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EUROGEN **2025**

16th Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications

September 16–18, 2025 – Lahti, Finland

www.lut.fi/en/eurogen-2025

MONDAY, SEPTEMBER 15

17:00–18:00 — Light Touch of Lahti: City Tour by Bus
As part of the Welcome Reception, a city tour by bus will be organized.

- Departure: Address: Vapaudenkatu 24, Lahti (next to Hotel Scandic)
- Conclusion: Lahti City Hall, followed by the reception

18:00–19:00 — Welcome Reception
Lahti City Hall, Address: Harjukatu 31, Lahti

TUESDAY, SEPTEMBER 16

8:00	Bus transportation from the conference hotels to the LUT University campus
8:00	*Registration takes place at the main entrance of LUT University* *Address: Mukkulankatu 19, Lahti*

OPENING AND PLENARY PRESENTATIONS, Auditorium 1

9:00-9:15	**Opening of the Conference** Welcome address by Jari Hämäläinen, EUROGEN 2025 Conference Chair Welcome address by Jaana Sandström, Vice rector of LUT University
9:15-9:45	**Plenary presentation by Dietrich Knörzer:** *30 Years of EUROGEN - Evolutionary Algorithms in Engineering and Computer Science* Chair: Tero Tuovinen
9:45-10:30	**Plenary presentation by David Greiner:** *Hybridizing Surrogate Modeling and Evolutionary Algorithms for Optimum Engineering Design Problems in Computational Engineering* Chair: Jari Hämäläinen

10:30-11:00	COFFEE BREAK

PARALLEL SESSIONS	**MINISYMPOSIUM ON** MACHINE LEARNING AND DATA-DRIVEN INNOVATIONS IN AERODYNAMIC OPTIMIZATION AND UNCERTAINTY QUANTIFICATION (I) proposed by Esther Andres Perez, Rodrigo Castellanos, Domenico Quagliarella Session chair: D. Quagliarella	**THEMATIC SESSION ON** TOPOLOGY OPTIMIZATION Session chair: Keita Kambayashi

11:05-11:25	DEVELOPMENT OF EFFICIENT EVOLUTIONARY ALGORITHMS BY EXTRACTING IMPLICIT KNOWLEDGE FROM THE OPTIMIZATION PROCESS **Zhili Tang**, Xin Zhao, Jacques Periaux	ON THERMODYNAMIC TOPOLOGY OPTIMIZATION WITH AN IMPLEMENTED THIRD MEDIUM REGULARIZATION SCHEME **Max von Zabiensky**, Dustin R. Jantos, Philipp Junker
11:25-11:45	GRADIENT-ENHANCED BAYESIAN OPTIMIZATION FOR AERODYNAMIC DESIGN **Emre Özkaya**, Long Chen, Nicolas R. Gauger	A FICTITIOUS PHYSICAL MODEL FOR VISIBILITY EVALUATION AND ITS APPLICATION IN ENGINEERING DESIGN **Xiao Huang**, Kaiwen Guan, Takayuki Yamada
11:45-12:05	A DATA-DRIVEN APPROACH FOR TURBULENCE MODELLING OF LAMINAR SEPARATION BUBBLES **F. A. D'Aniello**, G. Longobardo, P. Catalano, D. Quagliarella	TOPOLOGY OPTIMIZATION OF VISCOELASTIC COMPOSITES USING COMPLEX-VALUED HOMOGENIZATION **Hiroaki Deguchi**, Kei Matsushima, Takayuki Yamada
12:05-12:25	PROPELLER BLADES SHAPE OPTIMIZATION USING HYBRID GENETIC ALGORITHMS AND SURROGATE MODELS **J. Berrueco-Fernández**, I. Robledo, E. Andrés, R. Castellanos	

12:30-13:45	LUNCH

PLENARY PRESENTATIONS, Auditorium 1

13:45-14:30	**Plenary presentation by Cornelia Grabe:** The Potential of Data-Driven Turbulence Modeling for Industrially Relevant Aerodynamic Applications Chair: Tero Tuovinen

PARALLEL SESSIONS **14:35-16:00**	**MINISYMPOSIUM ON** CLEAR SESSION: CONTROL DESIGN FOR ENVIRONMENTAL ADVANCEMENT AND RESEARCH (I) proposed by S. Bezzaoucha, C. Choquet, É. Comte Session chairs: C. Choquet, É. Comte **Auditorium 1**	**THEMATIC SESSION ON** UNCERTAINTY QUANTIFICATION Session chair: Nuutti Hyvönen **Lecture hall A122**
14:40-15:00	OPTIMAL CONTROL FOR LAKE EUTROPHICATION: A DIRICHLET BOUNDARY CONTROL PROBLEM **É. Comte**, C. Choquet	ADAPTIVE BI-FIDELITY MONTE CARLO ESTIMATION FOR RANDOM ELLIPTIC PDES **Dustin Mühlhäuser**

15:00-15:20	POLYTOPIC APPROACH FOR STABILITY & CONTROL DESIGN OF SAINT-VENANT EQUATIONS Abderrazzak El Ammari, **Souad Bezzaoucha**, Catherine Choquet	CFD-DRIVEN ROBUST OPTIMIZATION OF TRANSONIC AERODYNAMIC SHAPES **Quentin Bennehard**, Marco Carini, Gregory Dergham
15:20-15:40	OPTIMIZING CROP IRRIGATION UNDER BIOLOGICAL AND OPERATIONAL CONSTRAINTS WITH METEOROLOGICAL UNCERTAINTY **Ruben Chenevat**, Bruno Cheviron, Alain Rapaport, Sébastien Roux	GAUSSIAN PROCESSES FOR UNCERTAINTY QUANTIFICATION AND FAST EMULATION OF CHEMICAL KINETICS **Sarah M. Askevold**, Ángel F. García-Fernández, Brianna Heazlewood, Suzie C. Abbs, Simon Maskell
15:40-16:00	A MACHINE LEARNING ALGORITHM FOR WATER QUALITY CONTROL **C. Choquet**, T. Pélissié de Montémont	A MULTIOBJECTIVE APPROACH TO EVALUATE SUITABLE BATTERY TECHNOLOGIES TO POWER HYBRID MEDIUM-RANGE AIRCRAFT **Nicolina Montella**, Domenico Quagliarella

16:00-16:30	**REFRESHMENTS**

PARALLEL SESSIONS **16:30-18:00**	**MINISYMPOSIUM ON** OPTIMIZATION MEETS INVERSE PROBLEMS Session chair: Tapio Helin **Auditorium 1**	**THEMATIC SESSION ON** ADJOINT-BASED SHAPE OPTIMIZATION Session chair: Rainald Löhner **Lecture hall A122**
16:35-16:55	RECOVERY OF TRANSVERSELY-ISOTROPIC ELASTIC MATERIAL PARAMETERS IN INDUCTION MOTOR ROTORS **Ville-Petteri Manninen**, Hanz Cheng, Tapio Helin, Timo Holopainen, Juha Jokinen, Andreas Rupp, Samu Sorvari	ADJOINT BASED SHAPE OPTIMIZATION FOR MULTIPHASE FLOWS WITH PHASE CHANGE DUE TO BOILING **Vishal Garg**, Wilfried Edelbauer, Gabor Janiga, Manolis Gavaises
16:55-17:15	QUASI-MONTE CARLO INTEGRATION FOR BAYESIAN DESIGN OF EXPERIMENT PROBLEMS GOVERNED BY PDES **Vesa Kaarnioja**, Claudia Schillings	ADJOINT-BASED SHAPE OPTIMIZATION IN SMOOTHED PARTICLE HYDRODYNAMICS **Eduardo Di Costanzo**, Niklas Kühl, Jean-Christophe Marongiu, Thomas Rung
17:15-17:35	ROBUST ACCELERATED PGET RECONSTRUCTION FOR SAFE DISPOSAL OF SPENT NUCLEAR FUEL **Tommi Heikkilä**, Sara Heikkinen, Tapio Helin	CAD-INTEGRATION FOR GRADIENT-BASED SHAPE OPTIMIZATION USING THE ALGORITHMICALLY DIFFERENTIATED PYTHONOCC LIBRARY **Mladen Banović**, Adam Büchner, Thomas E. Hafemann, Patrick Wegener, Arthur Stück

17:35-17:55	EDGE-PROMOTING SEQUENTIAL BAYESIAN EXPERIMENTAL DESIGN FOR X-RAY IMAGING Tapio Helin, **Nuutti Hyvönen**, Juha-Pekka Puska	AEROSTRUCTURAL OPTIMIZATION OF THE DLR-F25 TRANSPORT AIRCRAFT SUPPORTED BY ML-SURROGATES FOR CAD Xenofon S. Trompoukis, Varvara G. Asouti, Marina Kontou, **Kyriakos C. Giannakoglou**

18:10	Bus transportation to conference hotels.

WEDNESDAY, SEPTEMBER 17

PLENARY PRESENTATIONS, Auditorium 1

8:00	Bus transportation from the conference hotels to the LUT University campus
9:00-9.45	**Plenary presentation by Rainald Löhner:** *High-Fidelity Digital Twins: Detecting and Localizing Weaknesses in Structures* Chair: Kyriakos Giannakoglou
9:45-10:30	**Plenary presentation by Marko Mäkelä:** *Nonsmooth Optimization: From Theory to Methods and Applications* Chair: Emre Özkaya
10:30-11:00	**COFFEE BREAK**

PARALLEL SESSIONS	**MINISYMPOSIUM ON** ADVANCED METHODS FOR TOPOLOGY AND SHAPE OPTIMIZATION proposed by Daniela Masarczyk, Georgia Kikis Session chair: Daniela Masarczyk	**THEMATIC SESSION ON** ARTIFICIAL INTELLIGENCE IN OPTIMIZATION Session chair: David Greiner
11:00-12:30	**Auditorium 1**	**Lecture hall A122**
11:05-11:25	CFD-BASED RE-DESIGN OF GHIBLI ARC-JET NOZZLE **Roberto Carbone**, Antonio Schettino, Domenico Quagliarella, Jan O. Pralits	TOWARDS PREDICTIVE MAINTENANCE IN HYDROGEN STORAGE AND TRANSPORTATION USING AI AND MULTIOBJECTIVE DECISION SUPPORT **Robin van der Laag**, Michael Emmerich, Thomas Bäck, Yingjie Fan
11:25-11:45	CHECKERBOARD-FREE TOPOLOGY OPTIMIZATION USING POLYGONAL FINITE ELEMENTS WITH VORONOI TESSELLATIONS **G. Kikis**, B. Sauren, C. Birk, S. Klinkel	PHYSICS-INFORMED KOLMOGOROV-ARNOLD NETWORKS FOROSCILLATORY DIFFERENTIAL EQUATIONS **Michael Crocoll**

	Daniela Masarczyk, Minh T. Tran, Detlef Kuhl	**Francesco Fransesini**, Manuela Boscolo, Pier Paolo Valentini
12:05-12:25	THERMODYNAMIC TOPOLOGY OPTIMIZATION OF PHOTONICS **Sebastian Wolf**, Dustin R. Jantos, Philipp Junker	

12:30-13:45	**LUNCH**

PARALLEL SESSIONS **13:45-15:15**	**MINISYMPOSIUM ON** MACHINE LEARNING AND DATA-DRIVEN INNOVATIONS IN AERODYNAMIC OPTIMIZATION AND UNCERTAINTY QUANTIFICATION (II) proposed by Esther Andres Perez, Rodrigo Castellanos, Domenico Quagliarella Session chair: Domenico Quagliarella **Auditorium 1**	**THEMATIC SESSION ON** MULTI-OBJECTIVE OPTIMIZATION (I) Session chair: Jos Vankan **Lecture hall A122**
13:50-14:10	NEURAL NETWORK OPTIMIZATION FOR DATA-EFFICIENT GENERALIZATION IN SCIENTIFIC MACHINE LEARNING **Damiano Squillace**, Domenico Quagliarella, Umberto Iemma	COMPUTATIONAL PERSPECTIVES ON MULTI-OBJECTIVE HOME HEALTHCARE ROUTING AND SCHEDULING: FORMULATIONS AND CHALLENGES **Soumen Atta**, Michael Emmerich, Vítor Basto-Fernandes
14:10-14:30	MULTI-FIDELITY AIRFOIL SHAPE OPTIMIZATION WITH HYBRID GENETIC ALGORITHM **I. Robledo**, A. Vilariño, A. Miró , O. Lehmkuhl, R. Castellanos, C. Sanmiguel Vila	DISCUSSION ON THE EFFECT OF AIRFLOW-COORPERATION ON THE AEROSTRUCTURAL OPTIMIZED DESIGN OF A PASSACTIVE COMPLIANT MORPHING AIRFOIL **Keita Kambayashi**
14:30-14:50	SOLVING DISTRIBUTIONALLY ROBUST OPTIMIZATION PROBLEMS EFFICIENTLY VIA SURROGATE MODELS **Jan Rottmayer**, Long Chen, Nicolas R. Gauger	MULTI-CRITERIA OPTIMIZATION FOR BUILDING SPATIAL DESIGN **Ksenia Pereverdieva**, André Deutz, Tessa Ezendam, Thomas Bäck, Hèm Hofmeyer, Michael Emmerich
14:50-15:10		CAVITATION EROSION OPTIMIZATION IN A HIGH HEAD FRANCIS TURBINE USING EVOLUTIONARY ALGORITHMS **S. Stalikas**, E. Kontoleontos, V. Asouti, K. C. Giannakoglou

15:10-15:40	**REFRESHMENTS**

PARALLEL SESSIONS 15:40-17:05	**THEMATIC SESSION ON** SURROGATE AND REDUCED-ORDER TECHNIQUES Session chair: Cornelia Grabe **Auditorium 1**	**THEMATIC SESSION ON** MULTI-OBJECTIVE OPTIMIZATION (II) Session chair: Marko Mäkelä **Lecture hall A122**
15:45-16:05	AUTOMATIC AFFINITY DETECTION FOR CATEGORICAL VARIABLES IN SURROGATE-BASED OPTIMIZATION USING DIMENSIONALITY REDUCTION **Charlotte Beauthier**, Rajan Filomeno Coelho, Sylvério Pool Marquez, Caroline Sainvitu, Annick Sartenaer	INTERACTIVE MULTIOBJECTIVE OPTIMIZATION IN SUPPORT OF CLIMATE SMART FORESTRY **Juho Roponen**, Vili Kärkkäinen, Matias Nieminen, Bhupinder Saini, Veera Tahvanainen, Jari Vauhkonen
16:05-16:25	EFFICIENT SHAPE OPTIMIZATION OF TPMS HEAT EXCHANGERS VIA RBF-FD MESHLESS METHOD AND REDUCED ORDER TECHNIQUES **Fausto Dicech**, Riccardo Zamolo, Lucia Parussini	APPLICATION OF NATURE-INSPIRED OPTIMIZATION TECHNIQUES FOR AUTOMATED FINITE ELEMENT MODEL UPDATING OF A HISTORICAL MASONRY BELL TOWER **Shahin Sayyad**, Loredana Contrafatto, Simone Scalisi, Davide Li Rosi, Massimo Cuomo
16:25-16:45	CONSTRAINED GEOMETRIC OPTIMIZATION OF IMMERSED BOUNDARIES FOR MODELING HYDRAULIC DIODES **L. Groussy**, M. Belliard, P. Sagaut, O. Pantz	BENCHMARKING DISTRIBUTED OPTIMIZATION FORMULATIONS WITH A MULTIDISCIPLINARY FEASIBLE APPROACH FOR AERO-STRUCTURAL AIRCRAFT DESIGN **Fabian Volle**, Eric Schaar, Yann David
16:45-17:05	MULTI-FIDELITY OPTIMISATION STRATEGY BASED ON HYBRID METHODS Agustí Porta Ko, Sergio González Horcas, Jordi Pons-Prats, Gabriel Bugeda, **Jordi Ventura**	TOWARDS AERO-STRUCTURAL OPTIMIZATION USING THE NEW CFD SOFTWARE BY ONERA, DLR, AIRBUS (CODA) **Markus Widhalm**, Fabian Volle, Adam Büchner, Franziska Kasielke

17:15	Bus transportation from the LUT university campus to the hotels
18:30	Bus transportation from the conference hotels to the conference banquet
19:00–22:00	**Conference Banquet** in **Bistro & Bar *Kokka,*** Address Borupinraitti 4 Bus transportation to the conference hotels after the dinner

