# Digital Infrastructure in Astrophysics

## Report for the Ford and Sloan Foundation's Digital Infrastructure Research Program January 2020

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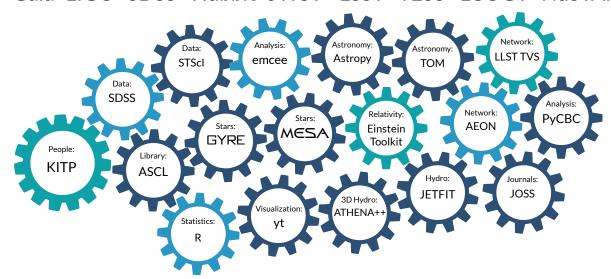
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## Gaia LIGO SDSS Hubble JWST LSST TESS LCOGT NuSTAR



## Laboratory Astrophysics

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## Contents

1	Ex	xecutive Summary						
2	Op	Open Digital Infrastructure in Astrophysics						
3	Vision and Execution of the Workshop							
4	Wo	Workshop Agenda and Focus Questions						
5	5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 5.11 5.12 5.13 5.14 5.15 5.16	e Digital Infrastructure Projects Considered GYRE - Rich Townsend Space Telescope Science Institute (STScI) Data - Arfon Smith Journal of Open Source Software (JOSS) - Arfon Smith emcee - Daniel Foreman-Mackey LSST Transients - Federica Bianco yt - Matt Turk R Astrostatistics - Gwendolyn Eadie SDSS Digital Infrastructure - Joel Brownstein TOM Toolkit - Rachel Street AEON Network - Rachel Street Astropy - Kelle Cruz ATHENA++ - Jim Stone Einstein Toolkit - Philipp Mösta PyCBC - Duncan Brown JETFIT - Andrew MacFadyen Astrophysics Source Code Library (ASCL) - Alice Allen MESA - Frank Timmes	55 66 77 88 88 99 100 111 111 122 133 134					
6	$\mathbf{S}\mathbf{y}$	nthesis	15					

## 1 Executive Summary

Astronomy, as a field, has long encouraged the development of free, open digital infrastructure (e.g., National Research Council 2010, 2011). Examples range from simple scripts that enable individual scientific research, through software instruments for entire communities, to data reduction pipelines for telescope operations at national facilities. As with the digital infrastructure of our larger society today (e.g., Eghbal 2016), nearly all astronomical research relies on free, open source software (FOSS) written and maintained by a small number of developers. And like the physical infrastructure of roads or bridges, digital infrastructure needs regular upkeep and maintenance (e.g., Eghbal 2016). In astronomy, financial support for maintaining existing digital infrastructure is generally much harder to secure than funding for developing new digital infrastructures that promise new science. Sustaining astronomy's digital infrastructure is a new topic for many, the sustainability challenges are not always widely known, and sometimes even formulating answerable questions can be formidable:

- What is the relationship between money and sustainability for community-driven, open-knowledge software instruments that enable transformative research in stellar astrophysics?
- At what points in a software instrument's lifecycle does an injection of financial resources help or hurt?
- Are science driven software instruments sustainable for the long term, say the next 40 years?

These questions are relevant from a science perspective because over the next decade astronomy will probe the rich stellar astrophysics of transient phenomena in the sky, including gravitational waves from the mergers of neutron stars and black holes, light curves and spectra from corecollapse supernovae, and the oscillation modes of stars. Laser Interferometer Gravitational-Wave Observatory (LIGO) and VIRGO have demonstrated the existence of binary stellar-mass black hole systems and continue to monitor the sky for gravitational waves from compact binary inspirals and asymmetrical exploding massive stars. Advances in detector technology, computer processing power, network bandwidth, software development tools, and data storage capability have enabled new sky surveys, such as the Sloan Digital Sky Survey, to create the most detailed three-dimensional maps of the Universe ever made. The stellar censuses of Gaia Data Release 2, containing about one billion stars, will provide the observational data to tackle a range of questions related to the origin, structure, and evolutionary history of stars in the Milky Way. This ongoing explosion of activity powers theoretical and computational developments, in particular the evolution of community-driven digital infrastructures for research and education. The scientific potential of these new observation capabilities will be unlocked largely through the efforts of developers and users in FOSS communities.

These questions are also central from a digital infrastructure perspective because software is an integral enabler of observation, experiment, theory, and computation and a primary modality for realizing the discoveries and innovations. Answers to these questions are also relevant from a potential funder's perspective because they fill a knowledge gap about FOSS digital infrastructures within domain-specific disciplines. To date, to our knowledge, there is little literature on the questions asked above for the domain-specific discipline of stellar astrophysics. Individual software instrument project principals may know their user, bibliometric, and funding profile history. However, this information is usually not openly shared or aggregated across a representative sample. Such aggregated information is likely to be of interest to potential funders who may seek an informed, holistic and effective strategy to any investment. Addressing this knowledge gap within the domain-specific discipline of stellar astrophysics is the topic of this report.

## 2 Open Digital Infrastructure in Astrophysics

The "Open Digital Infrastructure in Astrophysics" workshop was held June 4 - 5, 2019 at the Kavli Institute for Theoretical Physics (KITP) at UC Santa Barbara. The workshop's intent was to highlight open-knowledge digital infrastructures, software instrument communities, metrics for success, developer models, diversity efforts, funding profiles, and sustainability plans. The workshop strove to attain five strategic objectives that align with the Ford and Sloan Foundation's Digital Infrastructure Research program's broader goals:

- Serve as a focused forum for the principals of free and open source software projects within the fields of astronomy and astrophysics to share knowledge with each other;
- Explore innovative topics emerging within their respective software communities;
- Discuss emerging best practices across the software projects;
- Stimulate thinking on new ways of achieving long-term software sustainability;
- Share the aggregate information and experiences in a workshop report.

The 2-day workshop was held while the KITP programs "Better Stars, Better Planets: Exploiting the Stellar-Exoplanetary Synergy" and "The New Era of Gravitational-Wave Physics and Astrophysics" were in session. Participants in these two programs were encouraged to attend the workshop, in part by pausing their regular program schedules while the workshop was in session.

## 3 Vision and Execution of the Workshop

The Project Investigators (Timmes, Bildsten, and Townsend) discussed the vision, logistics, and execution of the workshop about once a week on average between February 2019 and June 2019. The vision was to host speakers who spanned a diversity of FOSS projects in stellar astrophysics:

- from single developers, through small teams, to large distributed alliance models;
- from user communities of a few, through hunderds, to thousands;
- from funding models of volunteers, though science/software grants, to Foundations.

