COMPUTATIONAL MECHANICS: THE NEXT DECADE

A Symposium on the Occasion of Prof. Rainald Löhner's 50th Birthday

March 27, 2009

Dewberry Hall, Johnson Center
George Mason University
Fairfax, VA
Foreword

Computational Mechanics has matured rapidly over the last 3 decades and has become a major engine of discovery and innovation in many areas of science and engineering. Computational Structural Dynamics (CSD), Computational Fluid Dynamics (CFD), Computational Electromagnetics (CEM) and Molecular Dynamics (MD) represent but a few of many research areas of computational mechanics that have blossomed into large disciplines.

The symposium seeks to cover a broad variety of topics, taking a high-level view across many disciplines. Every speaker was asked to talk for 1-3 minutes about the present, and to then focus explicitly on the coming decade.

The organizers are very grateful for the financial support of George Mason University and the Air Force Office of Scientific Research that made this symposium possible.
PROGRAM
Computational Mechanics: The Next Decade

Dewberry Hall, Johnson Center
George Mason University, Fairfax Campus

8:30- 9:00 **Welcome:**
President Merten
Rainald Löhner

9:00-10:20 **Session 1: Numerical Methods**

Advances in the Particle Finite Element Method (PFEM) for Problems in Sea, Earth and Fire
*Eugenio Oñate, Sergio R. Idelsohn, Riccardo Rossi*
CIMNE, Barcelona, Spain

Simulation Based Engineering: Challenges in Verification, Validation and Uncertainty Analysis
*Dominique Pelletier*
Ecole Polytechnique de Montreal, Canada

Development of a Discontinuous Galerkin Method for Computational Fluid Dynamics
*Hong Luo*
North Carolina State University, Raleigh, NC, 27695

Numerical Modeling of Fluid Instabilities in Laser-Driven Inertial Confinement Fusion (ICF) Capsules in the Small-Amplitude Limit
*Steven T. Zalesak*
Berkeley Research Associates and NRL, Washington, DC

10:20-10:40 **Coffee Break**
10:40-12:20: **Session 2: Government Perspectives**

**Computational Mathematics at AFOSR: Challenges and Future**

*Fariba Fahroo*
Air Force Office of Scientific Research (AFOSR)

**Computational Mechanics at DTRA: The Next Decade**

*M. Giltrud*
DTRA, Fort Belvoir, VA

**Understanding and Forecasting the Sun’s Impact on the Battlespace Environment**

*Jill Dahlburg*
Space Science Division, NRL, Washington, DC

**Missile Aerodynamic Performance Prediction**

*Alan Nicholson*
MSIC, Huntsville, AL

**The Next Decade in Supercomputing**

*R. Aubry, G. Houzeaux, M. Vazquez and J.M. Cela*
Barcelona Supercomputing Center, Barcelona, Spain

12:20-13:20: **Lunch**

13:20-14:40: **Session 3: Free Surface Hydrodynamics/Hydraulics**

**Do Analytical Methods Have A Future?**

*Francis Noblesse*
NSWC-CD, Potomac, MD

**The Future of CFD in Ship Hydrodynamics – Prediction and Optimization**

*Chi Yang*
Center for Computational Fluid Dynamics, GMU, Fairfax, VA

**Hydrodynamics vs. Hydraulics: An Old Controversy Yet to be Settled in Flow Simulation?**

*Gustavo C. Buscaglia*
University of São Paulo, Brazil
Vehicle Biomimetics at the Macro, Micro, and Nano Scale: Challenges for Computational Mechanics
William C. Sandberg
SAIC, McLean, VA

14:40-15:00: Coffee Break

15:00-16:00: Session 4: Bio/Medical Engineering

Computational Modelling of Human Respiratory System – An Overview
Perumal Nithiarasu
School of Engineering, Swansea University, Swansea, Wales, UK

Blood Flow Simulation: The Clinical Perspective
Christopher Putnam
INOVA Fairfax Hospital, Fairfax, VA

Clinical Applications of Computational Hemodynamics
Juan R. Cebral
Center for Computational Fluid Dynamics, GMU, Fairfax, VA

16:00-16:20: Coffee Break

16:20-17:40: Session 5: Fluid/Structure/Thermal Interaction

Damping the Flames: Fire Modeling for the Next Decade
Kathryn Butler
NIST, Gaithersburg, MD

Challenges in Integrated Structural Impact Analysis
Steve Kan
National Crash Analysis Center, GWU, Ashburn, VA

Modeling of Structural Response to Blast Loading
Joseph D. Baum
SAIC, McLean, VA 22102

Fifty Years Later: Outstanding Challenges and New Perspectives for Computational Mechanics
Charbel Farhat
Stanford University, CA

