ENERGETICS

AMMIN/DENERG - Hybrid-domain methods for Multiphysics modeling and control of advanced thermal metamaterials and energy systems

Funded By	Dipartimento DENERG Politecnico di TORINO [P.iva/CF:00518460019]
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Context of the research activity	The project will investigate AI-enhanced hybrid (physics-based + data-driven) approaches to model fluid flow, heat and mass transfer, interfacial effects, reactive phenomena in metamaterials (such as liquid foams) for advanced energy applications. Particularly, the research will explore the potential of current state-of-the-art AI methods to tackle the multi-scale and multi-physics nature of metamaterials, and how topological transitions affect thermal, reactive and acoustic propertied of metamaterials.
	Understanding complex fluid flow and heat transfer phenomena is key for the design and optimization of advanced energy systems, particularly those that are inherently characterized by highly non-linear, multi-scale or interfacial phenomena. Accurate modeling of such phenomena is particularly important in the context of novel systems and/or for emerging energy applications. Examples of such applications are: advanced and passive cooling strategies based on e.g. metamaterial-based thermal emitters; energy storage systems based on phase change materials (PCM) with engineering of the nano-structure, that require precise control of the small-scale dynamic morphology to optimize the power density; reactive systems, such as chemical and photo-chemical systems, whose performance is highly sensitive to e.g. local temperature, concentrations and flow conditions; smart systems for acoustic regulation, where advanced materials (metamaterials) can be adopted for sophisticated sound management. Detailed analysis of this latter sample set of energy systems often involves coupling of hydrodynamics, heat and mass transfer, interfacial effects and transient structural evolution at different scales, which renders modeling for such applications inherently challenging. Liquid foams, for example, with their evolving multiphase structure and tightly coupled thermal, hydrodynamic, and interface behavior, represent extremely challenging yet potentially very interesting emerging metamaterials for advanced energy applications. On these particular systems, previous understanding has been built in the context of the H2020 Sofia (Soap Film

Objectives	based Artificial Photosynthesis) project, where a novel biomimetic route to solar fuel production was explored based on soap films an foams. Besides this latter research line on fuels, additional possible applications of soap foams have recently been proposed, such as their use for acoustic applications. This latter idea has received recognition from the Compagnia di San Paolo within the project scheme Trapezio - Paving the way to research excellence and talent attraction, to which this research project is partly related. For these reasons, we propose here liquid foams as the starting test case for exploration of novel hybrid (data-driven combined with physics-based) modeling routes for metamaterials. Liquid foams represent indeed one of the best paradigmatic examples of complex materials to model, as they typically exhibit stiff mathematical characteristics and topological transitions, being extremely difficult to capture with conventional modeling and numerical methods. As of today, an accurate and (computationally) affordable multi-physics framework for their representation is still missing (despite some simplified approaches have been proposed). This research will therefore tackle this gap, starting from the thermal and acoustic properties of foams as a first methodological test case. Then, the acquired knowledge and developed methods could be applied also for the analysis of other advanced energy systems, where highly non-linear, multi-scale or interfacial effects are key for target performance metrics. The present research aims to explore the potential of the current state-of-the-art Artificial Intelligence (AI) methods to address the previously introduced modeling challenges for advanced energy systems. Particularly, among others, the following methods will be explored: Sequential Learning (SL) methods: suitable for the efficient optimization of systems governed by a large number of control parameters; Physics-Informed Neural Networks (PINNs), recently introduced, that allow to combine data-driven and physics-based modeling approaches for complex systems; Convolutional Neural Networks (CNNs), a particular type of neural networks for information extraction from images; Evolutionary algorithms, that allow flexible construction of surrogate models (typically via genetic programming, GP). These methods and variants thereof are primarily targeted to tackle different specific objectives of the expected activities. Therefore, a suitable modeling workflow based on different methods is to be designed to attain a robust analysis and optimization of the target system on a case-by-case basis. Hybrid methods will be also developed to target multiple objectives at a time. Focusing, as an example, on foams for illustrative purposes, a possible work plan to target such goals may involve the screening of different foam compositions and functionalization to achieve the target thermal or acoustic KPIs; the development of deep (CNN) models to analyze the flowing foams and relate their structure to thermal or acoustic response; the use of a GP to obtain a surrogate model for thermal or acoustic response as a function of the foam composition and structure.

Skills and competencies for the development of the activity	The candidate should have a solid background in thermodynamics, heat transfer and fluid dynamics. Familiarity with coding (Python, MATLAB, or similar) for scientific computing, and good analytical skills are desirable. Basic knowledge of AI methods and Machine Learning algorithms (Neural Networks) is a plus but not mandatory.