By March 2019 the PIs converged on a list of potential speakers to ask, and by April 2019 the invited speaker list was finalized. The workshop website, <a href="http://cocoubed.asu.edu/digital\_infrastructure\_astronomy">http://cocoubed.asu.edu/digital\_infrastructure\_astronomy</a>, went online in May 2019. It currently aggregates links to

- the recorded presentations, http://online.kitp.ucsb.edu/online/odia19/;
- live tweets made during the workshop, https://twitter.com/hashtag/OpenAstroInfra;
- the FOSS projects and communities represented at the workshop;
- efforts to conceptualize US Research Software Sustainability Institute http://urssi.us/;
- posts on the fundamentals of software sustainability https://danielskatzblog.wordpress.com/2018/09/26/fundamentals-of-software-sustainability/;
- a guide to sustainability models for research software projects https://github.com/danielskatz/sustaining-research-projects.

Table 1: Agenda for the Open Digital Infrastructure in Astrophysics Workshop

### Tuesday June 4, 2019

Time		Representative	Institution	Title
9:00	am	Rich Townsend	UW Madison	GYRE
9:45	am	Arfon Smith	Space Telescope	JOSS and STScI data
10:30	am	Coffee		
11:00	am	Daniel Foreman-Mackey	Flatiron Institute	emcee
11:45	am	Federica Bianco	Univ. of Delaware	LSST Transients
12:30	pm	Lunch		
2:00	pm	Matt Turk	Univ. of Illinois	yt
2:45	pm	Gwendolyn Eadie	Univ. of Toronto	R astrostatistics
3:30	pm	Break		
4:00	pm	Joel Brownstein	Univ. of Utah	SDSS Data Infrastructure
4:45	pm	Rachel Street	Las Cumbres Obs.	TOM Toolkit / AEON Network
5:30	pm	Workshop Dinner		

#### Wednesday June 5, 2019

Time		Representative	Institution	Title
9:00	am	Kelle Cruz	Hunter College	Astropy
9:45	am	Jim Stone	Princeton	ATHENA++
10:30	am	Coffee		
11:00	am	Philipp Mösta	Univ. of Amsterdam	Einstein Toolkit
11:45	am	Duncan Brown	Syracuse Univ.	PyCBC
12:30	pm	Lunch		
2:00	pm	Andrew MacFadyen	New York Univ.	JETFIT
2:45	pm	Alice Allen	Univ. of Maryland	Astrophysics Source Code Library
3:30	pm	Break		
4:00	pm	Frank Timmes	Arizona State Univ.	MESA
4:45	pm	Everyone		Open Discussion

## 4 Workshop Agenda and Focus Questions

Table 1 lists the invited speakers, their home institution, and their digital infrastructure project. The PIs encouraged the invited speakers to consider presenting quantitative and qualitative information, as appropriate, on the following 18 high-value questions and topics. In these questions, the word "instrument" was intended to be broadly interpreted to mean an open-source software instrument, an open data repository, or an open library.

- What does your FOSS instrument do?
- Who is your instrument's community?
- How many users does your instrument have, and how is this metric tracked?
- How is communication with your user base conducted, and at what frequency?
- What efforts are made to expand the user base?
- What are the longitudinal bibliometrics (citations, citations to citations, rankings, honors)?
- How often is an article published/distributed that describes new capabilities?

- What offshoots or spinoffs from the software instrument have arisen?
- Who is the developer community?
- What is the developer model?
- How are new developers attracted?
- How are developers retained?
- What efforts are made to build a diverse developer base?
- What is the past funding profile for your instrument?
- What new funding efforts are underway?
- Offer a definition of "sustainability" for your instrument.
- What efforts are being made to reach this definition of sustainability?
- Will your instrument be widely used by your community in 10, 20, 40 years?

## 5 The Digital Infrastructure Projects Considered

In this section we present data on the digital infrastructure projects studied.

#### 5.1 GYRE - Rich Townsend

Like a sound wave resonating in an organ pipe, sound waves can resonate inside a star. By measuring these wave frequencies, we can learn about a star's internal structure. This field, asteroseismology, has been reinvigorated in recent years thanks to the wealth of new observational data provided by NASA space-based instruments such as *Kepler* and now *TESS*. Interpreting these new observations requires the astronomer's analogue to the telescope: a stellar oscillation software instrument which calculates the frequency spectrum of an arbitrary input stellar model.

The free and open GYRE source code solves the system of equations governing small periodic perturbations to an equilibrium stellar state. GYRE is built on a robust and accurate numerical scheme, and makes efficient use of multiple cores and/or cluster nodes. The suite is written in Fortran 2008, with an object oriented architecture that is simple, clean, modular and adherent to modern coding best practices (https://bitbucket.org/rhdtownsend/gyre/wiki/Home).

GYRE's target community is stellar asteroseismologists. GYRE has currently attracted over 200 users world-wide. GYRE innovates by updating its community with an instrument paper describing major new software and science capabilities about every five years (Townsend et al. 2018; Townsend & Teitler 2013). These two instrument papers have been cited  $\simeq 150$  times and have a current citation rate of  $\simeq 65/\text{year}$ . The articles that cite GYRE have themselves generated  $\simeq 3,271$  citations, yielding a radius-of-influence of  $\simeq 3,271/150 \simeq 21$ , which suggests that GYRE helps generate articles that the broader astronomy community values. GYRE provides a portal for its community to openly share knowledge (http://www.astro.wisc.edu/~townsend/gyre-forums/), and offers  $\simeq 750$  archived and searchable posts of community discussions about stellar oscillations.

GYRE is maintained by two developers and five contributors who directly support a community of  $\simeq 110$  users and indirectly a community of  $\simeq 300$  users uses through GYRE's integration with MESA (see Section 5.17). The combination of these users downloaded the latest release of GYRE  $\simeq 400$  times. Development of GYRE and its community have been supported by a National Science Foundation (NSF) science award between 2009-2002 for \$428K, NSF digital infrastructure award

between 2014-2016 for \$76K, NSF digital infrastructure award between 2017-2021 for \$683K, and a NSF science award between 2017-2020 for \$317K.