THURSDAY, SEPTEMBER 18

8:00	Bus transportation from the conference hotels to the LUT university campus

PARALLEL SESSIONS	**MINI-SYMPOSIUM ON** PARTIAL DIFFERENTIAL EQUATIONS-GOVERNED MODELS AND OPTIMIZATION IN ENGINEERING APPLICATIONS proposed by Rabia Altunay, Jarkko Suuronen Session chair: Rabia Altunay	**THEMATIC SESSION ON** BAYESIAN OPTIMIZATION Session chair: Lassi Roininen
9:00-10:30	**Auditorium 1**	**Lecture hall A122**
9:05-9:25	COMPUTATIONAL METHODS FOR DESIGN OPTIMIZATION **Eero Immonen**	TOWARD SYSTEM-LEVEL CO-DESIGN: A MULTI-LEVEL SURROGATE FRAMEWORK FOR POWER CONVERTER COMPONENT OPTIMIZATION **Shuai Guo**, Qian Li
9:25-9:45	IDENTIFYING HIDDEN PARAMETERS IN CELLULAR AUTOMATA WITH NEURAL NETWORKS **Valery N. Ashu**, Zhisong Liu, Andreas Rupp, Heikki Haario	PARAMETRIC OPTIMIZATION OF RIGID BAFFLES ON LIQUIDFILLED TANKS SUBJECTED TO SLOSHING USING XFEM AND BAYESIAN OPTIMIZATION **Luc Laurent**, Antoine Legay, Christophe Hoareau
9:45-10:05	TOPOLOGY OPTIMIZATION OF PERSONALIZED DRUGS **Rabia Altunay**	OPERATOR-THEORETIC AND QUANTUM-INSPIRED FRAMEWORKS FOR DATA-DRIVEN MODELING OF NONLINEAR DYNAMICAL SYSTEMS **Joanna Slawinska**, Dimitris Giannakis
10:05-10:25	MATHEMATICAL MODELING OF DRUG DISSOLUTION **Jarkko Suuronen**	CORRECTING BIAS IN DYNAMICAL MODELS **Miracle Amadi**, Lassi Roininen

10:30-11:00	**COFFEE BREAK**

SESSIONS 11:00-12:10	**MINI-SYMPOSIUM ON** CLEAR SESSION: CONTROL DESIGN FOR ENVIRONMENTAL ADVANCEMENT AND RESEARCH (II) proposed by S. Bezzaoucha, C. Choquet, É. Comte Session chairs: C. Choquet, S. Bezzaoucha **Auditorium 1**

11:05-11:25	HOW TO SURVIVE SEVERE DISRUPTIONS IN ENERGY SYSTEMS **Ghazaleh Saboori**, Soumen Atta, Giovanni Misitano, Babooshka Shavazipour
11:25-11:45	MULTI-STAGE MULTI-SCENARIO MULTI-OBJECTIVE OPTIMIZATION FOR ADAPTIVE ROBUST ENERGY TRANSITION UNDER EEPUNCERTAINTY **Babooshka Shavazipour**
11:45-12:05	MULTI-OBJECTIVE LINEAR PROGRAMMING FOR ENVIRONMENTAL AND ENERGY COSTS IN RENEWABLE ENERGY SITE SELECTION WITH SPATIAL INTERACTION **Michael Emmerich**, Jonas Schwaab

PLENARY PRESENTATION and CLOSING OF THE CONFERENCE, Auditorium 1

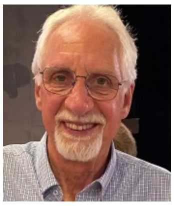
12:15 -13:00	**Plenary presentation by W. J. Vankan:** *Design and Optimization of HAR Composite Wings for SMR Aircraft – Multi-Disciplinary Analyses, Sizing, and Wind-Tunnel Experiments* Chair: Dietrich Knörzer
13:00-13:15	**CLOSING OF THE CONFERENCE** Speakers: Conference Chairs

13:15-14:00	**LUNCH**

13:30	Bus transportation to Helsinki airport. Note earlier departure time.

Speakers

Dr.-Ing. Dietrich Knörzer



Title of Plenary Speech:
30 Years of EUROGEN – Evolutionary Algorithms in Engineering and Computer Science

Dr.-Ing. Dietrich Knörzer holds a degree in Aerospace Engineering of the RWTH Aachen University. He worked as a research fellow in mathematical modelling in materials science at the RWTH Aachen University from 1980 to 1985 and got his PhD degree (Dr.-Ing.) in creep mechanics.

From 1985 he worked for the Airbus partner MBB in Hamburg/Germany (today Airbus Operations) on advanced technologies as hypersonic and hydrogen use for civil aircraft.

In 1989, he joined the Directorate General for Research of the European Commission in Brussels. Within the EU Research Framework Programmes, he worked as a senior scientific officer for research and innovation in aeronautics and transport. He was responsible for research activities mainly in aircraft design, flight physics and computational fluid dynamics.

He was the contact and project officer for scientific networks and research support actions related to aerospace. He was the scientific officer for the INGENET network with its EUROGEN short courses and conferences.

Since he retired from the European Commission in December 2016. Since he is active as an independent aeronautics expert and consultant, based in Brussels.

He is the vice-chair of the Stakeholders Advisory Board of the European Aerospace Science Network (EASN), the network of European universities performing aerospace research. Since 2021, he is a correspondent member of the AAE - the Air and Space Academy, Toulouse.

Speakers

Prof. David Greiner,
University of Las Palmas de Gran Canaria, Spain

Title of Plenary Speech:
Hybridizing Surrogate Modeling and Evolutionary Algorithms for Optimum Engineering Design Problems in Computational Engineering

Dr. David Greiner is an Associate Professor at the Civil Engineering Department and the Institute of Intelligent Systems and Numerical Applications in Engineering (SIANI) at the Universidad de Las Palmas de Gran Canaria (ULPGC), Spain. He holds a degree in Industrial Engineering (Mechanical) and a PhD in Intelligent Systems and Numerical Applications in Engineering.

Since 1995, Dr. Greiner's research has focused on optimal design in engineering applications using evolutionary algorithms. His extensive publication record includes over 120 works, encompassing JCR-indexed journal articles, edited books, book chapters, and presentations at national and international conferences. He has actively contributed to various national and international research projects, including the INGENET research network funded by the European Union (1997–2002). Additionally, he has held visiting scholar positions at Rensselaer Polytechnic Institute in the USA and the University of Jyväskylä in Finland.

Dr. Greiner has served as a reviewer for more than 30 JCR-indexed journals (including Elsevier, Springer, IEEE, and MDPI) and as an organizer or scientific committee member for numerous international conferences, such as EUROGEN, CMN, GECCO, IEEE-CEC, Civil-Comp Conferences, and ECTA.

Notably, he has served as General Chair for:
- EUROGEN 2013
- The XVIII Spanish-French School "Jacques-Louis Lions" on Numerical Simulation in Physics and Engineering (EHF 2018)
- The Spanish-Portuguese Congress on Numerical Methods in Engineering (CMN 2022)

Dr. Greiner has also held various administrative roles at ULPGC, including Vice-Dean of the Industrial and Civil Engineering School (2007–2013), Academic Secretary and Deputy Director at the SIANI Institute (2014–2017), and Director of Scientific Organization and Research at the Vicerrectorate of Research & Innovation (2017–2021).
Dr. Greiner's dedication to research, teaching, and scientific collaboration underscores his significant contributions to computational engineering and optimization techniques.

Speakers

Cornelia Grabe,
German Aerospace Center DLR, Germany

Title of Plenary Speech:
The Potential of Data-Driven Turbulence Modeling for Industrially-Relevant Aerodynamic Applications

Dr. Cornelia Grabe's presentation will explore the integration of adjoint-based methods and machine learning for data-driven approaches to turbulence modeling. These innovative methods promise higher prediction accuracy, improving the effectiveness of turbulence models in design and optimization—a topic closely aligned with the conference's focus on advancing computational engineering solutions.

Dr. Grabe earned her PhD from the University of Stuttgart in 2012. Following this, she joined the C²A²S²E department (Center for Computer Applications in Aerospace Science and Engineering) within the Institute of Aerodynamics and Flow Technology at the German Aerospace Center (DLR) in Göttingen as a postdoctoral researcher. Her work focused on developing CFD-compatible laminar-turbulent transition models for aircraft applications.

In 2017, Dr. Grabe became the head of the C²A²S²E department, and since 2023, she has also served as Deputy Head of the Institute of Aerodynamics and Flow Technology in Göttingen, overseeing aeronautical research and the development of numerical methods.

Dr. Grabe's expertise lies in the development of advanced computational tools for aerospace applications. Under her leadership, the C²A²S²E department has been at the forefront of developing compressible CFD solvers such as TAU and CODA, cutting-edge turbulence and transition models, multi-disciplinary analysis and optimization methods, reduced-order and surrogate models, and scale-resolving simulation methods. These tools are widely applied in aerospace industries and academic institutions across Europe, reinforcing her authority in the field.

Speakers

Rainald Löhner,
PhD, DSc, George Mason University, USA

Title of Plenary Speech:
High-Fidelity Digital Twins: Detecting and Localizing Weaknesses in Structures

Dr. Rainald Löhner is the head of the Computational Fluid Dynamics (CFD) Center at the College of Science, George Mason University, located in Fairfax, Virginia, near Washington, D.C. He earned his MSc in Mechanical Engineering from Technische Universität Braunschweig in Germany and holds both a PhD and DSc in Civil Engineering from the University College of Swansea, Wales.

Dr. Löhner's research interests encompass a wide range of fields, including numerical methods, field solvers, grid generation, parallel computing, visualization, pre-processing, fluid-structure interaction, shape and process optimization, digital twins, and computational crowd dynamics. His innovative codes and methodologies have been widely applied across diverse industries and research domains, such as:

- **Aerodynamics:**
  Analysis of airplanes, drones, cars, and trains.
- **Hydrodynamics:**
  Studies on ships, submarines, and underwater autonomous vehicles (UAVs).
- **Shock-Structure Interaction:**
  Simulation and assessment of dynamic stress effects.
- **Dispersion Analysis:**
  Urban area modeling for safety and environmental studies.
- **Haemodynamics:**
  Research on vascular diseases and blood flow dynamics.
- **Turbulence Studies:**
  Fundamental investigations of chaotic and turbulent flows.
- **Crowd Dynamics:**
  Modeling and optimizing evacuation strategies and the management of mass events.

Dr. Löhner has authored more than 800 scientific publications, including a widely respected textbook, *Applied CFD Techniques*. He also serves on the editorial boards of seven international scientific journals.

Speakers

Marko Mäkelä,
University of Turku, Finland

Title of Plenary Speech:
Nonsmooth Optimization:
From Theory to Methods and Applications

Professor Marko M. Mäkelä, a leading expert in applied mathematics, serves as Vice Head of the Department of Mathematics and Statistics at the University of Turku, Finland. He earned his Ph.D. in Computer Science from the University of Jyväskylä in 1990.

Nonsmooth optimization (NSO) is one of the most challenging areas in deterministic optimization, dealing with problems where the objective or constraint functions have discontinuous gradients. NSO has critical applications in diverse fields, including optimal control, engineering, computational chemistry, data analysis, and machine learning. Beyond these direct applications, smooth optimization techniques—such as decomposition methods, dual formulations, and exact penalty methods—often lead to NSO problems that are smaller in dimension or simpler in structure. Additionally, optimization problems that are analytically smooth may exhibit nonsmooth behavior numerically, further broadening the relevance of NSO.

Professor Mäkelä's research spans nonsmooth and nonconvex analysis, multiobjective optimization, and the application of these techniques to solve real-world industrial problems. His extensive expertise in the theory and practice of NSO makes his contributions invaluable to the field of computational mathematics.

Speakers

Dr. W. J. Vankan,
Netherlands Aerospace Centre, Netherlands

Title of Plenary Speech:
Design and Optimization of HAR Composite Wings for SMR Aircraft – Multi-Disciplinary Analyses, Sizing, and Wind-Tunnel Experiments

Dr. Jos Vankan holds an MSc in Mechanical Engineering and a PhD in Biomechanics from TU Eindhoven, the Netherlands. With over 25 years of experience as an R&D engineer, senior scientist, and principal scientist at the Royal Netherlands Aerospace Centre (NLR) in Amsterdam, he is a recognized leader in aeronautical research and development. He currently serves as a principal scientist in NLR's Aerospace Vehicles Division and is a member of the NLR Science Society, which ensures the scientific quality of the organization's work.
Dr. Vankan has been extensively involved in numerous international multidisciplinary aeronautical R&D projects over the course of his career. His expertise lies in multidisciplinary and multi-objective design optimization, with significant contributions in the following areas:

- **HAR Wing Design:**
  NLR R&D lead in the UPwing project, focusing on high-aspect-ratio (HAR) multifunctional wing design and advancements in novel control technologies.
- **Aircraft Concept Studies:**
  Lead researcher in studies on aircraft concepts and powertrain systems across various international research projects.
- **Composite Manufacturing Techniques:**
  Contributions to technology developments in thermoplastic composites manufacturing and assembly techniques, such as induction welding modeling, in recent research initiatives.
- **Aero-Structural Modeling:**
  Involvement in aero-structural modeling and design of composite fan blades for scaled wind-tunnel testing of turbofan engines.

Dr. Vankan's long-term dedication to advancing aeronautical technologies and his involvement in cutting-edge international projects make him a pivotal figure in the aerospace research community.

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Lahti, Finland, 16–18, 2025

MACHINE LEARNING AND DATA-DRIVEN INNOVATIONS IN AERODYNAMIC OPTIMIZATION AND UNCERTAINTY QUANTIFICATION

ESTHER ANDRES PEREZ*, RODRIGO CASTELLANOS+, DOMENICO QUAGLIARELLA†

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Keywords: data-driven models, aerodynamic analysis, machine learning, scientific machine learning

Abstract of the session

In recent years, the surge in data from computational sciences has underscored its potential to deliver insights and enhance predictive capabilities. In aerodynamics, extensive studies and optimizations yield large volumes of valuable data, creating an opportunity to advance data-driven and data-fusion models in engineering [1]. Yet, the integration of these models is still developing, with best practices only beginning to form.

Machine learning, including neural networks, offers a robust toolkit for tasks like clustering, dimensionality reduction, classification, and regression. However, processing and preparing aerodynamic and geometric data poses notable challenges. These tasks are often complex and objective-specific, leading to varied interpretations and applications of data-driven methods. Integrating machine learning techniques, commonly used in AI and Data Mining, promises substantial reductions in computational costs for aerodynamic analysis and uncertainty quantification [2]. These advanced methods open a pathway toward efficient, accurate solutions in aerodynamic design, despite ongoing challenges in data handling and model maturity.

This minisymposium aims to showcase new approaches and recent progress in applying machine learning and data-driven techniques for aerodynamic analysis and uncertainty quantification, with a focus on practical challenges and on the new opportunities that Scientific Machine Learning, i.e. the fusion of advanced Machine Learning techniques with Scientific Computing, offers for the development of increasingly efficient and effective analysis and design methodologies.

REFERENCES

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TOPOLOGY OPTIMIZATION OF VISCOELASTIC COMPOSITES USING COMPLEX-VALUED HOMOGENIZATION

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Keywords: Viscoelasticity, Topology optimization, Acoustic impedance, Homogenization method, Adjoint variable method, Wave attenuation

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Abstract

Viscoelastic materials, which exhibit both energy storage and dissipation, play a critical role in noise and vibration control. Unlike purely elastic materials, their mechanical behavior is characterized by complex-valued parameters, such as the complex Young’s modulus, to model internal damping. However, most existing topology optimization frameworks are formulated for real-valued material parameters, limiting their applicability to viscoelastic systems.

In this study, we propose a topology optimization method for viscoelastic-elastic composites based on complex-valued homogenization. The goal is to design microstructures that enhance wave attenuation by effectively combining elastic and viscoelastic phases. The material distribution within each periodic unit cell is described using a continuous density function, which interpolates between the elastic and viscoelastic material phases. Through complex homogenization, we compute the effective (homogenized) material constants that capture both wave propagation and attenuation characteristics.

A key contribution of this work is the derivation of sensitivity expressions for objective functions defined by either the real or imaginary part of the complex homogenized coefficients. We confirm the validity of these expressions by showing agreement between gradients obtained via the adjoint method and finite-difference-based sensitivity results. These findings lay the groundwork for the systematic design of viscoelastic microstructures with tailored damping properties, thereby contributing to the development of advanced materials for noise and vibration control systems.

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DEVELOPMENT OF EFFICIENT EVOLUTIONARY ALGORITHMS BY EXTRACTING IMPLICIT KNOWLEDGE FROM THE OPTIMIZATION PROCESS

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Keywords: Genetic algorithm, implicit knowledge, clustering, opposition-based learning, optimization efficiency

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Abstract

Typically, optimization methods applying machine learning are based on a series of existing datasets, these pre-prepared data containing prior knowledge will naturally greatly limit the exploration and exploitation capabilities during the evolutionary process. The optimization process itself generates a large amount of data, which contains a lot of useful information, such as the convergence of the population towards the dominant regions and the gradual contraction of the search space.

We propose a new idea that does not rely on a pre-prepared database with prior knowledge, but learns directly from the data generated in the optimization process and extracts the implicit knowledge in it to guide the optimization and thus improve the optimization efficiency. The population is dynamically divided through clustering operations and

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ON THERMODYNAMIC TOPOLOGY OPTIMIZATION WITH AN IMPLEMENTED THIRD MEDIUM REGULARIZATION SCHEME

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Keywords: frictionless contact, hyperelasticity, finite deformations, topology optimization

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Abstract

Topology optimization of hyperelastic structures is an ongoing challenge in which the large deformation of low-density elements, i.e. void regions, can cause numerical instabilities. The overall deformation field of the resulting optimized structure should not be impaired by those void regions. However, due to numerical stability issues, the residual stresses cannot completely vanish self-penetration is not desired either. Previous studies have shown several solution strategies to implement these aspects to the behavior of the void. Hereby the third medium method is most promising enabling (self-)contact of the structure. Most approaches require higher gradient theory within the finite element method. But one of the latest approaches regularizes the rotation of the void elements and thus enables the simulation of a contact problem using linear shape functions.