18:30-21:00: Reception
ABSTRACTS
The Particle Finite Element Method (PFEM) is a general numerical procedure for the analysis of problems in fluid and solid mechanics combining techniques from finite element and particle methods. The key feature of the PFEM is the use of a Lagrangian description to model the motion of the nodes in both the fluid and the solid domains. Surface nodes are viewed as particles which can freely move and separate from the main analysis domain representing, for instance, the effect of water drops or disgregated solid particles. The boundary of the analysis domain is defined at each step using the Alpha Shape method. A mesh connects the node defining the discretized analysis domain where the governing equations are solved using state of the art FEM. The PFEM is particularly suited for multidisciplinary problems in mechanics such as fluid-structure interaction situations accounting for large motions of the free surface and splashing of waves, heterogeneous fluid mixtures and non linear problems in solids accounting for large deformations with multiple frictional contacts, material fragmentation and thermal coupled effects.

In the presentation a wide range of examples of application of the PFEM are shown including the study of water streams on structures accounting for erosion of the foundation, the analysis of the failure of earth dams in overtopping scenarios, the stability of harbour structures under large waves, the analysis of mixing processes in fluids, the study of the melting and burning of objects in fire and the simulation of industrial forming processes.

References


Simulation based engineering: Challenges in Verification, Validation and Uncertainty Analysis

Dominique Pelletier

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Computer predictions are the basis of engineering decisions, they are the determining factor in product or system design, and they are the basis of scientific discovery. It is therefore natural to ask whether specific decisions can rely on the predicted outcome of an event. How accurate are the predictions of a computer simulation? What level of confidence can one assign a predicted outcome in the light of what is known about the physical system and the mathematical model used to describe it?

The science, technology and, in many ways, the philosophy of determining and quantifying the reliability of computer simulations has come to be known as Verification and Validation (V&V) is central to the success of CFD in the next decade.

Verification focuses on numerical analysis, the correctness of its implementation, and its correct application to simulate a “real” problem. Numerical accuracy is at the heart of Verification. Verification asks the question: Are we solving the equations right. Validation is an engineering activity focusing on the adequacy of the mathematical model used for a specific problem: Are we solving the right equations? Uncertainty analysis is concerned with problems whose data in know with limited accuracy and providing estimates of the uncertainty in the flow response due to the uncertainties in the input data.

The past five years have witnessed significant progress in these three fields. Rigorous procedures exist for code verification of complex flow models including the RANS equations with two-equation models of turbulence. In simulation verification, techniques have been demonstrated for determining which grids in a grid refinement study are in the asymptotic range of the numerical scheme and for providing uncertainty bands for the numerical accuracy. Procedures have also been devised to cascade input data uncertainties through a CFD code to yield uncertainty estimates of the flow response; very much like uncertainty analysis procedure used in experimental work.

Mastering these issues will reshape CFD. The controlled accuracy and the reliability of predictions will turn CFD into the powerful tool it was meant to be but so far has failed to become. However, many issues constitute formidable obstacles to this vision. For instance, successful techniques for 2\textsuperscript{nd} order time-stepping schemes become impractical for high-order time integrator. Similar observations hold for verification of high order space discretisation In 2-D, uniform refinement proceeds by subdividing a triangle into 4 self similar sub-triangles.
The 3-D analogue for a tetrahedral mesh leads to slivers or degenerate elements. Verification of higher order spatial discretisation is an unclear issue.

LES methods present special challenges for verification. The differential equations solved change with grid refinement because the sub-grid model in the PDE depends on the mesh size. Multi-scale physics and chemical reactions compound the difficulty. There is plenty of work for the next 10 years
Development of a Discontinuous Galerkin Method for Computational Fluid Dynamics

Hong Luo

Department of Mechanical and Aerospace Engineering
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Abstract

A discontinuous Galerkin (DG) method is developed for the numerical solution of the compressible Euler and Navier-Stokes equations on arbitrary grids. This DG formulation represents numerical polynomial solutions using a Taylor basis and consequently has a number of distinct, desirable, and attractive features and advantages from a practical perspective. Unlike the traditional iscontinuous Galerkin methods, where a Local Discontinuous Galerkin (LDG) formulation is usually used to discretize the viscous fluxes in the Navier-Stokes equations, this DG method uses Bhatnagar-Gross-Krook (BGK) scheme: a gas-kinetic viscous discretization, for the construction of numerical fluxes at the interfaces, which contains both convection and dissipation effects due to the intrinsic connection between the gas-kinetic BGK model and the Navier-Stokes equations. A weighted essentially nonoscillatory reconstruction scheme based on Hermite polynomials is developed and used as a limiter to eliminate spurious oscillations in the vicinity of the discontinuities. A fast, low-storage $p$-multigrid method is developed to obtain steady state solutions. The developed DG method has been used to compute a variety of both steady-state and time-accurate flow problems from low Mach number to hypersonic on arbitrary meshes. The numerical results demonstrate the superior accuracy of this discontinuous Galerkin method in comparison with a second order finite volume method and a third order WENO method, indicating its promise and potential to become not just a competitive but simply a superior approach than its finite volume and ENO/WENO counterparts for solving flow problems of scientific and industrial interest in computational fluid dynamics.
The problem we wish to address is that of accurately modeling the evolution of small-amplitude perturbations to a time-dependent flow, where the unperturbed flow itself exhibits large-amplitude temporal and spatial variations. In particular, we wish to accurately model the evolution of small-amplitude perturbations to an imploding inertial confinement fusion (ICF) pellet, which is subject to both Richtmyer-Meshkov and Rayleigh-Taylor instabilities.

