a zero bending stiffness, but an infinite in-plane stiffness. As a consequence, the problem reduces to a discrete geometry one, with a finite number of folds (lines of strain singularity), a finite mechanism with large rotations during the folding process, and a diffuse unilaterality to prevent the paper self-interpenetration

Several complex planar geometry problems have been studied from their complexity and design efficiency point of view, such as the color changing: starting from a single square of paper with one color on each of its sides, what are the feasible designs to make special patterns appear, without cutting nor gluing? The chessboard (8-per-8 checkered board) is one of the most challenging problems, especially when constrained by searching the most efficient design, i.e. with the less waste of paper. The complexity of a particular solution for a $n$-per-$n$ checkered board has been estimated with the smallest possible semiperimeter $s$ of the initial square of paper. Bounds are available: a first result in 2000 [3] gave $s = n^2$, and was suspected to be sharp. Nevertheless, a breakthrough in 2009 [2] provided a new bound: $s = ½\, n^2 + 8n + 8 - 5(n \bmod 4)$, smaller for $n \geq 16$. This polynomial complexity measures the difficulty to fold the pattern, so to check a solution. It is not the complexity of the design problem, i.e. the algorithmic problem of finding the solutions. Indeed, as soon as 1996, a simpler origami problem was proved to be NP-complete [1].

We propose herein the illustration of complexity on a pixel-matrix origami design. This is a complication of the chessboard: each board square should be able to change its color independently, using as many flapping mechanisms as necessary, but still using a single square sheet of paper with a minimal waste. We also discuss the ability of computer resources to help solving the design problem, together with a more or less deeper analysis by the human paperfolder (for instance using graph theory, with a 2-scale approach for the paper corrugation along the edge) to render the problem tractable, at least up to $n = 8$ [4].

## References

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# Day 2

# Tuesday, May 24

# Adaptivity in DPG methods for electromagnetics

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The *a posteriori* and *a priori* error analyses of discontinuous Petrov Galerkin (DPG) methods have matured in recent years [1]. DPG methods are derived using a combination of ideas in least-squares finite element methods and hybridized methods. They minimize a residual in a nonstandard, locally computable, dual norm. They are made easily implementable using "broken" test spaces, i.e., spaces of functions with no continuity constraints across mesh element interfaces. Broken spaces derivable from a standard exact sequence of first order (unbroken) Sobolev spaces are of particular interest. A characterization of interface spaces that connect the broken spaces to their unbroken counterparts is provided. We show that stability of certain formulations using the broken spaces can be derived from the stability of analogues that use unbroken spaces. This technique can be used [2] to provide a complete error analysis of DPG methods for Maxwell equations. Several related theoretical and practical issues will be addressed.

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# Non-intrusive coupling technique: from theory to practice.

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## ABSTRACT

In the last decade, many innovative modeling or solving techniques have been introduced in the field of computational mechanics. These techniques, such as enriched finite elements or multiscale modeling, make it possible to perform complex simulations that are out of reach of conventional finite element analysis (FEA) tools, in terms of computational or human costs. Although these techniques have proved their performance by extensive testing on academic applications, they are scarcely applied to actual industrial problems because they cannot be conveniently implemented into commercial FEA software packages. Therefore a scientific and practical challenge is to allow realistic simulation of complex industrial problems including all their physical and technological complexity.

The prerequisite of the proposed non-intrusive framework is to keep unchanged the global numerical model as well as the solver used for its treatment [1]. The improved models and software are introduced locally on subdomains (which can in the end cover the global model). Therefore two or several models are used concurrently, the untouched global model and local ones which are iteratively substituted where needed. The exchanges between the models are such that the data should be "natural" ones for the global model such as displacements and nodal forces. Possible applications are numerous [2] even though the approach as to be adapted depending on the context.

In this presentation we intend to focus on some recent works in order to illustrate the possibilities but also difficulties of the method based on our experience regarding:

- the extension of the method in explicit and implicit-explicit coupling in dynamics [3-4]
- the coupling between plate and 3D models for bolted and multi-bolted plates [5-6]
- the treatment of complex non-linear visco-plastic structures.