In the present work, the third medium approach with linear shape functions will be solved in a staggered manner using the Neighbored Element Method. Thereby the additional field of variables, which occurs due to the regularization of the rotation, does not relate to additional degrees of freedom within the finite element discretization but are instead updated by solving the partial differential equation with a generalized finite difference scheme. It will be shown that this solution strategy reduces the calculation time and results in a proper self-contact of the structure. Furthermore, the implementation of the Neighbored Element Method enables a convenient implementation of the thermodynamic topology optimization, since the solution scheme used for the density update is analogous to the solution for the void regularization. The effect of the third medium approach within the topology optimization will be shown in several numerical examples.

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GRADIENT-ENHANCED BAYESIAN OPTIMIZATION FOR AERODYNAMIC DESIGN

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Keywords: Bayesian optimization, surrogate modeling, design optimization

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Abstract

We present a multi-objective Bayesian optimization framework that integrates a derivative-enhanced Gaussian Process Regression surrogate model to efficiently explore the Pareto front in aerodynamic design problems. Classical Bayesian optimization methods often suffer from over-exploration and reduced performance, particularly as the dimensionality of the design space increases. Our framework addresses these challenges by incorporating arbitrary directional derivatives of multiple objective functions alongside their functional values, significantly improving prediction accuracy and model fidelity. By capturing underlying trends more effectively, the approach mitigates over-exploration and enables a more focused and efficient search for optimal trade-offs. To demonstrate its effectiveness, we apply the framework to benchmark aerodynamic optimization problems from the SU2 repository, targeting objectives such as drag minimization, lift maximization, and geometric constraints. Results show that selectively incorporating gradient information into the surrogate model substantially improves convergence rates and enhances the quality of the identified Pareto fronts. These findings highlight the potential of gradient-enhanced surrogate models to accelerate multi-objective aerodynamic design optimization while maintaining robust and accurate Pareto front approximations, even in high-dimensional settings.

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A FICTITIOUS PHYSICAL MODEL FOR VISIBILITY EVALUATION AND ITS APPLICATION IN ENGINEERING DESIGN

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Keywords: Visibility evaluation, Fictitious physical model, Finite element method, Topology optimization, Geometric features, Structural design

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Abstract

In many engineering applications, maintaining adequate visibility is essential for ensuring safety, usability, and operational efficiency. Scenarios such as construction sites, factory layouts, or automotive design demand unobstructed lines of sight to critical regions. However, enhancing visibility often requires geometric modifications—such as reducing material thickness or introducing cutouts—that may compromise the structural integrity of a design. This trade-off between mechanical performance and visibility presents a significant challenge in traditional design processes, which typically address these aspects sequentially through trial-and-error methods. Such workflows not only increase development time but may also yield suboptimal or impractical designs.

Given these challenges, it is imperative to develop a unified design methodology that concurrently optimizes structural performance and visibility. Unfortunately, there is currently no effective model for quantifying visibility without resorting to labor-intensive trial-and-error iterations, leaving a notable gap in structural design and optimization workflows. To address this issue, we construct a fictitious physical model, which yields a virtual scalar field whose distribution naturally reflects visibility conditions from multiple observation points. Moreover, by formulating the model within a level-set framework, we ensure seamless integration with established level-set-based topology optimization processes.

Finally, we validate the proposed model through a series of practical examples. The results demonstrate that the proposed model can be successfully incorporated into a topology optimization framework, achieving significantly enhanced visibility with only modest compromises in structural performance. We will present detailed numerical examples and offer a comprehensive discussion of our approach at the upcoming conference.

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A DATA-DRIVEN APPROACH FOR TURBULENCE MODELLING OF LAMINAR SEPARATION BUBBLES

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Key Words: *RANS turbulence modelling, data-driven, deep neural network, low-Reynolds number regime*

Abstract

The simulation of laminar separation bubbles (LSB) occurring in low-Reynolds number flows presents severe turbulence modeling issues. Indeed, LSBs are characterized by separation in laminar regime, while turbulence models are calibrated for flows separating in turbulent regime. Moreover, transition takes place in the separated region with a boost of turbulent kinetic energy, leading to the re-attachment of the flow.

This paper discusses the potential for a data-driven approach to address the issue of simulating laminar separation bubbles. Longobardo *et al*. [1] have proposed the field-inversion machine-learning (FIML) method, which involves a two-step process: the first step derives a functional correction of the turbulence model in the form of a spatially (or even spatio-temporally) varying field variable β whose value is determined through an inverse problem; once the unknown β correction is defined in terms of spatial variables, its functional form must be converted into an input-feature dependence through a machine learning algorithm (step 2).

The field inversion procedure allows, for a given high-fidelity simulation, the identification of a correction factor for the turbulence production term, which, once introduced as a field term in the $k - \omega - \gamma$ turbulence model, allows for significantly enhancing the RANS predictions of laminar bubble formation, bringing them closer to those produced by Large Eddy Simulations (LES). The field inversion procedure can create a map between the LES and RANS fields but cannot generate a correction field without an available high-fidelity solution. The present work aims to build an operator that generates the correction factor starting from the RANS local field data. Therefore, a deep neural network trained with the LES-RANS mappings obtained in a limited number of field inversion runs provides, for each single computational cell of a finite volume RANS solver mesh, the value of the correction factor β as a function of the values of the field variables and the spatial coordinates of the computational cell in question and of the neighboring ones. The deep network model adopted is DeepONet [2], which performs well in approximating nonlinear operators.

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TOPOLOGY OPTIMIZATION OF VISCOELASTIC COMPOSITES USING COMPLEX-VALUED HOMOGENIZATION

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Keywords: Viscoelasticity, Topology optimization, Acoustic impedance, Homogenization method, Adjoint variable method, Wave attenuation

Abstract

Viscoelastic materials, which exhibit both energy storage and dissipation, play a critical role in noise and vibration control. Unlike purely elastic materials, their mechanical behavior is characterized by complex-valued parameters, such as the complex Young's modulus, to model internal damping. However, most existing topology optimization frameworks are formulated for real-valued material parameters, limiting their applicability to viscoelastic systems.

In this study, we propose a topology optimization method for viscoelastic-elastic composites based on complex-valued homogenization. The goal is to design microstructures that enhance wave attenuation by effectively combining elastic and viscoelastic phases. The material distribution within each periodic unit cell is described using a continuous density function, which interpolates between the elastic and viscoelastic material phases. Through complex homogenization, we compute the effective (homogenized) material constants that capture both wave propagation and attenuation characteristics.

A key contribution of this work is the derivation of sensitivity expressions for objective functions defined by either the real or imaginary part of the complex homogenized coefficients. We confirm the validity of these expressions by showing agreement between gradients obtained via the adjoint method and finite-difference-based sensitivity results. These findings lay the groundwork for the systematic design of viscoelastic microstructures with tailored damping properties, thereby contributing to the development of advanced materials for noise and vibration control systems.

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PROPELLER BLADES SHAPE OPTIMIZATION USING HYBRID GENETIC ALGORITHMS AND SURROGATE MODELS

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Keywords: Aerodynamic Shape Optimization, Propeller Design, Hybrid Genetic Algorithms, Surrogate Modeling, Blade Element Momentum Theory.

Abstract

The optimization of aerodynamic components in aerospace applications increasingly relies on the integration of machine learning, surrogate modeling, and evolutionary algorithms to accelerate and enhance the design process[1]. However, achieving high-fidelity aerodynamic optimization at a reasonable computational cost remains a significant challenge. This study presents a novel approach to the aerodynamic shape optimization of propeller blades for fixed-wing, propeller-driven aircraft during cruise conditions, emphasizing enhanced propulsive efficiency. The methodology combines low-cost physics-based models, neural surrogate methods, and a state-of-the-art hybrid genetic optimization framework.

The aerodynamic performance of the propeller is evaluated using an in house **Blade Element Momentum Theory (BEMT)** solver, offering a low-fidelity, computationally efficient method that estimates thrust and power. Sectional airfoil performance— critical for capturing lift and drag characteristics—is obtained from **NeuralFoil**, a surrogate model implemented through **AeroSandbox** and trained on a comprehensive dataset combining simulation results with analytical and empirical models, enabling fast and reliable evaluations across varied airfoil geometries[2]. Design variables include the sectional chord and blade twist, and sectional airfoil shapes parameterized via the **Kulfan Class-Shape Transformation** method, which enables a compact, smooth, and flexible geometric representation across the blade span.

Optimization is performed using **HyGO (Hybrid Genetic Optimization)**, an in house Python-based toolbox that combines the global search capabilities of genetic algorithms with the local refinement efficiency of the Downhill Simplex (Nelder–Mead) method[3]. HyGO's hybridization strategy improves convergence while preserving diversity and robustness across high-dimensional, non-convex design spaces.

The integration of NeuralFoil ensures airfoil-level fidelity is preserved without introducing prohibitive computational expense and leveraging the knowledge of existing airfoil databases. Coupled with the BEMT, this framework provides a physics-based, cost-effective, and rapid evaluation capability. Meanwhile, HyGO effectively explores complex design spaces while efficiently exploiting local minima to identify high-performing geometries. In conclusion, this integrated framework enables efficient and reliable aerodynamic optimization of propeller blades, making it well-suited for early-stage propeller design phases in aerospace applications.

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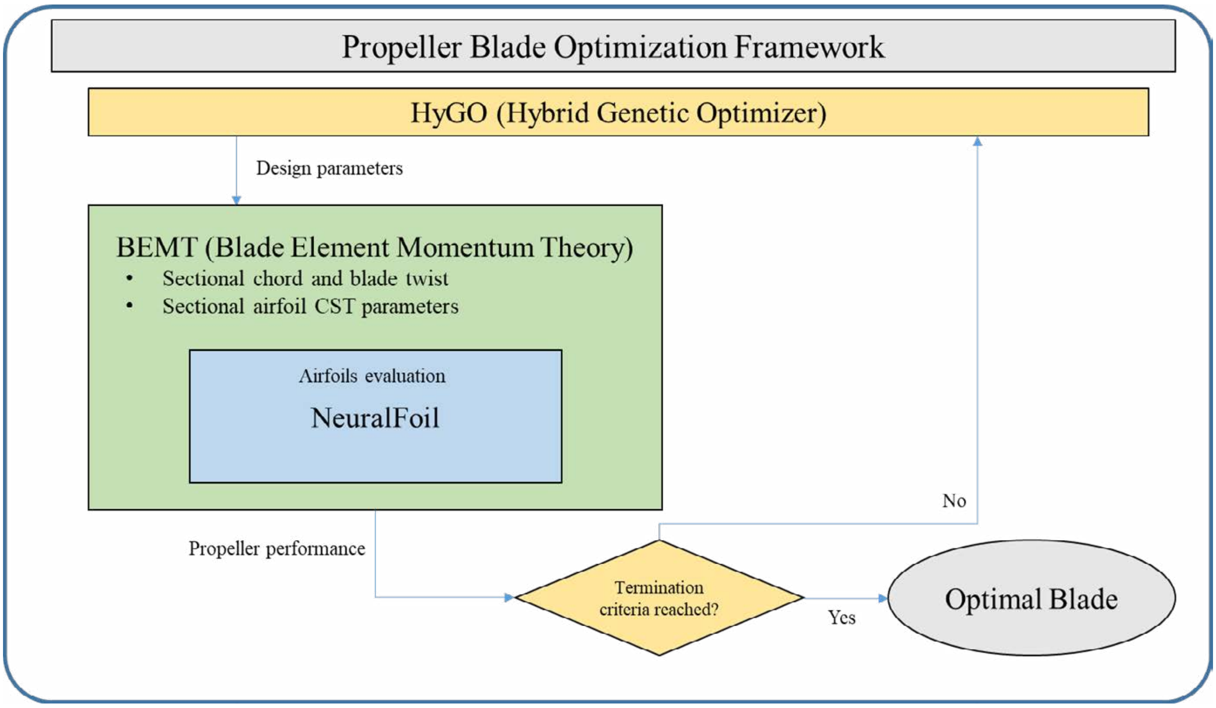

Figure 1. Flowchart for propeller blade optimization using in the integrated framework.

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CLEAR SESSION: CONTROL DESIGN FOR ENVIRONMENTAL ADVANCEMENT AND RESEARCH

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Keywords: control, modeling, sustainability, optimization, and robustness

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Abstract of the session

*The pressing challenges of environmental degradation call for innovative approaches in research and technology. This mini-symposium, titled "**CLEAR** session: **C**ontro**L** Design for **E**nvironmental **A**dvancement and **R**esearch", aims to bring together experts to discuss advancements in control theory and green engineering tailored to address environmental challenges.*

The focus will be on cutting-edge methods in control design, optimization, and system modeling for sustainable energy systems. Special attention will be given to managing pollution growth and stock, optimizing water allocation in irrigation systems, and ensuring ecological balance in lake ecosystems.
The goal is to demonstrate how results from theoretical mathematics, non linear control design approaches, and tools inspired by developments in artificial intelligence can be articulated to provide new solutions.
Key topics include:
- *Modeling and control of lake ecosystems for pollution mitigation and ecological preservation.*
- *Optimal and robust control strategies.*
- *Integration of environmental sustainability into control frameworks for water systems.*

The symposium aspires to foster interdisciplinary collaboration, bridging the gap between theoretical mathematical research and practical implementation.

Presentations of the session (totally 2 hours)

1. **Catherine Choquet, A machine learning algorithm for water quality control (25+5 min)**
2. **Éloïse Comte, Optimal control for lake eutrophication: A Dirichlet boundary control problem (25+5 min)**
3. **Souad Bezzaoucha, Polytopic approach for stability and control design of Saint-Venant equations (25+5 min)**
4. **Ruben Chenevat, Optimizing crop irrigation under biological and operational constraints with meteorological uncertainty (25+5 min)**

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OPTIMAL CONTROL FOR LAKE EUTROPHICATION: A DIRICHLET BOUNDARY CONTROL PROBLEM

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Keywords: Optimal control, Nonlinear PDEs, Dirichlet boundary control, Water pollution

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Abstract

Anthropogenic activities are constantly growing and affect the water quality resources.
One of consequences in lakes is the accumulation of nutrients (from watersheds activities), as phosphorus, which implies a cyanobacteria development and thus a perturbation of the ecosystem and a risk for human and animal health: it is called eutrophication.
We present a Dirichlet boundary control problem for the lake eutrophication, where we look for a trade-off between the benefits linked with the water contamination and the damages for the lake users. We consider the control as the input area of phosphorus from the watershed into the lake, which is only defined on the lake shore. The state problem is given by coupled nonlinear partial differential equations modeling the cyanobacteria concentration and the phosphorus stock dynamics.
We generally use a lifting of the control from the boundary into the whole domain for treated this class of control problem. We discuss the originality of the model and detail the shifting of the control. The well-posedness of the state problem and the existence of a global solution for the optimal control problem are proved.

C. Choquet and É. Comte, Optimal control of lake eutrophication. *Journal of Mathematical Analysis and Applications*, 528(2), 2023.

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ADAPTIVE BI-FIDELITY MONTE CARLO ESTIMATION FOR RANDOM ELLIPTIC PDES

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Keywords: uncertainty quantification, multi-fidelity Monte Carlo, neural networks, reduced models, finite element methods, parametrized PDEs

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Abstract

Monte Carlo (MC) estimation for random partial differential equations (PDEs) aims to estimate moments of a quantity of interest derived from the solution of the PDE. In this work, we derive an adaptive bi-fidelity Monte Carlo (ABFMC) estimator for the random Poisson equation in two dimensions. As the PDEs diffusion coefficient depends on both the spatial variable and a random variable, the solution is a random variable as well.

While the standard MC estimator approximates the expectation of the solution using independent and identically distributed samples, the ABFMC estimator combines high-fidelity and low-fidelity MC estimators. The high-fidelity estimator relies on finite element solutions, whereas the low-fidelity utilizes a neural network. Recognizing the reduced accuracy of the low-fidelity model, we demonstrate how the ABFMC estimator leverages its lower computational cost to achieve faster convergence rates than the standard MC estimator. In the process we prove the existence of a standard ReLu-neural network which is able to approximate the finite element solutions arbitrarily well, thereby justifying the use of a neural network as valid low-fidelity estimator.

Numerical experiments for different diffusion coefficients reveal that the mean squared error of the ABFMC estimator decreases at a significantly faster rate compared to the standard MC estimator for the same computational budget. More precisely, we observe that the ABFMC estimator achieves a convergence rate close to quadratic in the number of samples, whereas the standard MC estimator follows a linear convergence rate.

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POLYTOPIC APPROACH FOR STABILITY & CONTROL DESIGN OF SAINT-VENANT EQUATIONS

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Keywords: Polytopic approach, control design, shallow water flows, Saint-Venant equations.

