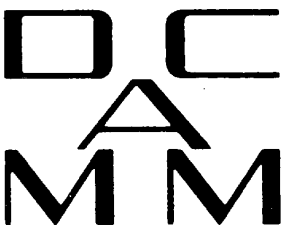
DANISH CENTER FOR APPLIED MATHEMATICS AND MECHANICS

The 2022 DCAMM Annual Seminar Speaker

in connection with the
100th anniversary of Frithiof Niordson
10 November 2022



TECHNICAL UNIVERSITY OF DENMARK -
AALBORG UNIVERSITY - AARHUS UNIVERSITY –
UNIVERSITY OF SOUTHERN DENMARK

DANISH CENTER FOR APPLIED MATHEMATICS AND MECHANICS

Scientific Council as of September 2022

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Chairman

Associate Professor Niels Leergaard Pedersen
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DCAMM Annual Seminar Speaker 2022

George Em Karniadakis
Professor of Applied Mathematics and Engineering
Brown University, USA

Title:

From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: QUO VADIMUS?

Abstract:
We will review physics-informed neural networks (NNs) and summarize available extensions for applications in computational mechanics and beyond. We will also introduce new NNs that learn functionals and nonlinear operators from functions and corresponding responses for system identification. The universal approximation theorem of operators is suggestive of the potential of NNs in learning from scattered data any continuous operator or complex system. We first generalize the theorem to deep neural networks, and subsequently we apply it to design a new composite NN with small generalization error, the deep operator network (DeepONet), consisting of a NN for encoding the discrete input function space (branch net) and another NN for encoding the domain of the output functions (trunk net). We demonstrate that DeepONet can learn various explicit operators, e.g., integrals, Laplace transforms and fractional Laplacians, as well as implicit operators that represent deterministic and stochastic differential equations. More generally, DeepOnet can learn multiscale operators spanning across many scales and trained by diverse sources of data simultaneously. Finally, we will present first results on the next generation of these architectures to biologically plausible designs based on spiking neural networks and Hebbian learning that are more efficient and closer to human intelligence.

DCAMM Special Invited Speaker 2022

Peter Gudmundson
Professor, Department of Engineering Mechanics
KTH Royal Institute of Technology, Sweden

Title:

Length scales and perturbation solutions –
application to plastic properties of particle reinforced materials

Abstract:
Perturbation analysis is a powerful tool to obtain simplified solutions that still are sufficiently accurate. Simple cases and results from previous research will exemplify the methodology. As an example, the plastic properties of particle-reinforced materials are analyzed in more detail. It is assumed that the volume fraction is small and that the reinforcing particles are so small that length scale effects of plastic deformation in the matrix must be considered. A strain gradient plasticity theory is applied in order to capture these effects. The theory includes a material length scale ℓ, that can be compared to the particle radii a. Perturbation based solutions are derived for the case $a/l \ll 1$ and for strain hardening also for the case $l/a \ll 1$. The so obtained closed form solutions for initial yield stress, strain hardening and cyclic plasticity are compared to extensive finite element simulations and to experiments. Excellent agreements to finite element solutions are found for $a/l \ll 1$. It is also found that the perturbation based solutions give quite accurate predictions for l/a of the order of one and that the model very well can capture experimental observations.

DCAMM Special Invited Speaker 2022

Norman Fleck
Professor, Department of Engineering
University of Cambridge, United Kingdom

Title:

The mechanics of the cathode of a Li ion battery

Abstract:
Li ion batteries discharge by the transport of Li ions from an anode (such as graphite or Li metal) to a cathode comprising ceramic particles that swell upon lithiation. The next generation of batteries comprise cathode particles in the form of single crystals made from layered nickel rich materials. Recently, optical microscopy has been performed that reveal the diffusion of Li within these single crystals ("Operando visualisation of kinetically-induced lithium heterogeneities in single-particle layered Ni-rich cathodes" by Chao Xu, Alice J. Merryweather, Shrinidhi S. Pandurangi, Zhengyan Lun, David S. Hall, Vikram S. Deshpande, Norman A. Fleck, Christoph Schnedermann, Akshay Rao, Clare P. Grey, Joule 6, pp. 1-12, 2022.) This allows for a direct comparison with a fully coupled chemo-mechanical model of Li diffusion, including the role of stress. Predictions reveals that the level of induced stress in the single crystals is sufficient to induce cracking when the particles are large and the rate of discharge (lithiation) is very fast (full battery discharge in 10 minutes). Additional simulations have also been performed to explore whether a micro-architectured cathode can be designed that does not swell at the macroscopic level despite significant swelling by the active material upon lithiation.

