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Caustics: A Python Package for Accelerated Strong Gravitational Lensing Simulations

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Summary

Gravitational lensing is the deflection of light rays due to the gravity of intervening masses. This phenomenon is observed at a variety of configurations, involving any non-uniform mass such as planets, stars, galaxies, clusters of galaxies, and even the large-scale structure of the Universe. Strong lensing occurs when the distortions are significant and multiple images of the background source are observed. The lens and lensed object(s) must be aligned closely on the sky. As the discovery of lens systems has grown to the low thousands, these systems have become pivotal for precision measurements in astrophysics, notably for phenomena including dark matter (e.g. Hezaveh et al., 2016; Vegetti & Vogelsberger, 2014), supernovae (e.g. Rodney et al., 2021), quasars (e.g. Peng et al., 2006), the first stars (e.g. Welch et al., 2022), and the Universe's expansion rate (e.g. K. C. Wong et al., 2020). With future surveys expected to discover hundreds of thousands of lensing systems, the modelling and simulation of such systems must be done at orders of magnitude larger scale than ever before. Here we present `caustics`, a Python package designed to facilitate machine learning and Bayesian methods to handle the extensive computational demands of modelling such a vast number of lensing systems.

Statement of need

The next generation of astronomical surveys, such as the Legacy Survey of Space and Time, the Roman Core Community Surveys, and the Euclid wide survey, are expected to uncover hundreds of thousands of gravitational lenses (Collett, 2015), dramatically increasing the scientific potential of gravitational lensing studies. Currently, analyzing a single lensing system can take several days or weeks, which will soon be infeasible to scale. Thus, advancements such as GPU acceleration and/or automatic differentiation are needed to reduce the analysis timescales. Machine learning will be critical to achieve the necessary speed to process these lenses. It will also be needed to meet the complexity of strong lens modelling. Literature on machine learning applications in strong gravitational lensing underscores this need (Brehmer et al., 2019; Chianese et al., 2020; Coogan et al., 2020; Karchev, Coogan, et al., 2022; Karchev, Anau Montel, et al., 2022; Mishra-Sharma & Yang, 2022). `caustics` is built with the future of lensing in mind, using `PyTorch` (Paszke et al., 2019) to accelerate the low-level computation and enable deep learning algorithms, which rely on automatic differentiation.

Several other simulation packages for strong gravitational lensing are already publicly available. The well-established `lenstronomy` package has been in use since 2018 (Birrer et al., 2021); `GLAMER` is a C++-based code for modelling complex and large dynamic range fields (Metcalf & Petkova, 2014); `PyAutoLens` is also widely used (Nightingale et al., 2021); `GIGA-Lens` is a specialized JAX-based (Bradbury et al., 2018) gravitational lensing package (Gu et al., 2022); and `Herculens` is a more general JAX-based lensing simulator package (Galan et al., 2022); among others (`GRAVLENS` Keeton, 2011; `LENSTOOL` Kneib et al., 2011; `SLITRONOMY` Galan et al., 2021; `paltax` Wagner-Carena et al., 2024). There are also several in-house codes developed for specialized analysis which are then not publicly released (e.g. Suyu & Halkola, 2010). The development of `caustics` has been primarily focused on three aspects: processing speed, user experience, and flexibility. Processing speed is comparable to the widely used `lenstronomy` when on CPU, and can be over 1000 times faster on GPU depending on configuration as seen in Figure 1. The user experience is streamlined by providing three interfaces to the code: configuration file, object-oriented, and functional. Flexibility is achieved by a determined focus on minimalism in the core functionality of `caustics` and encouraging user extension.