Abstract

The polytopic approach offers a powerful framework for addressing the stability and control design of systems with parameter-dependent dynamics, especially when these parameters vary within a known range. Applying this to the Saint-Venant equations, which are nonlinear partial differential equations (PDEs) modeling shallow water flows (such as in rivers, channels, or urban drainage), is a way to handle uncertainties and nonlinearities.
Indeed, the Saint-Venant equations describe the conservation of mass and momentum in open-channel flow. They are typically nonlinear and can be quite challenging for stability and control design due to their inherent nonlinearities and the presence of varying physical parameters such as water height, flow velocity, channel slope, and friction coefficients. These parameters are often subject to uncertainties and spatial-temporal variations, making classical linear control methods inadequate or overly conservative.
The polytopic approach helps by approximating these nonlinear PDEs with a set of linear parameter-varying (LPV) models, whose parameters stay within a convex polytope. The key advantage of the polytopic method is that by guaranteeing stability and performance at these vertex systems through Linear Matrix Inequalities (LMIs), one can ensure robust stability and control for all parameter variations within the polytope due to convexity properties. Furthermore, by seeking a common Lyapunov function valid for all vertices, the method ensures global stability over the entire operating range, which is essential for the practical control of water systems exposed to dynamic inflows, environmental disturbances, and structural uncertainties.
The polytopic approach thus provides a systematic and computationally tractable way to design controllers capable of regulating water levels, flow rates, or other objectives in open-channel flows while explicitly considering model uncertainties and nonlinearities through the convex hull of parameter variations. This makes it an appealing strategy for modern water management challenges, where safety, resilience, and efficiency are critical under uncertain and time-varying conditions.

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CFD-DRIVEN ROBUST OPTIMIZATION OF TRANSONIC AERODYNAMIC SHAPES

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Keywords: Robust Optimization, Uncertainty Quantification, Polynomial Chaos

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Abstract

Within the Computational Fluid Dynamics (CFD) community, the impact of uncertainties on flow simulation outcomes and CFD-driven optimization processes has become increasingly important. In industrial applications, uncertainties stemming from geometrical variations (e.g., manufacturing tolerances, wear and tear, flight deformation due to wing flexibility) and aerodynamic conditions are commonly assessed using non-intrusive stochastic approaches. However, these methods are severely limited by the curse of dimensionality, where the number of simulations required increases rapidly with the number of uncertain parameters, posing significant computational challenges even for dozens of uncertain parameters.
In this work we will show how efficient Uncertainty Quantification (UQ) methods, based on generalized polynomial chaos expansion can be employed to overcome this bottleneck. The use of a combination of compressed sensing [2][3] and gradient information [1] (efficiently computed thanks to the adjoint approach) allows us to greatly reduce the number of simulation needed to precisely assess the statistics of the quantities of interest (drag and lift for instance). Once these statistics (mean and standard deviation for instance) and their gradients can be computed with enough accuracy, they can be used in the definition of the objective and constraint functions of the robust optimization process to replace deterministic quantities. The considered approach will be demonstrated on two aerodynamic shape optimization test cases: a transonic airfoil for open-rotor design and a high aspect ratio transonic wing with an uncertain twist law [4]. A discussion on the trade-of between computational cost and accuracy of the robust optimization is illustrated, along with a comparison with deterministic optimization results.

This study is supported by the ONERA research project HORUS and by the European research project NEXTAIR project (GA N° 101056732). Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

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OPTIMIZING CROP IRRIGATION UNDER BIOLOGICAL AND OPERATIONAL CONSTRAINTS WITH METEOROLOGICAL UNCERTAINTY

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Keywords: Optimal control, Crop irrigation, State constraints, Non-deterministic system, Non-smooth dynamics.

Abstract

The development of effective crop irrigation strategies is a key element of water management in agriculture, seeking a necessary parsimonious use of resources, especially in the context of climate change. We consider a simple Controlled Crop Irrigation (CCI) model, written with non-autonomous and non-smooth dynamics, that includes a state constraint taking into account biophysical processes, a budget constraint representing the water quota for the cropping season, and a term modeling the rainfall events which are assumed to be instantaneous thus generating non-deterministic jumps in the soil moisture state variable. We investigate the problem of maximizing the final biomass production under such operating constraints while dealing with unknown long-term weather conditions. In order to aim for efficient irrigation strategies, we suggest to proceed in two steps. First, we look for an average optimal long-term strategy, involving the use of average cost control tools with impulsive dynamics. Second, we consider adaptive strategies locally in time that adjust the irrigation scenario according to short-term weather forecast. Then we combine these long- and short-term strategies while still fulfilling the global state and budget constraints. Such irrigation strategies are suitable for operational purposes, and can be tested on more complex crop models or assessed through an experimental framework.

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GAUSSIAN PROCESSES FOR UNCERTAINTY QUANTIFICATION AND FAST EMULATION OF CHEMICAL KINETICS

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Keywords: Gaussian Process, Chemical Kinetics, Machine Learning, Surrogate Model, Uncertainty Quantification.

Abstract

In recent years, machine learning methods have been used to perform calculations in a large variety of fields and applications. One such field is that of chemical kinetics, or the study of the rates, reactants and products of a set of chemical reactions. Chemical kinetics are traditionally described in terms of Ordinary Differential Equations and tackled using numerical techniques. These traditional methods can be computationally expensive and time consuming, particularly when the system of equations is stiff, i.e. there are some aspects of the reactions that are numerically unstable, leading to rapid variations in the solutions. For many applications, especially those that involve large numbers of predictions, speeding up the calculations involved would be desirable. Of course, the key is to find a balance between maximizing the speed while minimizing the size of the errors that accompany any use of approximation. However, it is not just important that the approximation error is minimized, but also that the size of those errors is quantified explicitly and that their size is itself accurately reported. Such "statistically consistent" reporting of uncertainty is crucial if there is a need to ensure that the accuracy is within tolerance and if both over-confidence and over-caution are to be avoided. One machine learning method that provides a statistically consistent notion of uncertainty is a Gaussian Process. Here we present a Gaussian Process method that predicts the outcome of a set of chemical reactions, given both the input species and environmental conditions such as temperature and pressure. This Gaussian Process model can be trained on a relatively small amount of high-dimensional data and provides predictions and the associated uncertainty faster than the numerical techniques that would otherwise be used. Indeed, results show that, running a commodity PC, using a Gaussian Process can provide estimates 20 times

faster than a traditional solver (Cantera), while remaining highly accurate and providing a statistically consistent quantification of that accuracy. In one example case we consider, 552 input-output pairs were used to train a Gaussian Process. The input-output pairs are related to the time-evolution of the mass fraction of each of the 31 species. The training took 4 minutes and 54 seconds. The prediction of a single pair took an average of 2.6 milliseconds, which is faster than Cantera, which took 63.8 milliseconds on average. The results are shown to be both accurate and statistically consistent. Furthermore, it is shown that altering the compromise between accuracy and run-time does not adversely impact statistical consistency. Future work plans to integrate the Gaussian Process into a hydrocode, a bigger system involving chemical reactions taking place in each of a number of cells with mixing between the cells: using a Gaussian Process in this context is hoped to help understand how approximation errors propagate in the hydrocode.

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A MACHINE LEARNING ALGORITHM FOR WATER QUALITY CONTROL

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Keywords: PDEs models, Graph theory, Combinatorial optimization, Reinforcement learning

Abstract

Most flow and contaminant transport models (at least the most realistic ones) are based on conservation laws translated into partial differential equations. Analytical solutions to these problems can rarely be calculated, especially when combined with a control strategy. Numerical simulation tools are therefore implemented. Whatever the method used, with or without a mesh, points are chosen in the spatial and temporal domains where the solution will be approximated. These points can be seen as nodes of a (large) graph whose edges, for the examples discussed here, represent physical characteristics and system control.

The method we propose consists in interpreting an optimal control problem as a graph optimization problem, its topological structure and the weighting of its edges. In particular, we have developed an algorithm based on the optimal permutation of the edges of the graph, which allows to converge, via gradient descent, to the minimum of any sufficiently regular loss function.

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Lahti, Finland, September 16–18, 2025

A MULTIOBJECTIVE APPROACH TO EVALUATE SUITABLE BATTERY TECHNOLOGIES TO POWER HYBRID MEDIUM-RANGE AIRCRAFT

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Keywords: medium-range hybrid aircraft, electrical propulsion, Dempster-Shafer theory, multiobjective optimization, energy density, imprecise probability, uncertainty quantification

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Abstract

The development of high-performance battery systems is a critical challenge for the advancement of hybrid-electric aircraft. This work aims to develop an optimization procedure capable of correlating the performance level required by design constraints to the time framework when this performance level will be available. In practical terms, the currently available maximum energy density of a given battery technology might not be enough for developing a competitive hybrid aircraft. Still, the same technology has some potential to provide the required energy density in the near future. Hence, it becomes essential to foresee in which temporal framework the technology improvements will make possible and readily available the required performance level.

In this work, we introduce a risk index that quantifies the probability that a given battery technology, characterized by a specific energy density, will not reach the required level of technological maturity within a given year. An optimization process is then developed, enabling a systematic trade-off between technological potential and associated risks, supporting strategic decision-making in the selection of energy storage solutions for hybrid-electric aviation. By quantifying the maturity risk of different battery technologies, this approach provides a structured decision support tool for aircraft designers and industries, facilitating the transition to feasible hybrid-electric propulsion systems.

The risk index is correlated to key battery parameters, such as energy density and maximum discharge rate, that directly influence the feasibility and efficiency of battery technologies for

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ADJOINT BASED SHAPE OPTIMIZATION FOR MULTIPHASE FLOWS WITH PHASE CHANGE DUE TO BOILING

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Keywords: adjoint method, shape optimization, multiphase flows, nucleate boiling, mixture model, objective function, RBF method

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Abstract

In the present work, an adjoint-based shape optimization method is developed for multiphase flows with phase change due to boiling for the applications such as optimization of the cooling efficiency in Battery Thermal Management System (BTMS) of the Electric Vehicles (EVs), power electronics and similar applications. To simulate the two-phase flow in the immersion cooling system, a mixture model is employed. This model utilizes mixture momentum and energy equations to govern the flow field and the enthalpy field, respectively. Additionally, a volume fraction equation is applied to describe the volume fraction of the liquid phase. Both the liquid and the gas phases are assumed to be incompressible whereas the mixture behaves as a compressible fluid. Laminar flow is assumed. The phase change is modeled with the Rohsenow correlation, since nucleate boiling is expected to be the dominating boiling regime. The optimization is done for a multi-objective function where the overall heat transfer and the overall pressure drop in the system are considered as the objective functions.
To propagate the boundary deformation into the volumetric mesh, a Radial Basis Function (RBF) method is used. To validate the presently developed adjoint based shape optimization method, the obtained sensitivities are compared with the finite difference sensitivities at selected boundary faces in the mesh subjected to deformation. For the testing of the developed adjoint method, two case studies with a 3D pipe and a C-shaped duct are considered. The adjoint based method for multiphase flows with phase change due to boiling is non-existent in the literature and is a novel contribution from the present work.

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RECOVERY OF TRANSVERSELY-ISOTROPIC ELASTIC MATERIAL PARAMETERS IN INDUCTION MOTOR ROTORS

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Keywords: Ensemble Kalman inversion, inverse eigenvalue problem, least squares minimization, linear elasticity, modal testing, and transversely isotropic material.

Abstract

In this talk, I will present two numerical algorithms; Sequential Least-Squares Programming and Ensemble Kalman Inversion (EKI), to recover the material parameters in eigenvalue problems arising from linear elasticity of transversely isotropic materials. Our considered application is the identification of elastic constants of a rotor core used in electric motors. The proposed approaches utilize vibration measurements of bending and torsional modes to infer these parameters.

Through a series of numerical experiments, we demonstrate that in noiseless conditions two pairs of bending modes are sufficient to accurately recover one to four elastic parameters. However, accurate recovery of all five parameters that characterize the elastic behavior of the core requires measurements of three pairs of bending modes and one torsional mode.

In addition, we examine the robustness of the inversion in the presence of multiplicative measurement noise. For simulated data corrupted with up to 1% of multiplicative noise, the EKI method can recover one to five parameter estimates with errors below 10% with three bending pairs and one torsional mode.

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Abstract

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QUASI-MONTE CARLO INTEGRATION FOR BAYESIAN DESIGN OF EXPERIMENT PROBLEMS GOVERNED BY PDES

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Keywords: Bayesian optimal experimental design, quasi-Monte Carlo method, sparse grid

Abstract

The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities in an experiment by optimizing the placement of measurements. The objective function in the resulting optimization problem involves a multivariate double integral over the high-dimensional parameter and data domains. For the efficient approximation of these integrals, we consider a sparse tensor product combination of quasi-Monte Carlo (QMC) cubature rules over the parameter and data domains. For the parameterization of the unknown quantities, we consider a model recently studied by Chernov and Lê (*Comput. Math. Appl.*, 2024, and *SIAM J. Numer. Anal.*, 2024) as well as Harbrecht, Schmidlin, and Schwab (*Math. Models Methods Appl. Sci.*, 2024) in which the input random field is assumed to belong to a Gevrey class. The Gevrey class contains functions that are infinitely many times continuously differentiable with a growth condition on the higher-order partial derivatives, but which are not analytic in general. We investigate efficient Bayesian OED for inverse problems governed by partial differential equations (PDEs) within this framework.

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ADJOINT-BASED SHAPE OPTIMIZATION IN SMOOTHED PARTICLE HYDRODYNAMICS

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Keywords: Smoothed Particle Hydrodynamics, Computational fluid dynamics, Adjoint-Based Shape Optimization

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Abstract

This paper introduces a numerical method for addressing adjoint shape optimization problems for applications in fluid dynamics under the influence of substantial changes in the simulation domain.

Interest in simulation-based optimal design methods is growing rapidly in industry, as companies seek to maximize performance and efficiency while minimizing development costs and development times. This is particularly true for transient applications characterized by complex, violent free surfaces, such as Pelton turbines.

Conventional mesh-based methods struggle with these applications due to extensive mesh adaptation requirements and the significant computational challenges of adequately tracking evolving free surfaces. In this context, particle-based, mesh-free Lagrangian numerical methods, such as SPH, offer significant advantages. Although primary simulations using SPH methods are already fully integrated into industrial workflows, the use of the adjoint SPH method for shape optimization is unknown.

To close this gap, we describe the derivation and implementation of a weakly compressible, unsteady, continuous-adjoint Riemann SPH solver that can be combined with any Lagrange-Euler formulation (SPH-ALE) to determine the design sensitivities of the cost functional to be minimized. The corresponding adjoint equations are derived from the weakly compressible isentropic Euler equations, discretized using the Riemann SPH-ALE method. Examples included refer to validation tests for simple problems using a force-based cost functional.

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ROBUST ACCELERATED PGET RECONSTRUCTION FOR SAFE DISPOSAL OF SPENT NUCLEAR FUEL

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Keywords: Nonlinear tomography, PGET, Iterative learning, Inverse problem

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Abstract

Passive Gamma Emission Tomography (PGET) is a nonlinear imaging method capable of accurately reconstructing the emission and attenuation profiles of radioactive spent nuclear fuel assemblies before their long-term underground disposal. The location and intensity of the emitted radiation is unknown, and only the attenuated and noisy signal can be measured, this is a very ill-posed problem and requires specialized reconstruction methods. By enforcing enough prior information about the geometry and physical properties of the given fuel assembly, it is possible to recover accurate emission and attenuation maps from the different fuel assemblies used in Finnish nuclear power plants.

In this work we experiment with accelerating the existing iterative reconstruction algorithm using machine learning methods. Due to the tight safety concerns of the application, the aim is to retain as robust and explainable algorithm as possible which we do by restricting the machine learning updates using the update steps from the traditional algorithm. This slows the convergence of the iterates but makes all tested methods very robust and well generalizable to data outside the limited training samples. Therefore the method tolerates even severe modeling errors and outliers in data.

By construction, it is also possible to go back to the traditional deterministic algorithm at any stage of the reconstruction pipeline, for example to confirm any unusual results.

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CAD-INTEGRATION FOR GRADIENT-BASED SHAPE OPTIMIZATION USING THE ALGORITHMICALLY DIFFERENTIATED PYTHONOCC LIBRARY

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Keywords: Gradient-based optimization, CAD-based optimization, Algorithmic Differentiation (AD), Geometric sensitivity, OpenCascade Technology / OCCT

Abstract

PythonOCC is a geometric modeling library that provides Python bindings for the widely-used OpenCascade Technology (OCCT) C++ kernel. To modularly integrate it into a gradient-based shape optimization framework, one requires the calculation of the so-called geometric sensitivities, i.e., derivatives of surface nodes with respect to the shape parameters – or their reverse-mode counterparts in workflows that are adjoint from end-to-end. To obtain this information, pythonOCC and OCCT are algorithmically differentiated by integrating the AD software tool ADOL-C (Automatic Differentiation by Overloading in C++) into their source code. For this purpose, a mixed-language AD approach is considered to allow the propagation of sensitivities from C++ to Python and vice-versa. The differentiated pythonOCC library is integrated – in the form of a CAD plugin – into a framework for multidisciplinary design and analysis (MDAO) based on the DLR's FlowSimulator HPC ecosystem. The CAD plugin provides an AD-enabled CAD link to all other components involved in an optimization chain. Moreover, it allows a robust and metadata-enabled mesh-to-CAD association between mesh objects (that can be domain decomposed) and the underlying CAD patches. This information is required to compute the geometric sensitivities, as well as surface displacements needed for mesh deformation. The framework integration of pythonOCC is demonstrated in a context of gradient-based shape optimization using an aerodynamic design problem of reduced complexity.