### 5.2 Space Telescope Science Institute (STScI) Data - Arfon Smith

The STScI helps humanity explore the universe with advanced space telescopes and ever-growing data archives. The Data Science Mission Office (DSMO) within STScI is responsible for maximizing the scientific returns from archives containing astronomical observations from 17 space-based missions and ground-based observatories. The scope of the DSMO includes Data Science (statistics, machine learning, algorithms, analytics and data mining) and all aspects of data management.

The James Webb Space Telescope (JWST) is a space telescope that is planned to be the successor to the Hubble Space Telescope (HST). The main focus of JWST data analysis tool development is to advance a set of high-quality FOSS libraries for working with JWST data, leveraging FOSS technologies where possible, In addition, the aim is to provide a set of high-performance visualization tools for exploring JWST data products, and provide a comprehensive suite of reproducible analysis captured as Juptyer notebooks.

The vision for these tools is to ensure that astronomers are equipped with software to analyze and interpret JWST efficiently from the start of the mission; reduce the necessity for astronomers to write data-analysis software, but make it easy to do so when necessary; provide a clear mechanism for astronomers to share expertise with each other and make it easy to share and re-use code; allow the community to easily contribute to and expand the capabilities of existing tools; improve repeatability and reliability of scientific results; and provide a clear offramp for those astronomers not wishing to make use of the tools developed by the mission.

The guiding principles for the JWST data analysis tools are that they should be FOSS, easy to install, well documented, easy to extend; able to support scripting and graphical user interfaces; built on stable, widely adopted languages and libraries; leverage existing source codes and algorithms, including some developed outside astronomy; allow for easy contributions by non-STScI staff; provide a consistent, coherent experience across all STScI-developed data analysis tools, regardless of scientific use case. Some of the FOSS developed to date include JWST-specific libraries, Astropy contributions (see Section 5.11), and contributions from the STScI community software initiative. The development model is internal development and See You On GitHub.

The Mikulski Archive for Space Telescopes (MAST) aims to maximize the scientific accessibility and productivity of astronomical data. Due to supporting several missions and observatories, the data products are heterogeneous and complex. MAST currently holds about 3 petabyte of data products, which is currently downloaded about once every 18 months. HST data currently generate  $\simeq 800$  articles/year, with  $\simeq 300$  articles/year from archival data. The earliest Hubble observations still yield publishable results almost three decades later.

The Data Science Mission Office's community is the world-wide astronomical community. Communication with users primarily occur via newsletters, mailing lists, and conferences. Long-term sustainability is the astronomy community being able to access (and interpret) data for decades to come. Funding for STScI comes from government contracts, mainly through NASA.

#### 5.3 Journal of Open Source Software (JOSS) - Arfon Smith

JOSS is a developer-friendly, open access journal for research software packages. It is committed to publishing quality research software with zero processing charges or subscription fees to authors.

JOSS is an academic journal (ISSN 2475-9066) with a formal, public, iterative peer review process that is designed to improve the quality of the software submitted (https://joss.theoj.org).

JOSS publishes articles about research software that: solves complex modeling problems in a scientific context (physics, mathematics, biology, medicine, social science, neuroscience, engineering); supports the functioning of research instruments or the execution of research experiments; extracts knowledge from large data sets; offers a mathematical library; or similar. JOSS submissions must be open source i.e., have an Open Source Definition (OSD) compliant license; have an obvious research application; be feature-complete (no half-baked solutions) and be designed for maintainable extension (not one-off modifications); not be minor "utility" packages, such as "thin" application programming interface (API) clients. JOSS currently publishes  $\simeq 30$  articles/month. Each article receives a Digital Object Identifier (DOI) and is indexed by the Astrophysics Data System (ADS), an online database of over eight million astronomy and physics articles from both peer reviewed and non-peer reviewed sources.

JOSS's community is academics writing open source software. Communication between editors, authors, and potential authors takes place in the open on Twitter, a blog, and GitHub. Offshoots include the sister journals Journal of Open Source Education and the Julia conference proceedings. JOSS is mainly funded by a grant from the Sloan Foundation and a volunteer editorial board. JOSS probably probably/hopefully not be needed in 5, 10, or 20 years as long-term sustainability is the academic credit model moving away from its exclusive focus on academic articles and citations.

The American Astronomical Society (AAS) Journals are arguably the top-tier forum for publishing significant new research in astronomy and astrophysics (https://journals.aas.org). In 2016 the AAS Journals adopted a policy that reflects the importance of software to the astronomical community, and the need for clear communication about such software which ensures that credit is appropriately given to its authors. The policy provides clear guidelines for citing software in all manuscripts, and supports the publication of descriptive articles about software relevant to research in astronomy and astrophysics (https://journals.aas.org/policy-statement-on-software/).

Since adopting this software policy an increasing number of software publications have appeared. However, many authors and readers would like the AAS Journals to provide a more detailed review of the software itself. Such a review might provide useful feedback to authors and provide readers with further assurance that software packages are of a "gold standard" quality.

In order to provide this service, the AAS Journals partnered with the JOSS in 2017. Authors submitting articles to the AAS Journals describing software published with a OSD-compliant license may choose to have their software reviewed in parallel at JOSS. Upon completion of both review processes, the AAS Journals indicate on the published article that the software has also been reviewed. The AAS Journals are paying a modest fee to JOSS for this service ( $\simeq \$50/\text{article}$ ), which helps support their operations and which is not passed on to authors, referees, or editors. The increasing number of authors who use this partnership between JOSS and the AAS Journals suggests the FOSS astrophysics community finds it a useful service.

#### 5.4 emcee - Daniel Foreman-Mackey

Probabilistic data analysis, which describes degrees of logical implication or subjective certainty, has transformed much of scientific research in the past decade. Many of the most significant gains have come from numerical methods for approximate inference, especially Markov chain Monte Carlo (MCMC). For example, many problems in astrophysics have directly benefited from MCMC

because the models are often expensive to compute, there are many free parameters, and the observations usually have low signal-to-noise ratios (Foreman-Mackey et al. 2013).

The emcee package is a Python implementation of a novel MCMC sampler that enables efficient Bayesian inference (https://github.com/dfm/emcee). Bayesian inference, as one probabilistic data analysis method, provides a powerful general basis for data analysis. The algorithm behind emcee has several advantages over traditional MCMC sampling methods and it has excellent performance as measured by the autocorrelation time (or function calls per independent sample).

