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Editorial: Computational science and STEM education

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Editorial on the Research Topic
Computational science and STEM education

In a growing revolution driven by information technology, computational science (CSc) is indispensable for solving complex problems. Thus, CSs has been recognized to be a vitally important application of computational capabilities to understand and solve complex problems in the real world [President's Information Technology Advisory Committee (PITAC), 2005]. In this regard, Yasar and Landau (2003) have proposed that the CSc represents the integration of applied mathematics, computer science, and applied sciences. Modeling skills are essential in applying CSc. All modeling is based on theoretical models derived from each scientific discipline, validated in each science domain. When executed by a computer, models that are configured as computational models allow us to solve mathematical models that give rise to simulations and computations that are often impossible without using today's computational capabilities (Tolk, 2018). Nowadays, the various tools of the CSc are essential to address scientific and engineering problems in an interdisciplinary way in areas such as chemistry, computational chemistry, cheminformatics, computational biology, bioinformatics, molecular biology, astrophysics, materials science, environmental sciences, engineering and manufacturing, nanotechnology, drug design and discovery, among others. Each discipline field has experienced a growing development in the last decade, driven mainly by new techniques for obtaining, processing, modeling and simulating data [President's Information Technology Advisory Committee (PITAC), 2005; Vetter et al., 2018].

The COVID-19 crisis has demonstrated the importance of educational specialization in science, technology, engineering and mathematics (STEM) to have a trained workforce in public and private laboratories, companies, governments, and organizations in general, which contribute to the resilience of societies (OECD, 2021). In this sense, STEM education must advance in integrating scientific and technological advances and developing skills to meet the needs of a society undergoing increasing technological changes. According to Blonder and Mamlok-Naaman (2020), the perspective of contemporary research and cutting-edge scientific knowledge should be included at all levels of science education, which would provide students with up-to-date scientific information and disciplinary knowledge. Nowadays, it is difficult to imagine the progress of knowledge generation in STEM, in its different disciplinary and interdisciplinary fields, without using some technological tool that optimizes a given process or supports the development of a potential solution (Cáceres-Jensen et al., 2021; Pernaa, 2022). Technological devices, instruments, and computers are tools for constructing knowledge and supporting materialization processes linked to scientific and computational thinking (Rodríguez-Becerra et al., 2020).

This Research Topic investigates educational innovations and new teaching and learning sequences to illustrate the design of learning environments aimed at addressing authentic—real-world—problems from an integrative and interdisciplinary approach to STEM education, as well as to summarize the evidence on computational literacy in science education. The Research Topic comprises six articles by 31 authors from six countries in North America, South America, and Europe. We will structure the editorial starting with a systematic review of computational literacy. Then, we continue with articles that show different perspectives on curriculum designs.

Braun and Huwer, employing a systematic review of scientific evidence on computational literacy integration into science education, state that the partial approach to computational thinking as a guiding idea is helpful as a starting point for identifying and taking a closer look at other concepts in parallel. However, researchers emphasize that it is essential first to consider science competencies or contexts and then to look for informatics competencies that can be effectively linked. In addition, they propose that there may be several relevant informatics competencies per unit of learning in science, not just one. This design type requires significant computational knowledge on the part of teachers, which implies that we need to train more science teachers in computer literacy.

Augmented reality in teaching and learning science sequences may be a valuable window to support students' visualization capacities. For instance, on the one hand, Merino, Iturbe-Sarunic et al. describe and analyse a teaching-learning sequence (TLS) that includes snails as an educational tool and integrates Augmented Reality (AR) for the design of STEM activities. In this curricular strategy, each disciplinary field of STEM is at the same level of extension and depth and promotes the development of specific skills as the students' capability to visualize. On the other hand, Merino, Marzábal et al., through an exploratory case study of a chromatography TLS that analyzed evidence from 38 undergraduate chemistry students', provides new evidence that, in general, display an advance in the visualization and levels of representation used by students after using AR, however, the differences in visualization capacity could be related to capacities to attribute meanings to the different forms of used into AR representation. The students showed a positive perception toward using AR artifacts, and they moved from simple macroscopic descriptions of observed phenomena—low sophistication—to explanations using microscopic representations of physicochemical processes of chromatography—high sophistication.

Elías et al. report a mixed-method study with two objectives. The first objective is to review the various definitions of digital and STEM skills for science teacher education. This review was conducted as a bibliographic study. The second objective is to determine future STEM teachers' perceptions of their STEM and digital skills. In addition, the article analyses the use of technologies in a chemistry teacher training program at a Chilean state university and reflects the findings of the reviewed skills categories. The second phase was conducted as a case study. This article is very useful for all working in STEM teacher education because it proposes up-to-date definitions of digital and STEM skills and discusses the relevance of their integration into STEM teaching and learning.

Computers using the software have made a significant contribution to the processing, analysis, and representation of data, as well as to computer modeling and simulation, as part of understanding phenomena and solving current scientific and socio-scientific problems. Some of these solutions even result in efficient and effective process automation. Computational science is an excellent opportunity to design learning environments that allow us to address authentic—real-world—problems in an integrative and interdisciplinary approach to STEM Education. In this regard, Johnston et al. describe a bioinformatics programme as an illustrative example of rational design and implementation of a module at an MSc level. Some distinctive elements used in the module implementation considered: (i) a mixed lecture/immediate computational practical approach; (ii) access to computational practical using virtual machines; (iii) a confident technical learning environment; (iv) authentic (real) research questions; (v) work-projects in interdisciplinary group research; (vi) collaborative and inter-communicated teams-work to generate transferable skills; (vii) ethics requirements of research and scientific communication; (viii) multi-faceted feedback and assessment.

Vater et al. explore the successes and challenges in implementing biomolecular modeling and designing remote computational research-based educational high school programs. In this regard, curriculum pace and the required mentorship effort are critical challenges in this kind of implementation.

Author contributions

JR-B and JP wrote this editorial. Both authors contributed to the article and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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