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EDGE-PROMOTING SEQUENTIAL BAYESIAN EXPERIMENTAL DESIGN FOR X-RAY IMAGING

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Keywords: X-ray tomography, optimal projections, Bayesian experimental design, A-optimality, D-optimality, adaptivity, edge-promoting prior, lagged diffusivity

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Abstract

This work considers sequential edge-promoting Bayesian optimal experimental design for X-ray imaging. The process of computing a total variation type reconstruction for the absorption inside the imaged body via lagged diffusivity iteration is interpreted in the Bayesian framework. Assuming a Gaussian additive noise model, this leads to an approximate Gaussian posterior with a covariance structure that contains information on the location of edges in the posterior mean. The next projection geometry is then chosen through A- or D-optimal Bayesian experimental design, which corresponds to minimizing the trace or the determinant of the updated posterior covariance that accounts for the new projection. The method is tested via numerical experiments based on simulated measurements.

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AEROSTRUCTURAL OPTIMIZATION OF THE DLR-F25 TRANSPORT AIRCRAFT SUPPORTED BY ML-SURROGATES FOR CAD

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Keywords: Aerostructural Shape Optimization, Continuous Adjoint, Machine Learning

Abstract

This paper presents a gradient-based shape optimization workflow for the aerodynamic and/or aerostructural optimization of an aircraft as well as the corresponding results computed in the EU funded NEXTAIR project. The workflow is supported by (a) the in-house GPU-enabled CFD code PUMA, solving the RANS equations with the Spalart-Allmaras turbulence model, (b) its continuous adjoint solver, with the complete linearization of the turbulence model equation, to compute the derivatives of the objective and constraint functions with respect to (w.r.t) the design variables, (c) a two branch λ-DNN (Deep Neural Network), as a replacement for the CAD-based parameterization of the aircraft, and (d) a structural analysis code, with its adjoint. The λ-DNN is trained on a set of point clouds lying on the aircraft surface, generated using various design variable sets (provided by DLR, a NEXTAIR partner) and used to predict the deformation of the wing, for each new set of design variables that occurs during the optimization, without having access to the CAD model of the aircraft. The optimization requires the derivatives of the aircraft surface coordinates w.r.t. the CAD parameters which are provided by differentiating the λ-DNN. The optimization workflow is used to optimize the high aspect ratio wing of the DLR-F25 transport aircraft model (by DLR), for minimum drag, under lift, pitching moment and structural constraints.

This work is part of the NEXTAIR project which is funded by the European Union (GA number 101056732).

constructs variable sub-populations. In addition to fitness value, the density of the individual's clustering is also used as another important criterion for selection. Combining the evolution on global population with independent evolution on sub-populations clustered in dominant regions to balance exploration and exploitation and also the opposition-based learning (OBL) with the contraction of search space, reducing the population size with the increase of evolutionary generation and the contraction of search space reduce significantly computational complexity.

Optimization experiments on thirteen test functions show that the improved efficient genetic algorithm (IGA) can find the global optimal solution faster in all cases. Compared with other algorithms, IGA not only improves optimal solution quality but also significantly reduces computational complexity, resulting in an optimization efficiency improvement by an order of 1~3. In addition, IGA also demonstrates its potential in solving optimization problems with large-scale decision variables.

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ADVANCED METHODS FOR TOPOLOGY AND SHAPE OPTIMIZATION

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Keywords: topology optimization, shape optimization, computational mechanics, numerical methods, engineering design, sustainability

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Abstract of the session

The growing emphasis on sustainability in engineering design, coupled with the rapid development of computational methods in engineering mechanics, has led to a rise in popularity of numerical structural optimization approaches. The optimization of shape and topology, which enable significant improvements in structural performance with respect to a range of predefined criteria, can be considered the most prominent among them. Both methods are accessible through a multitude of approaches and have undergone remarkable development in recent years.

This mini symposium aims to showcase the latest advancements in numerical structural optimization. The scope of the session includes, but is not limited to, innovative optimization methods, unusual application contexts or problem formulations, and novel parametrizations.

Researchers active in this emerging field are cordially invited to participate in a lively exchange of ideas. We look forward to your inspiring presentations and fruitful discussions in Lahti!

Recommended speakers

1. **Jun Wu (TU Delft), Title to be announced (20 min)**
2. **Tuan Minh Tran (Vietnamese German University), Title to be announced (20 min)**
3. **Dustin Jantos (Leibniz University Hannover), Title to be announced (20 min)**

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CFD-BASED RE-DESIGN OF GHIBLI ARC-JET NOZZLE

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Keywords: hypersonic, optimization, plasma wind tunnel, nozzle, internal aerodynamics

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Abstract

In collaboration with the Italian Aerospace Research Centre, this work aims to design the new expansion nozzle of their GHIBLI Arc-Jet, Nitrogen operating Plasma wind tunnel [1].
The facility is used to test materials for space/hypersonic applications, and the test zone is located after the nozzle discharge in the jet zone. The nozzle re-design task aims to improve the quality and reliability of tests through a more uniform flow in the test area with prevalently axial momentum flux and reduced reflection waves in the jet core to better approximate real operating conditions.

The current nozzle is a classic conic-divergent one that cannot satisfy those requirements completely. Furthermore, classic analytic nozzle design approaches, like the characteristics method, produce long divergent ducts, which are suboptimal [2] because of the viscosity effects associated with a significant boundary layer thickness growth, consequential total pressure loss increase, and potential flow core reduction.

The use of a contoured divergent and a viscous flow model, instead, allows seeking the optimal compromise between wave reflection control, flow pattern, and quality, core dimension, separations, or irregular boundary layer growth.
That region, in fact, interacts with the potential flow in the main duct. One of the effects is the local constriction of the flow area, which may lead, in some case, such as an abrupt growth of the boundary layer due to local flow separation, o compression effects that are not driven by the physical boundaries of the duct. Instead, they are caused by the development of the boundary layer, as the mean flow no longer follows the curvature of the nozzle but is instead guided by the shape of the boundary layer. This phenomenon can also result in angularity losses.

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TOWARDS PREDICTIVE MAINTENANCE IN HYDROGEN STORAGE AND TRANSPORTATION USING AI AND MULTI-OBJECTIVE DECISION SUPPORT

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Keywords: Predictive Maintenance, Hydrogen Infrastructure, Machine Learning, Artificial Intelligence, Multi-Objective Optimization, Energy Transition, Digital Twins

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Abstract

The hydrogen sector is rapidly becoming a key pillar of the global energy transition, requiring innovative maintenance strategies to ensure system security, reliability, and efficiency. Predictive maintenance, powered by artificial intelligence (AI) and data analytics, plays a crucial role in enhancing the safety and performance of hydrogen storage and transportation systems. We examine the use of advanced machine learning techniques and multi-objective optimization in predictive maintenance frameworks. Leveraging real-time data from sensors and Internet of Things (IoT) devices, machine learning models enable early fault detection, predictive analytics, and timely intervention before failures occur. Multi-objective optimization helps operators balance competing goals—cost, downtime, emissions, and safety—offering more sustainable and economically viable outcomes than traditional approaches. Key challenges include processing heterogeneous sensor data, ensuring model interpretability in safety-critical contexts, and addressing the scarcity of failure data, as most current datasets represent normal conditions. We explore solutions such as synthetic data generation, transfer learning, anomaly detection, and efficient real-time algorithms for large-scale hydrogen facilities operating under uncertainty. Finally, we highlight future research focused on developing adaptive, robust models for dynamic operational environments. Integrating AI with optimization offers a promising path toward intelligent, resilient, and economically sustainable hydrogen systems, supporting the global clean energy transition.

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CHECKERBOARD-FREE TOPOLOGY OPTIMIZATION USING POLYGONAL FINITE ELEMENTS WITH VORONOI TESSELLATIONS

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Keywords: topology optimization, polygonal finite elements, Voronoi tessellations, checkerboard modes

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Abstract

Topology optimization, commonly employed in mechanical and aerospace engineering, offers many advantages that can also benefit civil engineering, since it reduces the amount of material needed for a structure under a given constraint. The resulting optimized designs can be constructed thanks to the advances in additive manufacturing and the availability of high-performance materials that support the creation of innovative and complex geometries. However, a common issue that arises in topology optimization problems is numerical instability, which manifests as checkerboarding, mesh dependency, zig-zag boundaries, islanding, and layering. With respect to checkerboarding, which leads to alternating void and solid elements in certain regions, the main reason for the pronounced instabilities stems from the use of classical quadrilateral elements during topology optimization.

In this contribution the focus lies on the identification of the optimal material distribution within a structure to maximize its stiffness, which translates to minimizing its compliance. The Solid Isotropic Material with Penalization (SIMP) method in combination with the Optimality Criteria (OC) method is used for the optimization procedure. The initial linear elastic material tensor is degraded using the density values and a small remaining stiffness is applied for void regions in order to avoid singularities. It will be shown that the use of polygonal finite elements with Voronoi tessellations instead of classical quadrilateral elements effectively eliminates the unwanted checkerboard patterns. The application of polygonal elements in topology optimization has the additional advantage of allowing for an efficient local h-refinement and the representation of complex geometries of the design domains as well as their optimized versions. Here, the scaled boundary parameterization is used to discretize the polygonal mesh

and the displacements are approximated using linear interpolation functions along the boundary and in the direction of scaling, while the density remains constant within each polygonal element. The stability of the topology optimization problem when using polygonal finite elements with Voronoi tessellations can be proven by reformulating it as a mixed variational problem with the unknown displacements and densities as the two solution fields. The numerical instabilities of a mixed formulation are similar to the ones of the topology optimization problem and stem from the existence of spurious modes that manifest as checkerboard patterns. In this case, well-posedness can be proven if the coercivity on the kernel condition and the inf-sup, or Ladyzhenskaya-Babuška-Brezzi (LBB) condition are fulfilled.

A series of numerical examples are investigated in order to support the theoretical study of the stability. First, conventional finite element formulations utilizing quadrilateral elements are used for representing the design domain and the resulting optimized structure. In this case, significant instabilities are observed that manifest as checkerboard patterns. In a next step, polygonal finite elements with Voronoi tessellations are applied, which lead to an elimination of the checkerboard patterns and stable solutions. In addition, the optimized structures are compared to the solutions existing in literature.

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PHYSICS-INFORMED KOLMOGOROV-ARNOLD NETWORKS FOR OSCILLATORY DIFFERENTIAL EQUATIONS

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Keywords: machine learning, Kolmogorov-Arnold networks, oscillatory differential equations, PINNs

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Abstract

The idea behind Kolmogorov-Arnold networks (KANs) lies in the Kolmogorov-Arnold superposition theorem. KANs pose an alternative to the widely used multi-layer perceptrons (MLPs) as machine learning models.

The capabilities of KANs have been shown in many applications. We present some of the mathematical background for KANs, in particular the Kolmogorov-Arnold superposition theorem. We then discuss key advantages that KANs have over MLPs, such as interpretability and smaller network size. We also take a look at some of the functionalitites of the pykan code package, which offers an implementation of KANs for easy use. We see that due to the focus of the authors of the code package on the scientific usage of KANs, pykan can be a powerful tool for researchers in different fields. KANs in general and pykan in particular offer many advantages and we present possible resulting applications for KANs, that are not feasible with MLPs.

We conduct several numerical experiments for different problems, the main focus of these experiments is the solving of differential equations using KANs with a physics-informed neural network (PINN) setting. Some of the problems are chosen such that they have characteristics that are usually problematic for MLPs. One such property is, for example, an oscillatory component in the context of multi-scale problems. We compare MLPs to KANs for some of the chosen problems to get a better understanding of the advantages that KANs offer. The comparison shows that there are indeed situations, where the usage of KANs leads to favorable results. In particular, an oscillatory diffusion problem can be solved to a high precision using a KAN. An MLP struggles to show any sign of convergence for the same problem, even given significantly more training time.

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TOPOLOGY OPTIMIZATION WITH REINFORCED CONCRETE FOR RESOURCE EFFICIENT CIVIL ENGINEERING DESIGN

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Keywords: topology optimization, reinforced concrete, orthotropy, sustainability, multi material topology optimization

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Abstract

Mechanically efficient designs that can be realized in a resource-friendly manner represent a key component of the sustainable transformation of the building infrastructure. Numerical topology optimization, a versatile tool kit for drafting structures that are designed according to predefined criteria, is a promising method to support the form finding at an early stage of the structural design process. The task is interpreted as a material distribution problem in a finite element discretized design space. The static load profile of civil engineering structures is typically dominated by self-weight, which introduces a design-dependent load into the optimization problem. Previous studies [1] have shown that the minimization of compliance with a bound on the maximum volume fraction of material in the design space yields structures that are characterized by a load transfer by normal forces, which represents a beneficial load profile. Concrete, the most popular building material displays high compressive strength and brittle failure at comparably low tensile stresses [2]. This tensile/compressive strength anisotropy can be mitigated by the introduction of steel reinforcement.

The composite material is modeled as bundles of unidirectional steel fibers embedded in a concrete matrix. The constitutive tensor of the resulting material is obtained using the rule of mixtures and thus depends on the volume fraction of matrix and fibers [3,4]. The fibers reinforce the concrete in the direction of their orientation, which requires an anisotropic material model. This study aims to unlock the full potential of reinforced concrete using topology optimization. The material distribution, the orientation of the steel reinforcement, and

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STRUCTURAL OPTIMIZATION FOR FCC-EE INTERACTION REGION SUPPORT STRUCTURES

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Keywords: Structural optimization, lattice structure, minimal surface

Abstract

The structural optimization techniques have become crucial in engineering design, in particular for futuristic projects such as the Future Circular Collider, a high-energy circular collider. The structures analyzed in this work are the interaction region's main components supporting structures; the objective function is the mass reduction for all the optimization done.

The workflow proposed in this contribution has the scope to highlight the advantages of subdividing the structures into different functional areas before the optimization, instead of optimizing a global structure. The subdivision permits the selection of different optimization methods, using the one that is more appropriate to the sub-structure nature. The final result is a structure obtained by the composition of every single part optimized; this workflow allows obtaining a final structure combining different optimization methods for each sub-structure. It is important to correctly report the boundary conditions in each sub-structure, creating a congruent interface between the different sub-structures.

The structure analyzed has been divided into two parts, considering thickness variation, functional areas and mechanical constraints. Two methods have been chosen for the un-divided structure: the Solid Isotropic Material with Penalization and the generative design. The first approach requires a starting massive geometry and obtains the final shape with a step-by-step material removal following the objective function. The second approach starts from the geometric constraint and the objective function and evolves, creating different scenarios, using genetic algorithms for natural shapes' evolution, using Finite Element Analysis to control the constraints, and machine learning for better exploring the solutions. The subdivisions' number depends on the case under study, but the workflow remains valid. For the subdivided structure, in addition to the described method, the lattice structure with field-driven optimization has been contemplated, which consists of the stress map creation to formulate a thickness function for the lattice structure.

The results obtained confirm the advantages of subdivision before optimizing, in fact for the three constraint configurations analyzed, the optimization of the un-divided structure achieves a mass reduction of 67%, 68%, 70% respectively; in the other hand the resulting optimized structure from the subdivided model achieve a mass reduction of 78%, 76%, 73%, combining the generative design and the lattice structure.

To investigate more deeply the use of lattice structure for optimization, a workflow has been created to build an "ad hoc" lattice structure based on a minimal surface and using the hypercube as the initial domain. An iterative particle-spring dynamic model was used to generate the lattice, considering symmetry requirements related to boundary conditions. In comparison with the usual method for the minimal surface evaluation, using the Lagrangian equation, the proposed methodology allows to find the minimal surface configuration using iterative step of equilibrium, resolving the dynamic system at each step, using as equilibrating forces the sum of the forces dictated by the objective function and the reaction forces to respect the boundary condition. The lattice structure is then evaluated using homogenization techniques to characterize its mechanical properties. The lattice cell has been used as infill for a real part design, leading to 3D printing and testing the real mechanical behavior.

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THERMODYNAMIC TOPOLOGY OPTIMIATION OF PHOTONICS

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Keywords: Topology Optimization, Hamilton's Principle, Variation Calculus, Photonics

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Abstract

In the past decade, Junker and Hackl introduced a procedure based on Hamilton's principle to obtain the governing system of equations for topology optimization by the variation of a single Hamilton functional. This procedure is called Thermodynamic Topology Optimization (TTO) and was already implemented for many applications, such as anisotropic materials, tensile/compressive anisotropy, and plasticity.

We already extended this method to include the optimization of mechanical compliant mechanisms. To obtain this in a physical and thermodynamically consistent context, we used Betti's reciprocal theorem. In this study, we apply the concept of compliant mechanisms to electrodynamics. We replace the mechanical component in the Hamilton functional with an electromagnetic counterpart, which allows us to optimize a topology in such a way that it is able to focus light beams to a predefined point.

The key aspect of this work is the formulation of the Hamilton functional. We begin by presenting the Hamilton functional for electrodynamics including a density variable in a general way. Hamilton's principle is applied to derive the system of governing equations. This system comprises two physical equations and one equation for the density distribution. Here the physical equations are Ampère's law for the input and output of our problem. Then, we present the assumptions that allow us to reduce these to scalar Helmholtz equations in a two-dimensional space. The solution to this system of equations is obtained using the Neighbored Element Method (NEM), a hybrid approach combining the Finite Element Method for solving the physical problem and a generalized Finite Difference Method for solving the density distribution.