DCAMM Special Invited Speaker 2022

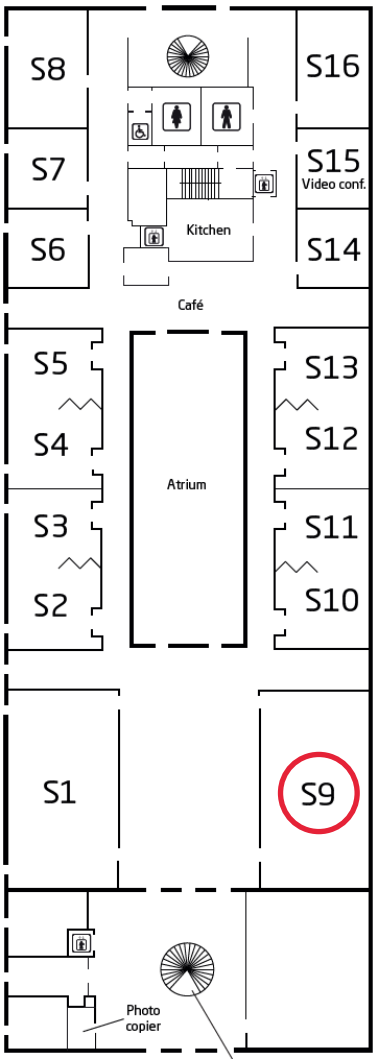
Claus B.W. Pedersen
Technical Director
Dassault Systèmes, France

Title:

Industrial Applications - Shell Models and Optimization Workflows

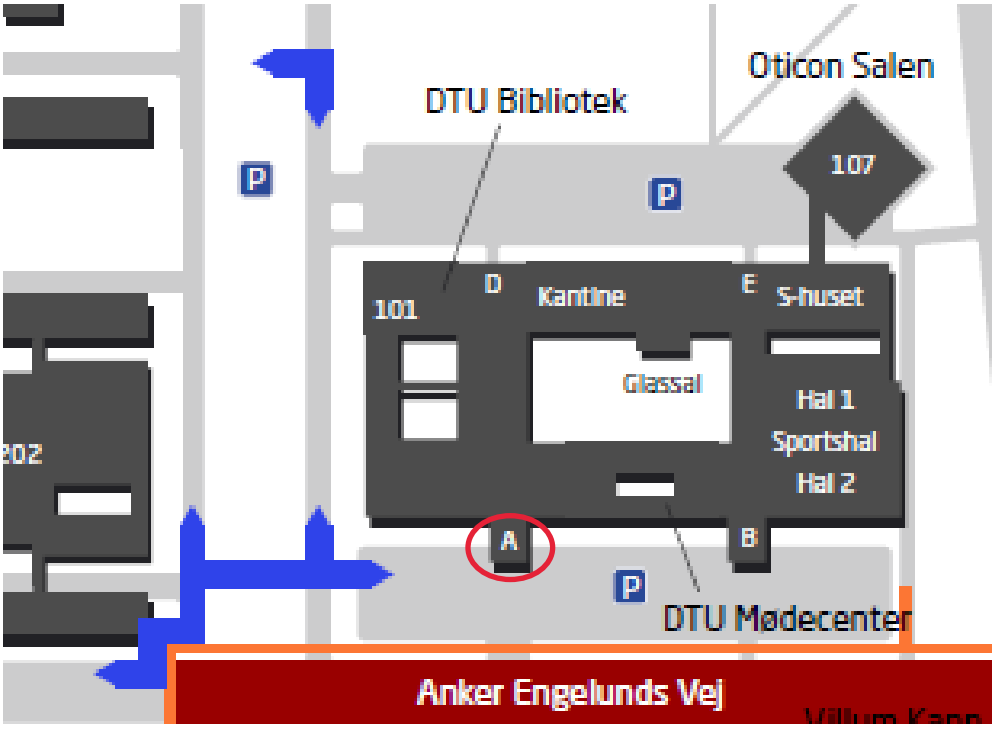
Abstract:
Due to sustainability, the Transport and Mobility (T&M) sector has started a transformation from conventional Fossil based systems to Electric Vehicles (EVs). Thus, we suggest to apply CAE workflows including shell modeling and non-parametric optimization approaches based upon adjoint sensitivities for addressing the challenges for deriving new and improved designs.
Initially, we show the mass minimization of a suspension component considering stiffness, strength and dynamic properties. The applied End-to-End optimization workflow includes automated CAD-reconstruction, concept variants for manufacturing constraints and additive manufacturing verification using a coupled thermal-stress process simulation considering continuously evolving convection and radiation surfaces during the manufacturing process.
Secondly, we construct a parametric skateboard shell model of the EV including the battery simulations applied to crash scenarios. Shell models are also applied to non-parametric crashworthiness bead and sizing optimization of the sheets for minimizing intrusions and head accelerations. Additionally, strength shell optimization is tackled using semi-analytic adjoint sensitivity analysis for non-proportional fatigue damage.
To conclude, we apply multiphysics modeling for optimizing the electrical machines of the EV drive train system having a major impact on the performance and overall comfort of the EVs.
Consequently, the present implemented modeling and optimization technologies can drive the T&M designs of the sustainable transformation.

