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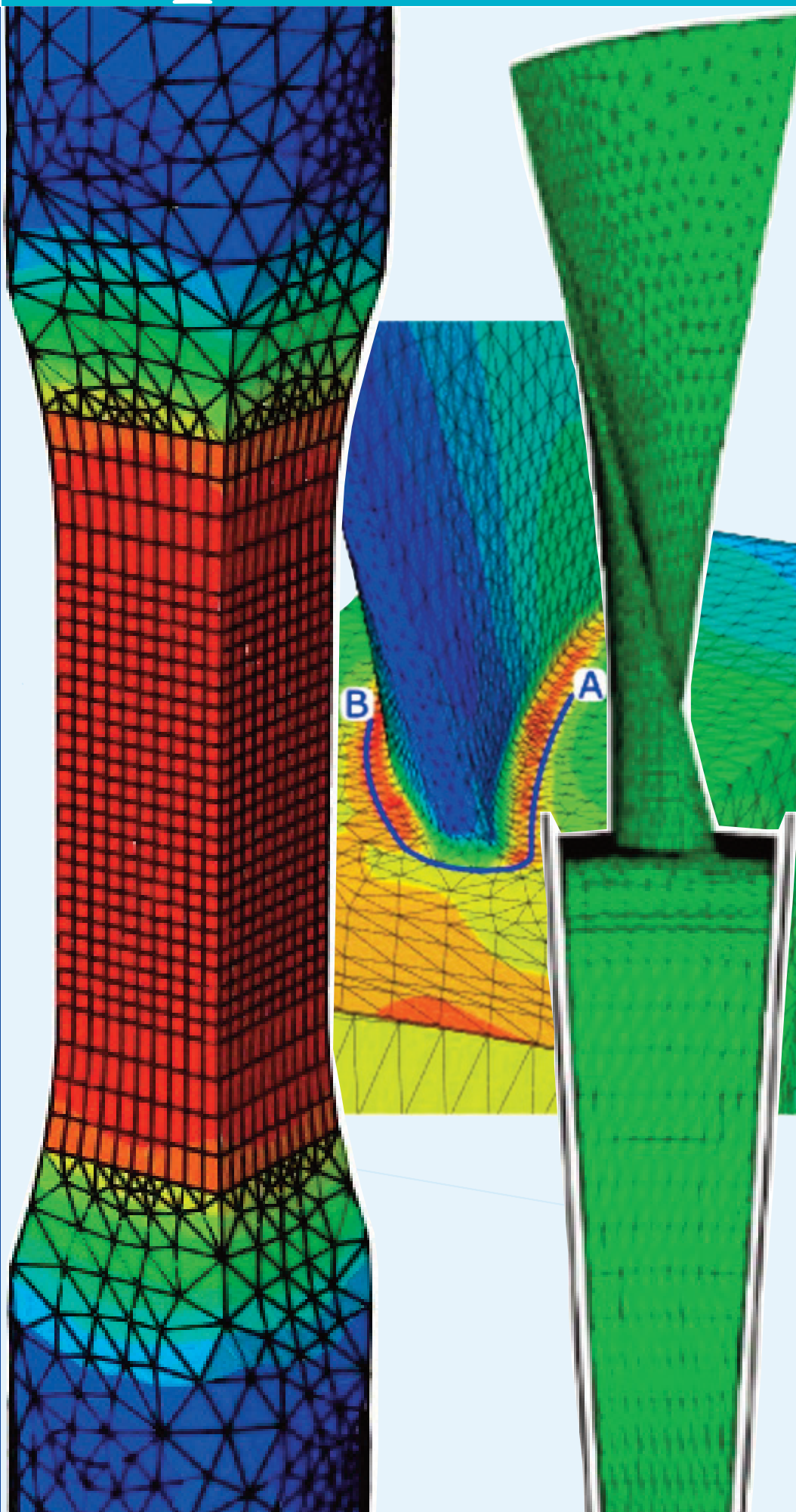
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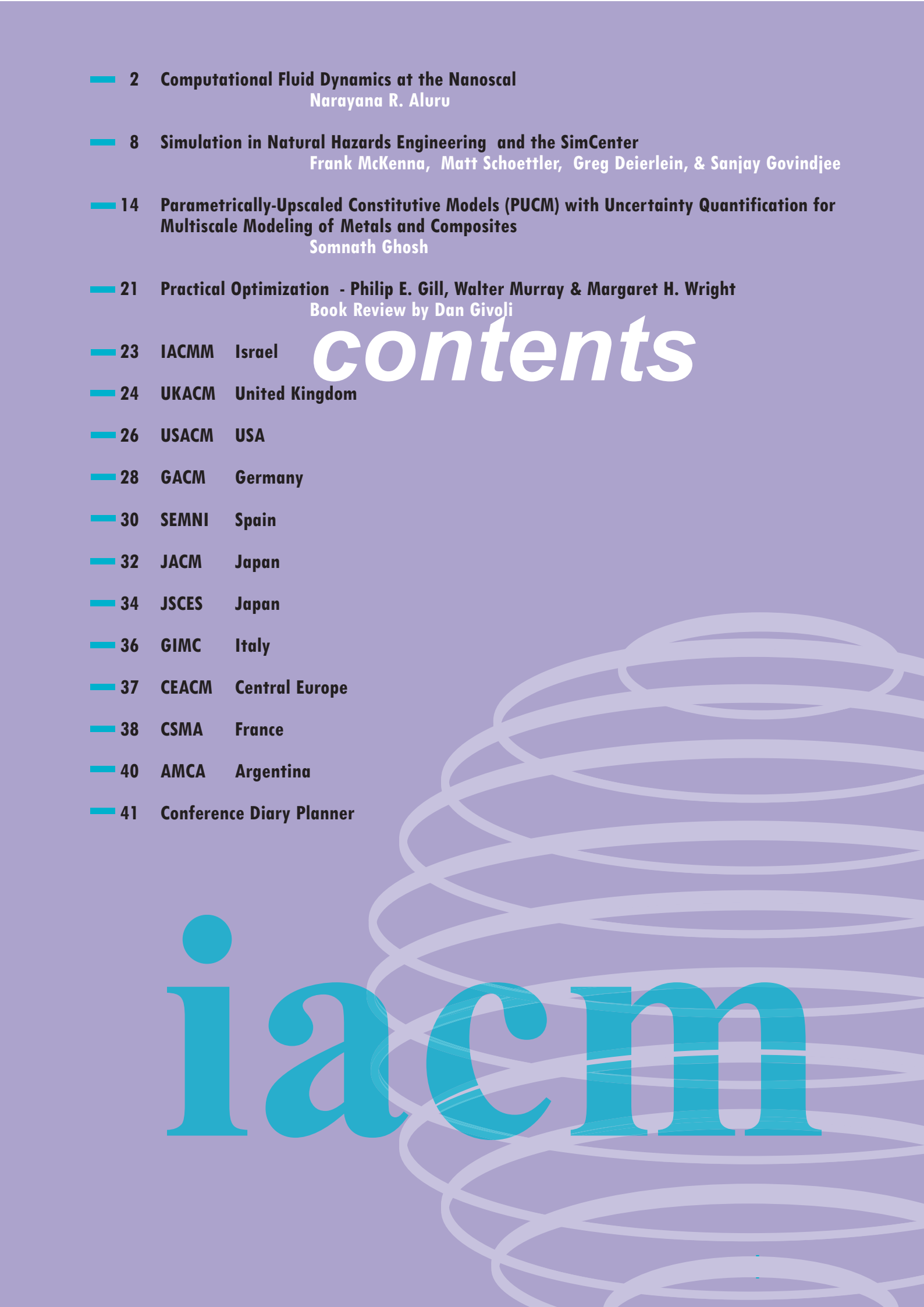
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Computational Fluid Dynamics at the Nanoscale

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Introduction

Computational fluid dynamics (CFD) has played a central role in enabling many important scientific and societal advances such as design of aircraft, understanding blood flow through arteries, electronics cooling for chip design, and simulation of complex manufacturing processes for product innovation. Classical CFD tools are built by solving the compressible and incompressible Navier-Stokes equations using a variety of sophisticated computational approaches. Often, depending on the application, the Navier-Stokes equations are combined with Maxwell's equations and their simpler forms to understand charged fluid transport. While compressible and incompressible Navier-Stokes equations are accurate for simulation of physical phenomena at larger length and time scales, an interesting question arises on the accuracy of these equations at the nanoscale. During the last couple of decades, fluid mechanics at the nanoscale (also referred to as nanofluidics) has gained a lot of prominence because of important applications such as clean water, clean energy, separations, nanomanufacturing, and selective transport of ions with important implications in disease diagnosis and drug discovery. As the critical dimension

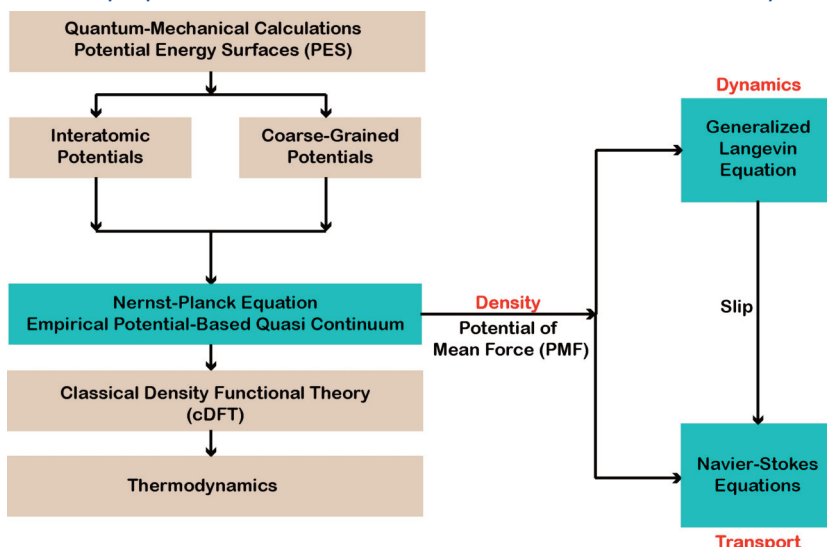
encountered in nanofluidics ranges from a few Angstroms to several tens of nanometers, important deviations from classical hydrodynamics are observed [1]. For instance, density fluctuations near the interface, size dependent fluid properties, restricted translational and rotational motions of molecules, charge inversion where the net charge density at an interface is opposite in sign to the prediction from classical theory, flow reversal where the fluid moves in the opposite direction as that predicted from the classical theory, breakdown of classical constitutive relations, and several other important phenomena have been observed at the nanometer scale. As a result, the use of classical CFD tools to simulate fluid physics at the nanometer scale has been questionable.

To overcome the limitations of the classical theories for nanoscale fluid transport, quantum and atomistic approaches are widely used. However, these approaches are limited to small length and short time scales, and it makes it difficult to use them in a design environment for applications involving nanoscale fluid transport. An alternative approach is to develop multiscale approaches seamlessly incorporating atomistic physics into continuum theories to enable rapid simulation of nanofluidic systems. Over the last 1-2 decades, efficient multiscale approaches have been developed to accurately simulate hydrodynamics at the nanoscale. These multiscale simulation tools provide a robust computational fluid dynamics environment for nanoscale fluids. The rest of this article describes a multiscale framework that accurately describes fluid physics at the nanoscale.

Figure 1:

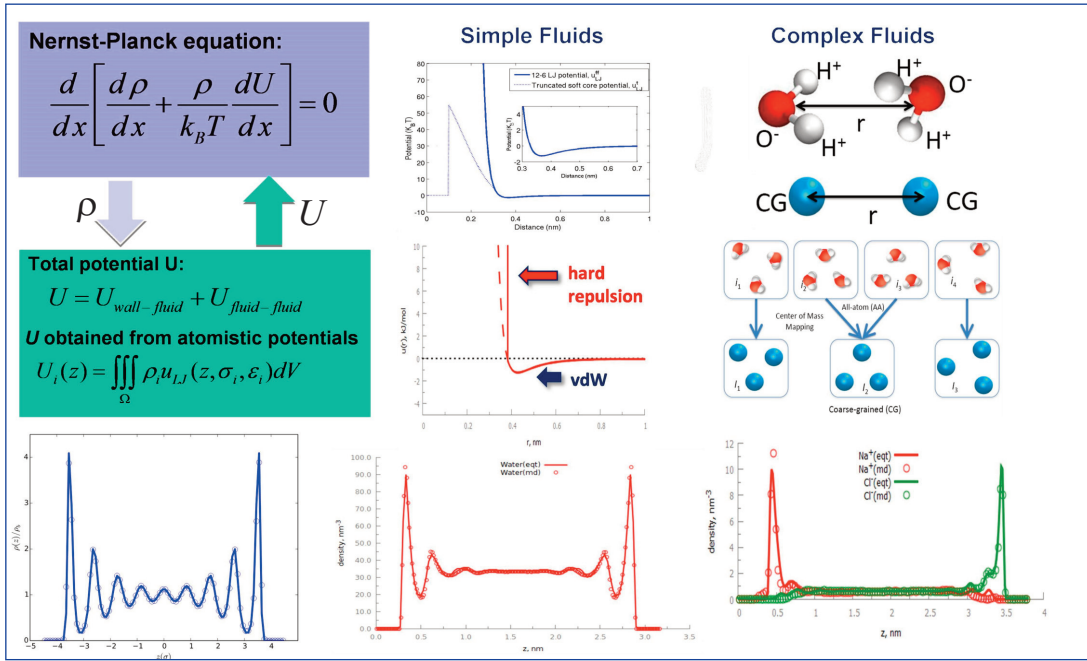
Multiscale framework for nanoscale computational fluid dynamics (CFD). Structure (e.g. density profiles), dynamics (e.g., diffusion) and transport (e.g. velocity) – the essential components of nanoscale CFD are shown in cyan color boxes.

The quasi-continuum framework can be combined with the classical density functional theory to compute the thermodynamic properties of fluids confined in nanometer channels and pores



II - Multiscale Framework

IACM Expressions readers will note that authors are requested to submit articles with no equations. With this in mind, the basic ideas in multiscale modeling of nanofluidics are introduced using pictures and the mathematical details can be found in the references. Simulation of nanoscale fluid transport, including coupling to electric fields as driving forces, can be essentially reduced to computing the structure of the fluid (the focus here is primarily on density, but other structural aspects of the fluid are also



important at nanoscale), dynamics (for simplicity, the discussion here will focus on diffusion, but other dynamical properties are also of interest) and transport, primarily referring to the velocity of the fluid. The multiscale framework to compute the structure, dynamics, and transport of nanofluidics is shown in Figure 1. To predict the structure of the fluid, the Nernst-Planck equation [2, 3] is used and the potential energy term in the Nernst-Planck equation is computed by using the atomistic potentials describing the atomic interactions in the fluid. The interatomic potentials and the coarse-grained potentials (as described in detail in Section III) can be obtained from quantum-mechanical calculations but this article will not delve into those details considering space limitations. Calculation of the structure is described in more detail in Section III. The solution of the Nernst-Planck equation provides the density profile as well as the potential of mean force (PMF) which serve as input to the generalized Langevin equation (for dynamics) and Navier-Stokes equations (for transport). The generalized Langevin equation is used to compute the trajectory of the fluid molecules using which the diffusion coefficient as well as the slip velocity of the fluid can be computed.

The calculation of dynamical properties is described in Section IV. The multiscale framework described here can also be used to compute thermodynamic properties and this is also concisely summarized in Section IV. Using inputs from the Nernst-Planck and generalized Langevin equations, the Navier-Stokes equations are solved to compute the transport properties of the fluid. This is described in more detail in Section V.

Figure 2:

(top left) Quasi-continuum framework to compute the structure of fluids;
(top middle) The fluid-fluid potentials are approximated by a soft-core (top) and hard repulsion (bottom);
(top right) Complex fluids (e.g., water) are represented by coarse-grained beads
(bottom left) comparison of density of argon from molecular dynamics (circles) and quasi-continuum theory (solid line)
(bottom middle) comparison of density of water from molecular dynamics (circles) and quasi-continuum theory (solid line)
(bottom right) comparison of density of ions (sodium and chloride ions) from molecular dynamics (circles) and quasi-continuum theory (solid line)

III - Structure

When a fluid is confined in a nanometer scale channel or pore, density inhomogeneity (layering of the fluid near the wall) is observed. The density oscillations, which arise due to the molecular interactions between the fluid with itself and with the wall, cannot be captured using classical theories. In addition, as shown in Figure 1, the density of a confined fluid is important to also understand dynamics and transport of the fluid. Instead of resorting to more expensive atomistic approaches, a quasi-continuum approach, where the interatomic potentials are directly integrated into the Nernst-Planck theory, can be used to compute the structure. The basic idea is shown in Figure 2. While quasi-continuum theories are prevalent in solid mechanics [4], for fluid mechanics it was first introduced in [5]. The potential energy term in the Nernst-Planck equation is computed using the atomistic interatomic potentials which are used to describe the fluid and wall in molecular dynamics – exceptions to this are discussed below. The various interactions

“The multiscale methods described here to compute the structure, dynamics, thermodynamics, and transport of fluids confined in nanometer channels and pores are a point of departure from the classical CFD tools that are widely used at macroscale..”

that contribute to the potential energy can be a function of the fluid density, so a simple iterative scheme is shown in *Figure 2* to self-consistently solve for the fluid density and the components of the potential energy. It is important to note that the potential energy dependence on density is highly nonlinear and good initial guesses (e.g., based on the Boltzmann distribution [6]) and effective nonlinear solvers are required to accurately compute the density profile.

Consider, first, simple fluids, which can be described by single-site isotropic pair potentials in atomistic simulations. In this case, van der Waals interactions [7] between fluid atoms (referred to as fluid-fluid interaction energy) and between the fluid and the wall (referred to as wall-fluid interaction energy) need to be considered. For most walls of interest, the wall-fluid interaction energy can be computed analytically by invoking the density of wall atoms (see [8] for more details). By invoking the density of a fluid, the fluid-fluid interaction energy can be computed by using the interatomic potential. However, the repulsive nature of the potential for short distances poses numerical difficulties. To overcome this, a mean-field approach, where a soft-core potential is used (see *Figure 2 (top middle)*) to approximate the repulsive part of the interatomic potential, a correlation-correction potential approach [9] where the pair correlation function is included in the formalism to overcome the mean-field approximation, and a fundamental measure theory where the repulsive part of the potential is approximated by a hard-sphere model (see *Figure 2 (top middle)*) are developed [10]. The unknown parameters in these approaches are determined by matching the potential of mean force (PMF) [11]. While all three approaches provide good accuracy, the fundamental measure theory-based approach is predictive and can be used for a variety of fluids with minimal effort (see *Figure 2 (bottom left)* for a typical result comparing molecular dynamics and quasi-continuum theory).

The quasi-continuum approach has also been extended to fluids with many-body interactions. For example, the charges on the oxygen and hydrogen atoms of water introduce electrostatic interactions which are long ranged. Since water molecules are represented by a density in the quasi-continuum approach, the charge information is not readily available. To address this challenge, each water is coarse-grained into a single spherical bead (see *Figure 2 (top right)*) and the interatomic potentials

describing water-water and water-wall are obtained by preserving some basic properties of the original all atom system. Some widely used approaches to develop coarse-grained (CG) potential for water and other complex fluids include iterative Boltzmann inversion (IBI) [12] – which preserves the bulk radial distribution function, force matching [13] – which preserves the forces between the all atom and CG systems, and relative entropy [14, 15] – which minimizes the information lost between all atom and CG systems. The CG potentials for water can be either directly incorporated or further coarse-grained before incorporation in the quasi-continuum framework. *Figure 2 (bottom center)* shows a typical result where the structure of water is compared between molecular dynamics and the quasi-continuum theory. The quasi-continuum framework can be extended to more complex fluids such as electrolytes, DNA, polymers, etc. For example, quasi-continuum treatment of electrolytes has been shown to effectively capture the charge inversion phenomenon (see [16]) which is missed by the classical theory.