The work concludes with numerical examples. On the one hand, we present a SIMP (Solid Isotropic Material with Penalization) approach, where the solution strongly depends on the

parameters of the Heaviside function. On the other hand, we demonstrate a penalization damping approach, which significantly improves the numerics and results.

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MACHINE LEARNING AND DATA-DRIVEN INNOVATIONS IN AERODYNAMIC OPTIMIZATION AND UNCERTAINTY QUANTIFICATION

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Keywords: data-driven models, aerodynamic analysis, machine learning, scientific machine learning

Abstract of the session

In recent years, the surge in data from computational sciences has underscored its potential to deliver insights and enhance predictive capabilities. In aerodynamics, extensive studies and optimizations yield large volumes of valuable data, creating an opportunity to advance data-driven and data-fusion models in engineering [1]. Yet, the integration of these models is still developing, with best practices only beginning to form.

Machine learning, including neural networks, offers a robust toolkit for tasks like clustering, dimensionality reduction, classification, and regression. However, processing and preparing aerodynamic and geometric data poses notable challenges. These tasks are often complex and objective-specific, leading to varied interpretations and applications of data-driven methods. Integrating machine learning techniques, commonly used in AI and Data Mining, promises substantial reductions in computational costs for aerodynamic analysis and uncertainty quantification [2]. These advanced methods open a pathway toward efficient, accurate solutions in aerodynamic design, despite ongoing challenges in data handling and model maturity.

This minisymposium aims to showcase new approaches and recent progress in applying machine learning and data-driven techniques for aerodynamic analysis and uncertainty quantification, with a focus on practical challenges and on the new opportunities that Scientific Machine Learning, i.e. the fusion of advanced Machine Learning techniques with Scientific Computing, offers for the development of increasingly efficient and effective analysis and design methodologies.

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MULTI-STAGE MULTI-SCENARIO MULTI-OBJECTIVE OPTIMIZATION FOR ADAPTIVE ROBUST ENERGY TRANSITION UNDER DEEP UNCERTAINTY

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Keywords: Sustainability, Scenario planning, Deep uncertainty, Dynamic robustness, Green energy systems, Multi-objective optimization

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Abstract

Real-life decision problems often involve multiple decision-making stages, conflicting objectives, and various sources of uncertainties, where most decisions need to be made without complete knowledge of all the parameters, probability distributions, outcomes, and consequences of the alternative solutions. In some cases, the experts do not know or cannot agree upon the appropriate models, probability distributions, or measuring the desirability of alternative outcomes. This condition defines deep uncertainty. Under deep uncertainty, using wrong probability distribution leads to failure. Scenarios, instead, should be used to evaluate the consequences of any solutions in different plausible futures and find a robust solution.

This talk introduces a multi-stage multi-scenario multi-objective optimization approach for adaptive robust decision-making under deep uncertainty. Then, we further describe how the proposed approach can be applied in complex strategic planning in renewable energy transition via a case study of the South African sugar-bioethanol supply chains. Indeed, the sustainability of the whole infrastructure and its transition is analyzed in such a way that the renewed system is sustainable, robust, and adaptable for a broad range of plausible futures. Three objectives are considered in this problem under six uncertain parameters. The results prove the economic profitability and sustainability of the project. The proposed approach can also be applied to other energy supply chain problems under deep uncertainty.

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NEURAL NETWORK OPTIMIZATION FOR DATA-EFFICIENT GENERALIZATION IN SCIENTIFIC MACHINE LEARNING

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Keywords: Scientific Machine Learning, Data-Efficient Training, Surrogate Modeling, Neural Network Optimization.

Abstract

In recent years, machine learning methodologies, such as neural networks, have become powerful tools for accurately predicting physical quantities after training on large datasets. However, achieving reliable results often requires vast amounts of data, posing significant challenges when the data comes from computationally intensive simulations, such as aerodynamic analyses, aeroacoustics predictions, or thermal-fluid studies in energy systems. To address this, scientific machine learning explores strategies such as introducing physical constraints into the learning process and optimizing neural network architectures to enhance data efficiency.

In this work, the objective is to establish a purely data-driven baseline by training a neural network to predict the pressure coefficient (C_p) distribution around an airfoil, considering variations in both geometry and angle of attack. Different network architectures are analyzed by modifying key parameters such as optimizers, learning rates, neuron counts and layer depths to evaluate their generalization capabilities when trained with limited datasets. Both the predictive performance and the resulting network configurations will serve as reference points for future comparative studies, aiming to assess the benefits of incorporating physical constraints and domain-specific knowledge into the learning process.

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COMPUTATIONAL PERSPECTIVES ON MULTI-OBJECTIVE HOME HEALTHCARE ROUTING AND SCHEDULING: FORMULATIONS AND CHALLENGES

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Keywords: Home Healthcare, Multi-objective Optimization, Routing and Scheduling, Pareto Optimality, A-posteriori Approaches, Evolutionary Algorithms, Mixed-Integer Linear Programming (MILP), Caregiver Assignment, Patient-Centered Logistics, Sustainable Healthcare Systems

Abstract

The Home Healthcare Routing and Scheduling Problem (HHCRSP) is a complex, multi-objective extension of the Vehicle Routing Problem, aimed at assigning and routing caregivers to patients' homes while balancing operational efficiency and personalized care. It involves diverse constraints such as caregiver skills, time windows, synchronized visits, and mandatory breaks. Traditional a-priori optimization methods limit flexibility by requiring predefined preferences. This study advocates an a-posteriori approach using a multi-objective MILP model and evolutionary algorithms (e.g., NSGA-III) to generate diverse Pareto-optimal solutions. This enables decision makers to explore trade-offs among objectives like travel cost, patient satisfaction, workload balance, and CO_2 emissions. Our framework supports scalable integration of difficult objectives such as caregiver well-being and service continuity. The proposed method promotes sustainable, efficient, and patient-centered decision-making in dynamic home healthcare environments.

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MULTI-FIDELITY AIRFOIL SHAPE OPTIMIZATION WITH HYBRID GENETIC ALGORITHM

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Keywords: Aerodynamic Shape Optimization, Airfoil design, Hybrid Genetic Algorithms, Multi-fidelity.

Abstract
The increasing power of high-performance computing has elevated high-fidelity Reynolds-Averaged Navier–Stokes (RANS) analysis from a validation step to a baseline tool in aerodynamic design at realistic flight conditions. Despite this progress, the prohibitive cost of numerous evaluations required by optimization algorithms hinders fully RANS-based design loops, particularly for large and complex search spaces [1]. Addressing this challenge, we present a **multi-fidelity airfoil shape optimization framework**[2] that combines the efficiency of the **XFOIL** potential-panel solver with the accuracy of high-resolution **RANS** simulations, using our in-house **Hybrid Genetic Optimiser (HyGO[3])**. HyGO implements a hybrid strategy featuring a two-tier evaluation loop per generation. First, the entire population is assessed using the computationally cheap XFOIL model for rapid, broad exploration. Subsequently, targeted exploitation uses high-fidelity RANS simulations to analyze promising regions from XFOIL.
Our goal is to maximize the mean aerodynamic **lift-to-drag (L/D)** ratio of airfoils defined by **12-CST** (Kulfan Class-Shape Transformation) parameters. Optimization considers performance at two key operating points: the **design cruise condition** ($\alpha = 1°$ and M=0.74) and a critical off-design **high angle of attack condition** ($\alpha = 10°$ and M=0.2), both at a Reynolds number of $\mathbf{Re = 6 \times 10^6}$. Geometric constraints are enforced to ensure minimum thickness and structural feasibility. To capture the distinct flow physics accurately in the high-fidelity step, we employ a **compressible Spalart–Allmaras RANS** solver for cruise and an **incompressible solver** for the off-desgin condition. Crucially, only 10% of individuals are evaluated with the high-fidelity RANS environment. This selective promotion drastically cuts computational time – by approximately an order of magnitude versus a pure-RANS approach – while effectively maintaining population diversity.
This work demonstrates that strategically managing model fidelity within an evolutionary algorithm framework delivers substantial aerodynamic gains across the operating envelope at an affordable computational cost, offering valuable guidelines applicable to other multi-condition or multidisciplinary optimization challenges.
Acknowledgments: Activity within the project **TIFON** (ref. PLEC2023-010251/MCIN/AEI/ 10.13039/501100011033), funded by the Spanish State Research Agency

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DISCUSSION ON THE EFFECT OF AIRFLOW-COORPERATION ON THE AEROSTRUCTURAL OPTIMIZED DESIGN OF A PASSACTIVE COMPLIANT MORPHING AIRFOIL

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Keywords: morphing wing, airfoil, compliant mechanisms, airflow-cooperation, static aeroelasticity, multiobjective optimal design, topology optimization

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Abstract

Morphing wings are expected to improve the flight performance of aircraft in response to the demand for more fuel-efficient aircraft to achieve carbon neutrality. A compliant morphing airfoil (CMA) is a concept that realizes continuous and smooth deformation of the airfoil outline through elastic deformation of the compliant mechanism that is one-piece flexible device. The challenging task is to simultaneously reconcile (compromise) the flexibility to deform and the rigidity to withstand aerodynamic forces, which would conflict with each other. Therefore, it would be important to design the CMA taking into account that it could be passively deformed by the airflow compared to a conventional airfoil. This research aims to develop a mathematical design method based on the design concept of "Let's get better at pass-actively deformation". As a way to achieve this, we consider an "airflow-cooperation" and clarify whether this function can be added to the CMA.

To discuss the possibility of adding an airflow-cooperation function, a CMA is designed based on a static aeroelastic deformation that simplifies the problem, followed by evaluating the aeroelastic properties. At first, a novel optimal design method is proposed that integrates static aeroelastic deformation analysis with topology optimization to simultaneously explore the external aerodynamic and internal structural performance of a deformable wing. The aeroelastic deformation is evaluated by a weak coupling of the aerodynamic panel and structural finite element methods. Based on this coupled aerostructural problem, design sensitivity is derived by the discrete adjoint variable method and utilized to explore the optimal structural topology. The design problem is a multiobjective design problem that simultaneously improve the lift coefficient of the deformed airfoil and the required input energy of the internal mechanism. Through numerical examples, the variation of the optimized solution with the magnitude of the effect of the interaction with the airflow is shown. Then, to investigate the effect of airflow-cooperation, we compare the aerostructural performance of the same optimized solution with and without static aeroelasticity. Based on the results, the possibility of adding airflow-cooperation function to the CMA will be discussed.

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SOLVING DISTRIBUTIONALLY ROBUST OPTIMIZATION PROBLEMS EFFICIENTLY VIA SURROGATE MODELS

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Keywords: DRO, surrogate-modeling, robust-optimization

Abstract

In distributionally robust optimization (DRO), one seeks decisions that perform well against the worst-case probability distribution within a prescribed ambiguity set. In many engineering applications - most notably aerodynamic shape optimization (ASO) - each evaluation of the performance function $f(x, \xi)$ (for example, a drag or lift coefficient computed by a high-fidelity computational-fluid-dynamics solver under operating condition ξ) is extremely expensive, often requiring minutes or hours per run. The canonical DRO problem

$$\min_{x} \max_{Q \in \mathcal{D}(P,\rho)} \mathbb{E}_{\xi \sim Q}[f(x, \xi)]$$

entails a double loop: an outer minimization over design variables x (typically nonconvex and high-dimensional) and an inner maximization over all distributions Q in the ambiguity set $\mathcal{D}(P, \rho)$. The inner loop alone requires many evaluations of the expectation $\mathbb{E}_{\xi \sim Q}[f(x, \xi)]$ and hence many calls to the expensive solver before the worst-case Q can be identified. The direct solution quickly becomes intractable when each f-evaluation invokes a full ASO simulation.

To overcome this bottleneck, we propose surrogate modeling of f as a function of ξ for each fixed design x. In the inner loop at a given x, rather than calling the high-fidelity solver at new ξ-samples, we query a pre-trained surrogate $\hat{f}_x(\xi)$ that approximates $f(x, \xi)$ to high accuracy over the support. This surrogate reduces the cost of estimating $\mathbb{E}_{\xi \sim Q}[f(x, \xi)]$ and its sensitivities with respect to Q by orders of magnitude, enabling efficient solutions of the inner maximization via first-order methods. Meanwhile, only a modest number of true solver calls are required to train the surrogate.

We demonstrate this surrogate-accelerated DRO workflow on an aerodynamic shape-optimization benchmark in which the uncertain parameters ξ represent the operating conditions such as angle of attack, and Mach number.

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MULTI-CRITERIA OPTIMIZATION FOR BUILDING SPATIAL DESIGN

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Keywords: building spatial design, multi-criteria optimization, solution diversity improvement, real-world applications

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Abstract

A building spatial design (BSD) defines the layout of spaces and the resulting internal and external walls and floors. Optimizing BSDs aims to enhance several objectives at the same time in a multidisciplinary framework. In our example, we study the simultaneous optimization of structural performance and thermal efficiency. Our use of models that allow non-orthogonal spaces entails large complexity of representations and their constraints, and concomitant difficulties in navigating the solution space in search of optima.

To solve such problems via evolutionary optimization, the Prism-Net search space representation was proposed. Prism nets are constructed from space-filling collections of triangular prisms defined by triangulations. Through the use of color parameters, these prisms can be grouped into spaces. This approach supports non-orthogonal geometries and allows for extensive topological variation. A hierarchical mutation operator has also been proposed, which has both continuous and discrete components, including those that change the topology of a BSD. However, at the moment, this approach has been applied exclusively to a toy problem, which does not allow us to judge the effectiveness of this mutation operator.

In this paper, we examined optimization on a real-world problem using a building design simulation environment (BSO toolbox) and calculating real-world effects. The use of NSGA-

II has shown that the proposed mutation operator performs exclusively local transformations. This leads to the fact that the Pareto front often consists of a single point, and the set of solutions in the final population is not diverse enough so that building design teams can benefit from this optimization process.

We have proposed a combination of improvements to the proposed algorithm to obtain more diverse solutions, despite the complexity of the task. In particular, we added a diversity-conservation (niching) technique to the optimization algorithm a broader mutation operator, to diversify solutions. This, in turn, allowed us to provide an optimized set of BSDs that has a high level of diversity, which may support early-stage building spatial design, and is a promising part of hybrid optimization, in which our optimization method is combined with simulations of co-evolutionary design processes.

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16th ECCOMAS Thematic Conference on
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Lahti, Finland, 16–18, 2025

CAVITATION EROSION OPTIMIZATION IN A HIGH HEAD FRANCIS TURBINE USING EVOLUTIONARY ALGORITHMS

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Keywords: cavitation erosion, hydraulic turbines, metamodel-assisted evolutionary algorithms, optimization

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Abstract

Cavitation is critical for the design of hydraulic turbines, as it can deteriorate efficiency and cause material erosion, an undesirable and costly consequence. Although erosion can be prevented by mitigating cavitation, it is rarely feasible to eliminate cavitation across the entire operating range. Since experimental assessment of erosion is time-consuming, CFD simulations can be utilized alternatively. This paper is based on a two-phase CFD solver, validated against experimental data from testing of hydraulic turbines and integrated into the GPU-accelerated software PUMA, developed by the PCOpt/NTUA. This solver, capable of predicting erosion, is used as the evaluation tool in an optimization with Metamodel-Assisted Evolutionary Algorithms (MAEAs), employing the EASY software developed by the PCOpt/NTUA. Hydraulic turbines involve several design variables and constraints. In this study, the optimization concerns a Francis hydraulic turbine with 36 design variables, which define the geometry of the blade's mean-camber surface. The MAEA which is essential for obtaining optimal solutions at a reasonable computational cost is additionally supported by the Principal Component Analysis (PCA). Both Single- (SOO) and Multi-Objective Optimization (MOO) problems are considered. The SOO problem targets min. cavitation erosion, by maintaining a constant efficiency, while the MOO copes simultaneously with the two contradictory objectives of min. cavitation erosion and max. efficiency.

The first author has received funding from the EU Horizon 2021 research and innovation program under the Marie Sklodowska Curie Grant Agreement No. 101072851 (MFLOPS).

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Lahti, Finland, 16–18, 2025

AUTOMATIC AFFINITY DETECTION FOR CATEGORICAL VARIABLES IN SURROGATE-BASED OPTIMIZATION USING DIMENSIONALITY REDUCTION

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Keywords: Surrogate-based optimization, Mixed-variable optimization, Evolutionary algorithms, Derivative-free optimization, Categorical variables, Affinity, Dimensionality reduction.

