Open Source for Science Fund

Open Source for the Life Sciences (OS4LS)

Letter of Intent Submission

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Section 1: Applicant Information

Question	Answer
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Have you previously received funding as a PI under the CZI EOSS program?	No
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Organization Type	Academic Institution

Section 2: Proposal Information

Question	Answer
Proposal Title	diffsol: Infrastructure for Mechanistic and AI Modelling

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<td>Short Summary</td>
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diffsol [1] (https://github.com/martinjrobins/diffsol) is an open-source Rust library for solving ordinary differential equations (ODEs) and semi-explicit differential algebraic equations (DAEs). Python bindings are available through pydiffsol, and interfaces for R and JAX are under development. diffsol has over 100 GitHub stars, receives approximately 300 downloads per day from crates.io, and is integrated into software serving pharmacokinetics and pharmacodynamics (Pmetrics, PKPD Explorer), cardiac electrophysiology (Myokit), battery modelling (PyBaMM), and systems modelling (Rumoca) communities.
diffsol provides a modern, composable, and high-performance foundation for numerical modelling. It supports a wide range of solver methods and features required for mechanistic modelling, including BDF, SDIRK, and Runge–Kutta solvers, multiple linear algebra backends, adaptive time-stepping, root finding, and forward and adjoint sensitivity analysis. While diffsol can already solve machine-learning models such as neural ODEs and latent ODEs, it currently lacks the scalable GPU execution capabilities required for efficient training and inference on large datasets.
This project will develop new capabilities that enable diffsol to serve as scalable computational infrastructure for AI-driven scientific discovery. Specifically, we will:
- Develop batched GPU solvers capable of solving large numbers of trajectories in parallel. Candidate technologies include cuda-oxide, cuTile (developed by NVIDIA), and CubeCL.
- Develop a GPU-native linear algebra backend supporting efficient batched execution and direct use from device code.
- Design these capabilities for interoperability with machine-learning frameworks and develop JAX bindings that allow diffsol solvers to be embedded directly within training and inference workflows.
- Develop benchmarks comparing diffsol with leading ODE libraries, including Diffrax, torchdiffeq, TensorFlow Probability ODE solvers, and DifferentialEquations.jl.
- Produce documentation, tutorials, and reference workflows for neural ODE and hybrid mechanistic/machine-learning models.
The overall goal is to enable diffsol to efficiently solve large numbers of ODEs and DAEs with varying parameters and initial conditions on single and multi-GPU systems while supporting forward and adjoint sensitivity analysis. Through scalable batched GPU execution and interoperability with modern machine-learning frameworks, diffsol will provide critical open-source infrastructure for AI-driven life-science research, allowing researchers to combine mechanistic biological knowledge with data-driven AI methods in neural ODE and hybrid modelling workflows. Applications include pharmacokinetic/pharmacodynamic modelling, disease progression modelling, systems biology, and patient-specific prediction.
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Expected Value	ODE/PDE models are fundamental tools across the life sciences, underpinning applications ranging from epidemiology and systems biology to PKPD and neuroscience. At the same time, growing biological datasets have increased the use of ML approaches such as neural ODEs and latent ODEs for modelling complex and irregularly sampled data. Existing ODE solvers within ML frameworks are typically optimized for ML applications and lack capabilities required for mechanistic modelling, such as support for DAE equations, sparse matrices, and a broad range of numerical methods. They are also tightly coupled to individual frameworks, limiting interoperability and reuse. Success for this project will be the availability of an open-source ODE/DAE library that combines the capabilities of traditional scientific computing with the scalability required for modern AI workflows. By adding batched GPU execution and interoperability with frameworks such as JAX, diffsol will enable efficient training and deployment of neural ODE, latent ODE, and hybrid mechanistic-ML models on large datasets. These improvements will immediately benefit downstream projects including Pmetrics, PKPD Explorer, Myokit, PyBaMM, and Rumoca. More broadly, diffsol will provide reusable infrastructure for AI-enabled life-science research, supporting large-scale model training, inference, and parameter estimation while allowing researchers to combine mechanistic biological knowledge with modern ML approaches.

Landscape Analysis	The differential equation software landscape is divided between traditional scientific computing tools and machine-learning frameworks. Traditional solvers such as SUNDIALS and MATLAB provide robust support for mechanistic ODE and PDE models, including sparse matrices and large-scale simulations, but have limited integration with modern AI workflows. In contrast, ML frameworks such as TensorFlow, PyTorch (torchdiffeq), and JAX (Diffrax) provide ODE solvers designed for neural ODEs and related models. These libraries integrate well with automatic differentiation and GPU acceleration but typically lack capabilities required for mechanistic modelling, including differential-algebraic equations, sparse matrices, and a broad range of numerical methods. The closest comparable project is DifferentialEquations.jl, part of the Julia SciML ecosystem, which successfully combines scientific computing and machine-learning capabilities but is largely restricted to Julia. diffsol occupies a complementary position by combining modern scientific-computing capabilities with interoperability across languages and ML frameworks. While less mature and smaller in user base than established alternatives, it is already adopted by software serving pharmacometrics, cardiac electrophysiology, battery modelling, and systems modelling communities. This project will add scalable GPU execution and ML integration, enabling broader use in AI-enabled and data-intensive life-science research.
Project Software Name	diffsol
Project Software Repository URL	https://github.com/martinjrobins/diffsol
Project Software Website URL	https://martinjrobins.github.io/diffsol/

Categories	Scientific computing, Hardware acceleration and scalability, Machine learning frameworks
Funding Track	Track 2: Foundational Libraries and Ecosystem Initiatives
Statement of PI Involvement	Confirm
Policies	Confirm

Thank you for your submission. Please reach out to info@os4science.org with any questions and reference your submission ID as noted above in the email subject.