IV - Dynamics, Thermodynamics

The dynamical properties of fluids (e.g., diffusion coefficient) at nanoscale can be different from their bulk properties. A straight-forward approach is to use molecular dynamics simulations. In molecular dynamics, the diffusion coefficient for the bulk fluid is usually determined by computing the mean-squared displacement (MSD) of the molecules, $\langle \Delta r(t)^2 \rangle$, as a function of time and fitting this behavior to the asymptotic time dependence predicted from the diffusion equation. For confined fluids, the diffusion coefficient can be anisotropic, i.e., the diffusion coefficient can be different along x-, y-, and z-directions. Furthermore, for inhomogeneous systems, where density layering is significant, molecules stay in the region of interest only for a finite time and then explore other regions. Thus, diffusion coefficient is expected to be different for different regions (spatial dependence of diffusion coefficient). Even though molecular dynamics simulations can be used to understand diffusion physics, they are expensive and limited to small systems.

The quasi-continuum framework can be combined with the memory function equation and generalized Langevin equation (GLE) (see *Figure 3 top*) to compute anisotropic and spatial variation of the diffusion coefficient [17]. In this multiscale approach, the density profile and the

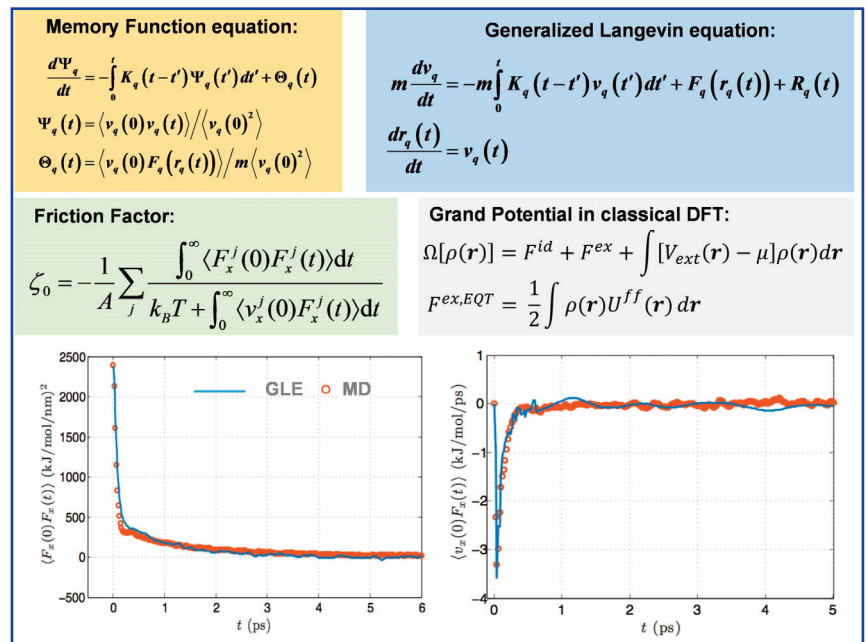
potential of mean force (PMF) are first computed by using the quasi-continuum theory. In a separate step, the memory function equation (see *Figure 3 top*), which is an integro-differential equation, is solved to determine the memory kernel. The dynamical variable (Ψ) describes normalized velocity autocorrelation function of a bulk fluid which is typically known, e.g., this can be obtained from molecular dynamics or experiments or via stochastic extension of the quasi-continuum theory. Once the PMF and the memory kernel are known, GLE can be solved to generate dynamic equilibrium trajectories of the fluid molecules. The generated trajectories can be used to compute quantities such as MSD and survival probabilities which can be used to estimate the diffusion coefficient. It is important to note that the solution of the memory function equation/GLE equation, with PMF obtained from the quasi-continuum theory, to obtain the diffusion coefficient is many orders of magnitude faster compared to the use of molecular dynamics. This is because the time step used in the generalized Langevin equation is much higher compared to that of the time step used in MD simulations.

A significant advantage of using the quasi-continuum/GLE approach, in addition to the fast calculation of the diffusion coefficient, is to estimate fluid-solid interaction properties such as the friction factor which can be used to calculate the slip velocity of a fluid on a solid wall. The friction factor, derived using linear response theory [18], is shown in *Figure 3 (middle)*. The expression for the friction requires the calculation of force autocorrelation and force-velocity cross correlation functions. Since forces and velocities as a function of time are obtained from the solution of GLE, the friction factor can be estimated easily. *Figure 3 (bottom)* shows force autocorrelation and force-velocity cross correlations for interaction of water with a silicon surface. The results from GLE compare well with those from MD. It is again important to note that the estimation of the friction factor using the GLE approach is orders of magnitude faster compared to using the molecular dynamics framework.

As shown in *Figure 1*, the multiscale framework can also be used to compute the thermodynamic properties of confined fluids. For fluids confined in nanometer channels and pores, the thermodynamic relationship between the grand potential and other thermodynamic properties such as entropy, temperature, pressure, etc. can be easily established. The classical density functional theory (cDFT) [19] provides a framework to

Figure 3:

(*top left*) Memory function equation to determine the memory kernel (K_q);
 (*top right*) Generalized Langevin equation (GLE) describing the dynamics of particles;
 (*middle left*) Mathematical expression to determine the friction (and subsequently the slip of the fluid) that relies on force autocorrelation and force-velocity cross-correlation;
 (*middle right*) Definition of grand potential in classical density functional theory (cDFT); the excess free energy is computed by using the quasi-continuum potentials;
 (*bottom left*) Comparison of force autocorrelation from GLE and molecular dynamics (MD);
 (*bottom right*) Comparison of force-velocity cross correlation from GLE and MD



determine the grand potential in terms of the equilibrium density of the fluid (see *Figure 3 middle*). The excess part of the intrinsic Helmholtz energy accounting for non-bonded interactions is often difficult to compute, but quasi-continuum potentials can be used to accurately determine the excess part of the Helmholtz free energy. Thus, by combining the quasi-continuum framework with cDFT, thermodynamic properties such as adsorption, local pressure tensor, surface tension, and solvation force, of confined fluids can be computed (see [9] for more details).

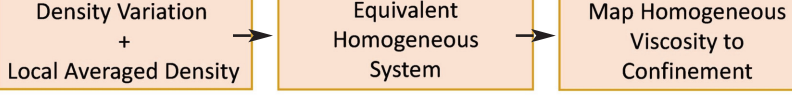
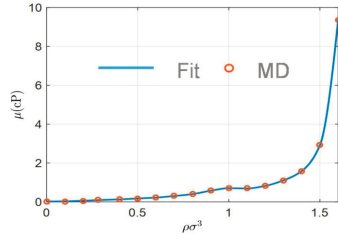
V - Transport

The governing equations for nanoscale transport are the Navier-Stokes equations (see *Figure 4 (top)*). The classical Navier-Stokes equations, however, do not always accurately describe transport at the nanoscale because of complex interfacial physics – for example, two well known effects are the slip velocity and interfacial viscosity. Fluid-surface interactions and the

Navier-Stokes Equations:

$$\frac{D\rho_m \mathbf{u}}{Dt} = -\nabla P + \nabla \cdot (\boldsymbol{\mu} \nabla \mathbf{u}) + \mathbf{f}$$

$$u_x \left(-\frac{L}{2} + \delta \right) = u_x \left(\frac{L}{2} - \delta \right) = u_s$$



and described in the previous section, the slip velocity is computed using the generalized Langevin equation. The approach to compute the spatially varying viscosity is summarized in *Figure 4* (middle). Using the density from the quasi-continuum theory, a local averaged density is first computed. The local averaged density is then mapped to a bulk homogeneous system and the viscosity of the corresponding bulk system is computed. The bulk viscosity, corresponding to the local averaged density, is then used as the local viscosity of the

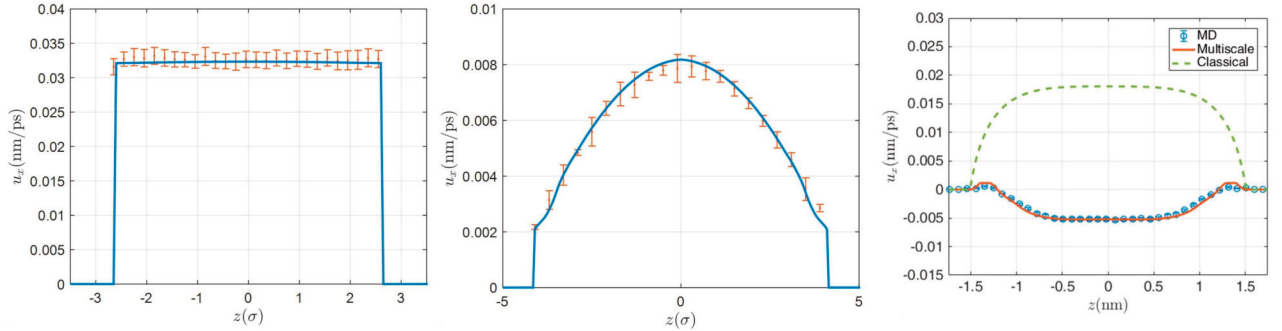


Figure 4:

- (top left)* Navier-Stokes equations along with the slip boundary conditions used for nanoscale transport;
- (top right)* Viscosity of water as a function of density
- (middle)* Approach used to determine viscosity of confined fluids
- (bottom left)* transport of water in graphene channels – solid line is multiscale simulation and error bars denote MD data
- (bottom middle)* transport of water in a silicon channel
- (bottom right)* electroosmosis of water; charge inversion causes flow reversal and multiscale theory accurately describes flow reversal

wall topology give rise to surface friction, which affects the collective motion of the fluid particles relative to the wall. The surface friction changes due to the potential corrugations, which changes due to the topology of the surface and the interaction potential between the fluid and the surface. It is important to account for surface friction effects which appear in the form of slip velocity in the transport model. It is also important to know where the slip velocity should be applied. Since there are essentially no fluid molecules at the wall, the slip velocity is applied at a distance from the wall where the density of the fluid is finite. This information is available from the quasi-continuum calculation of density profiles. The second aspect that is important is the viscous component of the flow. In macroscopic channels, viscosity is assumed to be constant in the entire channel. However, viscosity in confined channels can be different. Density layering near the surface introduces viscosity variation. As a result, viscosity can vary spatially in the nanochannel and it is important to account for this phenomenon. As shown in *Figure 1*

confined channel. This assumption works reasonably well for most nanochannels of interest. The bulk viscosity of most fluids as a function of density is known. In the absence of such relations, molecular dynamics can be used to compute density-viscosity relations. Shown in *Figure 4* (top right) is the density-viscosity relation for water. Once the various inputs to the Navier-Stokes equations are known (see *Figure 1*), the Navier-Stokes equations can be solved using well established methods to determine the velocity of the fluid.

The multiscale method described above has been used to investigate transport of a variety of fluids confined in nanometer channels [20]. Some representative results are shown in *Figure 4* (bottom). *Figure 4* (bottom left) shows the transport of water in a graphene channel. A significant slip velocity is observed in this system. The multiscale result (solid line) matches well with the molecular dynamics result (error bars). *Figure 4* (bottom middle) shows transport of water in a silicon channel where the slip velocity is not significant and viscous nature of the flow is observed in the central part of the channels. Again, a good comparison between multiscale method and molecular dynamics is observed. *Figure 4* (bottom right) shows an example where water and electrolytes are confined in a nanochannel. This is an example where charge inversion is observed, and the classical Navier-Stokes theory predicts that the water velocity is positive while molecular

dynamics predicts that the water velocity is negative. Multiscale theory, with inputs from the quasi-continuum theory for the density and the location of the slip velocity, the generalized Langevin theory for the slip velocity, and the local density approximation for the local viscosity, predicts that the water velocity is negative and the result matches reasonably well with the molecular dynamics result.

VI - Concluding Remarks

The multiscale methods described here to compute the structure, dynamics, thermodynamics, and transport of fluids confined in nanometer channels and pores are a point of departure from the classical CFD tools that are widely used at macroscale. Many important practical applications involve coupling of macroscale fluid mechanics with nanoscale fluid mechanics and efficient simulation of these problems is now possible via the multiscale methods described here. A number of issues such as the

development of coarse-grained potentials that are reliable at various thermodynamic states, seamless integration of structure, dynamics, thermodynamics and transport multiscale tools into one coupled computational environment, developing constitutive theories that are accurate and reliable at purely molecular limit, extraction of important transport parameters and properties such as slip and viscosity without resorting to coarse-grained theories are among the many challenges that will further push the frontiers on the development of multiscale methods for nanoscale hydrodynamics. ●

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Simulation in Natural Hazards Engineering and the SimCenter

by

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Introduction

Much of the world's population lives in regions susceptible to earthquakes, tropical cyclones (hurricanes), or other natural hazards, where the risks are exacerbated by aging buildings and civil infrastructure that often are not designed to resist the hazards. While knowledge and data gained through field observations and experiments are fundamental to addressing challenges associated with planning and design of resilient communities, computational simulations are seen as an essential component of the science and engineering needed to evaluate and mitigate the potential devastating effects of natural hazards, some of which are intensifying in magnitude and/or frequency due to climate change; further, risk exposure to all hazards is increasing due to population growth and urbanization (NHERI 2020).

To date, the primary focus of computational simulations with regards to natural hazards engineering (NHE) has been on applications for isolated purposes. Examples include:

1. *Hazard simulation (EVENT):*
This refers to direct modeling of the physics of a hazard, such as seismic wave propagation models for strong ground shaking, shallow-water solvers for coastal inundation, or Weather Research and Forecasting type models wrapped around Large Eddy Simulations for the multiscale assessments of wind flows.
2. *Asset response simulation (FEM):*
This typically involves simulating the response (displacements, accelerations, stresses, etc.) of an individual structure (building, bridge, utility pipeline, etc.) using the finite element method to determine the demand parameters for a given hazard EVENT.
3. *Damage and losses estimation (DL):*
This refers to predicting the resulting monetary losses and downtime for repairs given a FEM prediction of structural response of buildings or other infrastructure.

4. *Community recovery (REC):*

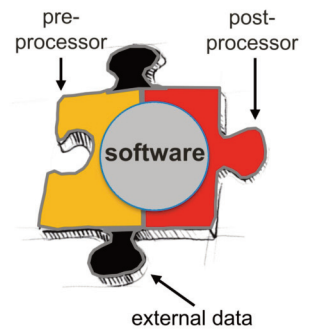
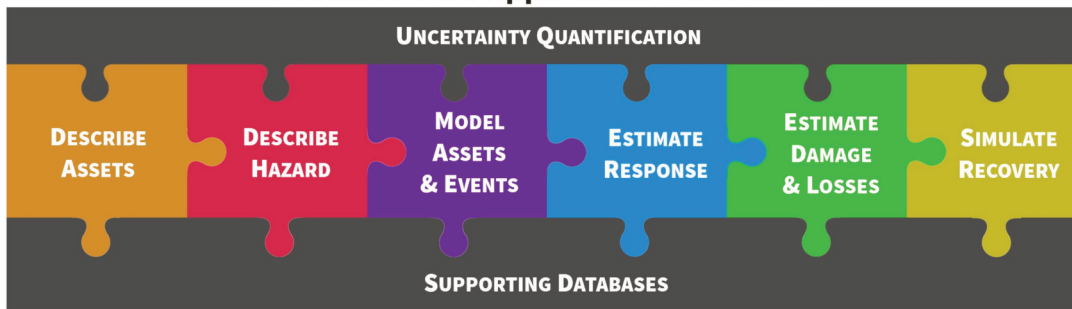
This refers to predicting population displacement, evacuation scenarios, and regional recovery for a given EVENT and subsequent DL.

The effects of natural hazards at a regional scale can be evaluated by simulating the hazard event, performing detailed analyses of localized response and damage of individual buildings and infrastructure components, and integrating the results through multi-scale analyses of regionally distributed communities and infrastructure systems. The manual effort needed to perform a comprehensive regional analysis, utilizing existing applications that individually solve just one step of the EVENT-FEM-DL-REC workflow, is time consuming, cumbersome, and error prone. Furthermore, such work requires expertise with the various applications. The consequence is that researchers have generally maintained a narrow focus on certain aspects of the problem. For example, researchers involved with earthquake simulation usually limit their investigations to predicting the maximum accelerations in a region, without going further to simulate the damaging effects of the motions. Moreover, there is limited collaborative work across the many disciplines that make up natural hazard engineering; and there is little connection between NHE researchers and those in urban planning and the social sciences. The result is a state of the art that is overly simplistic, and which misses the opportunities for comprehensive efforts to improve community resilience.

The Natural Hazards Engineering Research Infrastructure's Computational Modeling and Simulation Center (SimCenter) is a National Science Foundation (NSF) facility funded to provide open-source software that seeks to overcome this situation through the development of an application framework for creating targeted scientific workflow systems for NHE researchers. Scientific workflow systems are applications that allows users to create, launch, and monitor scientific workflows (i.e., in-silico workflows). In the SimCenter systems, the user defines the workflow in a desktop application and a backend application manages the running workflow by both

“Our goal is to support research that will enable dependable regional resilience assessments ... that reduce damage ... after an event, & ...improve community resilience.”

The SimCenter Application Framework



launching the different applications in the workflow and handling the flow of data between the applications.

While several general-purpose workflow systems exist, e.g., Taverna (Oinn et al., 2003), Kepler (Altintas et al., 2004), Pegasus (Deelman et al., 2015), etc., the SimCenter is developing domain specific systems for NHE with a focus on defining APIs for the different components of the workflow. For example, all EVENT applications accept a standardized JSON input and produce a standardized JSON output, permitting users to choose from a variety of EVENT applications provided by different researchers. The use of JSON allows applications to handle the standard API data requirements and to access additional application specific data. To accommodate the inclusion of new applications into the workflows, the SimCenter publishes APIs for application developers and writes pre- and post-processors for common applications as examples for developers. In addition, the SimCenter workflow systems provide simple graphical user interfaces (GUIs) that researchers can use to harness DesignSafe-ci provided HPC resources at the NSF funded Texas Advanced Computing Center (TACC) and to facilitate the use of Uncertainty Quantification (UQ) in a rigorous manner. As a SimCenter priority, UQ is automatically included in its scientific workflows, thus facilitating the characterization and propagation of uncertainties throughout the workflow.

SimCenter application framework

The application framework provided by the SimCenter, cf. Figure 2, consists of a collection of components (shaded rectangles) plus workflow systems (unshaded rectangles) that are built using these components, and several pre- and post-processors in the shaded SimCeA box, that invoke existing applications and interface with external web services.

Figure 1:
Modular SimCenter framework

Several of these components represent the four application types identified in the introduction: EVENT, FEM, DL, and REC. In addition to these four, the framework provides other components:

UQ: The UQ component provides an interface to software and routines for methods of uncertainty quantification (sampling, reliability, sensitivity), optimization and surrogate generation. Libraries being used include Dakota (Adams et al., 2014) and UQpy (Olivier et al., 2020), in addition to the SimCenter's own UQ engine.

CLOUD: A component that interacts with cloud-based resources. The current cloud component uses Tapis (Agave), a TACC Cloud API. The CLOUD API is designed such that other cloud components are easily integrated, allowing runs at any of the large cloud providers (e.g., Amazon Web Services, Google Cloud Platform, IBM Azure, etc.).

SAM: Structural Analysis Modeling (SAM) is the workflow component that includes rule-based, artificial intelligence (AI), and other types of applications to translate descriptive information about the built environment (e.g., building inventory) into information to create finite element or other types of models to simulate structural response to hazards.