Abstract

As numerous industrial applications must deal with continuous and categorical variables, our objective is to manage efficiently mixed variables within a surrogate-based optimization process. Since the construction of the surrogate models and the optimization search require the comparison of individuals with variables of several types, the approach followed here consists in defining a variant of the heterogeneous distance function, which natively uses specific metrics adapted to each variable type. In our approach, the overlap metric used for categorical variables is modified by introducing the notion of affinities between the possible values taken by a categorical variable (named "attributes"). Affinities between attributes can be interpreted as a weighted relationship between attributes. They are usually defined based on a physical intuition of the designer, who will tweak the distances between attributes in relation with their respective impact on the output responses, thereby modifying the topological representation of the parametric space. Practically, an automatic procedure is proposed to define these affinities by means of a dimensionality reduction algorithm called UMAP (Uniform Manifold Approximation and Projection). The principle of UMAP consists in detecting intrinsic topologies based on neighborhood distances. In our setup, samples with similar responses will be close, while samples exhibiting a very different behavior, with respect to these responses, will be far away, which leads to a clustering-based technique to identify affinities. Numerical results will be presented on test problems derived from structural and mechanical design frameworks to study the impact of the proposed strategy.

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INTERACTIVE MULTIOBJECTIVE OPTIMIZATION IN SUPPORT OF CLIMATE SMART FORESTRY

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Keywords: interactive multiobjective optimization, forestry, climate, software

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Abstract

In Finland, over half a million private individuals own the majority of the country's forests in commercial use. Any broad climate action targeting Finnish forests must therefore earn the voluntary cooperation of forest owners to succeed. Recognizing this challenge, we have brought together forestry researchers and multiobjective optimization experts to explore how forest owners' diverse preferences can be meaningfully incorporated into climate-smart forest management planning.

Towards this goal, we have developed an interactive multiobjective optimization tool that supports forest owners in finding a management plan that considers both climate goals and personal economic interests. The tool models stand-level management plans and presents the forest owner with Pareto optimal solutions balancing four key objectives: (1) carbon dioxide storage, (2) income from harvesting, (3) the net present value of the forest holding, and (4) the remaining timber stock at the end of the planning period.

We employ the interactive multiobjective optimization method NIMBUS, which allows users to iteratively express their preferences regarding the objectives. Based on the given preferences, new Pareto optimal solutions are generated in real time, enabling users to explore different trade-offs and progressively refine their understanding of desirable outcomes. To aid the decision-making, we have integrated customized map visualizations into the tool. These visualizations let forest owners immediately see what management actions would be undertaken at different stands at different stages of the plan.

Testing the tool with real forest owners has shown that an interactive, preference-driven exploration of management options—combined with clear, practical visualizations—helps the forest owners understand the costs and practical implications of climate smart forestry. Somewhat surprisingly, we observed that providing forest owners with intuitive information

about the climate impacts of their management choices was often sufficient to shift their behavior toward more climate-friendly practices.

Our work demonstrates the critical role that interactive multiobjective optimization, combined with user-centered visualizations, can play in encouraging individual forest owners to make their forestry management plans more climate-smart. By placing decision-making power in the hands of the forest owners by transparently illustrating the consequences of different choices, we can begin to bridge the gap between climate policy ambitions and individual action. This approach offers a promising pathway for promoting voluntary climate action in fragmented ownership contexts and showcases the value of decision maker-centered optimization tools in real-world environmental management challenges.

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Lahti, Finland, 16–18 September, 2025

EFFICIENT SHAPE OPTIMIZATION OF TPMS HEAT EXCHANGERS VIA RBF-FD MESHLESS METHOD AND REDUCED ORDER TECHNIQUES

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Keywords: Meshless Methods, Reduced Order Models, Shape Optimization.

Abstract

Triply periodic minimal surfaces (TPMS) recently gained attention as heat exchangers (HE) thanks to additive manufacturing. Their high surface-to-volume ratio, lightweight structure, and smooth geometry allow for the minimization of pressure loss while enhancing thermal performance. TPMS HE shape optimization is crucial to achieve the best possible results and requires multiple computational fluid dynamics (CFD) simulations for different geometrical configurations. CFD meshless methods are the perfect candidates for shape optimization, since they enable an automated simulation process, managing significant geometrical changes.

This work aims to compare the results of two multi-objective optimizations of a Schwarz TPMS HE unit cell. The first approximates the unit cell with a Radial Basis Function-generated Finite Difference (RBF-FD) meshless model, while the second approximates it with a non-intrusive Reduced Order Model (ROM). A ROM predicts full solution fields in near real-time, making it suited for many query applications, such as optimization. The TPMS HE ROM is trained on meshless solutions with consistent node distributions, without requiring geometrical mapping strategies. This synergy between meshless methods and ROMs minimizes both interpolation errors and further user supervision during the optimization.

The study is conducted under laminar internal flow conditions, with friction coefficient and Nusselt number as performance metrics to optimize. Therefore, both a pressure and a temperature ROM need to be trained. We then compare the Pareto frontiers obtained with the ROM-based optimization to the one obtained with a classical multi-objective optimization, both achieved with a fully automated process.

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APPLICATION OF NATURE-INSPIRED OPTIMIZATION TECHNIQUES FOR AUTOMATED FINITE ELEMENT MODEL UPDATING OF A HISTORICAL MASONRY BELL TOWER

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Keywords: Finite Element Model Updating, Genetic Algorithm, Particle Swarm Optimization, Operational Modal Analysis, Masonry Bell Towers

Abstract

Masonry bell towers, as a vital part of the historical assets of Italy, are highly prone to vibrations from human activities, such as motor-vehicle traffic and construction operations, as well as from bell ringing and seismic excitations. This study focuses on improving the accuracy of finite element models (FEM) for these slender masonry structures using advanced updating techniques. Finite element model updating (FEMU), framed as a minimization problem, is the process of calibrating model parameters based on the actual dynamic properties of a structure obtained from operational modal analysis (OMA), such as natural frequencies, mode shapes, and damping ratios. The purpose is to determine the optimal unknown parameters of the model, such as elastic moduli, mass densities, constraints, and boundary conditions, to minimize the objective function that quantifies the discrepancy between experimental and numerical modal properties. This research advances previous work on the medieval bell tower of San Giuseppe in Aci Castello, which relied on manual model updating through trial and error using experimental data. Here, manual FEM updating is replaced by nature-inspired optimization techniques to reinforce the accuracy and efficiency. The FEM of the bell tower, developed in OpenSeesPy, is calibrated employing Particle Swarm Optimization (PSO) and Genetic Algorithm (GA) to match natural frequencies and mode shapes obtained through OMA. The results demonstrate the effectiveness and efficiency of both algorithms in automating the updating process and improving the model accuracy. This study not only increases FEM reliability but also provides insights for further methodological improvements in structural health monitoring.

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BENCHMARKING DISTRIBUTED OPTIMIZATION FORMULATIONS WITH A MULTIDISCIPLINARY FEASIBLE APPROACH FOR AERO-STRUCTURAL AIRCRAFT DESIGN

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Keywords: Multidisciplinary analysis and optimization, MDAO, CFRP laminate tailoring, adjoint method, gradient-based MDO, multi-fidelity

Abstract

The aero-structural design of aircraft is an inherently multidisciplinary design optimization (MDO) task, in which aerodynamic shape and structural sizing of the aircraft are modified concurrently.

For this purpose, an MDO suite is been continuously developed by DLR, in which the structural optimization framework Lagrange, developed by Airbus Defence and Space, is coupled to DLR's computational fluid dynamics (CFD) code, TAU, within the high-performance computing (HPC) software integration framework FlowSimulator for accurately predicting the aircraft performance and providing sensitivities based on the adjoint method. A comprehensive loads and sizing process based on a linear aerodynamics model that is coupled to Lagrange's structural solver is also part of the MDO suite for efficiently considering large numbers of load cases and for providing sensitivities of the loads with respect to industry-relevant structural constraints [1].

Using single disciplinary optimizations, it was shown that the lift distribution and subsequently the aerodynamic performance of aircraft can be affected negatively when increasing the design freedom of the CFRP laminate parametrization for high-aspect ratio wings. Applying the MDO suite with the multidisciplinary feasible (MDF) optimization architecture, those effects can be captured and mitigated [2].

While the MDF optimization formulation has proven to work well in academia, it is frequently regarded as impractical in industry. To remedy this, distributed optimization methods were proposed that promise to reduce interdisciplinary interactions and offer more autonomy for the disciplines involved.

To evaluate their effectiveness, this paper benchmarks multiple distributed optimization methods against an MDF architecture. Among the methods investigated is a bilevel optimization architecture, in which a gradient-free system level optimizer imposes a fixed root

bending moment as a constraint on the aerodynamic shape optimization aiming to ensure inter-disciplinary consistency. The loads model responsible for structural sizing is used both with structural mass as an objective and the fuel burn as global objective function. This approach was proposed in [3].

A coordinate descent-based optimization as proposed in [4] is applied and extended to multi-fidelity aerodynamic models for performance prediction.

The optimization scenario chosen is a high-aspect ratio wing, civil transport aircraft configuration, the DLR F25, exhibiting strong interactions between aerodynamic performance and structural design.

Acknowledgement

Development of DLR-F25 was funded by the German Federal Ministry for Economic Affairs and Climate Action. This material is based upon work supported in part by the Clean Aviation Joint Undertaking and its members as part of the project Ultra Performance Wing (UP Wing, project number: 101101974). Co-funded by the European Union.

Disclaimer

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Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications
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A MULTI-FIDELITY OPTIMISATION STRATEGY BASED ON HYBRID METHODS

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Keywords: Optimisation algorithm, Multi-fidelity, Airfoil aerodynamics, Genetic algorithms, Hybrid methods, CFD

Abstract

A multi-fidelity optimisation strategy has been developed in the present work, and its performance is illustrated through a series of test cases. The strategy is based on hybrid methods such that two genetic optimisation algorithms are employed, each coupled to a different fidelity level with transfer of information between them. The aim is that the low fidelity model, being less accurate but with a lower computational cost, performs a comprehensive search along the design space guiding the high fidelity model to the optimum region. This strategy has been shown to reduce the computational time of an optimization through analytical test cases as well as numerical cases. The analytical cases have been used to tune the parameters that define the multi-fidelity strategy, while the numerical cases are employed to apply the method to engineering problems, focusing on the aerodynamic performance of an airfoil. The speed-up shows a certain dependency to the models relation, both regarding their similarity level as well as the relative computational cost. For cases exhibiting a significant dissimilarity between models, wherein the low fidelity model is notably inaccurate, the attained speed-up diminishes, and numerous instances demonstrate an absence of speed-up. However, for most cases, even with poor model similarity the optimisations are accelerated by an order of 2, while values up to 3–5 were found for higher similarity levels. Hence, the developed strategy shows a relevant decrease of computational cost of an optimisation procedure although its performance is affected by the models relative accuracy.

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CONSTRAINED GEOMETRIC OPTIMIZATION OF IMMERSED BOUNDARIES FOR MODELING HYDRAULIC DIODES

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Keywords: Shape Optimization, Lagrangian, Immersed Boundary Method, Penalized Direct Forcing, Passive systems

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Abstract

This framework is part of a research and development process on passive systems for current and future nuclear reactor safety. The aim of this approach is to improve the efficiency of a passive system by creating a geometric optimization process. In order to meet industrial needs, particularly in terms of cost (engineering time), two previous theses led to the development and introduction of a fictitious domain method in an in-house software [1]. This tool simulates turbulent two-phase flows around obstacles, while allowing easy modification of their geometries. The tool is based on an approach involving the "Penalized Direct Forcing" (PDF) method [2]. This method reduces the cost of generating new meshes for each new generated geometry.

The main objective of the current work is to carry out a geometric optimization process for passive safety devices based on hydraulic diodes, in order to maximize or minimize an objective function such as pressure drop (functionality of the flow limiter or advanced accumulator).

To achieve this, we propose an approach to get the shape derivative of the objective function compared to the immersed boundary with the introduction of the Lagrangian [3]. This approach is validated on a thermal test case then on a thermohydraulics case.

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TOWARDS AERO-STRUCTURAL OPTIMIZATION USING THE NEW CFD SOFTWARE BY ONERA, DLR, AIRBUS (CODA)

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Keywords: aero-structural optimization, gradient-based MDO, multi-fidelity, multidisciplinary

Abstract

In working towards a more climate-friendly air travel, multidisciplinary analysis and optimization (MDAO) capabilities based on high-fidelity methods for aerodynamics and structural mechanics are essential for the design of appropriate next-generation aircraft. In addition, optimization problems for industrially relevant use cases typically contain a vast number of design parameters and constraints in all disciplines being involved, which for reasons of efficiency requires the use of gradient-based methods that rely on the presence of accurate intra- and interdisciplinary gradients. Against this background, DLR and its partners are continuously developing a gradient-based MDO suite in multidisciplinary feasibility formulation (MDF) based on the application of RANS-based adjoint-ready computational fluid dynamics (CFD) solvers. So far, mainly the TAU solver of DLR in combination either with the LAGRANGE optimization framework of AIRBUS Defense and Space [1,2,3] or with NASTRAN as structural solver has been used. The FlowSimulator environment, which is being jointly developed by DLR, ONERA and AIRBUS and is specifically tailored for the simulation of CFD-based multidisciplinary applications on HPC systems [4], is applied as an overarching software integration framework for the elements of the MDO suite.

In addition to the optimizer, CFD solver and computational structural mechanics (CSM) solver (the former and latter are part of LAGRANGE), the suite includes (1) a differentiated reduced-order modelling approach to efficiently perform aerodynamic and structural shape variations; (2) a comprehensive loads analysis process based on fast low-fidelity aerodynamics which is capable of providing sensitivities of the loads with respect to structural constraints; and (3) an

aircraft performance analysis module suitable for evaluating the state and sensitivities of the elastic level flight-trimmed powered aircraft. The latter contains also the required standard tools for static CFD/CSM coupling methods such as CFD/CSM loads and deformation interpolation methods as well as an adjoint CFD mesh deformation method. The gradients are corrected to take into account the trim calculation that takes place in a sub-process.

To meet the current and future challenges in aircraft design, more advanced CFD capabilities are required, aiming at improved, accelerated, and more accurate simulations of MDAO applications than currently available with the existing legacy CFD solvers. This is the goal of the ongoing joint efforts of ONERA, DLR and AIRBUS in the development of the next generation CFD software CODA[1] [5]. Among the many innovative novel features of CODA, the most crucial for use in the context of MDAO is that, by exploiting techniques of automatic algorithmic differentiation (AD), it offers the possibility of a consistent and accurate discrete adjoint approach [6].

This paper shows the integration status of CODA within the described MDAO suite. Its application is demonstrated in optimizations of an industrially relevant benchmark test case with a high-aspect ratio wing. A detailed description of the components of the MDAO suite is presented in terms of which gradients are required for the chosen elastically coupled process. The integration with LAGRANGE and FlowSimulator is in the focus of this work, which will be demonstrated and evaluated using an exact algorithmic differentiation of CODA, which is currently carried out in forward mode in large parts.

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PARTIAL DIFFERENTIAL EQUATIONS-GOVERNED MODELS AND OPTIMIZATION IN ENGINEERING APPLICATIONS

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Keywords: optimization, numerical methods, partial differential equations

Abstract of the session

This minisymposium focuses on mathematical models governed by partial differential equations along with numerical methods and optimization techniques for tackling engineering challenges. The discussions cover computational approaches in fluid dynamics, drug dissolution, filtration, and transportation systems. One key method presented is homogenization, which alleviates the discretization burden in finite element methods. The importance of sophisticated computational tools is demonstrated in the design of personalized drugs. Also, efficient evolutionary algorithms and surrogate models are presented to accelerate the parameter optimization of computationally heavy models with a focus on the applications.

Presentations of the session (totally 2 hours)

1. **Miguel Angel Uribe Laverde, Evolutionary algorithms for bus rapid transit system (40+5 min)**
2. **Andreas Rupp, Continuous super-resolution for the simulation of multiscale porous materials (20+5 min)**
3. **Rabia Altunay, Mathematical modeling of drug dissolution (20+5 min)**
4. **Jarkko Suuronen, Optimal inverse design of personalized drugs (20+5 min)**

(Note that the first speaker may have a longer presentation than the other, or, you may propose 4 x 30 minutes, always reserve 5 minutes for questions and changes of the speakers).

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COMPUTATIONAL METHODS FOR DESIGN OPTIMIZATION

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Keywords: Optimal design, optimal control, computational design, CFD

Abstract

In past decades, advances in 3D physics simulation software and increasingly efficient access to high-performance computing systems have made computational methods a cornerstone of modern engineering design. Finite Element Analysis (FEA) is now routinely applied in structural design, while Computational Fluid Dynamics (CFD) plays a central role in the development of fluid-thermal systems. Nevertheless, current engineering practice still largely depends on resolving a limited set of design cases, manually selected by human experts.

This presentation has three key objectives. First, we show how computational methods can render the above-mentioned human-driven design process significantly more rigorous and systematic, resulting not only in improved design outcomes but also in more efficient use of the designer's time. Second, we demonstrate how various types of design variables—both discrete and continuous—as well as couplings between individual simulations and the optimization loop, can be effectively addressed, along with the complexities they introduce. Third, we showcase the breadth of modern computational design applications, with a particular emphasis on CFD-based optimization of structures, fluid systems, and flow control.