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# Adaptive mesh re-location for randomly fluctuating material fields

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Stochastic models with random material fields require adaptive meshing to properly resolve the features of each (deterministic) instance at a minimum computational cost. This is a challenging issue because, to be used in as a practical tool, the cost of the error indicators and the remeshing algorithms must be very small. This discards using any a posteriori error assessment technique and precludes remeshing from scratch at each instance.

We present an r-adaptivity approach for boundary value problems with randomly fluctuating material parameters solved through the Monte Carlo or stochastic collocation methods. This approach tailors a specific mesh for each sample of the problem. It only requires the computation of the solution of a single deterministic problem with the same geometry and the average parameter, whose numerical cost becomes marginal for large number of samples. Starting from the mesh used to solve that deterministic problem, the nodes are moved depending on the particular sample of mechanical parameter field. The reduction in the error is small for each sample but sums up to reduce the overall bias on the statistics estimated through the Monte Carlo scheme. Several numerical examples in 2D are presented.

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# On the limits of standard continuum mechanics models for very small objects

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The presentation shall illustrate some recently issues which have been solved to model the cold spray process. This process consists in making a coating by sending at high speed (typically 600m/s) very small spherical particulates (whose diameter is around 50 microns) of a material A onto a substrate of material B. The process researchers have found, by trial end error experimental testing, the appropriate conditions for which one obtains a good adhesion of the coating onto the substrate. Many metallurgical observations of these fabricated coatings permit to have an a posteriory idea of what happens to the material. But it is not predicitive. The object of this presentation is to propose a simulation method which helps some understanding of the physical phenomenons involved in such a process. The particles or the substrate experience huge strains when impact speeds are large (900 to 1000m/s). The standard finite elements fail because of too large element distorsions. Hence the SPH method is chosen for these computations. Moreover the observation is that adhesion occurs only if the particulates are small enough and the impact velocity is within a certain: there is no adhesion if the impact speed is too small or too large. The size effect indicates that adhesive forces have to be introduced to be able to be predictive for the size of the particulates to be used. A Dugdale model is proposed for adhesion modelling [1]. But this adhesion must only be activated if the interface is sufficiently sheared: otherwise the adhesion would occur for very small impact velocities. It must also stop if the material is damaged on one of the sides of the interface. This model shall be explained in details awithin the frame of 3D SPH method. Examples of application will show the importance of adhesion forces as well as the predictions of the speed range in case of Al particulates impacting a Cu substrate, as well as Al on Al or Cu on Cu impacts. These models have been implemented into the Europlexus software.

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# A computational framework for multiphysics and multiscale modelling of touch

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The sense of touch is the foundation for interaction with the world around us. Nevertheless, it remains the least understood of all human senses [1]. This is due to highly complex processes involved in generation of the sense of touch, which combine multi-disciplinary areas from biology, including both cellular and system levels; engineering, including tribology, electro-mechanics and computer simulation; neurophysiology and psychology. The main goals of the research undertaken in this work are: (i) the development of multiscale multiphysics computational platform to improve understanding of human touch, and (ii) its application to the virtual prototyping and optimisation of novel tactile displays [2,3].

A particular attention is given to the development, validation, and application of a computational framework for modelling tactile scenarios on real and virtual surfaces rendered by electrovibration technique. Electrovibration of tactile displays exploits the polarization of the finger pad, caused by an insulated high voltage supplied plate. This results in electrostatic attraction, which can be used to modulate the user's perception of an essentially flat surface and induce texture sensation. The framework features fully parametric model in terms of materials and geometry of the finger pad, virtual and real surfaces, and can serve as a tool for virtual prototyping and haptic rendering in electrovibration tactile displays.

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# The Thick Level Set (TLS) damage model for quasi-brittle fracture: an overview

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The TLS model was designed to allow for a smooth transition to fracture. It belongs to the family of the non-local damage models and thus introduces a length. The twist in the TLS is that it incorporates geometrical aspects: the shape of the localization zone is located by a level set.