BRAILS: Building Recognition using AI at Large Scale (BRAILS, Wang et al. 2019) is a SimCenter application dedicated to using machine learning (ML) to generate information about buildings in a region from multiple data streams, including imagery (satellite and street view images) and textual data (tax assessor data).

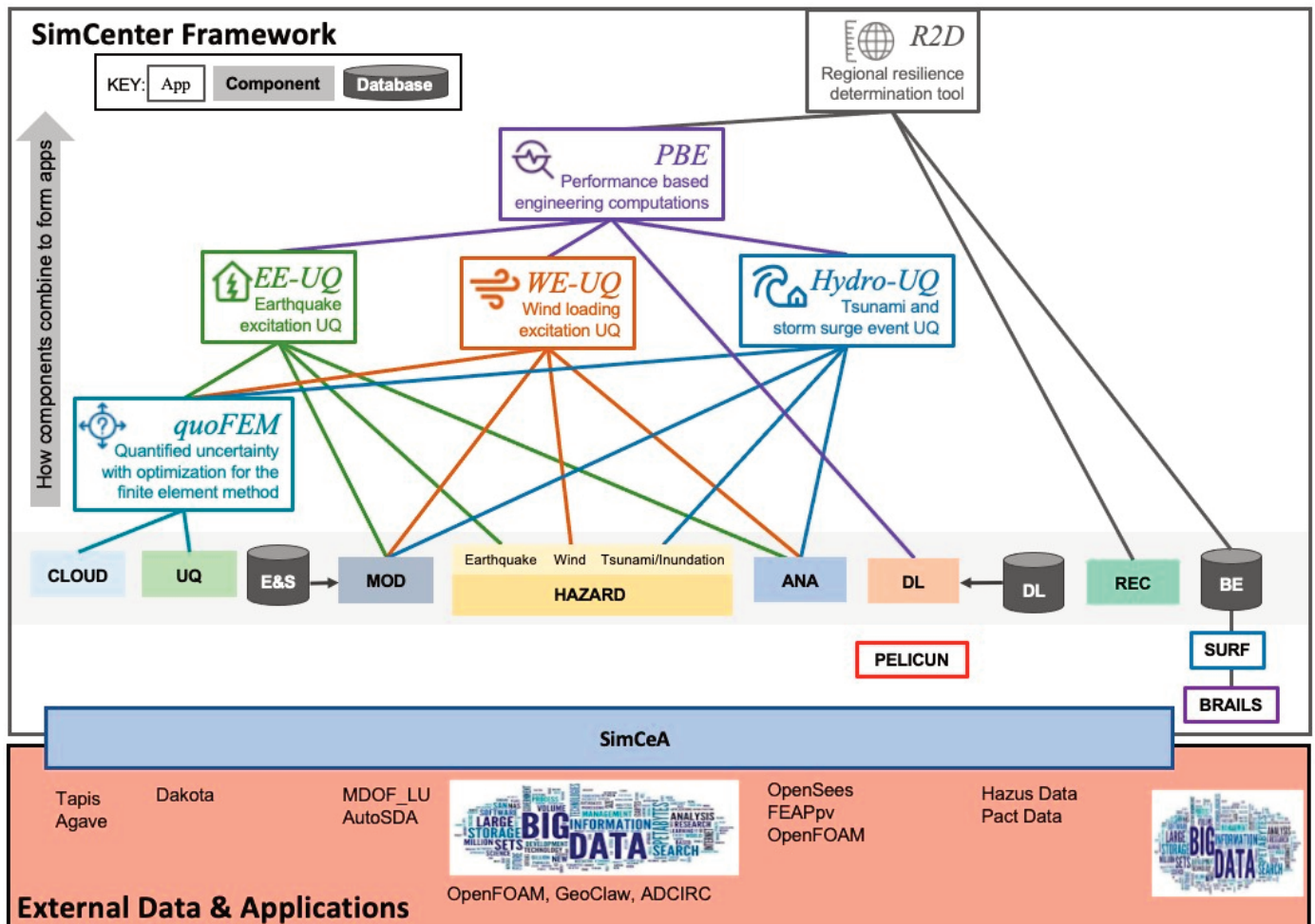


Figure 2:
SimCenter Framework Components and Applications

Central to NHE computations is a large amount of data about the built environment. Databases needed by the framework, the shaded cylinders in *Figure 2*, include:

BE – Built Environment Inventory: The BE consists of meta-data and data files that define the inventory of physical assets for regional simulations, including buildings, transportation components, utility infrastructure, etc. The data for the BE often comes from automated scraping of public websites and other on-line datasets.

DL Data: Databases of (probabilistic) fragility curves for damage and loss estimation for various types of assets subjected to the demands from various hazards (earthquake, wind, storm surge, etc.).

Exp/Sim Data: Databases of experimental and/or computational research data that is utilized for the machine learning SAM applications and code validation.

Finally, the unshaded boxes in *Figure 2* are desktop applications that pre-package

common workflows built from SimCenter framework components. These desktop applications facilitate launching workflows locally or on HPC resources as shown in *Figure 3*.

These applications include:

quoFEM: The Quantified Uncertainty with Optimization for the Finite Element Method application facilitates uncertainty quantification calculations by combining software systems for uncertainty quantification and optimization with FEA (and other) analysis codes. As shown in *Figure 2*, quoFEM is built upon the UQ and CLOUD resources of the framework.

EE-UQ, WE-UQ, and Hydro-UQ: These applications allow users to perform sampling, reliability, and sensitivity analyses for buildings subjected to input ground motions, wind flows, and hydrodynamic forces due to earthquake, wind, and storm surge/tsunami loading events. The tools play an important role under-pinning regional simulations, as reliable models of single structures are an integral part of high-resolution regional simulations. Research is crucially needed to improve wind and hydrodynamic simulation

capabilities, as at present they cannot reliably evaluate buildings and other structures subjected to turbulent wind and water flows.

PBE: The performance-based engineering application is an extensible workflow application to evaluate the damage, losses, and downtime of buildings or other assets to natural hazard events.

R2D: The Regional Resilience Determination Tool facilitates regional hazard scenario studies. The tool presently determines damage and loss for a region's building inventory for hurricane and earthquake events. The application is being expanded to include REC.

Workflow example with R2D

The R2D tool is the primary SimCenter application for regional scale simulations. *Figure 4* shows a comparison of results generated for a magnitude 7.0 earthquake impacting the San Francisco Bay area using R2D versus results from a large study organized by the US Geographical Survey (USGS). On the left side of *Figure 4* are results for an R2D simulation that utilized an SW4 (Petersson and Sjogreen, 2017) rupture simulation (EVENT) to individually shake 1.84 million buildings obtained by combining an UrbanSim (Waddell, 2002) database with Microsoft footprint data (Microsoft, 2020). Each building was modelled as a nonlinear shear building using MDOF-LU (Lu et al., 2014) with random variables assumed for structural stiffness, mass, and story yield properties.

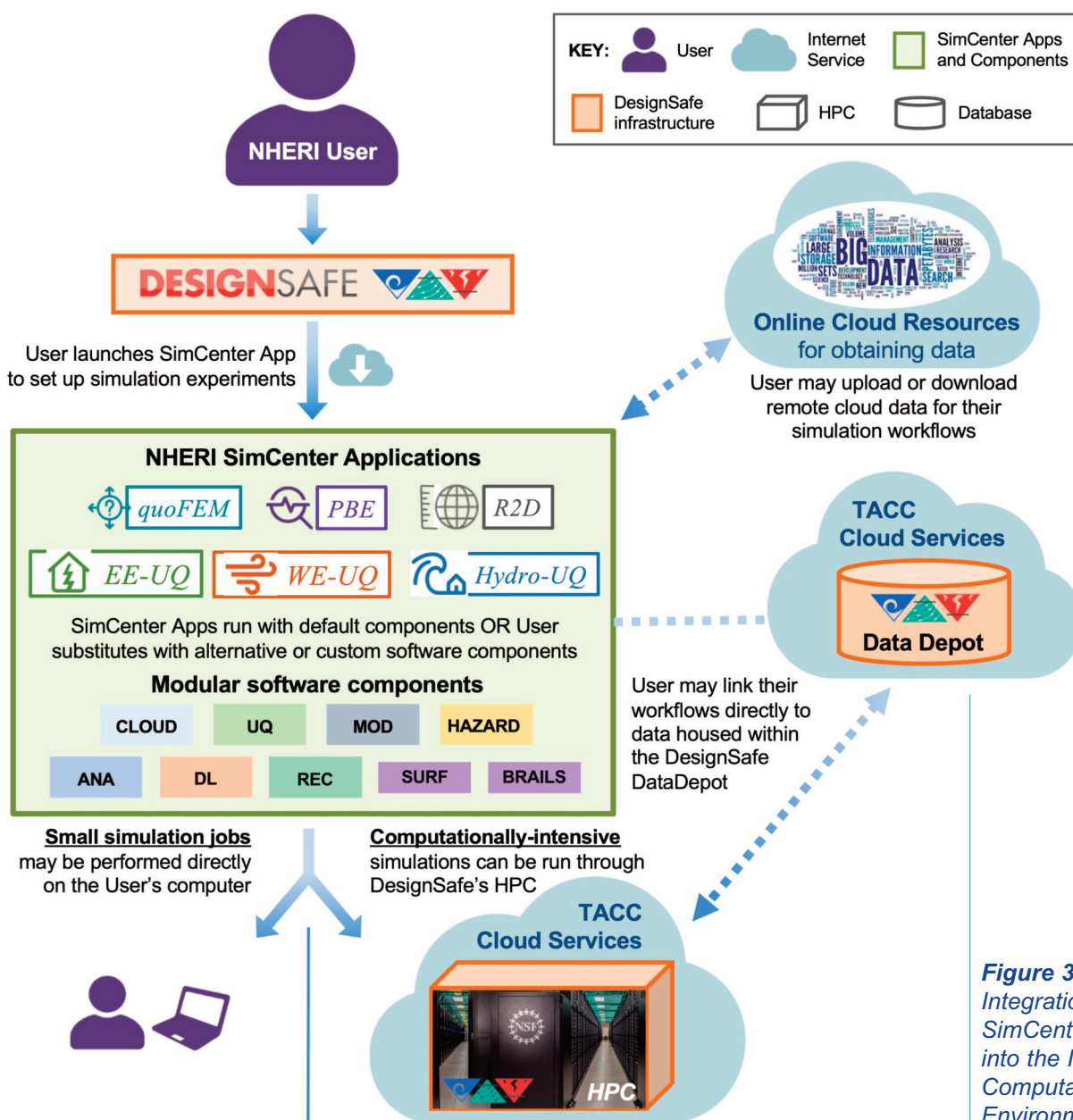
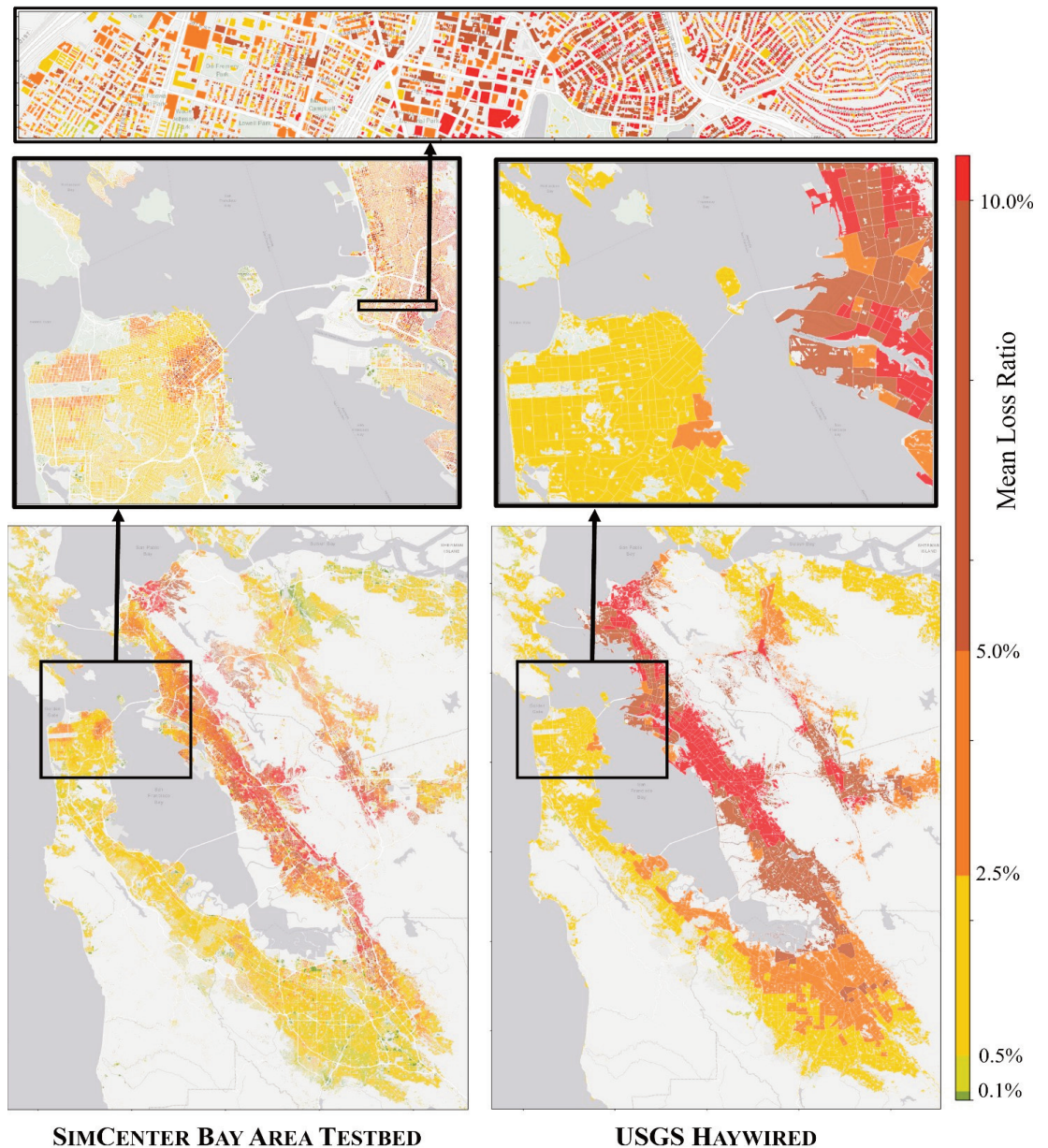


Figure 3: Integration of the SimCenter Framework into the NHERI Computational Environment

For a few dozen realizations, PELICUN (Zsarnóczy and Deierlein, 2020) was used to perform HAZUS-like (Schneider and Schauer, 2006; Kircher et al., 2006, Vickery et al, 2006) damage and loss estimates. The color shading represents the loss ratios for each building, calculated as the mean repair costs normalized by the building replacement value. On the right side of Figure 4 are the loss ratios reported in the USGS Mw 7.0 Haywired Earthquake Scenario (Hudnut et al, 2018) which represents results from a state-of-the-art risk analysis. Exposure and losses in the Haywired scenario were calculated using the HAZUS software. While it is instructive to compare results between the two studies, there are differences in the input data, scope, and goals of the studies which are important to keep in

mind. The models and results in the SimCenter study are preliminary, based on readily available information, and implemented by a small team over a couple months as an exercise to test R2D and its backend rWHALE. This contrasts with the multi-year multi-investigator Haywired study, whose goal was to inform earthquake planning and preparedness for the San Francisco Bay Area. An important distinction between the HAZUS-based Haywired study and the SimCenter workflow simulation is the level of resolution in the assessment and the propagation of various sources of uncertainty throughout the simulation. Whereas the HAZUS-based study aggregates building damage and losses based on census tract (postal code) data, the SimCenter workflow has resolution down to the building parcel level and can disaggregate losses within a building down to individual components on each floor (when such information is desired).

Figure 4:
Comparison of Building Loss Ratios from San Francisco Testbed – SimCenter (left), USGS-Haywired (right).



Concluding Remarks

The SimCenter provides an application framework for developing scientific workflow systems for NHE engineering that inherently take advantage of HPC and UQ. The SimCenter has released several applications using this framework, which presently aid NHE researchers to understand the effects and risks of natural hazards on the built environment. Our goal is to support research that will enable dependable regional resilience assessments to inform mitigation efforts that reduce damage to homes and businesses after an event, and thereby, improve community resilience.

Given the state of practice, contributions from researchers across disciplines are needed to realize this goal, and the presented open-source framework provides a common platform to mobilize these efforts. ●

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Parametrically-Upscaled Constitutive Models (PUCM) with Uncertainty Quantification for Multiscale Modeling of Metals and Composites

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“Explicit
dependence on the
microstructure,
significant
computational
efficiency,
and ease of
integrating with
commercial
software makes
the PUCM
a very
important tool
for structural
analysis and
material design.”

1 Introduction

Structural materials like metals and composites are typically characterized by heterogeneous microstructures containing nonuniform distributions of grains, colonies, fibers, particulates, and other features. Morphological and crystallographic characteristics strongly govern their mechanical behavior and failure response. For example, in polycrystalline alloys, variations in grain size, crystallographic orientations, microtexture, and slip-system resistance lead to large gradients in stresses and grain boundary dislocations leading to fatigue crack nucleation. Microstructure-based mechanistic modeling of representative volume elements (RVEs) using finite element (FE) or fast Fourier transform (FFT)-based solvers is a commonly accepted practice for analyzing the influence of microstructural descriptors on the overall material behavior. Pure micromechanical analysis becomes computationally prohibitive for structural-scale modeling, due to requirements of representing large degrees of freedom in the underlying microstructure. Macroscopic modeling with experimentally calibrated phenomenological constitutive models, on the other hand, have significant limitations due to inadequate connection with the material microstructure and underlying physics. This has prompted the development of multi-scale models for predicting the upscaled response of heterogeneous materials. These methods include mean-field homogenization [1], asymptotic homogenization methods [2,3,4], higher-order homogenization methods [5,6], FE² multi-scale method [7], reduced-order modeling [8], data-driven homogenization [9], data-analytics based reduced-order modeling [10,11] and data-science based approaches with machine learning [12,13]. There is a strong need for building accurate and efficient, physics-based multiscale models representing microstructural features and underlying mechanisms of deformation and failure. Physics-based constitutive relations, developed using data from experimentally-validated micromechanical simulations as upscaled transfer functions, are necessary ingredients of this endeavor.

1.1 Parametric Upscaling: The concept of *parametric upscaling* in constitutive models has been introduced by the Ghosh group in [14-23] to: (i) bridge length-scales through the explicit representation of lower-scale (microstructural) descriptors in higher-scale constitutive models, and (ii) overcome high computational costs incurred by many homogenization methods through an efficient computational platform. The physics-informed *Parametrically-Upscaled Constitutive Models* or *PUCMs* differ from conventional phenomenological models in their unambiguous depiction of constitutive parameters and their dependencies. The thermodynamically-consistent PUCMs, incorporate a parametric representation of lower-scale microstructural descriptors in higher-scale constitutive coefficients. These PUCM coefficients are expressed as functions of *Representative Aggregated Microstructural Parameters* or *RAMPs*, representing lower-scale descriptors of microstructural morphology and crystallography, e.g., texture and orientation distribution, grain, and reinforcement size, etc. Following the second law of thermodynamics, the general forms of PUCM equations are *a-priori* selected to reflect the fundamental deformation characteristics of aggregated micromechanics response of microstructural statistically equivalent representative volume elements or (SERVEs). Such deformation characteristics include objectivity, anisotropy, tension-compression asymmetry, hardening-softening behavior etc. The first law of thermodynamics, governing the mathematical theory of homogenization, is used to bridge length scales and express constitutive coefficients as functions of lower-scale RAMPs. Machine learning (ML) tools, e.g., symbolic regression and artificial neural networks (ANN) are essential for generating PUCM constitutive coefficients as functions of the RAMPs, using data-sets generated from micromechanical simulations. The PUCM framework provides a window for the ML tools to create meaningful physics-informed constitutive coefficients as functions of lower-scale descriptors. Since the windows are bound by thermodynamics, the requirement of a very large database is mitigated with this approach. The PUCMs are readily incorporated in FE codes like

ABAQUS through user-defined material modeling windows such as UMAT. A significantly reduced number of solution variables in the PUCM simulations, compared to micromechanical models, make them several orders of magnitude more efficient, but with comparable accuracy.

