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An interdisciplinary effort to integrate coding into science courses

The inclusion of computation in undergraduate STEM curricula varies widely, ranging from none at all to fully dedicated courses. We believe that building cyberinfrastructure skills within physical science courses would enhance domain-specific learning objectives and increase student understanding and engagement[1–3]. Programming within a science course, rather than in a standalone coding class, gives students a better understanding of the context for applying computational tools[4–6].

In line with this teaching strategy, we established Enhancing Science Courses by Integrating Python (ESCIP), a collaborative initiative that promotes the teaching of cyberinfrastructure skills within standard science courses. Python was chosen because it is a widely used, open-source programming language that is common to the scientific research community of physicists, chemists and astronomers, which are the disciplines supported by the Research Corporation for Science Advancement's Cottrell Scholars program. ESCIP has evolved from an initial team of eight early-career faculty members to a network of more than 177 scientists with an active Slack channel and a website with teaching resources.

Many faculty develop ad hoc notebooks for their own courses but do not have a place to share them more broadly. Our website currently hosts notebooks illustrating computation and modeling practices in chemistry, astronomy and physics courses. We encourage notebook submission (including via email or Slack) and provide contributor guidelines and a notebook template to help instructors adapt their content to a format that is easier for new colleagues to understand and adopt.

The establishment of ESCIP immediately prior to the COVID pandemic provided a platform where instructors could connect during a time when in-person laboratory activities were limited. Many repositories and communities – such as *Python in Chemistry*[7], *PICUP*[8], *Psi4Education*[9], *MERCURY*[10] and *chemcompute*[11] – support computational education that targets discipline-specific audiences, but ESCIP is intentionally cross-disciplinary. Exchanging ideas with teachers from other fields and schools gives a broad view of computing across the university-wide curriculum and helps to inform professors who may want to advocate for curricular changes at their own institution. Additionally, more diverse examples and feedback from teachers in other disciplines can help to improve accessibility for students from different backgrounds.

Between 2020 and 2024, ESCIP has hosted six workshops, in which 119 attendees shared teaching materials and developed new coding exercises collaboratively. Some workshop participants had already taught Python coding[12], while others were interested in getting started and sought to learn best practices from experienced colleagues. The NSF-funded Molecular Sciences Software Institute (MolSSI)[13] provided training for faculty members and postdocs to learn about Python libraries and tools that could be useful for undergraduate education, such as NumPy[14], pandas, seaborn, scikit-learn and RDKit. Lessons learned by the organizers of ESCIP workshops influenced the establishment of the Accelerating Curricular Transformation in the Computational Molecular Sciences (ACT-CMS), which is a faculty professional development program at the MolSSI that supports the integration of cyberinfrastructure skills into the molecular sciences curriculum. ACT-CMS also supports a Faculty Fellows program aimed at developing and sharing curricular resources.

One challenge discussed at the ESCIP workshop held in April 2023 was how best to leverage programming-based assignments using large language models (LLMs) that can generate code (for instance, ChatGPT) that can easily produce solutions to many standard problems. A number of scientists advocated using these tools to reduce the barriers to entry for programming, with the strategy of explaining whether or not the generated code is correct and why[15]. Students who have developed strong algorithmic thinking skills can also cross-check their own understanding with the results provided by ChatGPT to ensure accuracy and identify errors in logic or scientific understanding. Motivated by widespread interest in LLMs and AI-assisted coding, the theme of the 2024 ESCIP workshop was 'Teaching scientific computing at the dawn of AI'. One key takeaway was that students need support with learning prompt engineering to harness the power of their domain-specific expertise. Examples of effective strategies for including LLMs in assignments aimed at accelerating computational fluency and modeling were also discussed.

The ESCIP community aims to provide resources for teachers and students to develop broad cyberinfrastructure competency by emphasizing skills such as code reading, testing and editing, problem decomposition, and design strategies for program and function composition. Improved literacy in these areas will facilitate student engagement and learning, including in contexts where LLM code assistants are used in the classroom. One future direction of ESCIP is to create pedagogical materials that use free LLM assistants to teach cyberinfrastructure skills in science courses. Ideally, we will provide simple recipes to aid teachers to develop and adopt these tools in their own courses.

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References

1. McDonald A. R. Teaching programming across the chemistry curriculum: a revolution or a revival? In *ACS Symp. Series* (eds McDonald, A. R. & Nash, J. A.) Vol. 1387 (American Chemical Society, 2021).
2. Van Staveren, M. *J. Chem. Educ.* **99**, 2604–2609 (2022).
3. De Haan, D. O., Schafer, J. A. & Gillette, E. I. *J. Chem. Educ.* **98**, 3245–3250 (2021).
4. Phillips, A. M., Gouvea, E., Gravel, B. & Atherton, T. J. In *2022 Physics Education Research Conf. Proc.* 353–358 (American Association of Physics Teachers, 2022).
5. Sweet, C., Akinfenwa, O. & Foley, J. J. *J. Chem. Educ.* **95**, 384–392 (2018).
6. Rowe, P. M. et al. *J. Geosci. Educ.* **69**, 178–191 (2020).
7. McCluskey, A. R., Rivera, M. & Mey, A. S. J. S. *Nat. Chem.* **16**, 1383–1384 (2024).
8. Caballero, M. D. et al. *Phys. Teach.* **57**, 397–399 (2019).
9. Magers, D. B. et al. In *ACS Symp. Series* (eds McDonald, A. R. & Nash, J. A.) Vol. 1387, 107–122 (American Chemical Society, 2021).
10. McDonald, A. R. et al. *Int. J. Quantum Chem.* **120**, e26359 (2020).
11. Perri, M. J., Akinmurele, M. & Haynie, M. In *ACS Symp. Series* (eds Grushow, A. & Reeves, M. S.) Vol. 1312, 79–92 (American Chemical Society, 2019).
12. Fuchs, W., McDonald, A. R., Gautam, A. & Kazerouni, A. M. *J. Chem. Educ.* **101**, 3085–3096 (2024).
13. Nash, J. A., Mostafanejad, M., Crawford, T. D. & McDonald, A. R. *Comput. Sci. Eng.* **24**, 72–76 (2022).
14. Harris, C. R. et al. *Nature* **585**, 357–362 (2020).
15. Hocky, G. M. & White, A. D. *Digit. Discov.* **1**, 79–83 (2022).

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Competing interests

The authors declare no competing interests.