So far, most of the effort have been concentrated to quasi-brittle fracture. After restating the motivations for the new model, we review the results obtained in these past 5 years. Among other topics the following issues will be addressed:

- Capability of the model to reproduce properly size effects
- Predictive capabilities for crack onsets at notches.
- Theoretical issues regarding boundary conditions (with practical consequences!)
- Capability of the model to take into account concurrent local and non-local development of damage.
- Comparison with other non-local damage models
- Relationships with the cohesive zone model

Finally, a set of open issues will be detailed.

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# From Data to Knowledge: Combining Model Order Reduction and Machine Learning Techniques

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Parametric solutions make possible fast and reliable real-time simulations which, in turn allow real time optimization, simulation-based control and uncertainty propagation. This opens unprecedented possibilities for robust and efficient design and real-time decision making. The construction of such parametric solutions was addressed in our former works in the context of models whose parameters were easily identified and known in advance. Recently we addressed more complex scenarios in which the parameters do not appear explicitly in the model —complex microstructures, for instance. In these circumstances the parametric model solution requires combining a technique to find the relevant model parameters and a solution procedure able to cope with high-dimensional models, avoiding the well-known curse of dimensionality. Thus, we successfully combined model order reduction and nonlinear dimensionality reduction (kPCA, LLE, ...) for interpolating solutions, computational vademecums or for extracting the hidden model parameters in combination with the PGD (Proper Generalized Decomposition) for calculating the resulting parametric solution. [1, 2, 3]

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# Recent advances in nonlinear model reduction for design and associated uncertainty quantification

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This lecture will be organized in two complementary parts focused on advances in the construction of parametric, nonlinear, projection-based, reduced-order models that are suitable for design and design optimization, and a corresponding nonparametric probabilistic method for quantifying their uncertainties. In the first arena, this talk will present a scalable approach for nonlinear model order reduction that is based on: a clustering scheme for precomputed parametric snapshots that promotes simultaneously locality on the solution manifold, and low dimensionality; a stable, Petrov-Galerkin projection method based on local reduced-order bases constructed by compressing the clustered snapshots [1, 2, 3]; a family of hyper reduction methods tailored to the mathematical underpinnings of both of the constructed reduced-order models and their underlying high-dimensional counterparts [4] ; and an *online* solution strategy that blends appropriate interpolation schemes and Newton-like methods for delivering real-time performance [6]. Most importantly, this part of the lecture will present for the first time the results of two realistic case studies on the performance of this framework for parametric nonlinear model reduction for "what-if?" aerodynamic design scenarios. The first case study focuses on NASA's Common Research Model (CRM), which is representative of modern jet airliners. The second one focuses on the 2009 Volkswagen Passat, a midsize car. It will also contrast two approaches for training nonlinear reduced-order models and discuss their strengths and weaknesses for practical computations: the celebrated greedy method (for example, see [5]), and simple uniform sampling (for example, see [6]). In the second arena, this lecture will present a nonparametric probabilistic method for modeling various uncertainties associated with nonlinear reduced-order models, including model form uncertainties [7]. When experimental data is available, this approach can also quantify

uncertainties in the underlying high-dimensional parametric model. The main idea here is two-fold: to substitute the deterministic reduced-order basis with a stochastic counterpart; and to construct the probability measure of the stochastic reduced-order basis on a subset of a compact Stiefel manifold in order to preserve some fundamental properties of a reduced-order basis. The potential of this nonparametric probabilistic method for uncertainty quantification in general, and updating nonlinear reduced-order models in particular, will be demonstrated through several sample computational mechanics problems. Finally, the lecture will conclude with some perspectives on the synergy between model order reduction and uncertainty quantification, and their likelihood for becoming a game changer in computational mechanics, along the lines anticipated by Pierre Ladeveze and co-workers in their series of workshops on model reduction.

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# Multi-scale topological design: a Vademecum-based approach

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In the last decades, structural topological optimization has gained considerable interest in the Computational Mechanics community [1][2]. Though most of the current developments focus on single-scale structural topological optimization, in this work multi-scale topology optimization is considered. The micro-scale material topology is optimized to achieve the minimum macroscopic structural compliance. Computational material design at the micro-scale is then performed by using a level set method based on the topological derivative concept [4]. Despite the robustness of the algorithm, the direct solution of the problem is computationally unaffordable since a topology optimization problem has to be solved at every gauss point of the macro-scale.