1.2 Steps in Developing the PUCMs:

The steps are delineated in Table 1.

- Module 1 acquires data from microstructural characterization and mechanical testing for model calibration and validation.
- Module II first establishes microstructure-based *statistically equivalent* RVEs or SERVEs. Following this, image-based micromechanical models are calibrated, and micromechanical simulations of the SERVE are performed for validation with experiments.
- Module III begins with the creation of a database of evolving state variables from micromechanical simulations of the SERVEs with various microstructure and load combinations. Subsequently, the RAMPs of morphological and crystallographic descriptors, such as grain size, shape, orientation and misorientation distributions, are identified from detailed sensitivity analysis, e.g., Sobol analysis. Key RAMPs that affect the homogenized material response are identified.
- Module IV generates functional forms of PUCM constitutive coefficients as functions of RAMPs using machine learning tools, operating on an extensive database of RAMPs and corresponding homogenized state variables resulting from micromechanical simulations of the SERVEs. The PUCMs are incorporated in commercial FE software like ABAQUS and ANSYS through user-defined material modeling interfaces, for microstructure-sensitive structural response predictions. Finally, uncertainty quantification is built into the PUCM framework following a Bayesian inference formulation [16,19,20] to derive probabilistic microstructure-dependent constitutive laws of the macroscopic response.

A significantly reduced number of solution variables, compared to direct numerical micromechanical simulations, make PUCM-based simulations several orders of magnitude more efficient with good accuracy. The PUCMs have already found great interest in industry and government laboratories. The length-scale bridging can yield significant advantages in location-specific material design, while the speed achieved with

Module I <i>Experimental Data & Characterization</i>	Module II <i>Image-based Micro-mechanical Models</i>	Module III <i>Microstructural RAMP Identification</i>	Module IV <i>PUCM Calibration and Validation</i>
Acquire data on microstructures from EBSD/SEM maps	Generate statistically equivalent RVEs of microstructures	Create a range of virtual microstructures with various parameters	Database of homogenized micro-mechanical variables
Conduct mechanical tests for deformation and damage data	Calibrate micro-mechanical constitutive models	Identify critical distributions of micro-structural descriptors	Machine Learning for functional forms of RAMPs in PUCMs
Generate statistical functions of micro-structural descriptors	Validate image-based micromechanical models	Establish RAMPs for PUCM coefficients using Sobol analysis	Implement in macroscopic FE codes for validation
			Uncertainty quantification

Table 1: Steps in the development of the *Parametrically-Upscaled Constitutive Models* (PUCMs)

parametric upscaling is advantageous for many data-driven design algorithms.

Two applications of the PUCM framework are discussed in this article. The first is on the modeling of deformation and fatigue crack nucleation in structural components of polycrystalline titanium alloys. The second is on the use of parametrically-upscaled continuum damage mechanics (PUCDM) models for composite materials with nonuniform microstructural distributions.

2 Predicting Fatigue Crack Nucleation in Structural Components of Ti Alloys

Titanium alloys, such as Ti-7Al, Ti-64 and Ti-6242, are widely used in the aerospace industry, e.g. in turbine engine disks and aircraft panels. The fatigue life of these materials is strongly affected by various descriptors in their heterogeneous polycrystalline microstructure. These descriptors include crystallographic orientation and misorientation, as well as morphological features like grain size distributions as seen in the electron backscatter diffraction (EBSD) images of orthogonal surfaces of an extruded sample of alpha-phase hcp Ti-7Al alloy in *figure 1(c,d)*. The PUCM-based structural simulations along with post-processing by the *parametrically upscaled crack nucleation model* (PUCNM) developed in [17,18], are used to study the effect of microstructure on mechanical response and crack nucleation probability of a prototype turbine engine blade shown in *figure 1(a,b)*.

2.1 RAMPs: Constitutive parameters of PUCM equations have an explicit dependence on microstructural descriptors, which are expressed as functions of RAMPs. Sobol sensitivity analysis of the macroscopic response with respect to microstructural descriptors of near alpha-Ti alloys in [14,15, 17] has demonstrated that the crystallographic texture, lattice misorientation, and grain size distribution have considerable

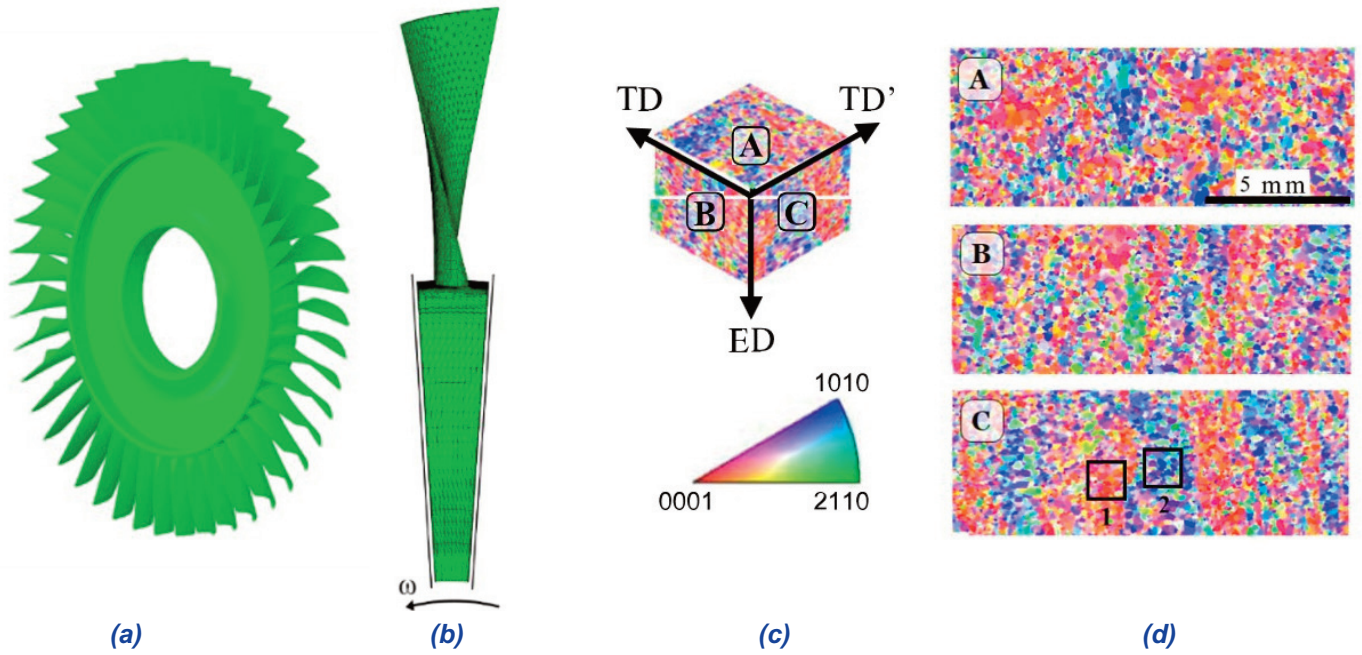


Figure 1:

Microstructure-sensitive structural-scale simulation results using the UQ-PUCM integrated in ABAQUS software:

- (a) a jet engine compressor disk-blade assembly with 42 blades;
- (b) FE model of an 80 angular segment containing one blade with roller constraints for axial symmetry;
- (c) EBSD images of orthogonal surfaces of an extruded Ti-7Al alloy showing the extrusion direction (ED) and transverse directions (TD, TD'),
- (e) inverse pole figure maps delineating microstructural crystallography and morphology as well as micro-textured regions (MTRs) elongated along ED [20]

influence on the homogenized elasto-plastic response. The corresponding RAMPs, used to characterize the microstructural distributions for these alloys are itemized below.

- **Texture Intensity Parameter and Material-Symmetry Axes (g_α, v_α):** These correspond to the eigenvalues and eigenvectors of the symmetric, second-order texture tensor $\mathbf{I}_{tex}$ that characterizes the aggregated crystallographic c -axis orientation of hcp crystals in a polycrystalline microstructure. $\mathbf{I}_{tex}$ is calculated as a weighted average of the crystallographic (0001) poles [14,17].
- **Lattice Orientation with respect to Material-Symmetry Axes ($OMA_{\alpha\beta}$):** This RAMP accounts for the effect of the distribution of crystallographic slip system orientations measured with respect to the material symmetry axes given by the eigenvectors v_α of the texture tensor. This RAMP represents the crystallographic orientation distribution in a reduced form, by measuring the density of the easy $\langle a \rangle$ -type slip systems with respect to the material symmetry axes, and governs the functional

dependencies of anisotropic plasticity.

- **Grain-pair misorientation parameter ($A_{\theta mis}$):** This RAMP represents the fraction of grain pairs with less than a threshold value of the misorientation angle θ_{mis} between their c -axes [114,17]. It reflects the ease of slip transfer across different grain boundaries in a polycrystalline microstructure, and governs the strain-hardening response.
- **Mean and standard deviation of the grainsize distribution (D^{μ_g}, D^{σ_g}):** The mean (D^{μ_g}) and standard deviation (D^{σ_g}) of a lognormal grain-size distribution constitute two RAMPs that influence the initial yield and subsequent strain hardening response in PUCMs.

The finite deformation PUCMs are selected to represent various mechanical response characteristics of Ti alloys such as anisotropy, tension-compression asymmetry, and strain-rate dependency etc. that are consistent with the micromechanical crystal plasticity simulations. Functional expressions of the constitutive parameters in terms of RAMPs using machine learning have been determined in [14-20].

2.2 Uncertainty Quantification and Propagation:

The constitutive relations are further augmented with uncertainty quantification and propagation to create a novel UQ-PUCM framework [16,19,20]. The explicit representation of microstructural variables in the PUCM constitutive equations makes them particularly suitable for incorporating uncertainties attributed to the following sources.

1. **Model reduction error (MRE):** This is an epistemic uncertainty stemming from the discrepancy between the machine

learning-generated, reduced-order functional forms of PUCM constitutive parameters and the microstructure-dependencies implicit in the micromechanical model.

2. *Data sparsity (DS)*: This is an epistemic uncertainty in the microstructure-dependent constitutive parameters due to the finite size of the micromechanics-based calibration dataset.
3. *Microstructural variability (MSV)*: This aleatoric uncertainty is due to the natural variability of the microstructure.

Uncertainties due to MRE and DS are accounted for by employing a Bayesian framework to calibrate the functional forms of constitutive parameters from crystal plasticity FEM-generated analysis data. MSV in this formulation is represented by a stochastic extension of the representative aggregated microstructural parameters or RAMPs. For computationally efficient propagation of uncertainty from the three sources to time-dependent material state and model output variables, a Taylor series expansion-based uncertainty propagation (UP) method is developed. *Figure 2(a)* shows the implementation of UQ/UP in the UQ-PUCM framework. This framework offers a comprehensive and computationally tractable multi-scale modeling framework, which addresses uncertainties relevant to both the calibration and prediction stages.

The UQ-PUCM is validated with experimental data on constant strain-rate tensile tests, performed on extruded Ti-7Al [17]. Consistent with the experiments,

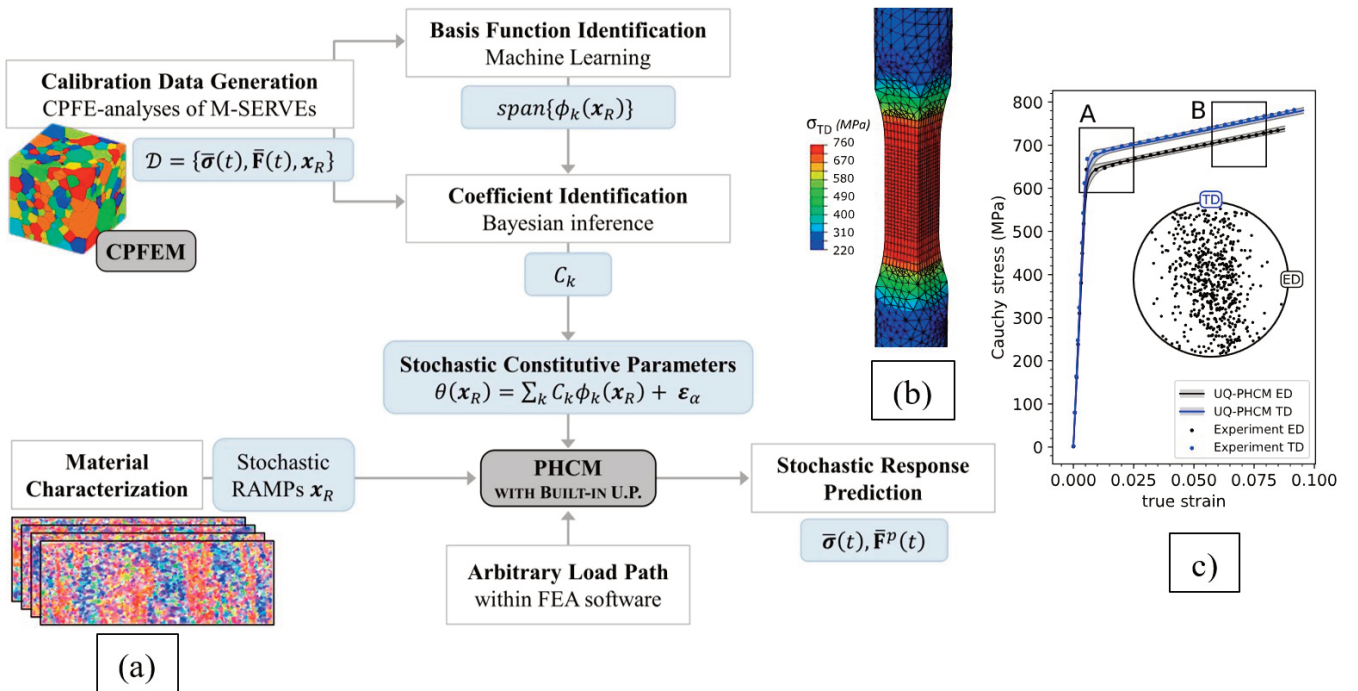
macroscopic FE models of the test specimens are generated with loading axes along extrusion (ED) and transverse directions (TD) of the material, as shown in *Figure 2(b)*. The RAMPs are calculated from EBSD characterization data in *Figure 1*, and are assigned to the FE mesh following a spatial sampling method. FE simulations are performed with UQ-PUCM integrated within the ABAQUS code. The predicted mean and 1σ intervals of the Cauchy stress at the gauge sections of both the ED and TD specimens are plotted and compared with experimental data in *Figure 2(c)*. The results show a larger uncertainty in the predicted response near the yield region with 1σ associated with the functional forms.

2.3 Multiscale Response and Fatigue Crack Nucleation in Turbine Engine Blades:

The PUCM-based FE model is used to model an angular segment of the turbine engine disk, shown in *figure 1(a,b)*. All the nodes in the model are subjected to centrifugal loading corresponding to an angular velocity (ω) of 7200 rpm for a total of 200 hours. This loading corresponds to approximately 6000 take-off operations each lasting 2 minutes and models the operating conditions of the disk.

Figure 2:

(a) Flowchart showing the flow of information and propagation of uncertainty in the development and prediction stages of UQ-PUCM, (b) macroscopic FE model of a tensile test specimen (TD) used in UQ-PHCM based ABAQUS simulations, showing the true (Cauchy) stress distribution at 8% strain, & (c) comparison of stochastic stress-strain response from UQ-PHCM simulations (solid lines and 1σ bounds), with experimental results (markers) along ED (black) and TD (blue)



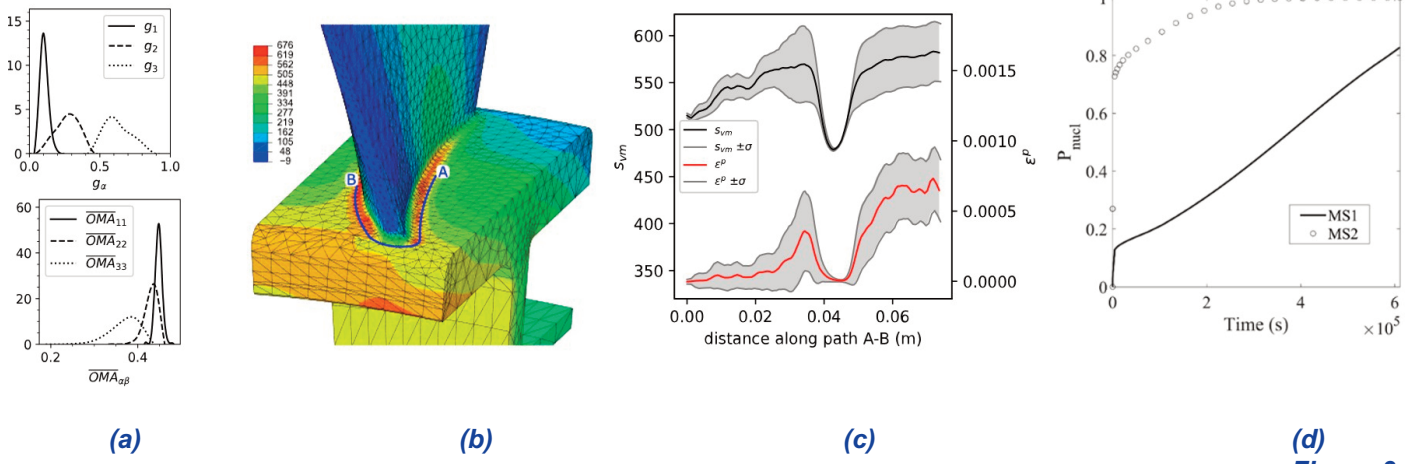


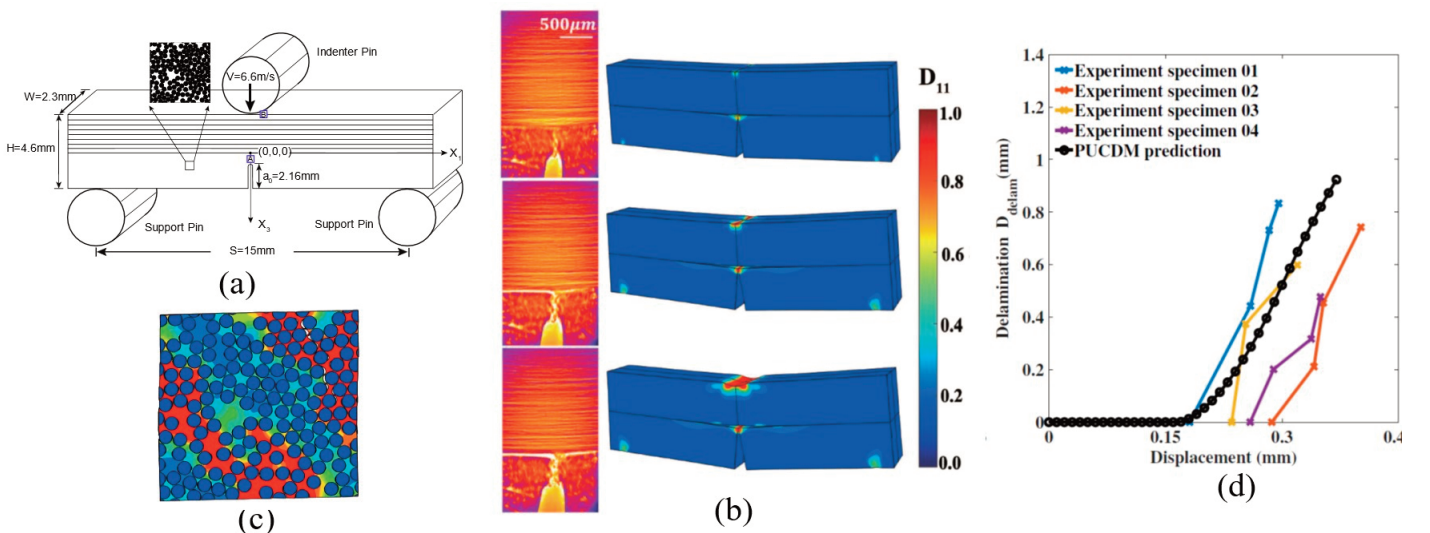
Figure 3:
 (a) Distributions of RAMPs calculated by sampling of EBSD scans for microstructure characterization data,
 (b) contour plot of $+3\sigma$ upper bound of stochastic von-Mises stress (MPa) after 200 hours of operation at $\omega = 7500$ RPM,
 (c) mean and $\pm \sigma$ bounds of the Von Mises stress and equivalent plastic strain along path A-B,
 (d) evolution of the crack nucleation probability (P_{nucl}) at two points along the path A-B with different models MS1 and MS2.