This modeling is difficult despite the expected linear evolution of the perturbations themselves, because these perturbations are embedded in a highly nonlinear, strongly-shocked, and highly complex flow field which in and of itself stresses numerical computation capabilities, and whose simulation often employs numerical techniques which were not designed with the proper treatment of small-amplitude perturbations in mind. We will review some of the techniques that we have found to be of use toward this end, including the imposition of a “differentiability condition” on the component numerical algorithms of the codes which implement such modeling, the appropriate representation of interfaces in an Eulerian hydrodynamics context, and the role of exact energy conservation.

Finally, we attempt to predict future advances in ICF capsule modeling in the next decade.
Computational Mathematics at AFOSR: Challenges and Future Directions

Fariba Fahroo

Air Force Office of Scientific Research (AFOSR)
Directorate of Mathematics, Information and Life Sciences

In this talk, a brief overview of the AFOSR Computational Mathematics portfolio along with the future directions and research needs will be presented. As the sole manager of the basic research in Computational Mathematics across the Air Force Research Laboratory, the portfolio is tasked with a dual goal: identifying and supporting the fundamental research needs in computation relevant to the air force as well as supporting cutting-edge advancements in algorithm development with potential broad impact. Application areas of interest to the Air Force’s future mission in air, space and cyber are as wide-ranging as unsteady aerodynamics, hypersonics, propulsion, directed energy, information science, and biological materials, processes and systems. To address the challenges common to these disparate applications, multi-scale, multi-physics modeling as well as uncertainty quantification have been identified as the general focus areas of research in the portfolio. Examples of specific challenges and approaches in these areas will be given to illustrate the portfolio’s perspective on how to meet these general challenges.
The battlespace environment extends far above the surface of the Earth. Of special importance are the outer layers of the Earth’s atmosphere, from altitudes 100 to 1000 km, where there is sufficient mass to impede the motion of Earth-orbiting spacecraft, and where layers of charged particles control the propagation of radio waves. Changes in atmospheric “drag” alter the orbits of the thousands of space objects in low Earth orbit (LEO) that are tracked by the U.S. Space Command. The ionosphere transmits, reflects, retards, and refracts kHz to MHz radio wave frequencies. As a result, fluctuations in the neutral and ionized environment can negatively impact Naval operations by disrupting communications and navigation, and by degrading radio accuracy, targeting precision, and orbit prediction. The Sun is the primary source of variations in the neutral and ionized upper atmosphere. Increasingly sophisticated models, data, databases, and forecasting indices are refining our understanding of the intricately interconnected Sun-Earth system, thereby improving the ability to predict this region’s impact on Department of Defense systems. This talk addresses current research and future directions in space experiments and associated extended battlespace environment modeling at the Naval Research Laboratory.
Missile Aerodynamic Performance Prediction

Alan Nicholson

MSIC, Huntsville, AL

For accurate prediction of missile performance, missile simulation programs require accurate aerodynamic data for the entire flight envelope which covers the full range of Mach numbers, roll orientations, angles of attack, altitudes, thrust conditions, and combinations of control surface deflections or control jet interactions that the missile will encounter. Currently, inviscid Computational Fluid Dynamics (CFD) techniques are being utilized in the computational equivalent of a wind tunnel - revolutionizing the quantity and quality of aerodynamic data provided for the modeling and simulation of missiles.

During the next decade, we all know that CFD techniques will continue to improve and computers will become more powerful which will allow us to perform more accurate aerodynamic analysis, faster. Because of this and for various other reasons I make the following predictions. We will see the death of wind tunnel testing and semi-empirical codes used for missile aerodynamic analysis. Aerodynamic databases used for missile simulation programs will dramatically increase in size, and then decrease as database optimization techniques mature. Use of six degree-of-freedom modeling coupled with CFD techniques will increase as computational resources become available. To improve accuracy especially for complex geometric configurations CFD techniques will be utilized over the entire trajectory to predict the aerodynamic heating of a missile. Flow through inlets and propulsive jets will be modeled using CFD to improve the accuracy of drag prediction. Viscous modeling techniques will be developed for inviscid computational grids which model the masking of protuberances, base drag, and separation effects to improve the accuracy of missile simulation aerodynamic databases.