To overcome this problem a Vademecum-based approach, inspired in [3], is used, and a discrete material catalogue is computed. Although building this catalogue implies a heavy computational effort a priori (off-line), its on-line consultation, along the material design process, allows solving the problem in a fast way. As proposed in [1], an alternated directions algorithm is used for solving the coupled multi-scale topology optimization problem. As a validation of the approach, some numerical examples are presented.

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# Synergies between the Constitutive Relation Error concept and PGD model reduction for simplified V&V procedures

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A permanent issue in science and engineering activities is the verification and validation (V&V) of mathematical and numerical models, which nowadays can attain very high levels of complexity. We focus here on the Constitutive Relation Error (CRE) concept which has been widely used over the last 40 years for robust verification [1] and validation [2] of Computational Mechanics models, in which the constitutive relation is a major component. The objective of this research work is to present new numerical tools, based on Proper Generalized Decomposition (PGD) and an *offline-online* strategy, that can be coupled to the CRE concept to make this latter fully implementable and exploitable for practical industrial applications. The PGD is a model reduction technique that has been extensively applied over the last decade to solve multi-parametric problems [3]. Its use into the CRE concept enables to decrease the computational cost and technicality associated with the construction of so-called admissible fields, leading to faster and cheaper V&V procedures. Numerical illustrations, addressing both model verification and model updating, are presented to assess the performances of the proposed approach.

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# Day 3

# Wednesday, May 25

# Modal Analysis of Vibrations of Internal Liquids Coupled with Structures. Computational and Reduced Order Models.

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We review the basic equations and corresponding variational formulations of the linearized vibrations of a liquid with a free surface contained in an elastic structure.

In hydroelastic standard situations, the liquid is considered as incompressible, gravity effects being taken into account through appropriate fluid-structure interface operator referred as *elastogravity* operator using a scalar field (pressure and/or displacement potential fields for the fluid) [1, 3].

Compressibility effects for the liquid can be introduced, neglecting gravity effects as in structural-acoustic problems, or taking into account those effects through some approximations [2].

Recently, we have analysed on a rigorous manner the basic equations of compressibility/gravity interactions: the fluid irrotationnality condition being replaced, in general, by a *plane-irrotationnality* equation.

We present here some basic appropriate corresponding variational formulations and its associated finite element / reduced order models.

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# Large time-step and coarse-mesh strategies suitable for problems with moving interfaces

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The aim of this presentation is to show that in many problems in which there are moving internal interfaces, one order of magnitude larger time-step can be used with an appropriate strategy[1,2]. Furthermore, finite element meshes much coarser than those used currently, may be acceptable with the same accuracy[1] .

The use of large time steps together with coarse meshes solves the same problem with the same accuracy by several orders of magnitude faster[1,2,3] .

Some patological examples of moving multi-fluids with internal interfaces, solved with fixed meshes are presented to demonstrate this assertion.

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# Enrichment in computational fluid-structure interaction

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Fluid-Structure Interaction (FSI) problems, as well as many other coupled multi-field problems, have received much attention in recent years and continue to attract more interest. The main reason is that they are of great relevance to many fields of engineering (civil, mechanical, aerospace, bio, etc.) and applied sciences. Similarly, the development and application of corresponding numerical simulation methodologies have received wide attention over the past decades. In this talk we will focus on the superior use of enrichments in computational fluid-structure interaction.

On the basis of a newly developed fixed grid approach for fluid-structure interaction, that is itself based on enriching standard finite element spaces, we will present two different extensions and advances. One extension is concerned with the ability to attach a deforming (ALE type) grid to the structure that allows high quality meshes in crucial areas of the flow domain (like boundary layer meshes). The embedding of these grids into the background grid is again done via function enrichments and enables to solve the complete flow domain on both meshes as a single field.

In a second part we will present a novel way of doing wall modelling for turbulent flows, again via a special enrichment of the continuous (FE) or discontinuous (DG) function spaces.

