JAX-DIPS: differentiable interfacial PDE solver for training neural network surrogate models

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Abstract

Ca. 100 words

This work presents a software package for solving elliptic partial differential equations with jump conditions across irregular interfaces using neural network surrogate models. The differentiable interfacial PDE solver, dubbed JAX-DIPS, is purely developed in JAX [**?**] and offers end-to-end differentiability from mesh generation to the higher level discretization abstractions, geometric integrations and interpolations, thus facilitating research into differentiable algorithms for developing hybrid PDE solvers. We release JAX-DIPS as an open-source software package under MIT license that is available for download at https://github.com/JAX-DIPS/JAX-DIPS

Keywords:
level-set method, free boundary problems, inverse problems, jump conditions, differentiable programming

Required Metadata

Current code version

Ancillary data table required for subversion of the codebase. Kindly replace examples in right column with the correct information about your current code, and leave the left column as it is.

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Nr.	Code metadata description	Please fill in this column
C1	Current code version	For example v42
C2	Permanent link to code/repository used for this code version	For example: *https* : *//github.com/mozart/mozart2*
C3	Code Ocean compute capsule	For example: *https* : *//codeocean.com/*2017/07/30/*neurospeech* − *colon* − *an* − *open* − *source* − *software* − *for* − *parkinson* − *apos* − *s* − *speech* − *analysis/code*
C4	Legal Code License	List one of the approved licenses
C5	Code versioning system used	For example svn, git, mercurial, etc. put none if none
C6	Software code languages, tools, and services used	For example C++, python, r, MPI, OpenCL, etc.
C7	Compilation requirements, operating environments & dependencies	
C8	If available Link to developer documentation/manual	For example: *http* : *//mozart.github.io/documentation/*
C9	Support email for questions	

Table 1: Code metadata (mandatory)

The permanent link to code/repository or the zip archive should include the following requirements:

README.txt and LICENSE.txt.

Source code in a src/ directory, not the root of the repository.

Tag corresponding with the version of the software that is reviewed.

Documentation in the repository in a docs/ directory, and/or READMEs, as appropriate.

1. Motivation and significance

Introduce the scientific background and the motivation for developing the software.

Explain why the software is important, and describe the exact (scientific) problem(s) it solves.

Indicate in what way the software has contributed (or how it will contribute in the future) to the process of scientific discovery; if available, this is to be supported by citing a research paper using the software.

Provide a description of the experimental setting (how does the user use the software?).

Introduce related work in literature (cite or list algorithms used, other software etc.).

2. Software description

Describe the software in as much as is necessary to establish a vocabulary needed to explain its impact.

2.1. Software Architecture

Give a short overview of the overall software architecture; provide a pictorial component overview or similar (if possible). If necessary provide implementation details.

2.2. Software Functionalities

Present the major functionalities of the software.

2.3. Sample code snippets analysis (optional)

3. Illustrative Examples

Provide at least one illustrative example to demonstrate the major functions.

Optional: you may include one explanatory video that will appear next to your article, in the right hand side panel. (Please upload any video as a single supplementary file with your article. Only one MP4 formatted, with 50MB maximum size, video is possible per article. Recommended video dimensions are 640 x 480 at a maximum of 30 frames/second. Prior to submission please test and validate your .mp4 file at $http://elsevier-apps.sciverse.com/GadgetVideoPodcastPlayerWeb/verification$. This tool will display your video exactly in the same way as it will appear on ScienceDirect.).

4. Impact

This is the main section of the article and the reviewers weight the description here appropriately

Indicate in what way new research questions can be pursued as a result of the software (if any).

Indicate in what way, and to what extent, the pursuit of existing research questions is improved (if so).

Indicate in what way the software has changed the daily practice of its users (if so).

Indicate how widespread the use of the software is within and outside the intended user group.

Indicate in what way the software is used in commercial settings and/or how it led to the creation of spin-off companies (if so).

5. Conclusions

Set out the conclusion of this original software publication.

6. Conflict of Interest

Please select the appropriate text:

Potential conflict of interest exists: We wish to draw the attention of the Editor to the following facts, which may be considered as potential conflicts of interest, and to significant financial contributions to this work. The nature of potential conflict of interest is described below: [Describe conflict of interest]

No conflict of interest exists: We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

Acknowledgements

Optionally thank people and institutes you need to acknowledge.

References

[1]

Please add the reference to the software repository if DOI for software is available.

Current executable software version

Ancillary data table required for sub version of the executable software: (x.1, x.2 etc.) kindly replace examples in right column with the correct information about your executables, and leave the left column as it is.

Nr.	(Executable) software metadata description	Please fill in this column
S1	Current software version	For example 1.1, 2.4 etc.
S2	Permanent link to executables of this version	For example: *https* : *//github.com/combogenomics/DuctApe/releases/tag/DuctApe* − 0.16.4
S3	Legal Software License	List one of the approved licenses
S4	Computing platforms/Operating Systems	For example Android, BSD, iOS, Linux, OS X, Microsoft Windows, Unix-like , IBM z/OS, distributed/web based etc.
S5	Installation requirements & dependencies	
S6	If available, link to user manual - if formally published include a reference to the publication in the reference list	For example: *http* : *//mozart.github.io/documentation/*
S7	Support email for questions	

Table 2: Software metadata (optional)