The stochastic material characteristics and RAMPs of the Ti-7Al alloy are shown in Figure 3(a). The ABAQUS FE simulations take approximately 85 minutes with 8 CPU cores. Figure 3(b) shows the contour plot of the stochastic von-Mises stress in the neighborhood of the blade support after 200 hours of operation. The variation of stochastic mechanical fields is studied along a path A-B in the contour plot along the base of the blade. The stochastic von-Mises stress and equivalent plastic strain along this path are plotted in Figure 3(c) with black and red lines respectively. The shaded areas correspond to the 1σ bounds of the fields. Analogous to the development of PUCMs, parametrical-

ly-upscaled crack nucleation models or PUCNMs have been generated in [17,18] from a database of the grain-scale probabilistic crack nucleation simulations developed in [25,26]. In [17,18], the probability of crack nucleation in PUCNMs is obtained at the macro-scale as a function of macroscopic mechanical variables such as stresses, plastic strain, and also the underlying RAMPs of the microstructure. The PUCNM corresponds to a macroscopic signature of fatigue crack nucleation in grains of the underlying microstructure. Figure 3(d) plots the evolution of the crack nucleation probability (P_{nucl}) at two points along the path A-B with different

Figure 4:

(a) Loading and specimen configurations for SENB experiments on double-ply composite beam,
 (b) PUCDM-based damage evolution and X-ray images for different applied displacements,
 (c) micromechanical damage evolution ahead of the notch-tip, and
 (d) comparison of the evolution of inter-laminar delamination as a function of the displacement



microstructures. As a result of higher plastic strain accumulation and the underlying RAMPs, one of the microstructures undergoes earlier crack nucleation ($P_{nuc}=0.95$) in comparison with the other. This study illustrates the potential of the PUCM and PUCNM-based simulations in giving insights into the microstructural influence on material response.

3 Parametrically-Upscaled Continuum- Damage Mechanics (PUCDM) Model for Multiscale Damage Evolution in Composites

Parametrically-upscaled continuum damage mechanics (PUCDM) models have been developed in [21-23] for multiscale modeling of damage and failure in composites with nonuniform fiber distribution. The PUCDM models incorporate data-driven techniques in a thermodynamical framework to explicitly represent parametric forms of key microstructural features and descriptors, in addition to evolving damage variables. A thermodynamically consistent damage potential is introduced in the space of the force conjugate of damage. Specifically, a fourth-order damage surface tensor P_{ijkl} is parametrically represented as functions of the evolving material damage states, as well as of key morphological descriptors of the composite microstructure in the form of RAMPs. The functional forms are developed using ANN algorithms, operating on a database of microstructure response variables from micromechanical simulations. The PUCDM models have demonstrated significant computational efficiency and accuracy in comparison with other multiscale approaches [21-23].

3.1 Identifying Representative Aggregated Microstructural Parameters (RAMPs):

The 2-point correlation function S_2^{fiber} is chosen to uniquely characterize the composite microstructures. However, this function cannot be directly used as RAMPs in the PUCDM model on account of the large number of data points representing this correlation. For efficient and unique parametrization of S_2^{fiber} for the RAMPs, the principal component analysis (PCA), is used to derive a low dimensional representation of high dimensional data. For a given data-set, PCA extracts a reduced number of features with a high variance. The original data-set can then be represented efficiently through the extracted principal components, computed as eigenvectors of the covariance matrix of the S_2^{fiber} data-set.

3.2 PUCDM-based Modeling of Single-Edge Notched Bending (SENB) Tests for Glass-Epoxy Composite Beams:

The PUCDM-based FE simulations of SENB experiments for [0,90] double-ply S-2 glass fiber/SC-15 epoxy matrix composite beams, shown in figure 4(a), are conducted. Damage predicted by the PUCDM model are compared with experimental measurements.

Figures 4(b) depict the contours of the PUCDM model damage tensor component D11 for different applied displacements, and the corresponding high-speed synchrotron X-ray images. The transverse crack in the bottom ply evolves towards the ply interface, and subsequently leads to delamination between the 0° and 90° plies. After the formation of a full transverse crack in the bottom ply, additional deformation primarily induces further inter-ply delamination and expansion of the damage zone in the top region, causing a rapid loss of the load-bearing capacity. Microscopic damage evolution at a point on the top surface of the beam is shown in figure 4(c). Matrix damage is the primary mode of macroscopic material degradation in this zone. The predicted crack lengths (inter-laminar delamination) are compared with the experimental measurements in figure 4(d), which falls within the range of experimental measurements.

In summary, this article demonstrates the significant potential of the *parametrically-upscaled constitutive models* for multiscale analysis of deformation and damage in metallic and composite materials. Explicit dependence on the microstructure, the capability of retrieving damage response across material length scales, significant computational efficiency, and ease of integrating with commercial software makes the PUCMs a very important tool for structural analysis and material design. ●

Acknowledgments:

The author acknowledges the contributions of his students Dr. D. Ozturk, Dr. S. Kotha and Dr. X. Zhang to the development of this framework.

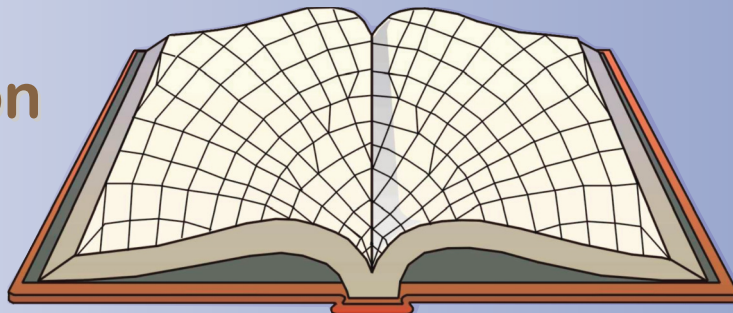
“...demonstrates the significant potential of the parametrically-upscaled constitutive models for multiscale analysis of deformation and damage in metallic and composite materials.”

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Practical Optimization

Philip E. Gill, Walter Murray &
Margaret H. Wright
SIAM, Philadelphia, USA, 2019



BOOK REVIEW

ISBN: 978-1611975598, 401 pages, soft cover, \$95 (List Price).

Contents: Preface; 1: Introduction; 2: Fundamentals; 3: Optimality conditions; 4: Unconstrained methods; 5: Linear constraints; 6: Nonlinear constraints; 7: Modelling; 8: Practicalities; Questions and answers; Bibliography; Index.

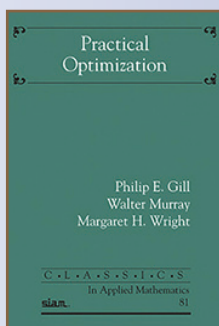
This 2019 edition appeared in the SIAM series Classics in Applied Mathematics. It is an exact reproduction of the original “Practical Optimization” book that was published in 1981 by Academic Press. Naturally a lot of research on optimization methods has been done since the book first appeared, but all the fundamentals covered here are still very relevant. The authors remark in the new Preface that even the basics of data science can be found in *chapters 7 and 8*.

Roughly, the book is divided into four parts. *Chapters 1 and 2* include mathematical preliminaries. *Chapter 3* provides a classification of optimization problems and (necessary and sufficient) optimality conditions for each type. *Chapters 4 to 6* are the heart of the book and present various optimization methods. *Chapters 7 and 8* discuss computational and implementational issues.

The book is very rich in information, sometimes in an encyclopedic scale (updated to 1981, of course). It includes algorithms and pseudo-codes, which allow the reader to better understand the methods presented, and to write her own codes. Some sections that are of a specific character are marked with * and can be skipped if desired. Many sections end with “Notes”, sometimes quite elaborate, as well as comments on the relevant bibliography. Each chapter starts with a quote of a well-known scientist or a public figure. My two favorite ones are both on p. 285: “*When one comes down to particular instances, everything becomes more complicated*” (Albert Camus, 1963), and “*You can get it wrong and still you think that it’s all right*” (John Lennon and Paul McCartney, 1965).

The book has a simple appearance, and it seems that no big effort was made to make it particularly attractive visually. There are a few black and white figures, mostly to illustrate the basic principles. Since it is a tradition of this Book Review section to display more exciting figures, we show here some illustrations from PhD theses on optimization methods, from recent years.

Chapter 1 is short and presents the general optimization problem. *Chapter 2* discusses fundamentals, like errors, condition number, LU factorization, finite differences, iterative processes, and more. *Chapter 3* provides a detailed classification of optimization problems and their optimality conditions. The optimization problems include the Unconstrained Problem (UCP), Linear Equality Constraints Problem (LEP), Nonlinear Equality Constraints Problem (NEP), Linear Inequality Constraints Problem



Philip E. Gill



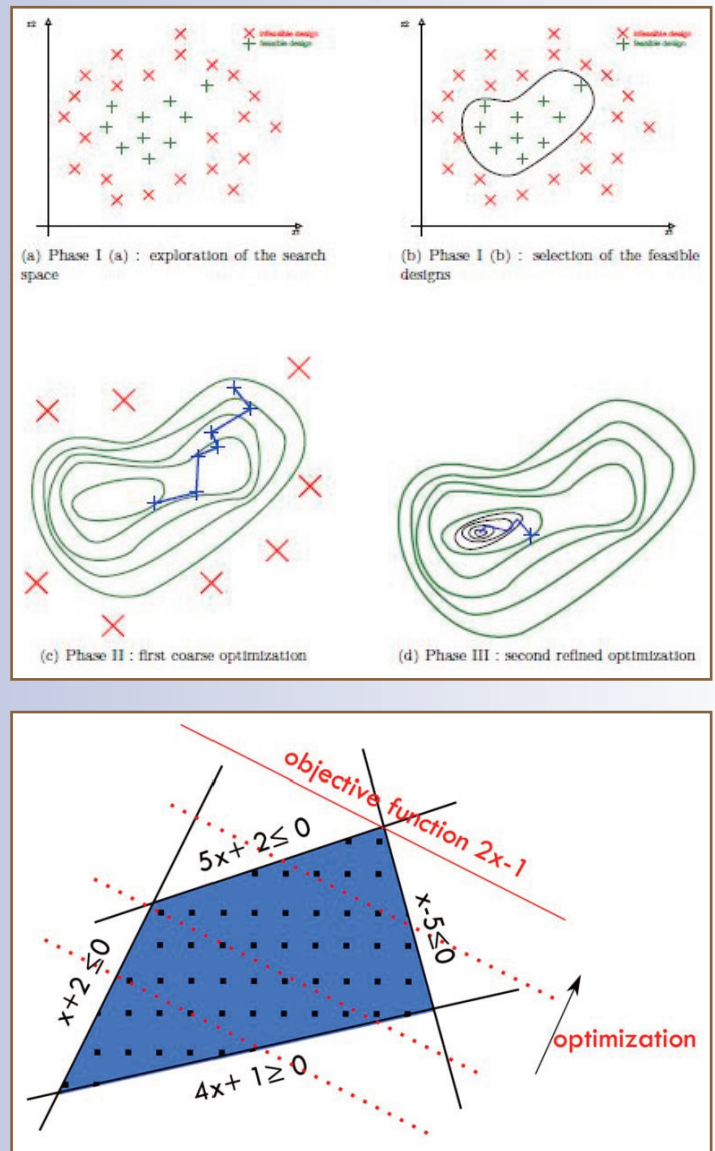
Walter Murray



Margaret H. Wright

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Figure 1:
Figure taken from the 2012 PhD thesis of Mathieu Balesdent, “Multidisciplinary Design Optimization of Launch Vehicles”, at the École Centrale de Nantes, showing the tactic of how to gradually zoom in on the minimizer



(LIP), Nonlinear Inequality Constraints Problem (NIP), Linear Programming (LP), Quadratic Programming (QP), and more.

Chapter 4 is dedicated to methods for unconstrained minimization. The order of the sections seems a bit peculiar – discussion on non-smooth functions appears before that on smooth functions, and the calculation of the step size comes before the determination of the search direction. Here and in other places in the book, the authors choose to go from the more general situation to the more basic one, and not in the opposite direction as in many other books. One may argue about the merit in this approach, but it seems that this was done here thoughtfully by the authors, as the whole book is written in a careful and didactic way. This chapter includes a discussion on sparse discrete Newton and on Conjugate Gradients, among other methods.

Chapter 5 concerns optimization under linear constraints and discusses LP and QP algorithms among other things. Chapter 6 discusses nonlinear constraints, including penalty and barrier function methods, augmented Lagrangian methods and others.

In Chapter 7, the authors give important practical advice on issues related to the optimization process. The same problem can be presented in more than one way, and one way may be more amenable to computation or more efficient than some others. The advice given here includes (a) ways to avoid unnecessary discontinuities, (b) ways to simplify or remove some of the constraints, and (c) the importance of good scaling. Chapter 8 deals with some numerical difficulties such as overflow, insufficient decrease in the merit function, lack of progress in the iterative process, and more. A nice sentence that appears on p. 324 is: “Ideally, the user should not need to perform a detailed investigation to determine why a routine has failed, since a good routine should provide some reason for an unsuccessful termination.”

In summary, this book is rich with information, and is excellent as a reference book on basic optimization methods. A bit surprisingly, it is not significantly outdated as one might expect from the fact that it was written 40 years ago. Yet, a teacher or a student looking today for a good textbook on optimization methods should probably look elsewhere. ●

Figure 2:
Figure taken from the 2016 PhD thesis of Maria Pires Pacheco, “Fast Reconstruction of Compact Context-Specific Metabolic Network Models”, at the university of Luxembourg, showing an example of linear programming

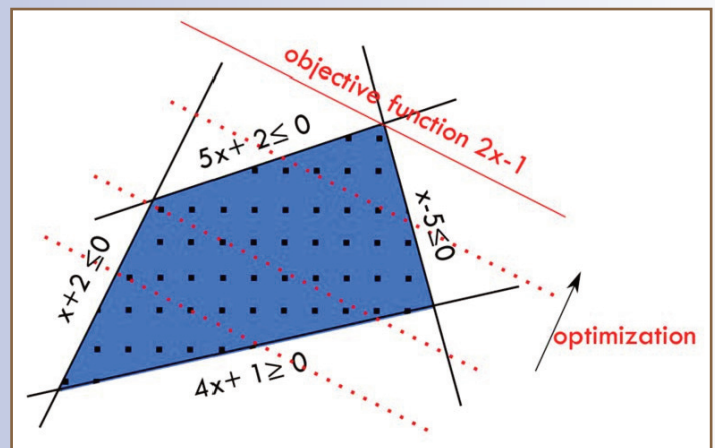
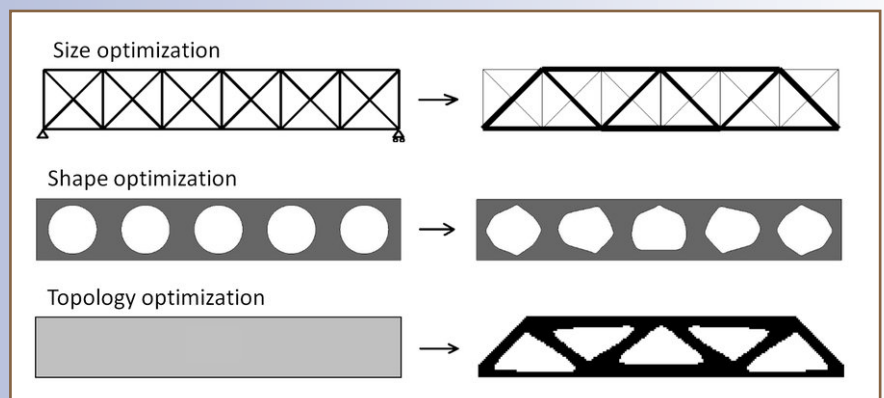


Figure 3:
Figure taken from the 2018 PhD thesis of Jan H.K. Haertel, “Design of Thermal Systems Using Topology Optimization”, at the Denmark Technical University, illustrating three types of optimization



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During the current year, the Israel Association for Computational Methods in Mechanics (IACMM) held one symposium due to the restrictions imposed by the Covid-19 pandemic. In particular, the **48th Israel Symposium on Computational Mechanics (ISCM-48)** was held on *November 11th 2021* at Technion – Israel Institute of Technology, Haifa, and the local organizers were Prof. Oded Amir and Prof. Mahmood Jabareen.

The interesting opening lecture was given by the invited speaker Prof. Shaul Markovitch from the Computer Science Department at Technion – Israel Institute of Technology, and titled "Are general-purpose autonomous robots coming soon?"

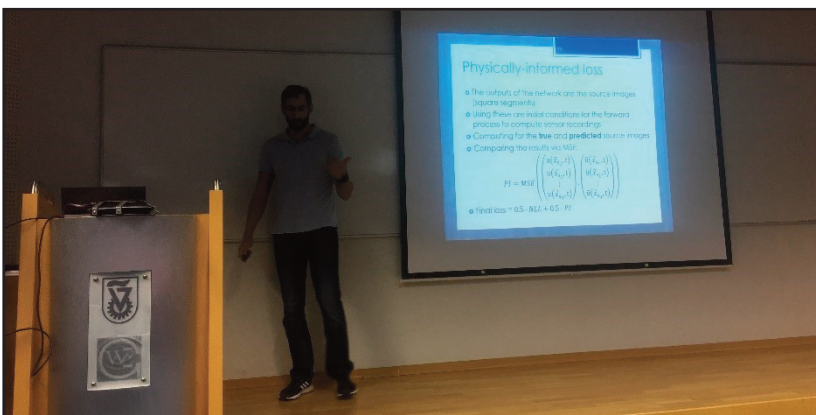
Figure 1 shows Prof. Markovitch with the IACMM executive council and the local organizers of ISCM-48. In his talk, Prof. Markovitch presented the current state of general-purpose robots and aspects of artificial intelligence. Also, Prof. Markovitch proposed the missing components that are needed for building such general purpose-robots.



Figure 1:
 Group photo of IACMM executive council, invited speaker and organizers of ISCM-48. Left to Right: D. Givoli, J. Tal, P. Bar-Yoseph, O. Amir, S. Markovitch, M. Jabareen, E. Priel

The 48th Israel symposium included 8 other lectures, presented by researchers from academia. These lectures spanned over a broad spectrum of computational mechanics topics such as machine learning, material modeling at different scales, structural topology optimization, buckling of plates, and more. The ISCM-48 was concluded by a tutorial lecture given by Dr. Yuri Feldman from the Department of Mechanical Engineering, Ben Gurion University – the title of his tutorial was "Recent trends and progress in the immersed boundary method." In his tutorial, Dr. Feldman presented the fundamentals of several basic formulations of the immersed boundary method. Also, Dr. Feldman, elucidated the latest progresses and challenges related to numerical simulation of various complex physical phenomena using the immersed boundary method.