The emcee package has been widely applied to probabilistic modeling problems in astrophysics with some applications in other fields. For example, the instrument paper describing emcee is currently in the Top 3 most cited articles in astronomy that were published in 2013 ( $\simeq 3100$  citations, citation rate of  $\simeq 1100/\mathrm{year}$ ). The articles that cite emcee have themselves generated  $\simeq 120,000$  citations, yielding a large radius-of-influence of  $\simeq 40$ , which strongly indicates the emcee package helps generate science articles that the broader astronomy community values.

emcee is currently maintained mostly by one developer with smaller contributions from  $\simeq 8$  contributors. Version 3.0 of emcee, to be released in 2020, is the first major release in about 6 years. It includes a full re-write of the computational backend, several commonly requested features, and a set of new ensemble implementations. To date, emcee has not been directly funded. Instead, development of the source code has relied on being part of a funded science effort.

#### 5.5 LSST Transients - Federica Bianco

A transient astronomical event, often shortened to "transient", is an astronomical object or phenomenon whose duration may be from seconds to days, weeks, or even years. This is in contrast to the timescale of the millions or billions of years during which the galaxies and their component stars evolve. Singularly, the term is used for intrinsic events such as supernovae, novae, dwarf nova outbursts, gamma-ray bursts, and tidal disruption events, as well as geometric events such as gravitational microlensing, transits, occultations, and eclipses.

The science community interested in the Large Synoptic Survey Telescope (LSST) is organized into Science Collaborations. Among those, the LSST Transients and Variable Stars Collaboration focuses on the transient sky (https://lsst-tvssc.github.io), which is one of the 4 primary science drivers of LSST (https://www.lsst.org/science). The collaboration is organized in 15 subgroups by common expertise and interests, that are delineating a roadmap to maximize the potential of the LSST survey in the discovery and characterization of the transient sky.

The LSST data reduction pipeline will deliver an alert package for every object in each image that exhibits a significant brightness or positional change. The shear scale of the survey leads to an anticipation of tens of millions of alerts per night and hence a computational challenge for astronomers to identify targets of specific interest for their science. In this context, "broker' refers to software which receives alert information, associates it with other data, performs classification functions according to numerous algorithms and criteria, and stores the information in a database. Brokers will provide interfaces to enable users to sort targets and alerts according to their own preferences. These users may be individual scientists, teams, or additional brokers. Brokers may also be accessed by the TOM software (See section 5.9), which is designed to automatically prioritize targets for a specific science goal, request follow-up observations, track progress, and analyze the results. To maximize the science return from LSST, the user interfaces to these brokers need to be carefully designed to address the needs of the community.

Financial support for the LSST's construction, operation, and its digital infrastructure, comes from the NSF, the Department of Energy, and private funding (e.g., Google, Simonyi Foundation) raised by the LSST Corporation, a non-profit 501(c)3 corporation formed in 2003.

#### 5.6 yt - Matt Turk

Conducting and analyzing computational simulations in astrophysics has grown increasingly sophisticated. The resultant data encompass many types of physical models, span tens of thousands of timesteps, and consume terabytes of storage with a variety of metadata schemes. As a result, analysis routines were often focused around specific problems, and specific simulation platforms that produced duplicated efforts, or incompletely analyzed simulations. yt was developed to alleviate these issues (Turk 2013; Turk et al. 2011).

yt is a community-driven, permissively-licensed, FOSS Python package for analyzing and visualizing volumetric data (https://yt-project.org). It supports structured, variable-resolution meshes, unstructured meshes, and discrete or sampled data such as particles. It is focused on driving physically-meaningful inquiry that meet the challenges of reproducibility, parallelization, and vast increases in data size and complexity. yt has been extensively applied in domains such as astrophysics, seismology, nuclear engineering, molecular dynamics, and oceanography. The yt software instrument article is currently one of the Top 50 most cited articles in astronomy and astrophysics that were published in 2011.

yt is unique in having a very large, active development team. Over the entire history of the project, 186 developers have contributed. Over the past twelve months, 35 developers contributed new code to yt. yt has one of the largest open-source teams in the world, ranking in the top 2% of all project teams on Open Hub. Development of yt is driven by a commitment to Open Science principles as manifested in participatory development, reproducibility, documented and approachable code, a friendly and helpful community of users and developers, and Free and Libre Open Source Software. yt is supported in part by the Gordon and Betty Moore Foundation (\$1.5M and \$350K between 2014-2019) and the NSF (\$85K, \$500K and \$1.65M between years 2014). yt is a also fiscally-sponsored project of NumFOCUS, a 501(c)(3) public charity, whose mission is to promote open practices in research, data, and scientific computing by serving as a fiscal sponsor for open source projects and organizing community-driven educational programs.

#### 5.7 R Astrostatistics - Gwendolyn Eadie

R is a programming language and FOSS environment for statistical computing and interactive graphical analysis (https://www.r-project.org). R and its libraries implement a wide variety of statistical and graphical techniques, including linear and nonlinear modeling, classical statistical tests, nonparametrics, multivariate regression and multivariate classification, time series analysis, and Bayesian inference, and others. R is extensible through functions and extensions, and the R community is known for its active contributions. Many of R's standard functions are written in R itself, which makes it easier for users to follow the algorithmic choices made. For computationally intensive tasks, C, C++, and Fortran packages can be linked and called at run time.

R is widely used among statisticians for developing novel statistical software and data analysis. Python currently dominates in astronomy and R is less common, perhaps because most astronomers are not (yet) usually trained in statistics. An advantage of R over Python is exposure to new developments in statistical methods as R is the language of statisticians. Astrostatistics is a discipline on the rise as it helps process the vast amount of data produced by automated scanning

of the cosmos, to characterize complex datasets, and to link astronomical data to astrophysical theory. For example, the Astrostatistics and Astroinformatics Portal (http://asaip.psu.edu) serves the cross-disciplinary communities of astronomers, statisticians and computer scientists. It is intended to foster research into advanced methodologies for astronomical research, and to promulgate such methods into the broader astronomy community. Packages have also been written to integrate R and Python within both the R environment and Jupyter Notebooks.

R is an official part of the Free Software Foundation's GNU project, which is a principal source of funding for the development, maintenance, and community-support of R. The R Foundation is a not-for-profit organization working to support the R project and other innovations in statistical computing (https://www.r-project.org/foundation/). The R Consortium is a group organized under an open source governance and foundation model to support the global community of users, maintainers and developers of R software (https://www.r-consortium.org). Its members include leading institutions and companies dedicated to the use, development and growth of R. Example of its community building efforts include supporting useR!, the annual meeting of the R user and developer community (e.g., https://user2020.r-project.org), and R-Ladies, a global organization whose mission is to promote gender diversity in the R community (https://rladies.org/about-us/).