State-of-the-art CFD techniques are and will continue to be utilized to rapidly and systematically provide accurate high-fidelity aerodynamic data for the analysis of missiles.
The Next Decade in Supercomputing

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Since almost half a century, Moore’s law, which predicts that the count of transistors integrated in the chip would double every eighteen months, has steadily driven the industry of computing hardware. However, even Gordon Moore noted in 2005 that: “It can’t continue forever. The nature of exponentials is that you push them out and eventually disaster happens”. From a programmer point of view willing to improve the range of problems to be solved by a computer, at least two new problems are appearing. First, it is almost impossible now to take further advantage of the parallelism at the instruction level. The various pipelines incorporated in the chips have been optimized to such a high level that no significant increase in instruction per cycle is possible, as seen from the last generation of processors released by the different constructors. The only way to take advantage of Moore’s law until it reaches its limit around 2020 is to put more cores in the chip. It is the reason why multicores or homogeneous architectures, have made there entrance in the personal computer market, and no single processors will be produced anymore. Second, the hardware devices responsible to maintain cache coherences are extremely power consuming, so that if the increase of cores in the chip seemed to offer a new solution, it is only provisional as the power consumption will soon be the bottleneck. At the Barcelona Supercomputing Center, strong emphasis has been put on a new generation of processor, the cell processor produced by IBM. As accelerators like GPU and FPGA appear in the market, the cell processor is the only processor which is a general purpose processor. It possesses an heterogeneous architecture without cache coherence, so that high flop counts are reached without excessive power consumption. This improvement comes however with the price that the programmer, instead of the processor, is responsible of a proper use of the memory. The uncertainties for the next ten years to come in supercomputing are then:

- How will the next generations of heterogeneous processors be constituted?
- Would some model programming exist for these architectures to relieve the programmer from the burden of losing portability?
Do Analytical Methods Have A Future?

Francis Noblesse

NSWC-CD

Analytical methods, based on a simplified (usually linearized) mathematical formulation and/or idealized geometries, were the dominant approach up until a fairly recent past, a couple of decades at most. Indeed, numerical methods capable of considering a complete formulation and complex geometries were not advanced enough to offer a feasible alternative until fairly recently. This situation has now undergone a nearly complete turn around, to the point that numerical methods (including unnecessarily complex methods) are occasionally used instead of simpler and more effective analytical methods because of a lack of familiarity with these “ancient” methods, indeed with the “analytical approach”.

The rapid rise of numerical methods and corresponding decline of traditional analytical techniques leads one to wonder whether there is a future for analytical methods. I obviously cannot answer that question, but it might be useful to consider it. Three main recommendations of analytical methods can be noted.

A major recommendation of analytical methods is that they typically yield relationships between essential variables associated with the problem under consideration. These relationships are sometimes extremely simple, even algebraic [e.g. 1], although they typically involve integrals or series that need to be numerically evaluated. Even so, the required calculations are typically very light in comparison to those involved in numerical methods. The relationships obtained from analytical methods often provide fundamental insight into a problem [e.g. 2].

Another important recommendation of analytical methods based on a simplified formulation is that they typically are efficient enough to allow parametric studies; studies that could not be performed using more complex numerical methods [e.g. 3]. Systematic parametric studies can provide invaluable insight, notably for design.

A third major recommendation of analytical methods is that they often are simple and efficient enough to be useful for design, notably at early stages and for optimization [e.g. 4]. Indeed, selection of a method of analysis requires consideration of a tradeoff between competing requirements with respect to accuracy and practicality. Specifically, practical tools that are simple to use and highly efficient, but need not be highly accurate, are required to quickly evaluate the very large number of alternative designs that typically need to be considered for early (concept and preliminary) design and for optimization. On the other hand, detail design and design evaluation involve many fewer choices and require more accurate computational tools, for which efficiency and ease of use are less important.
So, is there a future for analytical methods? That future will vary with problems; e.g., it may be quite different in mechanics of solids and fluids, and even in aeronautics and ship hydrodynamics. The answer to the question will also depend both on the ability of analytical methods to move up the “accuracy ladder” and the ability of computational methods to become more practical and efficient; notably to be suitable for broad parametric studies from which simple analytical relations can be deduced. Competition between the two approaches, like all competition, in fact is a good thing that can only benefit both types of methods; and as always the best methods will ultimately survive. Let us then meet again and reconsider the question in 10 years!

The Future of CFD in Ship Hydrodynamics – Prediction and Optimization

Chi Yang

CFD Center, Dept. of Computational and Data Sciences
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With the rapid development of computer hardware and software, large-scale computational simulations are making significant contributions to many important areas of ship hydrodynamics. Computational fluid dynamics (CFD) in particular is proving to be extremely useful in the hydrodynamic analysis and design of ships. The future of the CFD in ship hydrodynamics is to improve available CFD tools and integrate them in a comprehensive simulation environment to predict and study ship behaviors at sea and perform hydrodynamic design optimization of the ship hulls.