During the ISCM-48th, a competition for the best presentation was held and the



winner Mr. Adar Kahana, a PhD student from the Department of Mathematics at Tel Aviv University. The title of Mr. Kahana's talk was "Deep-learning method for locating sources in underwater acoustics with high noise." Figure 2 shows Mr. Kahana during his talk. ●

Figure 2:
 Mr. Kahana, the winner of the ISCM-48 competition for the best presentation, during his talk



Re-elected UKACM president

During the Executive Committee meeting of UKACM, held on 14th April 2021, it was announced that Prof Rubén Sevilla has been unanimously elected to continue as President of UKACM until December 2024.

UKACM 2021 Conference

The 2021 conference took place on 14-16 April 2021. Organised by Dr Marco Discacciati (Loughborough University), the conference followed an online format, with 78 participants delivering live talks.

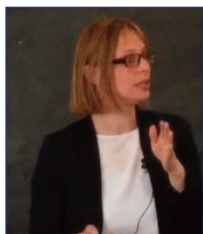
UKACM School

As it is tradition in UKACM, a School was organised before the start of the conference. This year two topics were covered in the UKACM School.

- Model Order Reduction methods.
(Prof. Elías Cueto and Dr Alberto Badías, University of Zaragoza, Spain)
- 'Weak form' in many flavours. Sustainable development of research code for complex engineering problems
(Dr Lukasz Kaczmarczyk and collaborators, University of Glasgow, UK).

UKACM Plenary Speakers

Three plenary lectures at the conference were delivered by the following distinguished researchers:



Prof Paola F. Antonietti
(Politecnico di Milano, Italy)
Numerical models for earthquake ground motion and seismic risk assessment



Prof Elías Cueto
(University of Zaragoza, Spain)
On the role of machine learning in computational mechanics



Prof Joaquim Peiró
(Imperial College London, UK)
A variational approach to high-order curvilinear mesh generation and adaptation for compressible flows

UKACM Conference Awards

The following delegates received the three UKACM conference awards:

- Fabiola Cavaliere from Universitat Politècnica de Catalunya and Swansea University received the Mike Crisfield Prize for the paper "A nonintrusive reduced order method for the NVH assessment and automotive structural dynamics".
- Eki Febrianto from Cambridge University received the prize to the best presentation by a post-doctoral researcher for the paper "The statistical finite element method for physics-informed digital twins".
- Massimo Sferza from the University of Nottingham received the prize to the best presentation by a PhD student for the paper "Global-local multidisciplinary optimisation of aircrafts".

UKACM Conference Proceedings

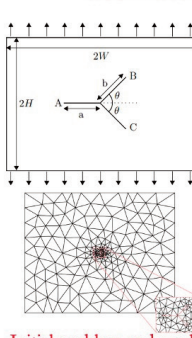
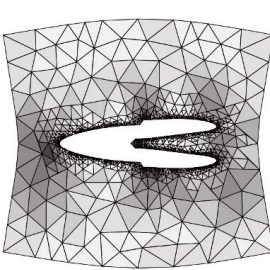
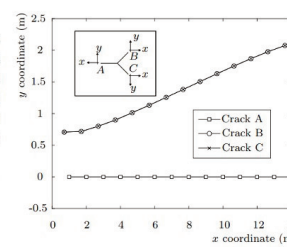
The proceedings of the 2021 UKACM conference can be accessed at https://repository.lboro.ac.uk/projects/UK_Association_for_Computational_Mechanics_UKACM_Conference_2021/113478

2021 Roger Owen PhD Thesis Award

The winner of the 2021 Roger Owen PhD Thesis Award was Dr Robert Bird. ●

Research highlight

A hp-adaptive discontinuous Galerkin finite element method for accurate configurational force brittle crack propagation

Initial problem and mesh.

Final hp-adapted mesh with displacement distortion applied and polynomial order shown.

Machine precision for propagation paths using a novel domain independent configurational force calculation.



Durham University

EPSRC
Engineering and Physical Sciences Research Council



Robert Bird (rbird@jc.ac.uk) – UKACM Roger Owen's thesis prize winner Durham University, UK	Supervisors: Dr W.M. Coombs (w.m.coombs@durham.ac.uk) Dr S. Giani (stefano.giani@durham.ac.uk)	Funders: EPSRC: EP/M507854/1 EC: 734370 (BESTOFAC)
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UKACM 2022 Conference



University of Nottingham
UK | CHINA | MALAYSIA

UKacm
UK Association for Computational Mechanics
2022



The 2022 UKACM conference will be organised by Dr Jelena Ninic, Dr Matteo Icardi and Dr Kristoffer Van Der Zee, from the University of Nottingham. The Conference and School will take place between 20th-22nd of April 2022.

The following invited speakers will deliver a plenary lecture in the UKACM 2022 Conference:

- Prof. Dr.ir. Dr.h.c. René de Borst, University of Sheffield
- Prof. Dr.-Ing. Stefanie Elgeti, Vienna University of Technology
- Prof. Dr.-Ing. Dominik Schillinger, Leibniz Universität Hannover
- Dr Emilio Martinez-Paneda, Imperial College London

The school will focus on:

- Computational phase-field modelling - Dr Kris van der Zee
- Immersed finite element methods - Prof. Dr.-Ing. Dominik Schillinger
- Optimization - Dr Ender Özcan

This conference will also mark the start of the 30th Anniversary of UKACM. ●

USACM Holds 16th National Congress on Computational Mechanics as Virtual Event

The 16th U. S. National Congress on Computational Mechanics (USNCCM16) was held as a fully virtual event July 26 - 29, 2021. The conference was widely received by the computational mechanics community with over 1240 conference registrants that represented 36 countries. USNCCM16 also had 459 student participants (459) and a record number of women researchers (181) who participated.

USNCCM16 offered a strong technical program with 73 minisymposia that comprised 269 technical sessions. Over 1075 technical abstracts were presented during the four days of the conference. The Congress featured four Plenary and six Semi-plenary lectures that covered the broad spectrum of Computational Mechanics. Special efforts were made to preserve the in-person flavor of interaction with the technical sessions being broadcast live. Several networking features were also available.

Other highlights of the conference included:

- A series of mid-day talks celebrating the 30th year of holding USNCCMs. The featured speakers were Professors Bob Taylor, J. Tinsley Oden, and Tom Hughes who presented reflections and history of USACM.
- A minisymposium honoring Prof. J. Tinsley Oden's contributions to Computational Mechanics.
- The USACM-FRG and FRC-IACM held a Women's Networking Event featuring Dr. Jian Cao as a guest speaker and presented several awards for Best Female Presentation (see frgusacm.org for the list of winners).
- Over 30 posters were presented virtually in a student poster competition. The winners were announced during the Closing Ceremony and their names can be found at 16.usnccm.org/poster_competition.

A panel discussion on Navigating the Emerging Landscape of Computational Mechanics featuring experts from academia, national laboratories and federal agencies was held. Another panel discussion on the Role of Computational Mechanics in Industry, discussing the fostering of fruitful mechanics collaborations between academia, national labs, and industry, and the opportunities for students in industrial careers that leverage computational mechanics was presented.

To read more about this discussion, go to the USACM website, usacm.org. ●

USACM Upcoming Events *further details at usacm.org*

- **The Role of Mathematical and Computational Modeling in Cancer Research**, January 10-12, 2022, (virtual conference), sites.google.com/usacm.org/bio-mcr/home
- **Conference on Uncertainty Quantification for Machine Learning Integrated Physics Modeling (MLIP)**, August 18-19, 2022, Arlington, VA, sites.google.com/usacm.org/uq-mlip/home
- **Meshfree and Novel Finite Elements with Applications**, September 25-27, 2022, Berkeley, California; mfem2020.usacm.org
- **Isogeometric Analysis**, November 6-9, 2022, Banff, Canada; iga2022.usacm.org
- **17th U. S. National Congress on Computational Mechanics**, Albuquerque, New Mexico, July 23-27, 2023, 17.usnccm.org ●

USACM 2021 Awards



John von Neumann Medal – Jacob Fish,

Columbia University

For his sustained and seminal contributions to the field of multiscale computational science and engineering and for its major impact on industry

The Belytschko Medal – Gordon Johnson,

Southwest Research Institute

In recognition of pioneering and lasting contributions to high-rate computational solid dynamics, particularly constitutive models for metals and brittle materials and explicit methods for finite element and meshfree particle analysis



Thomas J.R. Hughes Medal – Qiang Du,

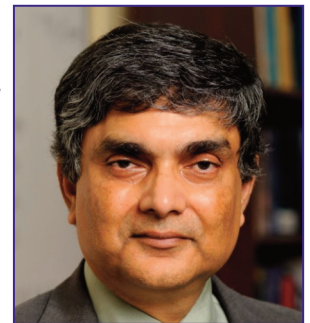
Columbia University

For his numerous innovative contributions to computational physics and computational fluid mechanics, and his unwavering service to the scientific computing community

J. Tinsley Oden Medal – Somnath Ghosh,

Johns Hopkins University

For outstanding fundamental contributions to Computational Mechanics of Materials through the development of innovative methodologies in spatio-temporary multi-scale modeling of heterogeneous materials transcending the Mechanics and Materials communities



Gallagher Young Investigator Medal – John Evans,

University of Colorado-Boulder

For contributions to isogeometric analysis, structure-preserving discretizations, multiscale and stabilized methods, and immersed methods with application to fluid mechanics, structural mechanics, and fluid-structure interaction

USACM Fellows

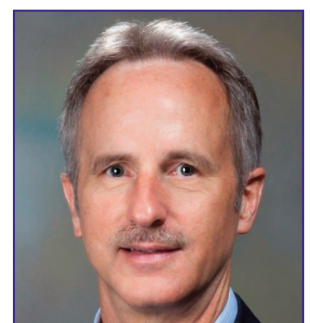


Harold Park, Boston University

For important contributions to atomistic/continuum coupling methods, computational modeling of surface effects on nanomaterials, long timescale methods for atomistics, the mechanics of two-dimensional materials, and computational soft matter mechanics.

James Stewart, Sandia National Laboratories

For leadership and service to the USACM community, especially in the area of uncertainty quantification and data-driven modeling. ●



New GACM Board

At the annual General Assembly held at the end of last year, the new GACM board was elected for the next four-year term. The new board is composed of the following members:

M. Behr (RWTH Aachen, president), **G. Meschke** (RU Bochum, vice president), **M. Kaliske** (TU Dresden, previous president), **S. Klinkel** (RWTH Aachen, treasurer), **T. Münz** (Dynamore GmbH), **S. Leyendecker** (FAU Erlangen-Nuremberg), **C. Birk** (U Duisburg-Essen), **L. Scheunemann** (U Duisburg-Essen, junior researcher), **N. Hosters** (RWTH Aachen, general secretary)

At this point, we would like to take the opportunity to thank the past president, **Michael Kaliske**, for his dedicated service over the past four years.

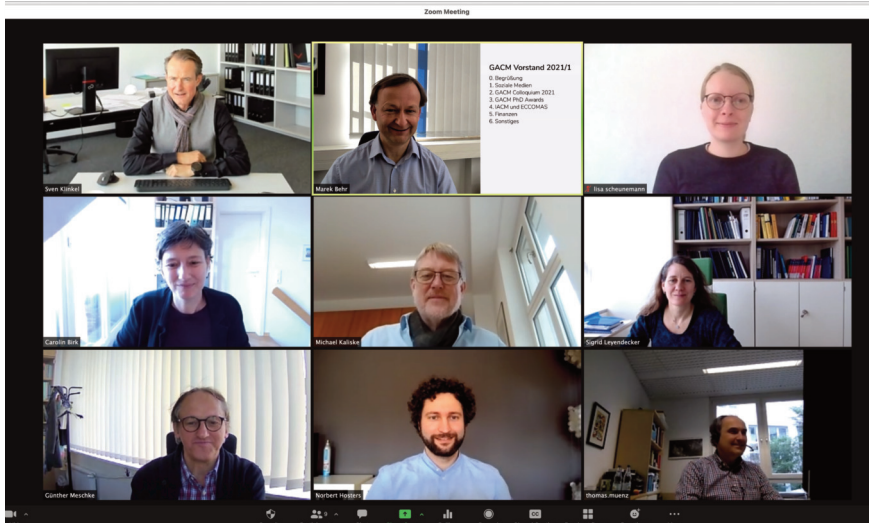


Figure 1:
First Board Meeting

9th GACM Colloquium on Computational Mechanics 2022 Essen, Germany

Colloquium Chairpersons

D. Brands, H. Gravenkamp, L. Scheunemann, C. Schwarz, A. Schwarz

The *9th GACM Colloquium on Computational Mechanics for Young Scientists from Academia and Industry* will take place from **September 21 to 23, 2022 in Essen, Germany**. The colloquium is jointly hosted by the Institute of Structural Analysis of Plates and Shells and the Institute of Mechanics at the University of Duisburg-Essen.

The GACM Colloquium is a biennial conference that brings together young researchers in the field of computational mechanics. This event provides excellent opportunities for students and postdocs to present their work, to acquire new knowledge in the field of numerical modeling in engineering and science, and to establish a network of colleagues and peers. The colloquium consists of mini-symposia — organized by selected young scientists — as well as a poster session and several plenary lectures.

We are pleased to announce the plenary lectures given by Prof. Swantje Bargmann (BU Wuppertal), Prof. Laura De Lorenzis (ETH Zürich/TU Braunschweig), Prof. Marc-André Keip (U Stuttgart) and Prof. Otto von Estorff (TU Hamburg).

We would like to invite you to attend the 9th GACM Colloquium. Detailed information will be announced here: <https://colloquia.gacm.de/>.

GACM Best PhD Award

In 2012, GACM has successfully established an award for young academics, namely the GACM Best PhD Award. It is our great pleasure to announce that the outstanding doctoral thesis of **Dr.-Ing. Maximilian Grill** is honored with this award for the year 2020.

The thesis **"Computational Models and Methods for Molecular Interactions of Deformable Fibers in Complex Biophysical Systems"** of Maximilian Grill was conducted at Technical University of Munich and has been performed under the academic supervision of Prof. Wolfgang Wall.

The award will be officially conferred at the next GACM Colloquium in Essen in 2022.

Dr. Grill's PhD thesis was concerned with novel models and methods for molecular interactions of deformable fibers such as van der Waals adhesion, electrostatic effects, and steric repulsion. Bringing together fundamental concepts from the disciplines of molecular biophysics and computational mechanics in a novel, unprecedented way, Dr. Grill's work develops conceptually new methods that allow to investigate so far intractable problems in real biological systems on the nano- and microscale. Several examples of such applications are presented in his thesis.

The key idea of the methodological part is to describe the molecular two-body interaction in a dimensionally reduced manner, which is inspired from and thus fully consistent with using beam theory as a model for the slender deformable fibers. This paradigm shift from atom-atom to section-section interaction potentials (SSIP) leads to a beam-beam interaction formulation, which is the first of its kind and yields a speedup of more than three orders of magnitude. In the important case of very short-ranged interactions, Dr. Grill showed that this can even be taken one step further by using section-beam interaction potentials (SBIP) to achieve an additional 4x speedup. Both, the first principles of molecular interactions as well as geometrically exact 3D beam theories, involve a high mathematical complexity and are still highly active fields of research. Dr. Grill selected and combined the latest and most promising techniques in his thesis. For the analytical derivation of the pivotal SSIP and SBIP laws (starting from the first principles), Dr. Grill succeeded to find accurate, simple expressions for the challenging four- or even five-dimensional integrals over both interacting bodies (at arbitrary distance and mutual orientation). His choice to consider generic interaction potential laws and different scenarios such as short- and long-ranged interactions additionally increased the mathematical complexity, yet significantly extends the versatility of the novel approaches. This is demonstrated by the variety of applications. To mention one last aspect, Dr. Grill resolved the critical numerical issues associated with the characteristic singularity of molecular interaction laws at zero separation by developing a highly effective, tailor-made regularization scheme. ●



Figure 2:
Dr.-Ing. Maximilian Grill
Best PhD Award

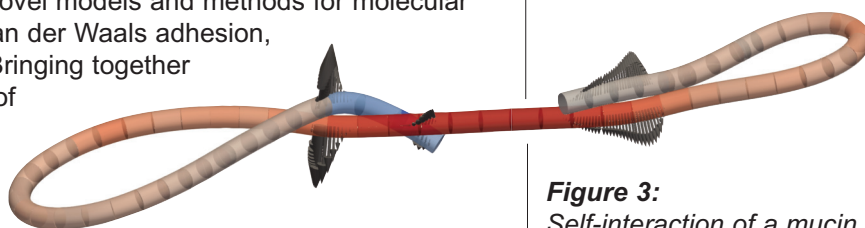


Figure 3:
Self-interaction of a mucin
filament carrying a complex
line charge distribution

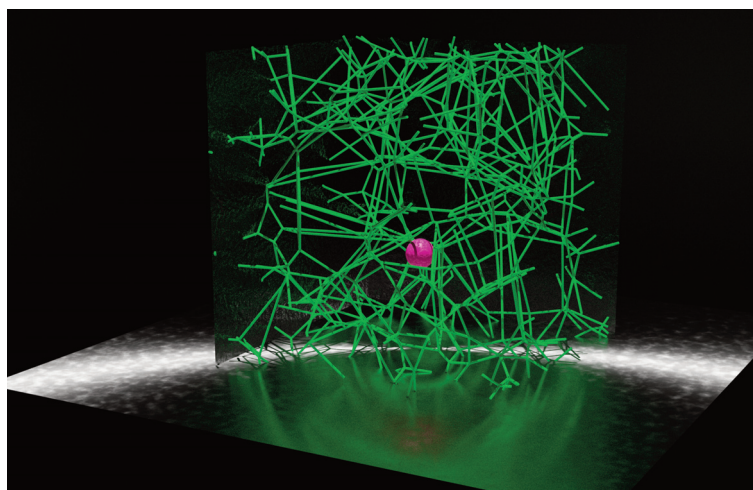


Figure 4:
Hindered diffusion of a
charged nanoparticle through
a biopolymer fiber network

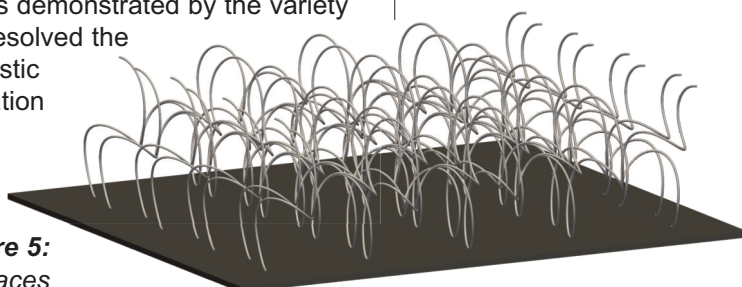


Figure 5:
Pulling off two adhesive, nanofiber-grafted surfaces

SEMNI Juan C. Simó award 2021

SEMNI has awarded its annual Juan C. Simó prize during its last executive meeting. The awardee will receive his prize during the gala dinner ceremony of the joint Spanish-Portuguese Conference on Numerical Methods, CMN, to be held in Las Palmas de Gran Canaria next 2022.