The Comprehensive R Archive Network (CRAN, https://CRAN.R-project.org/) is the official, regulated, peer-reviewed repository of R. CRAN has a set of policies on package submissions and updates; these policies provide a standardized format for R packages, help files, and example code, as well as required testing and compatibility with future R distributions (https://cran.r-project.org/web/packages/policies.html). For example, when a new version of R is released, if a package no longer works then the maintainer is required to update their package. If no update is completed within a certain amount of time, then the package is archived. CRAN aggregates a collection of sites which carry identical material, consisting of the R distribution(s), the  $\simeq 14,000$  contributed extensions, documentation for R, and binaries. While R is available in Jupyter Notebooks, RStudio is the most popular user interface for R (https://rstudio.com/), and R Shiny is a popular tool for developing interactive figures and graphs (https://shiny.rstudio.com/).

#### 5.8 SDSS Digital Infrastructure - Joel Brownstein

Astronomy sky surveys are research projects to capture uniform data about a region of the sky. SDSS has a long history of operating advanced data acquisition, innovative data management, world-class archival storage, and scientific visualization practices. The breadth and depth of science fostered by SDSS's community-organized approach (https://www.sdss.org) have advanced our understanding of the cosmos, and spurred innovative technical and analytical approaches to challenges in systems development, data management, and pipeline development and implementation. SDSS has generated over 8000 refereed articles, currently over 600 refereed articles/year, and  $\simeq 330,000$  citations. The road to success was not without lessons about how to conduct big, collaborative, data-based scientific projects.

SDSS data is accessed through the Catalog Archive Server (CAS), the Science Archive Server (SAS), or direct data file access via globus online, http by wget or curl (Cherinka et al. 2019; Weaver et al. 2015). CAS offers catalog level data and interactive tools to browse through SDSS images with links to associated spectra and catalog data about the objects on the images. SAS is the primary interface to all of the original images, raw data from North and South Observatories, and includes all of the spectra, intermediate and final results, and is accessed at rates exceeding 10 TB of downloads and 50 million web hits per month. It provides tools to interactively view

and download SDSS spectra, download images of SDSS fields, and generate mosaics of those fields. Storage at SAS crossed the 1 petabyte level in 2019. The final Data Release of SDSS-IV is scheduled for July 2021, and will include all APOGEE-2, eBOSS and MaNGA spectra observed during SDSS-IV, as well as all final data products and catalogs SDSS-V will start observations in summer 2020, with its first data release expected two years later. Surveys in SDSS-V include Milky Way Mapper, Local Volume Mapper and Black Hole Mapper. A challenge for the near-future is developing and maintaining a sustainable and innovative science archive.

Funding for the Sloan Digital Sky Survey IV has been provided by the Alfred P. Sloan Foundation, the U.S. Department of Energy Office of Science, and the Participating Institutions. The Sloan Foundation was an early supporter of the SDSS in 1992 and has invested  $\simeq \$60 \mathrm{M}$  across 16 grants, with another \$16M grant recently approved to continue SDSS through at least 2024 (https://www.sciencephilanthropyalliance.org). The project is widely considered one of the big success stories in science philanthropy. The Sloan Foundation has provided  $\simeq 20$ –25% of the SDSS costs at each phase of its implementation. The balance has been funded mainly by Participating Institutions that join as members. Each member typically contributes  $\simeq \$1$  million over five years, which allows its faculty, researchers, and students to get early access to SDSS data. The project now has over 54 university partners who contribute most of the funding for SDSS.

#### 5.9 TOM Toolkit - Rachel Street

Astronomical surveys are producing ever increasing catalogs of new discoveries at ever faster rates. Astronomers have found it necessary to build database-driven systems – called Target and Observation Managers (TOMs) – for powerful, programmable control over all aspects of astronomical observing schedules and data products. TOM systems offer users a powerful way to display and interact with targets and their data through a web browser. These systems can also submit requests for observations directly to networked, robotic telescope facilities to harvest the data products. When coupled with analysis software, TOMs are capable of conducting entirely automated follow-up programs, including rapid responses to national and international alerts.

Building a TOM system previously required specialist expertise in database and software development, thus generally restricting TOMs to a subset of large projects. The TOM Toolkit is a FOSS software package centered around a highly flexible database, designed for astronomical data and to be customized by the user to accommodate science-specific parameters and data products. Developed by professional software engineers in collaboration with scientists at Las Cumbres Observatory (https://lco.global/tomtoolkit/), the TOM Toolkit can be used as a stand-alone package to build a TOM from scratch or as a library of useful functions. The Toolkit comes with a widerange of functions to support observing programs and is designed to be extendable with community contributions. The TOM Toolkit is designed to make it easy to develop plugins to interface with external software and resources, such as additional telescope facilities. Development of the TOM Toolkit is supported the Zegar Family Foundation (\$450K between 2018 and 2020) Heising-Simons Foundation (\$650K between 2018 and 2020).

#### 5.10 AEON Network - Rachel Street

Modern astronomical surveys can deliver tens of thousands of new discoveries every night, alerted within minutes. Yet many will require additional observations in order to understand the physical phenomena and maximize the scientific return. Observatories supporting this critical follow-up must be capable of responding on similar timescales and with a flexibility governed by the demands

of the science. The Astronomical Event Observatory Network (AEON, http://ast.noao.edu/data/aeon) is a collection of world-class telescope facilities which can be accessed on demand, at the touch of a button. At the heart of the network, the Las Cumbres Observatory is joining forces with the National Optical Astronomy Observatory (NOAO), Southern Astrophysical Research (SOAR) and Gemini telescopes to build a network for rapid, flexible, programmable access to world-class telescope facilities in the forthcoming the LSST era (see Section 5.5).

Astronomers will be able to request observations from any participating facility using the programmable and customizible interface supported by the TOM Toolkit, as well as through the facility's own system. Telescopes in the network have agreed to some or all of their time being available in highly flexible queue-scheduling, so that observations can be requested at any time, and conducted on timescales driven by the science goals. The combined network will offer access to imaging and spectroscopic instruments on telescopes of a range of apertures distributed across the world. Each facility retains control over the fraction of its time that is executed in AEON mode, and telescope nightly operations need not be fully robotic to participate. Development for the successful first phase of the AEON project was provided by the NSF through the NOAO (e.g.,  $\simeq \$300$ K for the SOAR interfaces), with planning for the next phase currently underway.