A virtual marine basin will be further developed to complement model testing in real basins for hydrodynamic predictions of ship behaviors at sea in the next decade. The European Union funded an integrated four-year project called VIRTUE (The Virtual Towing Tank Utility in Europe) in 2005, which aims at the development of largely enhanced CFD tools and an integration platform to meet the requirements of future ship design and hydrodynamic analysis (http://www.virtual-basin.org/). The model basins, academia, CFD software providers and consultants can be expected to work together in the future, as the working model established in VIRTUE, to improve the state-of-the-art CFD tools and design better communication platforms to improve communications between CFD tools and other sources required to generate and store information for a comprehensive product data model.

Modern and integrated tools will allow complete analysis and optimization of hydrodynamic performance of new ships at different design stages. Four different virtual tanks, which are associated with corresponding physical tanks, will be further developed to provide the required information in the resistance, seakeeping, maneuvering and propulsion aspects of hydrodynamic analysis in ship design. A significant amount of the overall effort will be devoted to the improvement of the accuracy and flexibility of CFD tools. This will lead to better and more reliable CFD predictions in all areas of interest which are expected to close the existing “quality gap” between numerical and experimental investigations at model scale. The progress can also be expected in large-scale simulation to complete numerical modeling and simulation of ship behavior both at full scale and in real sea conditions.

The integrated CFD tools can be found very useful at the early and preliminary design stage. The CFD tools will be better integrated with optimization tools and hull representation tools. The CFD tools will not only be used for prediction and analysis, but also for hydrodynamic optimization. Multi-objective hydrodynamic optimization will be performed at early design stage to produce new hull forms. The future of CFD in ship hydrodynamics will move in parallel on both prediction and optimization.
Hydrodynamics vs. Hydraulics: An old controversy yet to be settled in flow simulation?

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The field of fluid flow simulation has evolved, as many other fields of science, along two quite independent paths. One of these paths, certainly the most familiar to the CFD community, evolved from the discretization of the governing equations under different approximations, such as the potential flow model used in early aerodynamics simulations. This evolution path is strongly linked to numerical techniques for solving partial differential equations, which constitutes both a blessing and a curse. A bless, because it has been possible to establish a rigorous theory that supports the available methods, and because a precise framework exists to borrow techniques from vast areas of applied mathematics. A curse, because this evolution path has always been limited to the simulation of phenomena for which a PDE model exists, with very little ability to incorporate information from experiments or from the user’s expertise. In a sense, this more mathematical path corresponds to the Hydrodynamics side of the well-known Hydrodynamics/Hydraulics controversy of which the D’Alembert Paradox is the most famous example.

The flow simulators that are most widely used in industry, however, have evolved following a quite different path, which could be seen as the "hydraulics path". I am referring to lumped-parameter models of which typical examples are HYSYS (aspentech.com), Flowmaster (flowmaster.com), FluidFlow3 (fluidflowinfo.com), FlowNex (flownex.com), among many others. In these codes complex systems can be set up, of which individual elements can be a pipe, a turbine, a centrifugal pump, or even a three-phase-flow chemical reactor. These codes do not rely, for obvious reasons, on PDE models. Instead, they are based on global conservation laws and on empirical closure laws, typically very simple ones that depend on a reduced set of parameters that can be determined by experiments. As inaccurate as these closure laws may be, it is unquestionable that lumped-parameter flow simulators provide a global, dynamical, fully-coupled picture of fluid systems which respects the main underlying conservation principles, justifying their popularity.

In many technological situations it is more important to account for the global balances and dynamics than with local details. In these situations, which are rather ubiquitous in process engineering for example, lumped-parameter models are as irreplaceable as CFD models are in flows governed by 3D effects, such as aerodynamics or blunt-body heat transfer. In this way, both CFD and lumped-parameter simulators have flourished in the last decades, producing an impressive record of successful applications in their respective niches.
Notwithstanding, there exists a wide class of applications for which neither lumped-parameters nor CFD models are suitable. Some components cannot be reasonably approximated by a lumped-parameter model, while for others a solvable PDE-based model simply does not exist. In this presentation, I will provide a few real-life examples and elaborate on the need of a robust, flexible and automatic framework for plugging CFD models into lumped-parameter codes. I will discuss some of the mathematical and algorithmic challenges involved. Further, I will succinctly review some progress along this research direction made recently in collaboration with P. Blanco and J. Leiva. The next decade will arguably witness the development of a new generation of codes that will blend the capabilities of the two main flow simulation paradigms currently available. This will settle this apparent dichotomy in flow simulation codes, which much resembles, and is to some extent related to, the historical hydrodynamics/hydraulics controversy.
The last two decades have seen exciting technology developments resulting from the push towards autonomous unmanned vehicles. MEMS sensor and actuator technology, functional nanomaterials design, novel battery technology, and onboard microprocessor computing are among the drivers that have provided the impetus. Complementing the specific component and vehicle technology developments has been the investigation by the biological community of Nature’s successes in the air, on the ground, and on and under the sea. At the macro-scale there have been extensive investigations of the aerodynamics of flapping wings, hovering aerodynamics of birds and insects, optic flow and object avoidance aerodynamics, leading edge flow control by cetaceans, unsteady hydrodynamics of precise low-speed controllability of pectoral fin swimmers, and the sure-footed, high-speed locomotion of crawling insects and crustaceans in an obstacle-strewn terrain. Extending down to the micro-scale have been the investigations of the gravity-defying surface adhesion of the gecko, the self-cleaning of leaf surfaces and, continuing down to the atomic–level, the interactions between single biomolecules and their surrounding fluid and their resulting conformational changes, shown below, in a shear flow as they move near a wall (Atomic hydrodynamics of DNA; coil-uncoil-coil transitions in a wall-bounded shear flow, Physical Review E 78, 061910 (2008)).