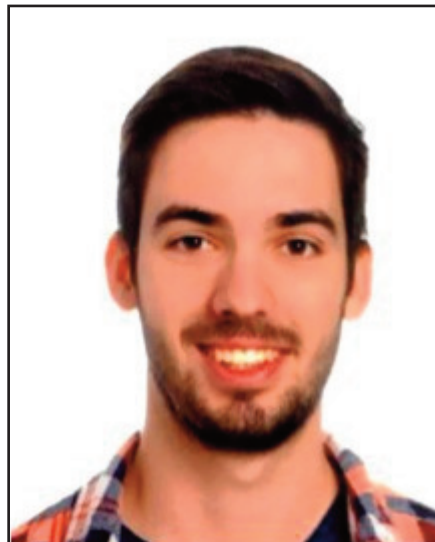
SEMNI's prize to young researchers commemorates the legacy of the late Professor Juan C. Simó in the field of numerical methods. The committee was formed in this occasion by Ignacio Romero (president), Manfred Bischoff (University of Stuttgart), Antonio Gil (University of Swansea), Alessandro Reali (University of Pavia) and Laurent Stainier (University of Nantes).

In this occasion, the awardee is **Dr. Marcos Latorre** (Yale University), for his contributions to computational nonlinear solid mechanics with emphasis on applications to cardiovascular biomechanics and mechanobiology.

The Committee has valued the breadth of his research activities and the variety and extent of his national and international research collaborations. ●

SEMNI best PhD award 2021

The SEMNI best PhD thesis award committee, composed by Francisco Montáns (President, Polytechnic University of Madrid), Marino Arroyo (University of Catalan), Estefanía Peña (University of Zaragoza), Esther Reina (Servile University) and Rena C. Yu (University of Castilla-La Mancha), selected the following doctoral thesis defended during 2020 for the best PhD award:



Dr. Alberto Baldías Herbera, University of Zaragoza, "Simulated reality: physics-based mixed and augmented reality for intelligence augmentation", supervised by David González and Icíar Alfaro . ●

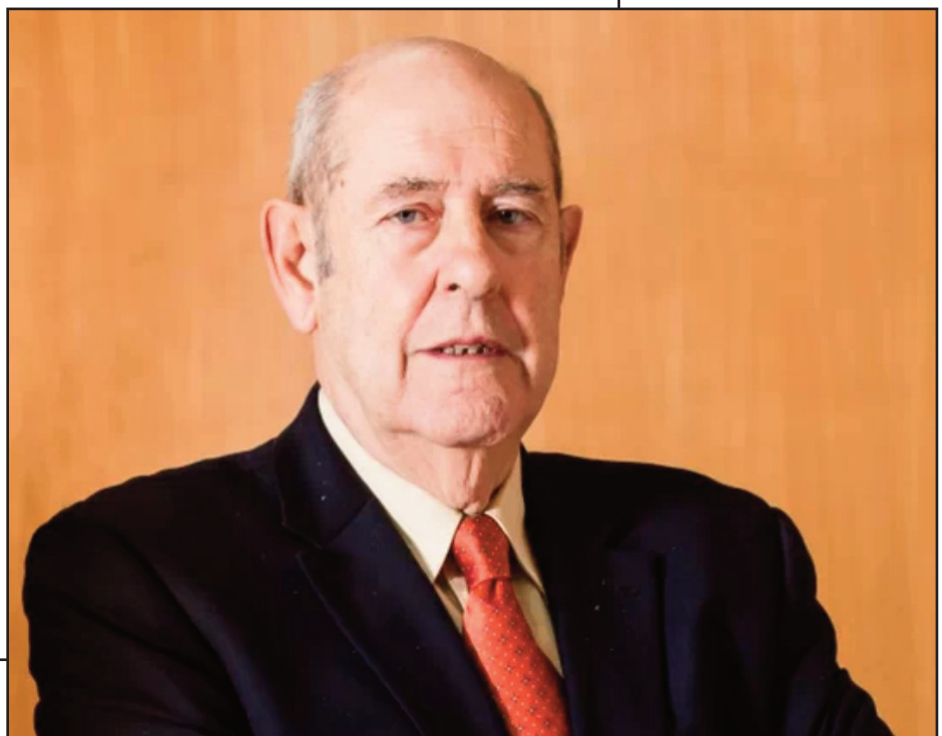
Memoriam: Manuel Casteleiro

It is with great sadness that SEMNI informs the death of Professor Manuel Casteleiro. He died on April 22, 2021, at his home in A Coruña at 74. A Civil Engineer from the Polytechnic University of Madrid, Casteleiro got a Master and Ph.D. from the University of Wisconsin-Milwaukee and Northwestern University in the USA, respectively. Upon his return to Spain in 1975, he became a professor at the Civil Engineering School, the Polytechnic University of Catalonia (UPC). He contributed actively and significantly to the establishment and consolidation of the new school. During this period, he also served as vice-rector for teaching staff, director, and founder of the Department of Applied Mathematics III. In 1992 he moved to the University of A Coruña, Galicia. His talent, experience, and vision left their mark on this new institution, of which he was also vice-rector, and was crucial in the founding stage of this new school, of which he was director between 2005 and 2013. Upon retirement in 2017, he continued to work as an emeritus professor until a few weeks before his death.

Manolo, fondly known by his family and friends, was an extraordinary instructor who greatly influenced the formation of more than 40 promotions of engineers in the two schools to which he dedicated his life. A brilliant researcher with international fame, he promoted numerical methods and their applications in engineering and trained scientists who today lead top-level research groups. He fostered the promotions of CIMNE (the International Center for Numerical Methods in Engineering) and SEMNI (the Spanish Society of Numerical Methods in Engineering). In the 90s, he also led a fruitful alliance with APMTAC (the Portuguese Association of Theoretical, Applicational, and computational Mechanics) for the joint organization of the national congresses of both countries.

For the members of SEMNI, Manolo not only chaired SEMNI between 2003 and 2008, but he is also a reference figure in our community. He has inspired many members with his leadership, example, and charisma. He served our society with dedication and had been a dear companion for all its members. In 2017 he received the Olgiard C. Zienkiewicz award, the highest recognition of SEMNI for his research career.

Great personalities are usually beacons that shine beyond the purely professional. Manolo was an inspiring man. Those of us who were lucky enough to work with him learned a lot from his side. We will miss him and remember him. May he rest in peace. ●



The Japan Association for Computational Mechanics (JACM) is a union of researchers and engineers working in the field of computational mechanics mainly in Japan. The JACM is a loosely coupled umbrella organization covering 29 computational mechanics related societies in Japan through communication with e-mail and web page (<https://ja-cm.org/index-e.html>). The number of individual members is about 330. JACM members actively participate in the IACM activities.

The JACM elected a new executive council in March 2021. Hiroshi Okada continues to serve as the president of JACM for next three years. The former secretary general, Professor Ryuji Shioya, continues his service as the vice president. The new executive council members for 2021–2023 are as listed below:

President:

Professor Hiroshi Okada, Tokyo University of Science, hokada@rs.noda.tus.ac.jp, http://www.rs.noda.sut.ac.jp/me/laboratories/okada_laboratory.html

Vice Presidents:

Professor Ryuji Shioya, Toyo University
shioya@toyo.jp, <http://www2.toyo.ac.jp/~shioya/shioya.html>

Professor Kenji Takizawa, Waseda University
Kenji.Takizawa@waseda.jp, <https://www.jp.tafsm.org/>

Secretary General:

Professor Yuichi Tadano, Saga University
tadano@me.saga-u.ac.jp, http://sentan.me.saga-u.ac.jp/profile_tadano_eng.html



Figure 1:

Hiroshi Okada (President), Ryuji Shioya (Vice President), Kenji Takizawa (Vice President), Yuichi Tadano (Secretary General), April 2021–March 2024.

On July 29, 2021, the 2021 JACM annual meeting and award ceremony were held online. In this year, JACM inducted ten new honorary members. Before the award ceremony, new honorary members were introduced. They have distinguished records of researches and services to computational mechanics related professional societies. The new honorary members are:

Figure 2:

Professor

Thomas J. R. Hughes
(The University of Texas
at Austin)
making his short speech



Professor Ichiro Hagiwara (Professor Emeritus, Tokyo Institute of Technology and Distinguished Professor, Meiji University), Professor Koichi Hashiguchi (Professor Emeritus, Kyushu University and MSC Software), Professor Thomas J. R. Hughes (The University of Texas at Austin), Professor Hiroshi Kanayama (Professor Emeritus, Kyushu University), Professor Masanori Kikuchi (Professor Emeritus, Tokyo University of Science), Professor Yutaka Miyake (Professor Emeritus, Osaka University), Professor Noriyuki Miyazaki (Professor Emeritus, Kyushu University and Kyoto University), Professor Tayfun E. Tezduyar (Rice University), Professor Takashi Yabe (Professor Emeritus, Tokyo Institute of Technology).

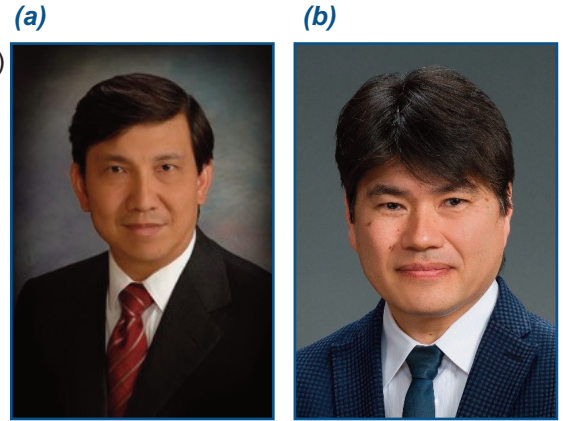
Each of new honorary members gave a short speech, after their introductions (Figure 2, Professor Thomas J. R. Hughes making his short speech).

Following the introduction of the new honorary members, the award ceremony took place. There are three categories of JACM Awards. They are the JACM Computational Mechanics Award which is the highest award, JACM Fellows Award and the JACM Young Investigator Award.

Professor Jiun-Shyan (J. S.) Chen (University of California, San Diego) and Professor Shu Takagi (The University of Tokyo) (Figure 3).

Figure 3: Computational Mechanics Award:

(a) Professor Jiun-Shyan (J. S.) Chen
 (University of California, San Diego) and
 (b) Professor Shu Takagi (The University of Tokyo)



The recipients of the JACM Fellows Award were Professor Taiji Adachi (Kyoto University), Professor Atsuya Oishi (Tokushima University), Professor Akiyuki Takahashi (Tokyo University of Science), Professor Shinya Taketomi (Saga University) and Professor Amane Takei (Miyazaki University) (Figure 4).

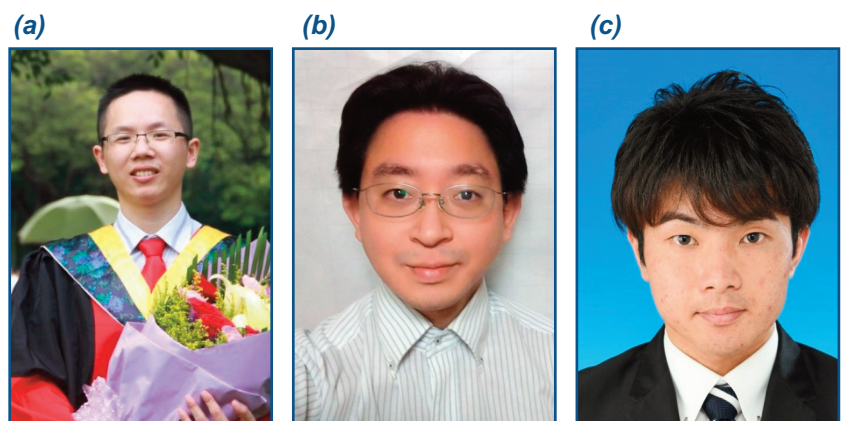


Figure 4: Fellows Award:
 (a) Professor Taiji Adachi (Kyoto University), (b) Professor Atsuya Oishi (Tokushima University),
 (c) Professor Akiyuki Takahashi (Tokyo University of Science), (d) Professor Shinya Taketomi (Saga University) and
 (e) Professor Amane Takei (Miyazaki University)

The winners of JACM Young Investigator Award were Professor Shunhua Chen (Sun Yat sen University), Dr. Daisuke Hotta (Meteorological Research Institute, Japan Meteorological Agency) and Professor Yuto Ootoguro (Tokyo University of Science) (Figure 5).

Figure 5: JACM Young Investigators Award:

(a) Professor Shunhua Chen
 (Sun Yat-sen University),
 (b) Dr. Daisuke Hotta
 (Meteorological Research Institute, Japan
 Meteorological Agency)
 and (c) Professor Yuto Ootoguro
 (Tokyo University of Science)



At the end of the 2021 JACM meeting, we took a group photo (Figure 6). Although I believe that the 2021 JACM meeting was a memorable event for all the participants, I hope to have our 2022 meeting in person. ●

Figure 6:

Group Photo (All the participants)





WCCM-APCOM2022

The 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics (WCCM-APCOM 2022) will be held in Yokohama, Japan, July 31 to August 5, 2022 (<https://www.wccm2022.org>).

The WCCM-APCOM Congress is co-organized by The International Association for Computational Mechanics (IACM) and The Japan Society for Computational Engineering and Science (JSCES) in cooperation with The Asian Pacific Association for Computational Mechanics (APACM) and Japan Association for Computational Mechanics (JACM).

The plans to hold an “on-site” congress with featured plenary and semi-plenary speakers, over 400 mini-symposia with keynote lectures, exhibitions from various sponsors, and other wonderful events, expecting the end of COVID-19 crisis until then.

Key days (for the time being)

2021 November 15:	Deadline for Submission Abstracts
2022 March 1 - May 10:	Early registration period
May 10:	Deadline for speaker registration
May 10:	Deadline of physical or virtual attendance selection
May 31:	Deadline for submission of extended abstract
June 1 - July 6:	Video submission period

“On-site” or “Online” conference?

The local organizing committee believes that face-to-face conference at the venue is the best way to know/communicate each other and to expand future personal connections over the world, in particular for young researchers. Based on this philosophy, the WCCM-APCOM 2022 is organized as the “on-site” conference at the moment. However, the format is subject to change according to situation of the COVID-19 pandemic. ●

Figure 1:
PACIFICO YOKOHAMA, the
conference venue of the
WCCM-APCOM 2022



The JSCES Grand Prize 2020

Prof. Jiun-Shyan Chen (Figure 2) of University of California, San Diego, received the JSCES Grand Prize 2020 for his outstanding contributions in the field of computational engineering and sciences. The awarding ceremony and his special lecture were held during the annual conference 2021 (online). The awarding ceremony and the special lecture of **Prof. Antonio Huerta** (Figure 3) of Universitat Politècnica de Catalunya, the awardee of JSCES Grand Prize 2019, were also held together since the annual conference 2020 was canceled due to COVID-19. ●



Figure 2:
Prof. Jiun-Shyan Chen



Figure 3:
Prof. Antonio Huerta

AIMETA 2021 Conference *Postponed to 2022*

The Italian Association of Theoretical and Applied Mechanics (AIMETA) postponed its conference, AIMETA 2021, to September 2022. The conference will be held in Palermo (Sicily, Italy). More information and the conference dates will soon be available at the following link

<https://www.aimeta.it/index.php/notizie/191-congresso-aimeta>

GIMC Best PhD Thesis Award

The GIMC Best PhD Thesis Awards committee, composed by Massimo Cuomo (Università di Catania), Lorenza Petrini (Politecnico di Milano), Alberto Salvadori (Università di Brescia) and Giuseppe Vairo (Università di Roma Tor Vergata), selected the following theses, defended in 2020, as the best Theses in Computational Solid and Fluid Mechanics:

- Dr. Giulia Bertaglia, Università di Ferrara, “1D augmented fluid-structure interaction system with viscoelasticity: from water pipelines to blood vessels”. This thesis was also selected as candidate to the ECCOMAS PhD Award,
- Dr. Francesco Liguori, Università della Calabria, “Optimal design and numerical modelling of imperfection sensitive shell structures”.

News from AIMETA groups

The AIMETA groups of Biomechanics (GBMA), Computational Mechanics (GIMC) and Mechanics of Materials (GMA) have organized the on-line event “Giovani alla ricerca” held on **7-8 June**.

“Giovani alla Ricerca” has moved from the desire to give space and visibility to the younger researchers of the three groups, in a period of limited scientific relationship due to the Covid pandemic, offering them an opportunity for sharing ideas, comparisons and critical discussions. In particular, the meeting has allowed to present to the scientific community, the best PhD Theses discussed in the two years 2020-2021 rewarding those young people who, despite the difficulties of these days, have continued to work effectively in the fields of Biomechanics, Computational Mechanics and Mechanics of Materials.



2021 News from CEACM

URL: <http://www.gf.unsa.ba/web/>

The CEACM counts the following Central European countries (in alphabetical order): Austria, Bosnia and Herzegovina, Croatia, Czech Republic, Hungary, Slovakia and Slovenia. In 2021, CEACM has elected a new Executive Committee that consists of the President, Adnan Ibrahimbegovic, the Vice-President, Janos Logo and the Past-President, Bernhard Pichler.

The scientific activities of CEACM in 2021 concern short courses and a scientific conference ECCOMAS MSF 2021, jointly organized by University of Split, University of Sarajevo and UT Compiegne.

The short course, entitled “Current Research on Solids & Fluids: Computations, FE Code Coupling, Model Reduction, Probability...” (URL: <http://gf.unsa.ba/eccomas-msf-2021/index.php/preconference-course/>), was held just before the conference, June 27-29, 2021. The course participants were doctoral students from CEACM and other European countries. The course lecturers: A. Ibrahimbegovic (UTC), H.G. Matthies (TUBs), N. Limnios (UTC), A. Ouahsine (UTC), J.L. Perez-Aparicio (UPV) and F. DeVuyst (UTC) provided an extensive review of numerical models for computational solid and fluid mechanics, modern developments in model reduction, probability aspects and uncertainty quantification, coupling with thermal, electric and magnetic fields and their interactions.

In 2021, CEACM sponsored a scientific conference ECCOMAS MSF 2021 –Multiscale Computational Methods for Solids and Fluids, which was held in Split, June 30- July 2, 2021. This was the 5th conference in series organized by Adnan Ibrahimbegovic, this time in collaboration with Mijo Nikolic, professor at University of Split. The meeting attracted close to hundred scientific presentations, with total of 208 contributing authors. The conference was held in hybrid format with 30% of participants present onsite and the remaining online. The conference provided a platform for exchange among leading specialists in analysis and design of complex engineering structures and systems, coming from aerospace, civil and mechanical engineering, material science, and in the design and analysis of numerical algorithms from applied mathematics. The main goal was elaborating the multi-field and multi-physics approach, which has significantly modified previously firm frontiers among these traditional engineering disciplines. A series of introductory distinguished lectures on the first day of this conference were scheduled with: H. Matthies and D. Dinkler from Germany, P. Ladeveze, R. Ohayon and A. Ibrahimbegovic from France, J.L. Perez-Aparicio from Spain, P. Pimenta and A. Couthino from Brazil, C. Hellmich from Austria and P. Travalusci from Italy. Ten different Mini-Symposia were organized covering various topics on: Resilience, Fracture, Experimental Aspects, Environment, Internal Flows, Multi-phase flows, Steel Structures, Isogeometric and Discrete elements. The ECCOMAS MSF 2021 Proceedings are available for download at (URL: http://gf.unsa.ba/eccomas-msf-2021/Eccomas_MSF_2021.pdf). ●



Figure 1:
ECCOMAS MSF
2021 Conference
onsite participants



Figure 2:
ECCOMAS MSF
2021 Conference
final meeting of
organizing committee



14th WCCM
iacm & Ecomas Congress 2020
Virtual Congress 11-15 January, 2021

14th. World Congress on Computational Mechanics (WCCM XIV) and **8th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2020)**

Chair: Pr. Francisco Chinesta
Co-chairs: Pr. Rémi Abgrall, Pr. Olivier Allix, Pr. David Néron, Pr. Michael Kaliske
Local organizing committee: Pr. Rémi Abgrall, Pr. Olivier Allix, Pr. Delphine Brancherie, Pr. Francisco Chinesta, Dr. Luc Laurent, Dr. Cécile Oliver-Leblond, Pr. David Néron



Prof. Remi Abgrall
University of Zurich



Prof. Olivier Allix
ENS Paris-Saclay



Prof. Delphine Brancherie
Université de Technologie de...