#### 5.11 Astropy - Kelle Cruz

The Astropy Project is a community-driven effort to develop and maintain a FOSS package that contains much of the core functionality and common tools required across astronomy (https://www.astropy.org). These core functions include support for different file types, unit and physical quantity conversions, celestial coordinate and time transformations, world coordinate systems, containers for representing gridded as well as tabular data, and a framework for cosmological transformations and conversions (Astropy Collaboration et al. 2018, 2013). One goal is to avoid duplicated efforts for these common core tasks, and to provide a robust framework upon which to build more complex interoperable tools. The Astropy Project also hosts an ecosystem of affiliated packages that are not necessarily developed by the core development team, but share the goals of Astropy, and often build from the core package's code and infrastructure.

Astropy has been extraordinarily well-received by the astronomy community. The first software article (Astropy Collaboration et al. 2013) is currently in the Top 3 most cited article in astronomy and astrophysics that were published in 2013. The second software article (Astropy Collaboration et al. 2018) is presently also in the Top 3 most cited astronomy and astrophysics articles that were published in 2018. The Astropy Project is also unique in having a very large, active team. Its unqualified success is made possible by the efforts of  $\simeq 200$  team members that perform numerous important roles. These roles encompass a broad scope of responsibilities ranging from direct package development to communication, distribution, and managerial activities.

The Astropy Project has the ability to accept financial contributions from institutions or individuals through NumFOCUS, a 501(c)(3) public charity whose vision is an inclusive scientific and research community that utilizes actively supported open source software to make impactful discoveries for a better world. The Astropy Project has received \$900k in funding from the Moore Foundation.

#### 5.12 ATHENA++ - Jim Stone

Numerical methods are essential for exploring of a wide range of applications in astrophysical fluid dynamics. The development of accurate and capable algorithms, along with a description of

their implementation on modern large-scale parallel computer systems, is crucial for progress in this field. Athena++ is a software instrument for performing such astrophysical magnetohydrodynamic simulations. Athena++ itself is a complete re-write of the Athena software instrument. Currently, the instrument paper describing Athena (Stone et al. 2008) ranks within the Top 60 most cited papers ( $\simeq 500$  citations,  $\simeq 60$  citations/year) in astronomy that were published in 2008.

Athena++ is an example of application scientists developing software to solve science problems (see Section 5.14 for another example). It is developed using continuous integration tools (e.g., Jenkins, Travis CI) and maintains strict adherence to C++ standards. As a result, Athena++ has been run on everything from a laptop to the very largest machines (e.g., Felker & Stone 2018; White et al. 2016). The package is currently developed by 4 core team members, who collectively do  $\simeq 90\%$  of the commits, and about 8 significant contributors (https://princetonuniversity.github.io/athena/). While the package is not intended to provide a service to the community, the first user meeting was held in April 2019 at the University of Nevada, Las Vegas and attended by  $\simeq 60$  (mostly young) participants interested in computational fluid dynamics. Athena++ has a recent download rate of  $\simeq 300$  time per month by its user base. Development and maintenance of Athena++ has been funded by science grants. To date, there has been no funding for code development or professional support for its  $\simeq 100,000$  lines of code. Athena++ will likely survive as a software instrument only as long as it remains a useful tool for doing science problems.

#### 5.13 Einstein Toolkit - Philipp Mösta

Scientific progress in the field of numerical relativity has always been closely tied to the availability and ease-of-use of enabling software and computational infrastructure. The Einstein Toolkit is a community-driven FOSS platform of core computational tools to advance research in relativistic astrophysics and gravitational physics (https://einsteintoolkit.org). The aim is to provide the core computational tools that can enable new science, broaden the community, facilitate inter-disciplinary research, and take advantage of emerging petascale computers and advanced digital infrastructure. A large portion of the current Toolkit is made up of over 100 community-developed components for computational relativity along with associated tools for simulation management and visualization. The software instrument paper describing the Einstein Toolkit (Löffler et al. 2012) currently has  $\simeq 230$  citations and a citation rate of  $\simeq 40/\text{year}$ , with individual components that the Toolkit having their own bibliometrics.

The Einstein Toolkit is currently used by  $\simeq 240$  users in  $\simeq 50$  numerical relativity groups in the USA and Europe, with most of users coming from  $\simeq 10$  research groups. These researchers use the Toolkit framework and generally deploy their own proprietary components for applications. Many of these users do not directly collaborate on science problems, and in some cases compete. However, these groups agree that sharing the development of the underlying infrastructure is mutually beneficial for every group and the wider community as well. The Toolkit does not itself develop software. A distributed developer model ( $\simeq 350$  commits by  $\simeq 20$  team members within the past year) maintains core support of the Toolkit with partnerships to  $\simeq 7$  core developers who contribute and coordinate together on development. Official stable releases occur every 6 months.

Funding for the development and maintenance of the Einstein Toolkit include a NSF Physics at the Information Frontier Grant (2006-2015) to Georgia Institute of Technology, California Institute of Technology, Louisiana State University, and Rochester Institute of Technology at  $\simeq \$160 \text{K/yr/institution}$ . Current funding includes a NASA Theoretical and Computational Astrophysics Network centered at Rochester Institute of Technology ( $\simeq \$1.6 \text{M}$  between 2018-2021). Cur-

rent challenges identified include finding the balance between curation and innovation, longevity and sustainability on decadal timescales, and staying relevant on modern, evolving High Performance Computing infrastructures.

#### 5.14 PyCBC - Duncan Brown

The LIGO and Virgo detectors are large-scale experiments designed to directly detect gravitational waves, from, for example, merging black holes (e.g., Abbott et al. 2016). LIGO is large-scale NSF funded project involving thousands of people and hundreds of institutions. The Gravitational Wave Open Science Center (https://www.gw-openscience.org/about/) provides calibrated data from these observatories, along with access to tutorials and software tools (Vallisneri et al. 2015).