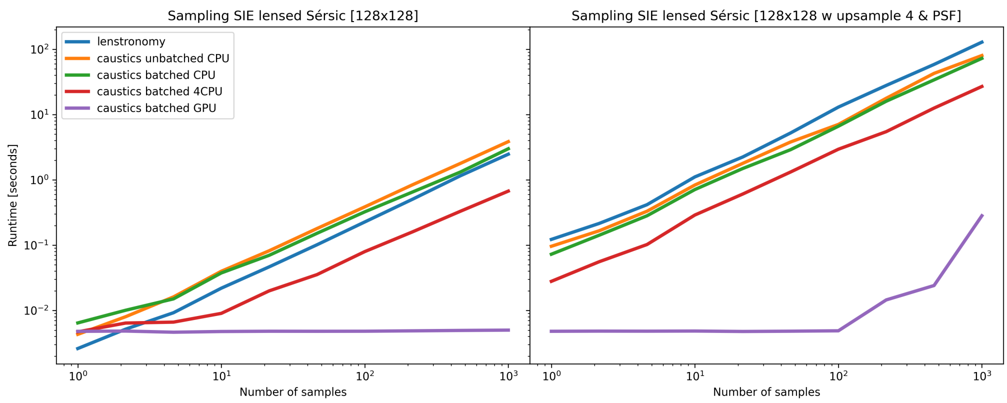

Figure 1: Runtime comparisons for a simple lensing setup. We compare the amount of time taken (y-axis) to generate a certain number of lensing realizations (x-axis) where a Sérsic model is lensed by an SIE mass distribution. For CPU calculations we use an Intel Gold 6148 Skylake and for the GPU we use a NVIDIA V100. All tests were done at 64-bit precision. On the left, the lensing system is sampled at 128-pixel resolution only at pixel midpoints. On the right, a more realistic simulation includes upsampled pixels and PSF convolution. From the two tests we see varying performance enhancements from compiled, unbatched, batched, multi-threaded, and GPU processing setups.

`caustics` fills a timely need for a differentiable lensing simulator. Several other fields have already benefited from such simulators, for example gravitational wave analysis (Coogan et al., 2022; Edwards et al., 2024; K. W. K. Wong et al., 2023), astronomical image photometry (Stone et al., 2023), point spread function modelling (Desdoigts et al., 2023); time series analysis (Million et al., 2024), and even generic optimization for scientific problems (Nikolic, 2018). With `caustics` it will now be possible to analyze over 100,000 lenses in a timely manner (Hezaveh et al., 2017; Perreault Levasseur et al., 2017).

Scope

`caustics` is a gravitational lensing simulator. The purpose of the project is to streamline the simulation of strong gravitational lensing effects on the light of a background source. The primary focus is on all transformations between the source plane(s) and the image plane through the lensing plane(s). There is minimal effort on modelling the observational elements of the atmosphere or telescope optics. A variety of parametric lensing profiles are included, such as: Singular Isothermal Ellipsoid (SIE), Elliptical Power Law (EPL), Pseudo-Jaffe, Navarro-Frenk-White (NFW), and External Shear. Additionally, it offers non-parametric representations such as a gridded convergence or a potential field and pixelized sources.

Once a lensing system has been defined, `caustics` can then perform various computational operations on the system such as raytracing through the lensing system, forwards and backwards. Users can compute the lensing potential, convergence, deflection field, time delay field, shear, and magnification. All of these operations can readily be performed in a multi-plane setting to account for interlopers or multiple sources.

With these building blocks in place, one can construct fast and accurate simulators used to produce training sets for machine learning models or for inference on real-world systems. Neural networks have become a widespread tool for amortized inference of gravitational lensing parameters (Hezaveh et al., 2017) or in the detection of gravitational lenses (Huang et al., 2021; Petrillo et al., 2017), but they require large and accurate training sets that can be created quickly with `caustics`. The simulators are differentiable, enabling algorithms such as recurrent inference machines (Adam et al., 2023) and diffusion models (Adam et al., 2022; Remy et al., 2023).

The scope of `caustics` ends at lensing simulation, thus it does not include functionality to optimize or sample the resulting functions. Users are encouraged to use already existing optimization and sampling codes such as `scipy.optimize` (Virtanen et al., 2020), `emcee` (Foreman-Mackey et al., 2013), `dynesty` (Speagle, 2020), `Pyro` (Bingham et al., 2019), and `torch.optim` (Paszke et al., 2019). Interfacing with these codes is easy and demonstrations are included in the documentation.

Further, `caustics` does not implement simulators for all possible lensing problems (AGN microlensing, multi-source lensing, supernova time-delay cosmography, etc.). Instead it is formatted much like `PyTorch` where one constructs a class (Module) and builds a forward model function by calling individual (often functional) components defined within `caustics`. In this way it can always be adapted to the specific needs of a lensing problem.

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