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Editorial

Introduction of *COMPES*: Finding directions in energy and computational science

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Energy is the material foundation on which we rely for survival and development, and the level of energy consumption and utilization is an important indicator of national economic development and people's living standards. The energy system is highly complex; it includes facilities, technology, and knowledge systems related to energy resource endowments, production, storage and transportation, consumption, as well as elements including government, energy enterprises, energy consumers, energy policies and regulations. Due to the urgent need to reduce carbon emissions, slow down the abnormal worsen of global climate, and achieve a balance between environmental protection and economic development, energy transition has been a focus of both scientific research and social attention in the past decades (Lu et al., 2022). The current energy transition is a process of gradually replacing carbon-intensive traditional fossil fuels (coal, oil, and natural gas) with low-carbon non-fossil fuels (especially renewable energy) (Zhang et al., 2022). However, energy transition does not necessarily mean a complete absolutization of fossil fuels, but rather a shift in the ways and routes of fossil energy utilization (Afra et al., 2023). The core of the future development of fossil energy is to create an upgraded scenario of the fossil energy industry and to promote efficient, low-carbon, green and sustainable development of fossil energy, and fundamentally promote efficient and clean development and utilization of the whole energy system (Zhang et al., 2024). Especially, the current fast-changing international political situation has brought new challenges to the energy transition procedures, while the necessity of conventional energy development has received increasing attentions with regard to the stable supply and maturely developed technologies (Zhang et al., 2023). Thus, studies on either the conventional fossil energy or the new energy should all be encouraged and welcomed. We have now established a new journal, Computational Energy Science, abbreviated as *COMPES*, to facilitate the exchange and dissemination of original research results and state-of-the-art reviews pertaining to both the conventional and new energy, to bring together researchers in the aforementioned fields to highlight the current developments of energy studies in both theory and methods, to exchange the latest research ideas, and to promote further collaborations in the community.

The first aim of this journal is to promote studies on the computation-based energy science. Numerical computation utilizes computers to simulate real energy processes and solve complex numerical systems (Chen, 2007). The core part of numerical simulation can be roughly divided into four steps: model construction, numerical solution, result analysis, and visualization (Cui et al., 2022). Numerical computation is significantly more effective than experimental research methods, allowing users to safely, quickly, and time-effectively improve

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the cognitive level and further explore on computers (Sun and Zhang, 2020). The power of computation-based energy science is reflected in complex layout modeling, solving complex physical-chemical coupled problems and visualizing the dynamic evaluation process (Sun and Wheeler, 2005). Engineering operations in the energy industry can also be supported by numerical simulations, including production prediction, injection and local pressure control (Jin and Firoozabadi, 2015), enhanced recovery, oil-gas-water separation and pipeline dispatching. Especially, AI developments for state-of-art energy applications are welcomed, including reservoir digital twin construction, flow and transport modeling and simulation in the geothermal energy system and CCUS process, hydrogen storage and transportation, and many others.

This journal also aims to highlight the advances in energy-based computational science. The unconditionally energy stable property, required by the second law of thermodynamics, has been proved in a number of numerical models and algorithms, which further exhibit a better performance in computational efficiency and robustness compared with less stable numerical schemes (Wheeler et al., 2020). As a result, energy stability has attracted increasedy attentions in model construction and algorithm implementation in computational science, especially for solving problems considering complex multi-component, multi-phase, multi-physics or multi-scale systems (Myint and Firoozabadi (2015)). This journal will focus on algorithms designed with energy functionals and energy norms as the main thread and related computational science (especially fully robust numerical algorithms based on discrete energy stability). In addition, the new field of thermodynamic computing is to discover universal laws based on non-equilibrium thermodynamics/statistical mechanics for all information processing (computing) systems, including the popular artificial neural network architectures.

The short name of this new journal is designed to be *COMPES*, which is pronounced as compass, an instrument for finding directions. The energy landscape and the computational landscape are accelerating rapidly. We wish that this journal could help the community to find future research directions in energy and computational science, with the aid of AI techniques and dialectically following the energy transition popularities.

Conflict of interest

The authors declare no competing interest.

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