PyCBC is one of those FOSS software instruments (https://pycbc.org). PyCBC's algorithms can detect coalescing compact binaries and provide Bayesian estimates of the astrophysical parameters of detected sources (e.g., Biwer et al. 2019; Nitz et al. 2017). The software enables accessing the open gravitational wave data through the Open Science Grid (OSG, https://opensciencegrid.org) and the Extreme Science and Engineering Discovery Environment (XSEDE, https://www.xsede.org) computational platforms. PyCBC was used in the first direct detection of gravitational waves by LIGO and is used in the ongoing analysis of LIGO and Virgo data. PyCBC was featured in Physics World (Smith 2017) as a good example of a large collaboration of application scientists developing software to solve science problems that published its research products and its software. PyCBC has been mentioned in 186 articles since 2014, including five ranked as top-cite 1000+, four ranked top-cite 500+, and nine articles with over 100 citations (data from INSPIRE-HEP). The binary-merger search method described in Usman et al. (2016) has over 160 citations.

PyCBC is developed on GitHub by about 6 core developers and about 70 contributors (roughly 90% male, 10% female) who directly support a community of  $\simeq 200$  users. Communication between developers and users mainly occurs through Slack, which also serves as a repository of the discussions with over 160,000 messages. PyCBC's funding model for development and maintenance is mainly through the science that it enables, although there has been support through the NSF Advanced Cyberinfrastructure program (\$500K between 2014 - 2019). The core science funding is through the NSF Gravity program (\$900K between 2014-2019), the Albert Einstein Institute (\$1M between 2014-2019), and awards to United Kingdom and European Union investigators.

#### 5.15 JETFIT - Andrew MacFadyen

Jets are collimated beams of matter ejected from an astronomical object. Relativistic jets occur when the beams of matter are accelerated close to the speed of light. Examples of objects that feature high-energy jets include supermassive black holes in the center of galaxies, X-ray binaries, gamma-ray bursts, and protostars. JETFIT is a software tool to fit observational data of jets to numerical simulations. JETFIT is an example of application scientists developing software to solve curiosity-driven science problems. It has a community of 2 or 3 researchers who constitute both the developers and the users of this FOSS. It is hosted on GitHub, and there is no help desk, community forum, outreach campaign, or email listserv. Science-driven development of JETFIT and the RAM (Relativistic Adaptive Mesh) hydrodynamics package has been assisted, at times, by science funding from the NASA SWIFT mission (\$15K), the NASA NASA Astrophysics Theory Program (\$300K for 3 years), and the NSF (\$300K for 3 years).

#### 5.16 Astrophysics Source Code Library (ASCL) - Alice Allen

The ASCL is an online registry of scientist-written software used in astronomy or astrophysics research (https://ascl.net). The primary objectives of the ASCL are to make the software used in research more discoverable, more available, and more transparent (Allen & Schmidt 2015; Allen et al. 2018; Shamir et al. 2018). Entries in the ASCL include the name, description, author of the software, a unique ASCL ID, and either a link to a download site for the software or an attached archive file for the software so the code can be downloaded directly from the ASCL. A link to an article describing or using the software is usually included to demonstrate that the software has been used for research in the refereed literature. ASCL entries are indexed by the SAO/NASA Astrophysics Data System (ADS) and Web of Science's Data Citation Index. Software can thus be cited in a journal article even when there is no citable article describing the software. Additionally, ADS can link some articles which use software to the software entries, enabling an easier examination of the computational methods used. ADS also tracks citations to ASCL entries, assuming the citations are suitably formatted, which can help authors of research software for whom citations are an important metric.

Started in 1999, ASCL initially required software to be deposited. Most software authors were reluctant to adopt this model, which stagnated ASCL's growth. ASCL dropped this model in 2010, although software deposits are still accepted, and transitioned to the current model of providing download locations. ASCL subsequently grew from  $\simeq 40$  entries to about 2100 today. The percentage of software that have been cited grew from  $\simeq 7\%$  in 2014 to  $\simeq 34\%$  in 2019. Citations in the refereed literature to ASCL entries increased by  $\simeq 59\%$  between 2017 and 2018, while the number of entries increased by  $\simeq 35\%$ . This suggests a growth in the use of ASCL over and above the growth in the number of ASCL entries (Allen et al. 2018). Finally, author submissions grew by  $\simeq 31\%$  over the same time period.

ASCL is currently supported by the Heidelberg Institute for Theoretical Studies ( $\simeq$  \$6K/year), the NASA Astrophysics Data Analysis Program ( $\simeq$  \$162K for two years), in-kind contributions from Michigan Technological University for internet hosting, and in-kind contributions from the University of Maryland Libraries for DOI minting.

#### 5.17 MESA - Frank Timmes

The Modules for Experiments in Stellar Astrophysics (MESA) source code is a set of FOSS modules for stellar astrophysics that can be used on their own, or combined to solve the coupled equations governing 1D stellar evolution. The MESA Project's community is stellar astronomers and astrophysicists. The MESA Project has grown from  $\simeq 100$  users in 2012 through  $\simeq 800$  users in 2015 to over 1000 users world-wide. It currently accounts for about 1/2 of all stellar models published in the modern literature. The MESA Project innovates by updating its community with an instrument article describing major new software and science capabilities about every two years. MESA I (Paxton et al. 2011) is currently ranked within the Top 5 most cited articles in astronomy and astrophysics that were published in 2011. MESA II (Paxton et al. 2013) is in the Top 10 most cited articles published in 2013, MESA III (Paxton et al. 2015) is in the Top 10 most cited articles published in 2015, and the recent MESA IV (Paxton et al. 2018) is in the Top 25 most cited articles published in 2018. The articles that cite MESA have themselves generated  $\simeq 45,000$  citations, yielding a radius-of-influence of  $\simeq 15$ , which suggests that MESA helps generate articles that the broader astronomy community values.

The MESA Project provides two portals to openly share knowledge. MESA-Users offers

 $\simeq 10,000$  archived and searchable posts of community discussions about stars. The website http://mesastar.org offers a Zenodo backed portal to build provenance by sharing tools and guidance. Currently there are  $\simeq 400$  contributions by the community, for the community. A Software Development Kit builds the instrument across a variety of Unix-based platforms. The offshoot MESA-Docker simplifies the run-time requirements with only minor overhead from running in a container, and is useful for new users and Windows users. Another spinoff is MESA-WEB (http://mesa-web.asu.edu), a cloud-based resource for education that has served 4000+ models to  $\simeq 600$  unique users in  $\simeq 3$  years of operation.