Prof. Francisco Chinesta
ESI GROUP Chair, ENSAM...



Dr. Luc Laurent
Conservatoire national des...



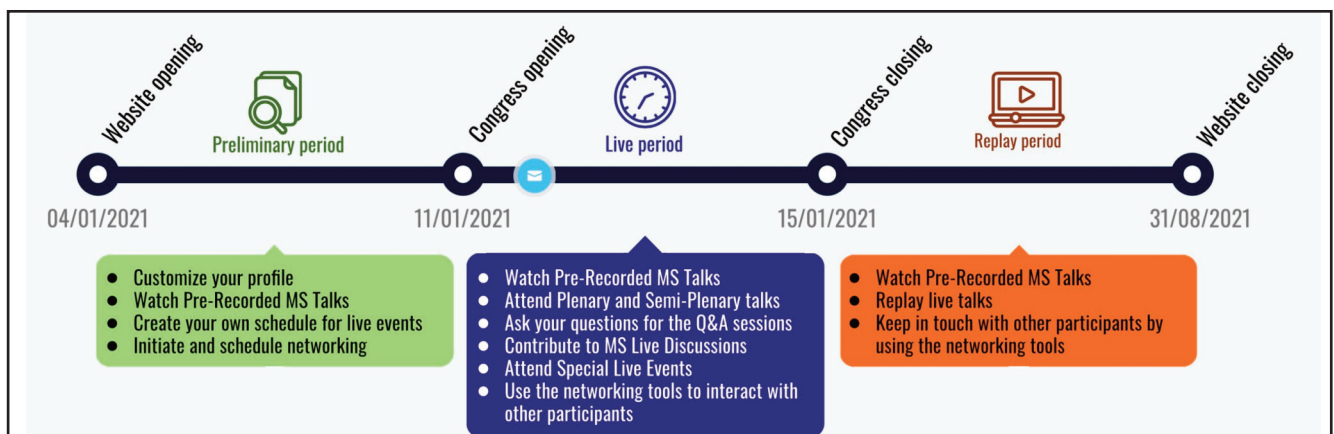
Prof. David Néron
ENS Paris-Saclay

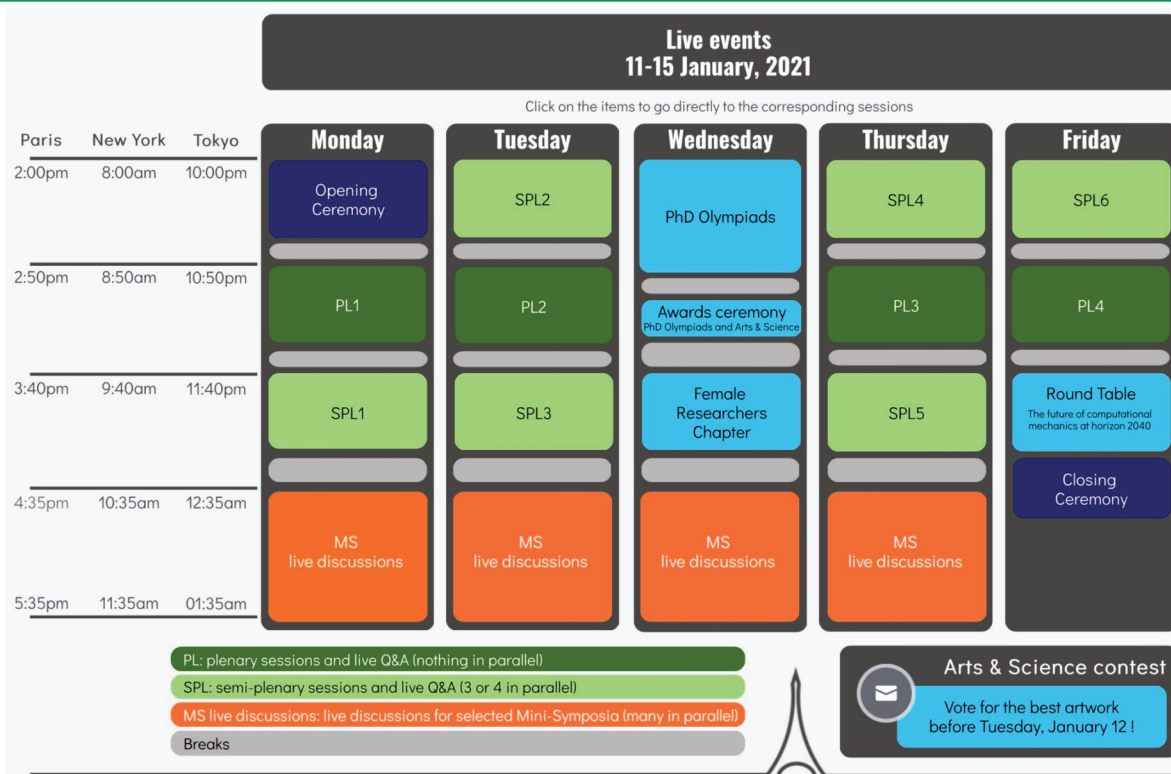


Dr. Cécile Oliver-Leblond
ENS Paris-Saclay

The joint 14th World Congress in Computational Mechanics and ECCOMAS Congress was planned to take place in Paris in July 2020 with more than 5000 presented papers. The tragedy of the covid-19 pandemic has made impossible to organize the ECCOMAS-WCCM congress in its standard face-to-face format. The organizing committee finally proposed the first ECCOMAS-WCCM congress organized in a fully digitalized format.

This very special event received an enthusiastic response from all the community, bringing together more that 3000 participants of 30 countries, over 280 mini-symposia (MS) corresponding to almost 2500 presented papers. The presentations were pre-recorded, making them accessible to a wider audience than in the traditional format. They were available online, along with all the special events organized during the congress week, till end of August 2021.





The week of the congress (January 11-15, 2021) was the occasion to organize a series of special events going from the traditional plenary (4) and semi-plenary lectures (24) to more special events as the ECCOMAS young investigators event, the IACM Female Chapter event or the round table on future challenges in computational mechanics. All along the congress week, daily live meetings around a plenary conference, 4 semi-plenary conferences and discussion sessions dedicated to mini-symposia were offered. They were the occasion of very rich and fruitful live discussions. Quite unusual was also the Art and Science contest, organized by the ECCOMAS young investigators, consisting in a virtual exposition hall.

A virtual conference has its share of successes and sometimes small disappointments. In any case, it allows to learn a lot about this new format for a conference of this size.

It is obvious that live participation is limited by the daily tasks of the participants. We expected that the fact that the website remained open after the conference would compensate for any loss of participants during the week of the conference, but the numbers are a real message of encouragement with live participation that may have exceeded 1000 in the plenaries and 400 in the semi-plenaries. This is the order of magnitude of a standard conference with, in addition, something that was appreciated: the exchanges through the chat and the discussion led by the chairs.

On the other hand, the researchers had the possibility to follow all the conferences that interested them, which is normally not possible when 50 sessions are held in parallel. More than 400 presentations were viewed more than 20 times. Regarding the live discussions on the mini-symposia, the participation ranged from 20 to 200 people and the presence of experienced researchers in these moments of exchange was a great success.

Finally, more than 7000 messages were sent either in public (3000) or in private (4000). These figures show that a virtual congress can nevertheless be a moment of exchange. It goes without saying that direct contact with colleagues and friends is irreplaceable.

The proposed format was embraced by all the community to create a very special, enthusiastic and successful scientific event. ●

Contributions from AMCA members to fight against COVID-19 in Argentina.

CFD helps to reduce COVID-19 transmission in massive transport¹¹ **Damian Ramajo & Santiago Corzo****AMCA regular members**Centro de investigación
en métodos computacionales
(CIMEC)–CONICET–UNL –
Santa Fe, Argentina

COVID-19 is the worse pandemic of XX1st century. At least two factors promoted the fast spread of the disease: firstly, the high connection of people around the world. Secondly, the people living in crowded big cities. Massive transport media have played a significant role in virus transmission. However, recent numerical and experimental studies have shown that travel by airplane should be safe even for long time trips because the laminar descending airflow as well as the use of High Efficient Particulate Arresting (HEPA) filters lead to adequate renewal air ratios. These technical features added to strict boarding and on-board protocols seem to be enough to reduce the risk of airborne virus transmission.

On the other hand, the scenario is completely different in urban buses, trains and subways, where the average trip is relatively short, but the distance between passengers is lower, the Heat, Ventilation, Air Conditioning systems (HVAC) recirculate most of the cabin air, and filters are ineffective to retain viruses. One positive and, three negative factors that clearly increase the transmission risk. The best solution seems to be to enhance the air renewal ratio by re designing the HVAC systems, loosing energy efficiency, but improving safety conditions. Although it

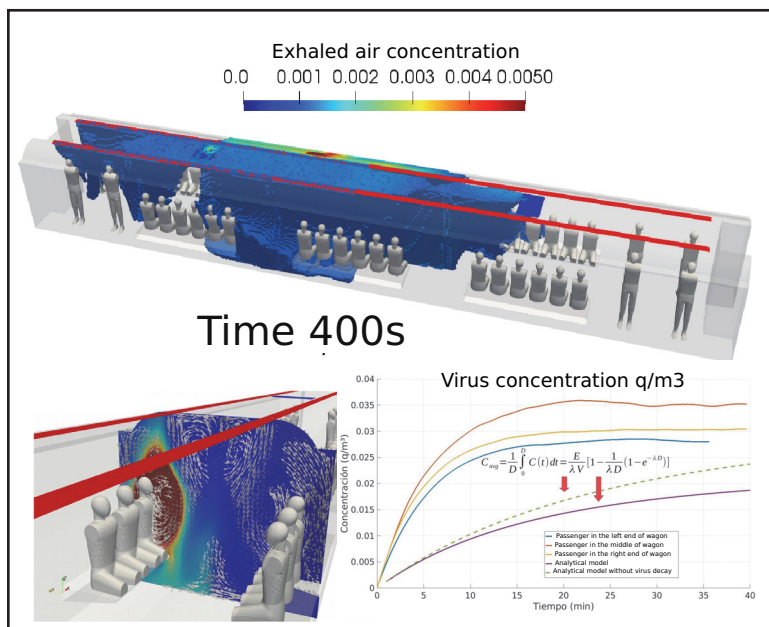
is obvious the role of HVAC on virus dissemination, it is also clear that the local virus concentration around the infected passenger will be reduced by spread it along all the room. Taking into account that a certain dose should be inhaled to contract disease, it could be benefit for passengers close to the infected.

Since mid 2020 we have performed CFD simulations with OpenFOAM to give guidelines for improving the safety in transport media. *Figure 1* displays the simulation of virus transmission in the Buenos Aires city subway. The air exhaled by a passenger in the central zone is quickly aspirated by the outlet air vent and disseminated covering more than a half of the wagon after 400 s. That is, around 0.1% of the indoor air comes from the infected passenger.

Simple transmission models allows us to estimate the virus concentration considering perfect mixing assumptions. These models give us the average virus concentration, which is in general in a good agreement with CFD results. But the main advantage of CFD is the capacity to visualize the local concentrations, which can be two or three times higher than the average ones. *Figure 1* on the bottom right displays the average, and local virus concentration in the wagon. As noted, the central zones (zones 2, 3 and 4) reach to concentration values two times more than the average. As shown, analytical models are useful for preliminary estimations, but the improvement on the current HVAC systems should be supported by detailed CFD modeling.

Cover to sneeze or cough. The wide range of particle sizes exhaled by a person during respiratory activities represents a great challenge for the study of disease transmission mechanisms. The trajectory of ballistic droplets after sneeze or cough is also affected by the indoor airflow. For large droplets larger than 300 μm the droplets follow parabolic trajectories based on the inertia force, but most of droplets are smaller than 100 μm and evaporate almost completely. As

Figure 1:
Concentration of the
air exhaled by a infected
passenger in the
subway wagon.
Effect of the HVAC on
virus spread. Concentration
of virus at different zones

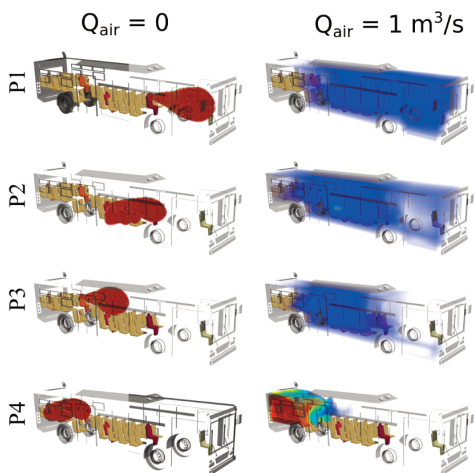


shown in *Figure 2*, they are easily dragged by the airflow, traveling more than 4 m before deposition on the floor and horizontal surfaces.

Remain silent. A speaking person produces between 5 and 20 more aerosols than a silent breathing person. *Figure 3* shows the exhaled air concentration caused by a person speaking for one minute. As noted, the HVAC system promotes rapid spread of virus, but locally reduces its concentration.

Opening the windows. The opening the windows in urban buses is the best choice in terms of air renewal. *Figure 4* displays the outflow and inflow CFD results for a bus moving at 40 km/h. The pressure drop at the external front part of the bus promotes high incoming flow through the rear windows and outgoing flow through

Figure 3:
Concentration of the air exhaled by a speaker for one minute in different zones of the bus with (right) and without (left) HVAC



the front windows. As a consequence, 7s, 12 s and 26 s are needed to replace the indoor air at 20 km/h, 40 km/h and 60 km/h, respectively. These times are very promising if we consider that a typical HVAC system with a renewal ratio of 25% it needs more than 235 s to achieve that.

Conclusions. CFD simulation is a very powerful tool for understanding and improving the safety of massive transport media. The energy efficiency and comfort but also the health concerns should be included in the design of modern buses, trains and subways. Meanwhile, the opening of windows, the maximization of the renewal ratio of HVAC systems and the inclusion of efficient filters is mandatory. ●

Figure 2:
Spread of droplets after sneezing of a passenger placed in different zones of the urban bus

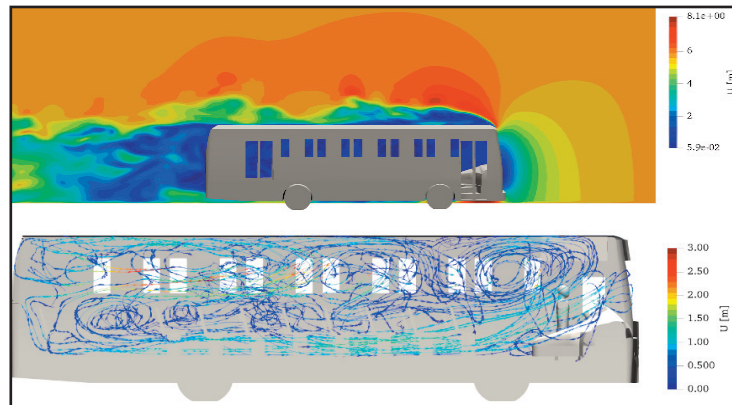
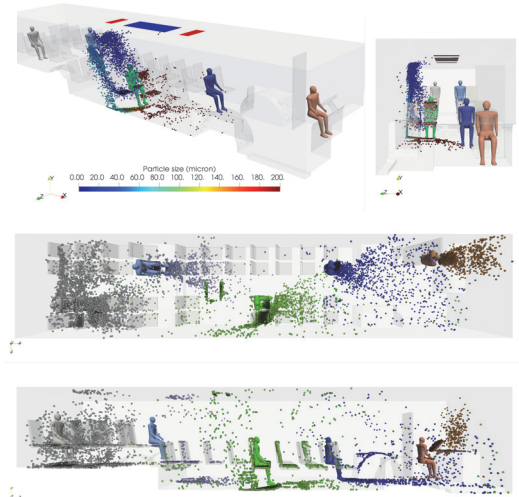


Figure 4:
Outflow and inflow induced by opening the windows of a bus traveling at 40 km/h

MECOM 2021

XXXVII Argentine Congress on Computational Mechanics

Resistencia, Chaco, Argentina.

Dear AMCA Members,

We like to inform you that the thirty-seventh edition of the Argentine Congress of Computational Mechanics will be celebrated from 1st to 5th November 2021, fully online. We invite you to join us once again in a new edition of our Association Congress. You could check for information updates in the website <https://amcaonline.org.ar/mecom2021>.

Best regards,

Dr. Ing. Javier Mroginski
Organizing Committee President

Dr. Ing. Guillermo Castro
Scientific Committee President



conference diary planner

1 - 5 Nov 2021 **MECOM 2021 - XXXVII Argentine Congress on Computational Mechanics**

Venue: Chaco, Argentina

Contact: <https://amcaonline.org.ar/mecom2021>

10 - 12 Jan 2022 **The Role of Mathematical and Computational Modeling in Cancer Research**

Venue: Virtual Conference

Contact: sites.google.com/usacm.org/bio-mcr/home

4 - 6 April 2022 **EMMC – 18th European Mechanics of Materials Conference**

Venue: Oxford, UK

Contact: <http://www.emmc18.org>

20 - 22 April 2022 **2022 UKACM Annual Conference**

Venue: Nottingham, UK

Contact: <https://www.ukacm2022.ukacm.org/>

16 - 20 May 2022 **CSMA 2022 - 15th National Colloquium in Structural Design**

Venue: Giens, France

Contact: <https://csma2022.sciencesconf.org/>

6 - 8 June 2022 **CSME 2022 - The Canadian Society for Mechanical Engineering International Congress**

Venue: Edminton, Canada

Contact: www.csmecongress.org

4 - 8 July 2022 **11th European Solid Mechanics Conference**

Venue: Galway, Ireland

Contact: <https://www.esmc2022.org/>

31 Jul - 5 Aug 2022 **WCCM-APCOM 2022 - 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics**

Venue: Yokohama, Japan

Contact: <https://www.wccm2022.org>

18 - 19 Aug 2022 **MLIP - Uncertainty Quantification for Machine Learning Integrated Physics Modeling**

Venue: Arlington, VA, USA

Contact: sites.google.com/usacm.org/uq-mlip/home

September 2022 **AIMETA - Italian Association of Theoretical and Applied Mechanics**

Venue: Palermo, Sicily, Italy

Contact: <https://www.aimeta.it/>

25 - 27 Sept 2022 **MFEM2020 - Meshfree and Novel Finite Elements with Applications**

Venue: Berkeley, California, USA

Contact: mfem2020.usacm.org

6 - 9 Nov 2022 **IGA2022 - USACM Thematic Conference - Isogeometric Analysis**

Venue: Banff, Canada

Contact: iga2022.usacm.org

25 - 29 July 2021 **USNCCM16 - 16th U.S. National Congress on Computational Mechanics**

Venue: Chicago, Illinois

Contact: <http://16.usnccm.org/>

6 Dec 2022 **11th JACM Computational mechanics Symposium**

Venue: Japan

Contact: <https://ja-cm.org/index-j.html>

23-27 July 2023 **17th U. S. National Congress on Computational Mechanics**

Venue: Albuquerque, New Mexico, USA

Contact: 17.usnccm.org

21 - 26 July 2024 **WCCM/PANACM - 16th World Congress on Com. Mechanics & 4th PANACM Congress**

Venue: Vancouver, Canada

Contact: <https://www.cacse-accsq.ca/>

7 - 10 Dec 2025 **APCOM 2025 - The 9th Asian Pacific Congress on Computational Mechanics**

Venue: Brisbane, Australia

Contact: <https://www.apacm-association.org/>