Advanced Modeling, Scientific Computing & Data Analysis with Open SageMath

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Abstract. Our contribution addresses the computational challenges in physics and STEM education posed by advanced models. We introduce SageMath, a Python-based CAS software that integrates numerous open-source packages. We illustrate two pivotal modeling features: the desolve_odeint procedure for fast and accurate numerical solutions of differential equations and the LMFIT library for fitting their parameters directly with experimental data. As a professional science tool, SageMath demonstrates potential in education, enabling the model of complex real-world situations and bridging the gap between professional and educational computational tools.

Digital tools for computational modeling

Building models of physical phenomena is undeniably one of the key competencies and outcomes of scientific literacy and STEM education. However, when we consider classroom computational modeling in physics education and the digital tools we should use to train, develop, or strengthen modeling skills, the answer is not so clear. According to [1], fundamental tools include open programming languages (e.g., Fortran, C, Java, or Python), spreadsheets (Excel, Google Sheets, GeoGebra), graphical modeling (STELLA, Dynasys, Modus, or VnR), and also complex interactive environments with strong visualization support (Coach, Tracker, GeoGebra, Modellus, VPython, or Easy Java Simulations). PER continues to explore and examine the effectiveness of these various options historically brought in the development of digital technologies. In our contribution, we present another powerful candidate from complex environments, SageMath Jupyter notebooks, with which we now have 8 years of experience [2].

Advanced models, computations & data analysis in SageMath Jupyter notebooks

More than a decade ago, researchers, scientists, and professionals typically used scientific computing environments like Mathematica or MATLAB in real science and practice. In 2014, physicists and data scientists F. Perez and B. Granger initiated the ambitious Jupyter project (jupyter.org) to develop a powerful, universal, and open virtual interactive scientific environment. Today, Jupyter is the most widely used technology for performing scientific calculations, open data analysis, processing, and reporting. It has also become a crucial educational tool in STEM education, bridging the gap between professional and educational tools. One version of these notebooks is Jupyter Notebooks with SageMath (sagemath.org) as the computational kernel (see [2]), which integrates more than a hundred open-source programs and libraries. Now it provides

- numerical and symbolic manipulations as a powerful CAS calculator
- real-world problems advanced modeling via inverse problems & nonlinear optimization
- reliable sources of scientific data, including open databases of math, physical and material constants, or chemical and biological data
- data literacy tools for effective data processing and analysis (e.g., Python or R libraries)
- programming capabilities in Python but also R, Octave, Julia, Fortran, etc.
- advanced visualization and interactivity via dynamic multimedia presentations (which can be interactively modified also while presenting, unlike PowerPoint), interactive widgets (equivalent to Java applets or scripts), or dynamic HTLMs
- AI chatbots (e.g., AI Jupyternaut assistant [3] using LLMs like ChatGPT or Claude)

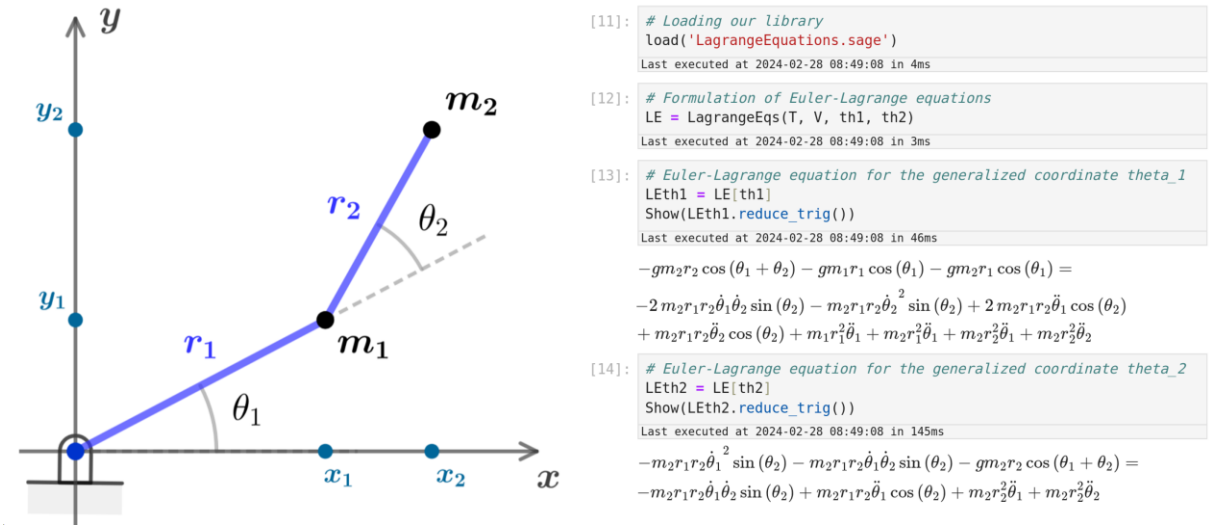

Fig. 1. Modeling a robotic arm (on the left) using Lagrange equations automatically generated in SageMath by elementary CAS commands hidden in our own LagrangeEquations.sage library (on the right).

The power of SageMath can be better appreciated through specific STEM illustrations. In Fig. 1, we see the modeling of a robotic arm [4] using energy instead of the more complicated classical approach using forces. After constructing the arm model using kinetic energy T and potential energy V, the subsequent algebraic manipulations (such as differentiation, which is not physics), leading to the Lagrange equations, can be performed automatically by SageMath as a CAS. The resulting equations of motion can be very quickly and accurately solved numerically using the Sage command desolve_odeint with static or interactive visualization. For fitting with experimental data, the library LMFIT, based on nonlinear optimization, can be used to directly fit parameters of the formulated models without the need to know their analytical solutions, as it is traditionally needed and can be done only in linear cases with respect to the estimated parameters.

Thanks to SageMath, our students [5] in projects can successfully model a variety of complex real STEM situations, such as the fall of a polystyrene ball in studying microplastics in the environment, the Apollo 8 flight to the Moon (using Hamiltonian equations), quantum engineering (LED lasers), molecules via Wilberforce pendulum, myth busters experiments, robots in the 4th industrial revolution, the human heart via Van der Pol oscillator, the nonlinear pendulum in the frame of chaos theory, or smartwatches charging pads based on resonance in RLC circuits.

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