DTU: 12:00 – 17:30



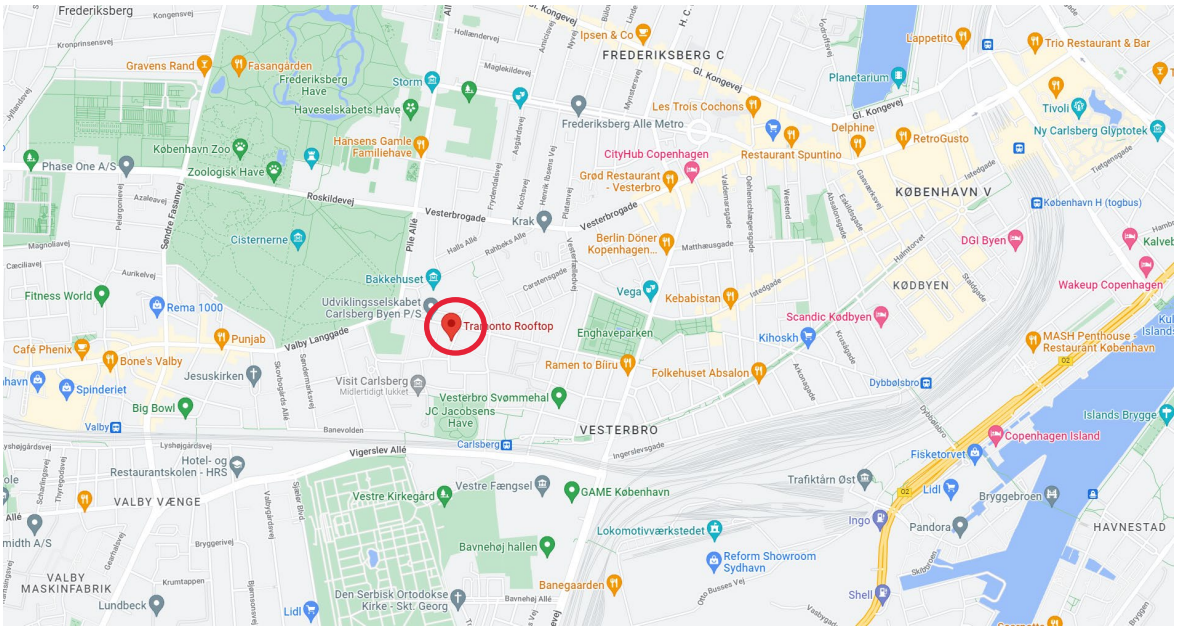
Left:
Map of DTU Meeting Center.
DCAMM Annual Seminar Speaker Event in connection with the 100th anniversary of Frithiof Niordson in **room S9**.

Below:
Map of DTU building 101.
Use entrance A to DTU Meeting Center (Mødecenter).



Copenhagen: 18:00 – 21:30

Restaurant Tramonto
Carlsbergbyen,
Bryggernes Plads 7, 1799 Copenhagen V



The programme of DCAMM's Annual Seminar Speaker in connection with the 100th anniversary of Frithiof Niordson

12:00 -- 13:00	**Lounge**	**Lunch: Sandwiches and beverages**
13:00 -- 13:10	**S09**	**Welcome by the chairman**
		<u>DCAMM Annual Seminar Speaker 2022</u>
13:10 -- 14:00	**S09**	**Professor George Em Karniadakis** ***From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: QUO VADIMUS***
		<u>DCAMM Invited Speakers</u>
14:00 -- 14:40	**S09**	**Professor Peter Gudmundson** ***Length scales and perturbation solutions - application to plastic properties of particle reinforced materials***
14:40 -- 15:10	**Lounge**	**Coffee break**
15:10 -- 15:50	**S09**	**Professor Norman Fleck** ***The mechanics of the cathode of a Li ion batteri***
15:50 -- 16:30	**S09**	**Technical Director Claus B.W. Pedersen** ***Industrial Applications - Shell Models and Optimization Workflows***
16:30 -- 17:30	**Lounge**	**Refreshments: Beers and soft drinks**
17:30 -- 18:00		**Bus transport to restaurant in Copenhagen**
18:00 -- 21:30		**Dinner at Restaurant Tramonto** **Carlsberg Byen, Bryggernes Plads 7, 1799 Copenhagen**

Lounge: Ground floor in front of S09 at DTU Meeting Center