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# Parameter Estimation via Conditional Expectation — A Bayesian Inversion

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When a mathematical or computational model is used to analyse some system, it is usual that some parameters resp. functions or fields in the model are not known, and hence uncertain. These parametric quantities are then identified by actual observations of the response of the real system. In a probabilistic setting, Bayes's theory is the proper mathematical background for this identification process.

Typical deterministic procedures include such methods as minimising the mean square error (MMSE), leading to optimisation problems in the search of optimal parameters. As the inverse problem is typically ill-posed — the observations do not do contain enough information to uniquely determine the parameters — some additional information has to be added to select a unique solution, typically through Tikhonov-regularisation. In a probabilistic setting the ill-posed problem becomes well-posed [1]. This is achieved at a cost though. The unknown parameters are considered as uncertain, and modelled as random variables (RVs). The result of the identification is a probability distribution, and not a single value, and the computational work may be increased substantially, as one has to deal with RVs. It is well known that the Bayesian update is theoretically based on the notion of conditional expectation. Here we take an approach which takes this not only as a theoretical basis, but also as a basic computational tool [2]. This may be seen as somewhat related to the "Bayes linear" approach which has a linear approximation as its basis [3].

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# Putting Mechanical Content in DVC: Toward 4D Mechanical Correlation

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The goal of the present study is to illustrate the full integration of sensor and imaging data into numerical procedures for the purpose of identification of constitutive laws and their validation. The feasibility of such approaches is proven in the context of *in situ* tests monitored by tomography. The bridging tool consists of spatiotemporal (i.e., 4D) analyses with dedicated (integrated) correlation algorithms.

A tensile test on nodular graphite cast iron sample is performed within a lab tomograph. The reconstructed volumes are registered by resorting to integrated digital volume correlation (DVC) that incorporates a finite element modeling of the test, thereby performing a mechanical integration in 4D registration of a series of 3D images. In the present case a non-intrusive procedure is developed in which the 4D sensitivity fields are obtained with a commercial finite element code, allowing for a large versatility in meshing and incorporation of complex constitutive laws. Convergence studies can thus be performed in which the quality of the discretization is controlled both for the simulation and the registration.

Incremental DVC analyses are carried out with the scans acquired during the *in situ* mechanical test. For DVC, the mesh size results from a compromise between measurement uncertainties and its spatial resolution. Conversely, a numerically good mesh may reveal too fine for the considered material microstructure. With the integrated framework proposed herein, 4D registrations can be performed and missing boundary conditions of the reference state as well as mechanical parameters of an elastoplastic constitutive law are determined in fair condition both for DVC and simulation.

# From damage to fracture in dual-phase microstructures: a statistical analysis using a FFT-based microscale solver

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Modern automotive applications call for high-performance materials that optimally combine strength and ductility. Multi-phase materials (e.g. dual-phase steels) constitute the key ingredient towards reaching this objective. The in-depth understanding of the interaction between the phases in terms of the resulting mechanical properties, damage nucleation and fracture propagation are therefore of great importance.

This contribution focuses on a methodology that enables a statistical analysis of the two-phase mechanical interaction in a dual-phase steel [1, 2]. The key aspects addressed are: (i) A binary idealization of the microstructure morphology, which at high resolutions matches experimental micrographs. This idealization allows to investigate a large ensemble of microstructures with considerable statistical variations; (ii)An efficient FFT-based spectral solver, which naturally incorporates the nonlinear material behaviour and large deformations. The consistent linearization used thereby closely resembles FE procedures. A key ingredient is the elimination of the linear auxiliary problem that obscured the treatment of nonlinear problems in the past; (iii) A systematic study of different morphologies and microstructural parameters, enabling the identification of the average distribution of phases around fracture initiation sites; (iv) The transition from damage initiation to propagation, including the interaction between previously nucleated damage sites; (v) Application of the proposed method to high-resolution real microstructures.

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## Thanks for your participation!

## Hoping that you had a pleasant and fruitful workshop, have a nice trip back and see you soon !

Views of the future ENS Cachan building after the move to the Campus of Paris-Saclay University in 2019 (Renzo Piano Buildings Workshop, Architects)