These examples are but a very few of the very many biological investigations that have provided glimpses into Nature’s strategies for effective operation in challenging environments.

The aspiration to create vehicles with similar capabilities to sense and respond to their environment demands that we address a myriad of challenges,
both physical and computational, in order to adapt Nature’s strategies to our purposes. In the air, Nature’s evolved solutions for controlling and landing its vehicles in extreme environments is on display daily. Can we understand stall control and the precise perching of an eagle on a slender branch or the stationary hovering and abrupt vertical shifts of a dragonfly above a wind-swept pond? And if we succeed in understanding the unsteady aerodynamics what must we also learn about material dynamic response characteristics and control logic if we are to build vehicles with similar capabilities? On the ground can we combine in some way the characteristics of the gecko and the cockroach? Under the sea can we understand how drag is reduced and vorticity production, shedding, and force vectoring is controlled by flapping dynamics, and if we do, can we create the new materials, sensors, and actuators necessary to embody that functionality in swimming vehicles? These questions will be explored and implications and challenges they pose for computational mechanics will be discussed.
Numerical modelling of human airways is gaining interest among the computational mechanics scientists due to increasing diseases and disorders faced by the human population. For example, one third of the population in the UK complains about breathing problems at some point in their life. Though many of these complaints are trivial, the resources required to address this issue are not small. Life threatening diseases such as COPD also consumes a large portion of the healthcare budget due to its intensive nature. Many of the disorders, such as vocal-cord paralysis, nasal airway blockage and sleep apnoea, are nowadays commonly treated in western countries. Due to lack of clear understanding and the need for better diagnostic methods and treatments, modelling of the respiratory systems is seriously considered. In addition to providing an overview of current status of the topic, this presentation will also discuss two possible approaches for modelling human respiratory system.

Human respiratory system consists of both upper and lower parts. Upper part of a respiratory system consists of nose and part of the trachea. The lower part consists of the lower part of the trachea and the lung geometry. Both the upper and lower parts of the respiratory system contain complex flow passages and non-conventional fluid-structure interaction. Studying the upper part provides information on various disorders such as sleep apnoea, nasal passage blockage and vocal cord paralysis. Modelling the lower airway provides better understanding of lower airway related diseases, including COPD. Studying the respiratory system as a whole will also be useful in designing devices for mechanical ventilation, drug delivery etc.

In this presentation, two modelling approaches will be described. The first one uses patient-specific scans to construct geometries to model the flow, and the second approach uses a one dimensional modelling procedure to study the fluid and structure interaction of the lower airways. Since 3D modelling of the lower airways on a regular basis is difficult, the one dimensional approach offers an alternative option. Patient-specific modelling approach includes image processing, meshing and studying fluid dynamics along with appropriate boundary conditions. One dimensional approach involves a combination of one-dimensional equations and appropriate technologies to account for boundary conditions and bifurcations.

References


Clinical Applications of Computational Hemodynamics

Juan R. Cebral
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Over the last decade, advances in medical imaging and computational modeling have allowed the construction of patient-specific models of the hemodynamics in human arteries. These models are important for three main purposes:

a) better understanding of the underlying mechanisms responsible for the pathogenesis, progression and outcome of vascular diseases,

b) improving patient evaluation and diagnosis, and

c) personalization and optimization of treatment plans.

It has been shown that image-based computational fluid dynamics models are capable of representing the in vivo conditions and that they can be used to link hemodynamic variables to clinical events and observations. However, before these techniques can be applied routinely in clinical practice, several milestones have to be reached. In order to achieve these goals, the years to come will see developments in the following directions:

- Development of clinical databases of patient-specific models that can be used for statistical testing of hypotheses about vascular diseases and to identify risk indices that can improve patient evaluation.