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Lahti, Finland, 16–18, 2025

TOWARD SYSTEM-LEVEL CO-DESIGN: A MULTI-LEVEL SURROGATE FRAMEWORK FOR POWER CONVERTER COMPONENT OPTIMIZATION

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Keywords: Gaussian Process Regression, Bayesian Optimization, Converter Design Optimization, Power Electronics, Surrogate Modeling

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Abstract

For a power converter system, converter-level virtual prototyping presents significant challenges due to the iterative nature of optimizing interdependent components. A change in specifications for one component often necessitates re-optimization of other components. This iterative design process becomes particularly demanding as component-level optimization itself is inherently complex, usually characterized by mixed-integer design variables, complex nonlinear constraints, and irregular feasible design spaces. Traditional optimization methods struggle with this iterative process, especially when relying on expensive Finite Element Analysis (FEA) simulations to verify performance and constraint satisfaction. As a result, they often fall short in delivering high-quality designs within reasonable computational budgets.

To address these challenges, a multi-level surrogate-based optimization framework is proposed in the current work, which is specifically tailored for component-level optimization in the context of converter-level co-design. Our approach not only optimizes individual components but also prepares for the rapid re-optimization needed during converter-level integration.

At the component level, the proposed framework enables efficient design optimization by first constructing a Gaussian Process Regression (GPR) surrogate model tailored to accurately capture constraint boundaries through a limit-state-aware active learning strategy. This pre-trained model then initiates a Bayesian optimization process with a feasibility-weighted acquisition function, employing Monte Carlo sampling to propose promising candidates with

discrete, coupled design variables and an adaptive multi-region bounding-box search to efficiently refine them.

Crucially, to enable efficient converter-level co-design, the proposed framework incorporates an "informed search" strategy that builds a meta-surrogate model by mining knowledge from previously solved component design cases. This meta-model predicts performance boundaries for new component designs with changed specifications, allowing for rapid adaptation without starting optimization from scratch. By eliminating unproductive search regions early, it greatly enhances efficiency whenever component requirements change.

The approach was validated with a heat sink design problem involving 11 mixed-integer, coupled design variables. The design objective was to minimize heat sink weight while satisfying geometric and thermal constraints defined by two specified heat sources. To emulate changing design specifications in converter-level co-design, 50 different combinations of heat source values were randomly generated as inputs to the optimization framework. In 44 out of 50 test cases, the proposed approach yielded lighter heat sink designs, achieving an average 32% weight reduction compared to a baseline genetic algorithm, while reducing computational time by an order of magnitude. Furthermore, the informed search strategy accelerated the process an additional 20-fold, with no loss in optimality.

Overall, the proposed design framework presents a highly efficient and scalable optimization pipeline that directly tackles the iterative nature of converter-level co-design, paving the way for practical solutions to real-world converter design optimization challenges.

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IDENTIFYING HIDDEN PARAMETERS IN CELLULAR AUTOMATA WITH NEURAL NETWORKS

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Keywords: Cellular automata, Convolutional Neural Networks, Parameter Estimation

Abstract

Cellular Automata (CA) are powerful discrete models used to simulate complex systems that exhibit emergent behavior, such as urban growth, fluid dynamics, biological pattern formation, and epidemic spread. Despite their simplicity, CA models can produce highly intricate dynamics from local rules. However, uncovering the hidden parameters that drive these behaviors particularly those related to spatial and temporal evolution remains a major challenge. These hidden parameters determine crucial characteristics such as interaction rules and cell transition behaviors. Identifying them is essential for interpreting model outputs, validating simulations, and applying CA to real-world scenarios where the governing rules are not directly observable.

This study investigates the use of Convolutional Neural Networks (CNNs) to identify hidden jump parameters in a two-dimensional CA model. We propose a custom-designed CNN architecture tailored for parameter classification using raw CA-generated grid states as input. Unlike traditional approaches that rely on exhaustive simulations, our method learns to infer hidden parameters directly from spatial patterns. The jump parameter in our model dictates the neighborhood size and movement rules of individual cells, significantly influencing the evolution of the CA.

The CNN was trained and tested on synthetic datasets generated by running CA simulations across a range of domain sizes (from 25 × 25 to 150 × 150 grids) and iteration depths (0 to 50). We observe that larger domain sizes yield higher classification accuracy, as they offer more spatial context for learning meaningful features. Similarly, CA iterations up to a moderate depth improve performance, but beyond a certain threshold, additional iterations provide diminishing returns. This indicates that early temporal information is most informative for jump parameter identification.

Our model achieves an accuracy of 89.31% when utilizing both the temporal and spatial evolution in the training, outperforming traditional architectures like LeNet-5 and AlexNet in both predictive performance and inference speed. While AlexNet reached slightly higher peak accuracy in some configurations, our architecture was significantly more efficient, making it suitable for real-time applications and large-scale simulations. The CNN learns to exploit spatial correlations and morphological patterns in CA states that correlate with specific parameter settings something difficult to achieve with conventional statistical or rule-based methods.

These results demonstrate the promise of deep learning as a tool for parameter identification in discrete dynamical systems. Beyond accuracy, the lightweight nature of the model enables its deployment in interactive simulation environments or embedded systems where computational resources are limited.

Future work will extend the approach to identify multiple hidden parameters simultaneously, explore three-dimensional CA models, and evaluate transfer learning strategies for generalizing across different CA rule sets. This line of research opens new possibilities for integrating machine learning with traditional simulation frameworks to better understand and control complex systems.

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PARAMETRIC OPTIMIZATION OF RIGID BAFFLES ON LIQUID-FILLED TANKS SUBJECTED TO SLOSHING USING XFEM AND BAYESIAN OPTIMIZATION

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Keywords: sloshing, XFEM, Bayesian Optimization, Gaussian Process

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Abstract

Design of liquid-filled tanks is a critical concern for transport engineering manufacturers. One main concern is to develop such system by considering sloshing [1] in order to avoid dramatic behavior when the tank is subjected to dynamic loads. In order to reduce the impact of sloshing, one can consider a passive way that consists in adding baffles inside the tank. This work proposes an efficient parametric optimization strategy to design optimal baffles by considering two main tools: (i) a dedicated solver based on XFEM [2] designed to solved linearized sloshing vibrations and (ii) a Constrained Bayesian Optimization [3] based on Gaussian Processes and an iterative enrichment enables to localize the global optimum by minimizing the number of solver calls. The strategy is applied to 2D and 3D rigid, partially filled tanks. The effects of the baffles are presented and discussed such as the efficiency and accuracy of the solver. Finally, optimization convergence is discussed with respect to the whole computation time.

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Topology optimization of personalized drugs

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Keywords: topology optimization, Eikonal equation, Stochastic Reduced Order Method

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Abstract

We introduce a non-parametric topology optimization method for designing personalized drugs. We aim to design a multi-material drug composition that yields a target release profile. The release mechanism relies upon the Noyes-Witney equation which is converted on the Eikonal equation formalism. The topology optimization is implemented with a continuous relaxation approach which permits computing the objective function gradient with the help of the discrete adjoint method. We address material parameter uncertainties with the Stochastic Reduced Order Method (SROM) which is a computationally effective method for performing robust topology optimization (RTO). We demonstrate the applicability of the proposed method of designing multi-material drugs with various distinct target release profiles such as linear and pulsed release.

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Operator-Theoretic and Quantum-Inspired Frameworks for Data-Driven Modeling of Nonlinear Dynamical Systems

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We present a data-driven operator-theoretic framework for the analysis and reduced-order modeling of nonlinear dynamical systems. Rooted in Koopman operator theory and enriched with kernel-based learning techniques, this approach constructs finite-dimensional approximations of infinite-dimensional evolution operators, allowing nonlinear dynamics to be studied and forecasted via linear evolution in a learned space of observables.

The framework admits a spectral decomposition that enables interpretable and compact representations of spatiotemporal dynamics. Variations based on **vector-valued observables** support the modeling of coupled subsystems and multivariate fields. By embedding nonlinear evolution into linear operator flows, the method captures dominant patterns and enables structure-preserving dimension reduction, without relying on intrusive solvers or explicit governing equations.

Among several Koopman-based predictive schemes developed within this framework, one of the most recent advances is a **quantum-inspired formulation**, in which the evolving state is represented by a data-driven analog of a **density operator**, and observables evolve under a Koopman operator in the spirit of **Heisenberg dynamics**. This formulation naturally incorporates **uncertainty quantification**, and forms the basis for a nonparametric **data assimilation** scheme. Evolution and measurement operators are constructed empirically using time-ordered observations, represented as matrices in a data-adaptive basis learned through delay-coordinate embeddings and kernel methods.

The framework is particularly well suited for systems where only partial observations are available, or where modeling from first principles is intractable. By learning the evolution dynamics directly from data, it provides a flexible and interpretable alternative to black-box machine learning approaches, while retaining connections to functional and spectral analysis. **Moreover, it offers a systematic pathway for developing subgrid-scale modeling strategies, including closure schemes and parameterizations, by capturing the influence of unresolved dynamics through the evolution of coarse-grained observables.**

Current research efforts are focused on designing algorithms to implement this framework on quantum-like platforms and quantum computers, leveraging the operator structure and spectral evolution to align naturally with quantum computational primitives. These directions aim to exploit quantum architectures for scalable, data-driven dynamical modeling in high-dimensional systems.

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MATHEMATICAL MODELING OF DRUG DISSOLUTION

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Keywords: drug, release, parameter estimation, level-set method, finite element method

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Abstract

We discuss the computational aspects of modeling drug release. There are numerous different drug compositions for both tablet and implant designs. The compositions include polymers, hydrogels, matrix composites, multi-layered structures, and many others. Due to the great number of drug formulations, the physical mechanisms of the release of the active pharmaceutical ingredient (API) are versatile. Some of the drugs may release the API from their surface via progressive erosion, while other drugs may release the API through diffusion, or both. We present erosion and diffusion-based computational models for modeling the drug release. Our erosion model is based on the Eikonal equation and the level-set method, which are numerically robust methods for tracking time-dependent domains with topological changes. The diffusion-driven release is approximated by the diffusion equation coupled to the time-dependent boundary of the drug through the level-set equation. A sophisticated finite element implementation is used to solve the diffusion equation, while the level-set equation and the Eikonal equation are solved using the finite difference method. We fit some experimental data to our forward models to showcase the advantages and limitations of the proposed models.

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CORRECTING BIAS IN DYNAMICAL MODELS

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Keywords: Dynamical models, Model bias correction, Stochastic Modelling, Optimization, MCMC methods, Parameter identification

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Abstract

Dynamical models are often biased due to simplifications in their structure, limiting their ability to accurately represent real-world phenomena. Addressing these biases is important especially when optimization and predictive accuracy are the focus. This study presents a stochastic modeling framework that integrates both deterministic and stochastic components to improve model accuracy. We illustrate this approach using a case where a non-seasonal dynamical model is corrected to incorporate seasonal variations typically observed in real data, using an additive stochastic process. However, such corrections introduce challenges related to parameter identifiability, which require robust prior models and advanced sampling techniques, as standard MCMC methods like Metropolis-Hastings often fail to efficiently explore the posterior distribution in these settings. This approach can be used in any application involving biased dynamical models.

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CLEAR SESSION: CONTROL DESIGN FOR ENVIRONMENTAL ADVANCEMENT AND RESEARCH

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Keywords: control, modeling, sustainability, optimization, and robustness

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Abstract of the session

*The pressing challenges of environmental degradation call for innovative approaches in research and technology. This mini-symposium, titled "**CLEAR** session: **C**ontro**L** Design for **E**nvironmental **A**dvancement and **R**esearch", aims to bring together experts to discuss advancements in control theory and green engineering tailored to address environmental challenges.*

The focus will be on cutting-edge methods in control design, optimization, and system modeling for sustainable energy systems. Special attention will be given to managing pollution growth and stock, optimizing water allocation in irrigation systems, and ensuring ecological balance in lake ecosystems.
The goal is to demonstrate how results from theoretical mathematics, non linear control design approaches, and tools inspired by developments in artificial intelligence can be articulated to provide new solutions.
Key topics include:

- *Modeling and control of lake ecosystems for pollution mitigation and ecological preservation.*
- *Optimal and robust control strategies.*
- *Integration of environmental sustainability into control frameworks for water systems.*

The symposium aspires to foster interdisciplinary collaboration, bridging the gap between theoretical mathematical research and practical implementation.

Presentations of the session (totally 2 hours)

1. **Catherine Choquet, A machine learning algorithm for water quality control (25+5 min)**
2. **Éloïse Comte, Optimal control for lake eutrophication: A Dirichlet boundary control problem (25+5 min)**
3. **Souad Bezzaoucha, Polytopic approach for stability and control design of Saint-Venant equations (25+5 min)**
4. **Ruben Chenevat, Optimizing crop irrigation under biological and operational constraints with meteorological uncertainty (25+5 min)**

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HOW TO SURVIVE SEVERE DISRUPTIONS IN ENERGY SYSTEMS

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Keywords: Energy, Deep uncertainty, Robustness, Resilience, Anti-fragility, Multiobjective decision-making, Shocks, Unpredictable events

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Abstract

Energy systems are increasingly subject to many disruptions, such as natural disasters, pandemics, wars, and depletion of natural resources. These increase the vulnerability of energy systems. Indeed, due to the unpredictable nature of disruptions, precise information is lacking. Thus, most of the decisions related to energy systems are made under uncertainty. The level of uncertainty can be so high that the decision outcomes become uncountable, and their probabilities are not definable, or the experts cannot agree upon one decision. This is considered deep uncertainty.

To address deep uncertainty, contemporary research has focused on the development of systems to cope with severe disruptions, withstand volatility and uncertain environments, and even thrive in such contexts. However, there are research gaps when addressing deep uncertainty, and it is not clear which of the established strategies, such as robustness, resilience, and anti-fragility, are the best suited and when to be utilized to address deep uncertainty. As these strategies are meant to support decision-makers in handling potential disruptions in energy systems, identifying high-performing strategies is crucial.

In this talk, we will present the results from a systematic literature review, which surveys concepts and approaches that have been used to address disruptions under uncertainty in energy systems. The primary contributions of this study are the identification and classification of energy systems, disruption sources, and types and sources of uncertainties. We also provide an extensive list of strategies suggested to deal with disruptions in energy systems, compare the most favorable ones, and briefly review their advantages and disadvantages. Finally, we identify research gaps and offer guidelines for addressing disruptions in energy systems by discussing the most promising approaches to enhance the robustness, resilience, and anti-

fragility of these energy systems under deep uncertainty. These results will help researchers and practitioners alike to choose the most suitable one to address deep uncertainty and disruptions in energy systems.

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MULTI-STAGE MULTI-SCENARIO MULTI-OBJECTIVE OPTIMIZATION FOR ADAPTIVE ROBUST ENERGY TRANSITION UNDER DEEP UNCERTAINTY

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Keywords: Sustainability, Scenario planning, Deep uncertainty, Dynamic robustness, Green energy systems, Multi-objective optimization

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Abstract

Real-life decision problems often involve multiple decision-making stages, conflicting objectives, and various sources of uncertainties, where most decisions need to be made without complete knowledge of all the parameters, probability distributions, outcomes, and consequences of the alternative solutions. In some cases, the experts do not know or cannot agree upon the appropriate models, probability distributions, or measuring the desirability of alternative outcomes. This condition defines deep uncertainty. Under deep uncertainty, using wrong probability distribution leads to failure. Scenarios, instead, should be used to evaluate the consequences of any solutions in different plausible futures and find a robust solution.

This talk introduces a multi-stage multi-scenario multi-objective optimization approach for adaptive robust decision-making under deep uncertainty. Then, we further describe how the proposed approach can be applied in complex strategic planning in renewable energy transition via a case study of the South African sugar-bioethanol supply chains. Indeed, the sustainability of the whole infrastructure and its transition is analyzed in such a way that the renewed system is sustainable, robust, and adaptable for a broad range of plausible futures. Three objectives are considered in this problem under six uncertain parameters. The results prove the economic profitability and sustainability of the project. The proposed approach can also be applied to other energy supply chain problems under deep uncertainty.

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Multiobjective Linear Programming for Environmental and Energy Costs in Renewable Energy Site Selection with Spatial Interaction

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Keywords: Integer Linear Programming, Renewable Energy Site Selection, Spatial Interaction

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Abstract

Site selection for renewable-energy assets—wind turbines, solar arrays, and the networks that connect them—must reconcile economic and ecological goals. At the same time decisions are at high stakes so that large optimality gaps, potentially arising from using heuristic solvers, cannot be afforded, and the use of exact methods is thus encouraged. Electricity-transport costs rise with the spatial dispersion of sites, while biodiversity objectives often depend on keeping habitat patches physically linked. Both concerns introduce non-linear spatial-interaction terms that are difficult to handle for exact optimisation tools. This paper tests how far standard integer linear programming (ILP) solvers can be stretched to return provably Pareto-optimal plans when those interactions are linearised. We compare two strategies. The first approximates transmission cost by assigning each chosen site to a cluster centroid and penalising its radial distance. The second embeds an explicit network: within every cluster we build a minimum spanning tree (MST) over the selected sites and penalise the tree's total length, enforcing connectivity through a single-commodity flow formulation. We provide compact ILP models for both formulations and benchmark them on synthetic instances designed to mimic real-world geography. Results indicate that the centroid model is an order of magnitude faster but can understate true transmission expenses, whereas the MST model, though computationally heavier, captures them with high fidelity and remains tractable at the region scale. We also sketch how MST-style connectivity constructs could be repurposed to strengthen ecological corridors and offset the habitat fragmentation risk posed by new energy infrastructure.