The MESA Project is currently developed by a team of 16, of which 2 are women ( $\simeq 12\%$ ). The percentage of women developers is smaller ( $\simeq 20\%$ ) than recent demographics of physics and astronomy theory Ph.D graduates. The MESA Summer School, which averages  $\simeq 36\%$  women participants (e.g.,http://cococubed.asu.edu/mesa\_summer\_school\_2019/), offers a week of extensive hands-on labs to gain familiarity with MESA software instruent and learn how to make better use of MESA in their own research. The Summer School cadre of instructors, TAs and participants (now over 250) are creating their own MESA user infrastructure at  $\simeq 40$  institutions around the world. The MESA Project focuses on supporting young scientists who are also skilled at developing community software instruments to obtain high-profile graduate fellowships (6), named postdoc fellowships (6), and tenure-stream positions (5). The MESA Project has been supported by funding from the NSF Software Infrastructure for Sustained Innovation program with \$500K between 2013-1016, and \$2.1M between 2017-2021.

## 6 Synthesis

Figuring out how to support digital infrastructure may seem daunting, but there are plenty of reasons to see the road ahead as an opportunity.

 $Nadia\ Eghbal$ 

Roads And Bridges: The Unseen Labor Behind Our Digital Infrastructure

The projects described above span a range of science (from observations through data pipelines to simulations), development models (from one person, through small teams, to large distributed alliances), user communities (from a few to thousands), and funding models (from volunteers to institutional science grants). Nevertheless, it is important to state that this sample is limited and incomplete in terms of the science spanned and projects studied. Any opinions, findings, conclusions or recommendations expressed below should be weighed against these intrinsic imperfections.

Returning to the research questions posed in the Executive summary,

- What is the relationship between money and sustainability for community-driven, open-knowledge software instruments that enable transformative research in stellar astrophysics?
- At what points in a software instrument's lifecycle does an injection of financial resources help or hurt?
- Are science driven software instruments sustainable for the long term, say the next 40 years? a potential funder should consider its desire to nurture a culture of free, open-source, open-knowledge software sharing in astronomy. Investments should be in a potential funder's wheel-house: a focus on cutting-edge basic science, a committment to sustaining software instruments that accelerate discovery, a desire to facilitate the participation of many diverse researchers, and a desire to realize an opportunity to fundamentally transform astronomy.

Determining how much money is useful at a given stage of an individual FOSS project's lifecycle will nearly always be a challenge. Supporting both up-and-coming and well-established software instruments requires a degree of patience and a willingness to take risks. One key to success is to ensure the relevant scientific community is at the helm and fully engaged with the software project. The success of the projects should be based on their open-source, open-knowledge principles, their capability to enable open-ended discovery, their integration of diversity and inclusion considerations throughout a project, and their capacity to allow new questions in astronomy that were unable to be addressed due to closed-source, closed-knowledge practices.

It is often easier to fund innovation-driven research and much more difficult to fund maintenance and community support. For example, software development efforts in stellar astrophysics are usually contained within innovative research proposals. One common approach is to describe the software development as a sub-aim of research focused on astrophysical discovery. It can be easy to overlook that developing community-driven software instruments involves many tasks that are not related to new capabilities, but on improving the existing software and supporting the user community. These essential tasks may not be innovative or directly related to writing source code, but they are critical to improving the quality of the software instrument and to building a robust, productive relationship with users. These essential efforts include updating the software instrument in response to continuous changes in hardware infrastructure; refactoring the software to improve its usability, maintainability, reliability, efficiency, correctness, robustness, extensibility or interoperability; fixing bugs and writing associated test suites to ensure that these bugs don't reappear; writing and updating source code documentation and users tutorials; managing public releases; actively supporting the user community by promptly providing advice, best practices, and guidance; managing new feature contributions from users; recruiting and nuturing new developers; building and maintaining the business case for the software project; helping core developers land permnant positions; disseminating information of community interest such as job opportunities within the field and announcements; building the community through summer schools, workshops, or seminars; managing project infrastructure including source code repositories, web sites, mailing lists, wikis, social media feeds, Docker containers, and software development tools; and being agile in the face of new experimental or observational scientific discoveries. A thriving open-knowledge software project takes a village, whose activities take time, commitment, and financial resources.

Software projects being considered for a potential funder's support should go through a rigorous internal review process and an external peer-review process. Questions that a potential funder may want to see addressed when considering support of a software project include:

- What does the software do? What are its key capabilities and novel features?
- Who is the target audience for the software?
- What is an estimate of the size of the market for the software? What is the software's current market penetration?
- To what extent does the software fill a recognized need within a community to advance basic science research?
- Are there other FOSS projects that have similar functionality? What makes the software different from others, what is unique?
- How many person-hours, funded and unfunded, have been invested to date to bring the software to its current state?

- What is the source code's license? Does the software project demonstrate a sufficient commitment to free, open-source, and open knowledge principles?
- What tangible metrics will be used to measure the success of the software project?
- To what extent has the software project demonstrated agility to new science discoveries and/or the changing needs of its the user community?
- Hardware changes. Compilers change. Libraries change. To what extent is the software adaptable to new technologies?
- To what extent are provenance, reproducibility, composability, and interoperability part of the software project's activities?
- To what extent does the software project address diversity and inclusion within its user community, developers, and leadership?
- Is there a demonstrated commitment to work with other software projects within the community's software ecosystem?
- How long does it usually take to go from proof-of-concept prototyping of a new software element to dissemination into the user community?
- Has the software project been funded in the past? What was the impact of that funding?
- How does the software project define sustainability?
- To what extent are the current resources no longer adequate?
- Why should funders help this software project thrive?

To report on its progress, each year the software project's principals send a summary of its progress relative to what was planned. Each project comes with an appropriate set of metrics - adding new capabilities to the software, refactoring the instrument to the ever-evolving hardware, community engagement, achieving scientific research objectives, or publishing a certain number of software instrument papers. The funder should review the progress made each year and towards the end of a funding phase, determine whether to consider funding for another phase.

In determining funding for initial or future phases, a funder should ask whether the software instrument will still be relevant over the period of the project as the landscape of astronomical research changes and evolves; whether the research questions to be enabled by improvements to the software instrument are likely to remain at the forefront of astronomy during this period; whether the project leadership team and plan remain strong; whether plans for software access, storage, archiving, and dissemination continue to be on the leading edge; whether the project has made substantial strides in terms of diversity and inclusion; and whether there is continuing demand for the software instrument from the relevant research community.

As the figure on the cover page suggests, the builders of digital infrastructure in stellar astrophysics – be it for telescopes, data pipelines, or theoretical models – are deeply interconnected to each other and technically very talented. They have already built the core platforms that power much of modern astronomy. They just need help to keep the gears rolling so they can continue doing what they do best.

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