- Development of disease models that can be used to test hypotheses about the fundamental mechanisms governing the initiation and progression of vascular diseases.

- Development of complex multi-scale coupled models linking the different factors involved in vascular diseases such as hemodynamics, thrombosis, vascular wall biomechanics, mechano-biology and mechano-transduction, and the extra-vascular environment.

- Improvements in the speed and simplicity of image-based modeling and solver performance in order to use these techniques in the clinic to obtain information that is otherwise unavailable.

- Development of faster solution techniques in order to make larger and more complex models practical for clinical investigations.

- Development of techniques to perform virtual interventions in order to predict the outcome of medical treatments and improve current treatment planning.

- Performance of clinical studies using longitudinal data in order to link predictions and clinical end points and outcomes.

In conclusion, this is an exciting field that requires multi-disciplinary collaboration and that can have a significant impact on the way medicine is practiced today and result in better patient care.
Damping the Flames: Fire Modeling for the Next Decade

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National Institute of Standards and Technology
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The complexity of fire makes its behavior very difficult to predict. The heat and volatile gases given off by a burning object depend on its composition, physical nature, and geometry, the oxygen content of the air, and the presence of water and other fire suppression agents. Fire phenomena take place over scales ranging from the nanoscale effects of particles and chemistry, through the microscales of flame front thickness and bubble generation, to the macroscales of heat and mass transfer through a room, over multiple floors of a building, across a neighborhood, or through a forest. While we are capable of answering many questions about heat transport, smoke movement, and the effects of ventilation and sprinklers with today’s computational tools, the answers to other questions remain out of reach.

Tools exist to represent some fire-related phenomena in the rich variety of fuels found in our homes, workplaces, and vehicles. Solid phase 1D models have been developed to describe chemical degradation, charring, and intumescence, and simple 2D models are available to characterize flame spread over flat surfaces. The use of thermoplastic materials, which are employed in products like mattresses, upholstered furniture, and molded objects such as electronic housings and automobile parts, is growing due to their low cost, good mechanical properties, and ease of manufacture. However, computational methods have only recently given us the ability to model the melting and dripping of these materials. When a drip pool ignites, the feedback between the pool fire below and the burning object above increases the heat flux to other objects in the room and can cause rapid growth of the fire. Certain nanoparticles and barrier fabrics eliminate the dripping of thermoplastics, and nanoparticles can reduce their flammability through increased charring. More advanced models that capture nanoscale to mesoscale effects will aid in the development of safer materials, and incorporation of solid phase models into computational fluid dynamics (CFD)-based analysis systems will result in more realistic representation of fires.

Models are only as good as the data entered into them. Gaps in our knowledge of mechanical properties, chemical kinetics, thermal properties, and other parameters prevent us from solving the problem of predicting behavior of materials in large-scale fires from their behavior in small-scale tests. Close collaboration between modelers and experimentalists is therefore required to develop the test methods that will fill these gaps.

We do not currently have the means to predict the failure of structures due to fire, including crack propagation, buckling, and connection failure. New modeling techniques and insights that enable monitoring of developing structural weaknesses would save lives of both firefighters and occupants.
Computational models of fires now run much slower than real-time. This is satisfactory for investigating fires that have already happened and for testing the adequacy of fire protection in buildings that have already been designed. Creation of models and machines that run faster than real-time will make many new applications possible, including the direction of firefighters on the scene, the incorporation of fire protection into the design cycle of ships and buildings, and the addition of wildfire winds to weather prediction.

Many countries around the world now permit a performance-based approach to designing new buildings, in order to encourage innovation without sacrificing safety. This adds a new impetus to advance the capability, accuracy, and speed of the modeling tools available to the fire protection engineer.
Challenges in Integrated Structural Impact Analysis

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Over the past decade, large-scale simulation has been successfully used in structural impact applications, such as automotive crash analysis and aircraft engine containment analysis. In automotive industries, computer simulation analysis based on finite element method has become routine practice for vehicle structure/component design, crashworthiness evaluations and structural optimizations. With the advancement in computer hardware technology and more affordable hardware resources, system level optimization has also become possible in many of these applications. While recent advancement in impact analysis breaks down many technical barriers, new challenges still remain. For example, most of material failure models used in structural impact analysis are application dependent. In order to achieve the level of accuracy, reliability, and robustness of analysis results, new material failure models must be developed.

Traditional material failure models, based on simple tensile or compression tests, cannot address complex state of stresses during material failure in different applications. New material models need to incorporate different material failure modes such as uni-axial tensile and compression, bi-axial tensile and compression, shear and torsion. Material coupon tests should be designed to validate these corresponding failure modes. In addition, these material failure models should include strain rate effect, temperature effect and damage accumulation. Furthermore, in order to isolate the problem of mesh dependency in finite element models, mesh regularization scheme should be applied to these failure models. The model with these capabilities should be able to provide more reliable and robust simulation results with predictive capability for different impact conditions and impacting geometries. Applications, such as aircraft fan blade-out and engine containment analysis, can greatly benefited by these material failure models in order to simulate the events of fan blade-out, fan-casing interaction and rubbing, fan blade-to-blade interaction more accurately. During the fan-blade-out event, un-balanced rotational fan response causes additional loading to engine/fan shaft and its supporting structures, thus cause additional loading on aircraft wing structures, which could lead to catastrophic wing structural failure. With more reliable and robust material failure models, the interactions between fan blade and fan casing, between engine shaft and its supporting system, between engine and wing structure will be better understood during the engine fan blade-out event.

With the increase use of advanced materials such as high strength steels, composite materials, and plastics in automotive and aerospace applications, research efforts will be focused on developing material models that take account not only their material characteristics but also their material history during their manufacturing and fabricating processes, and their failure mechanism in micro structural level.
Modeling of Structural Response to Blast Loading

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Our research objective over the past fifteen years was to develop, validate, verify and apply a coupled CFD/CSM methodology capable of accurately modeling structural response to blast wave loading. The coupled algorithm combines the Computational Fluid Dynamics (CFD) FEFLO code and the Computational Structural Mechanics (CSM) codes GA-DYNA3D and SAICCSD via an embedded approach, where the CSM objects float through the CFD domain. This combination enables an easier and more accurate prediction of the physical processes typically modeled by our group, namely: weapon HE detonation, case cracking and fragmentation, airblast and fragment propagation and impact on the responding target, the loaded structural response to the loading and blast wave propagation past/through the failing target.

While we enjoyed good success modeling the fairly focused set of physical processes our customers are interested in, we have observed that models capable of accurately describing several different physical processes must be included. Among these are:

1. Material properties. Modeling of such granular material as concrete continues to pose a challenge. Further complexities are introduced by such coating materials as polymers, ceramics, weaved Kevlar, etc. While waiting for better material information, development of a discrete approach, at least for concrete, might be worthwhile;

2. The requirement to model blast response of structures backed by incompressible materials, such as water or jelled substances, requires replacing the compressible module in the CFD code with a combined compressible and incompressible modules;

3. Blast interactions with structures also require the modeling of long-term response, not just structurally, but thermally. Hence, material ignition and fire must be modeled. Thus, we must incorporate couple thermal codes, as well as advanced material modeling (e.g., material temperature dependence) within the CSM code;

4. Modeling of reactions, whether within the non-ideal explosive, or the response of substances within the targeted structures, requires incorporating a time-dependent chemical dynamics solver. Because of the stiffness of the equations solved, compromises must be sought between affordability (CPU, customer requirements and patience) and accuracy; and

5. Modeling of particulate behavior either under high pressure, high-temperature environment, such as inside a cased weapon, or medium-pressure, hot environment in the attacked facility, requires the modeling of particle phase transition for solid (from macro to nano size), liquid or jelled materials.

In summary, development of the required methodologies for modeling the complete range of physical processes envisioned will most likely carry us to the 60th birthday celebration, at which time we should hopefully provide a better review.
FIFTY YEARS LATER: OUTSTANDING CHALLENGES AND NEW PERSPECTIVES FOR COMPUTATIONAL MECHANICS

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Fifty years after Sir Löhner was born, and despite his numerous and impressive technical contributions to the field of computational mechanics, high-fidelity time-dependent numerical simulations remain so computationally intensive that they cannot be used as often as needed, or are more often used in special circumstances than routinely. This is the case, for example, for turbulent CFD computations at high Reynolds numbers. Consequently in many engineering fields, the impact of Computational Mechanics on time-critical operations such as (conceptual) design, design optimization, and control, to name only a few, has not yet fully materialized. For such operations, this full impact will perhaps be enabled during the next decade by advanced reduced-order modeling (ROM) methods — that is, methods that find approximate realizations using smaller computational models — which can faithfully reproduce the essential features of the larger computational models at a fraction of their computational cost, and most importantly, are capable of capturing the critical behavior of the engineering systems of interest. In this talk, new methods for constructing linear and nonlinear fluid, structural, or fluid-structure interaction ROMs based on Galerkin and Petrov-Galerkin projection schemes will be presented. The concept of a database of ROMs will be motivated, and an innovative interpolation method for adapting pre-computed ROMs to parameter changes in near real-time will be highlighted. This interpolation method is based on appropriate manifolds, their tangent spaces, and concepts from differential geometry. The lecture will conclude with a brief reporting on the successful application of all discussed computational methodologies to the support of the aerodynamic design of a Formula 1 car and the flutter flight testing of a fighter aircraft. These two real-life examples highlight the potential of the developed ROM methodologies for bridging Computational Mechanics to time-critical applications and modern assistive technologies.