

# Improving Interoperability in Scientific Computing via MaRDI Open Interfaces

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## Summary

Computational scientists often face two obstacles while conducting numerical experiments:

- **Multiple programming languages** are used for numerical solvers
- Multiple solvers have **different interfaces** for the same problem types

Combination of solvers, thus, could lead to significant programming effort on scientist's side: writing bindings and adapting interfaces takes time. MARDI OPEN INTERFACES aim to improve interoperability in Scientific Computing by alleviating these obstacles by replacing pairwise bindings between languages and implementations with decoupled bindings.

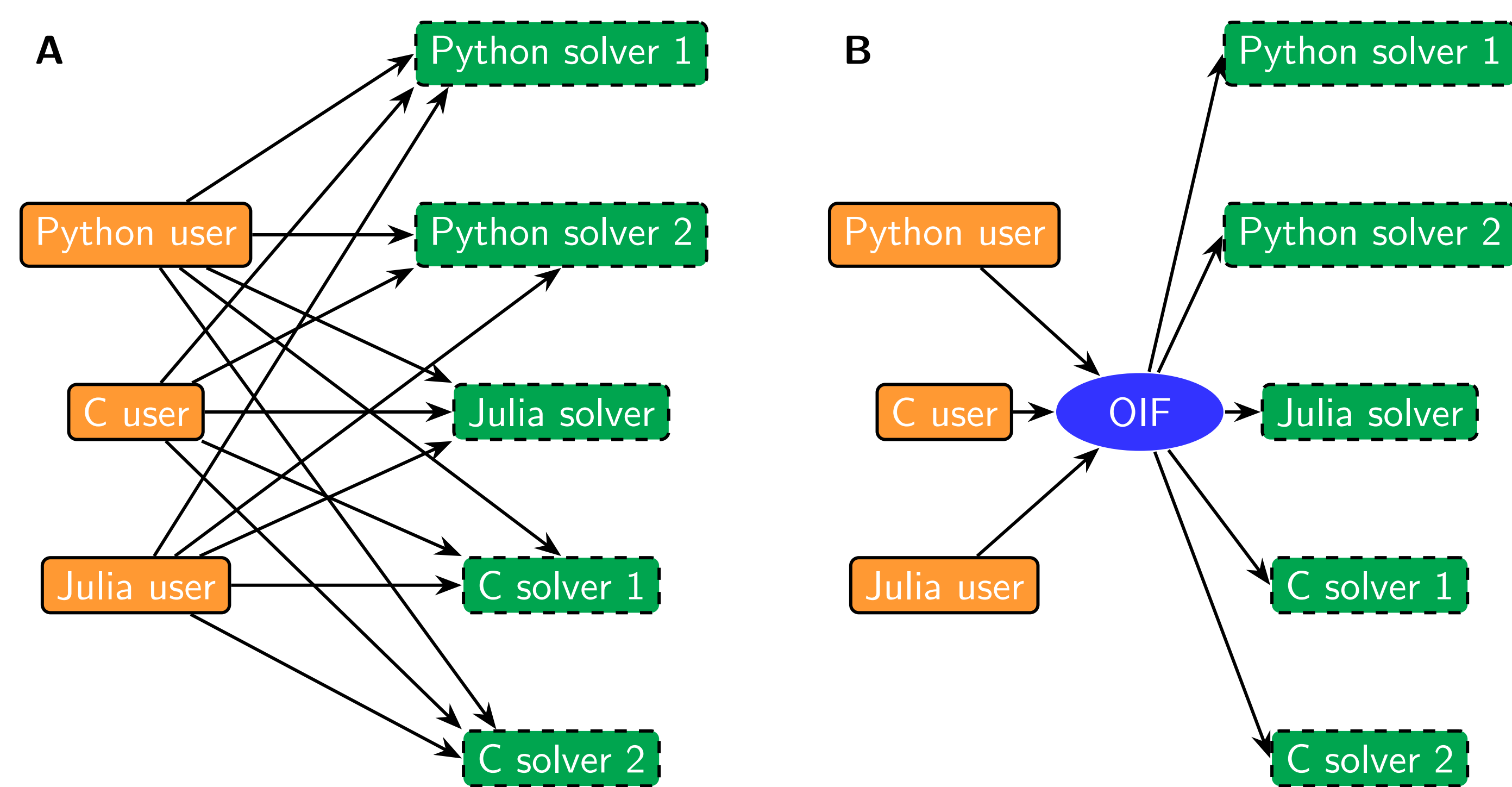


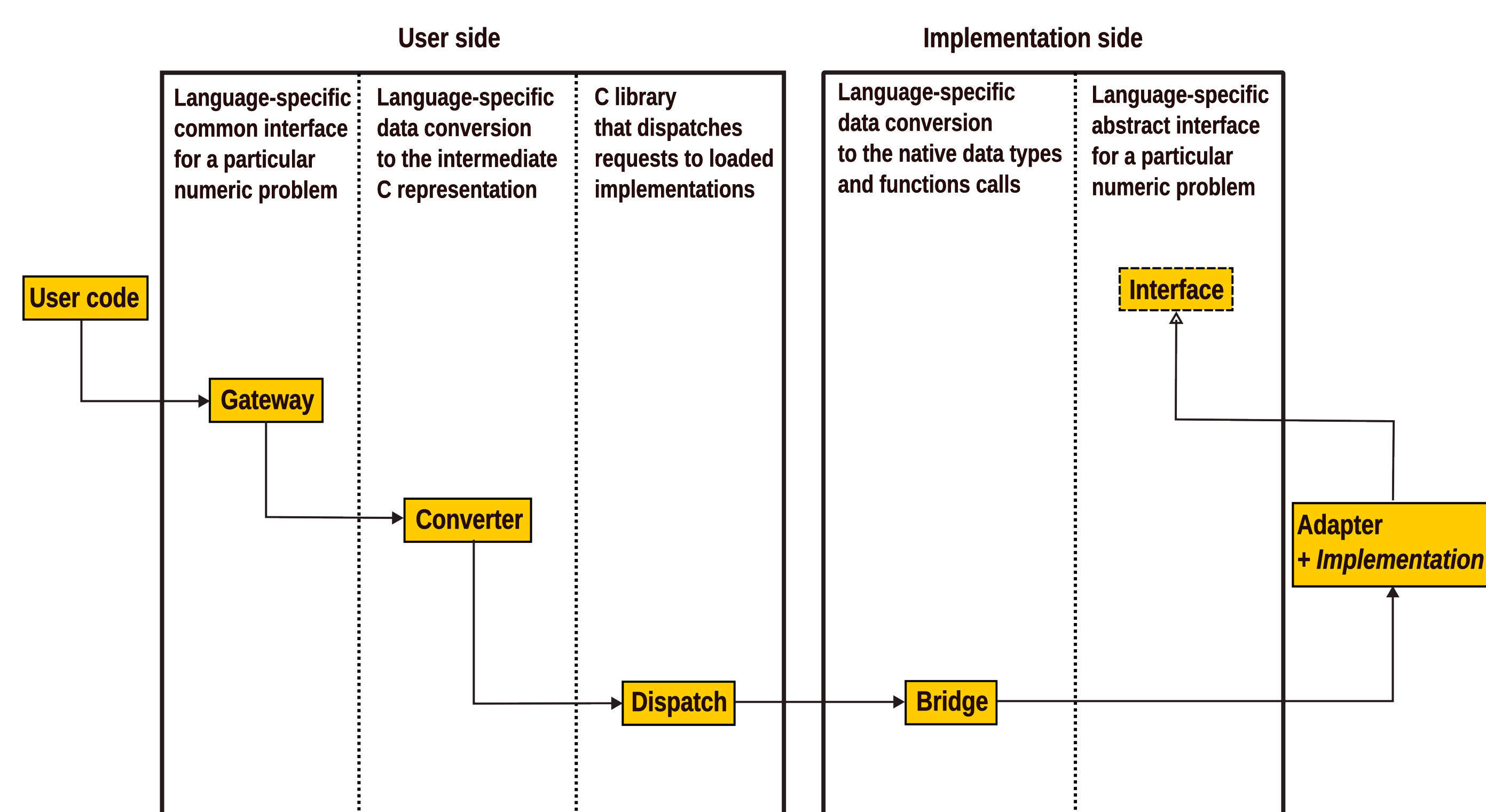
Figure 1: Schematic comparison of two approaches to the problem of multiple languages/multiple implementations. **A** Standard pairwise bindings **B** Bindings via MARDI OPEN INTERFACES.

## Objectives

- Develop library that passes data between languages automatically
- Develop generic interfaces for typical numerical problems
- Encourage the community to program against these interfaces

Similar to software packages such as PYMOR (Milk, Rave, and Schindler, 2016), SUNDIALS (Gardner et al., 2022), or PRECICE (Chourdakis et al., 2022), we aim to abstract out discrepancies between different solvers, so that computational scientists would spend less time connecting them.

## Software Architecture and Data Flow



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## Example usage

Consider the inviscid Burgers' equation problem:

$$\frac{\partial u}{\partial t} + \frac{\partial (u^2/2)}{\partial x} = 0, \quad t \in [0, 2], \quad x \in [0, 2]$$

$$u(t, 0) = 0.5 - 0.25 \sin(\pi x) \quad \text{and} \quad u(t, 2) = u(t, 0),$$

which we integrate using an open interface for Initial-Value Problems (IVP) for ordinary differential equations.

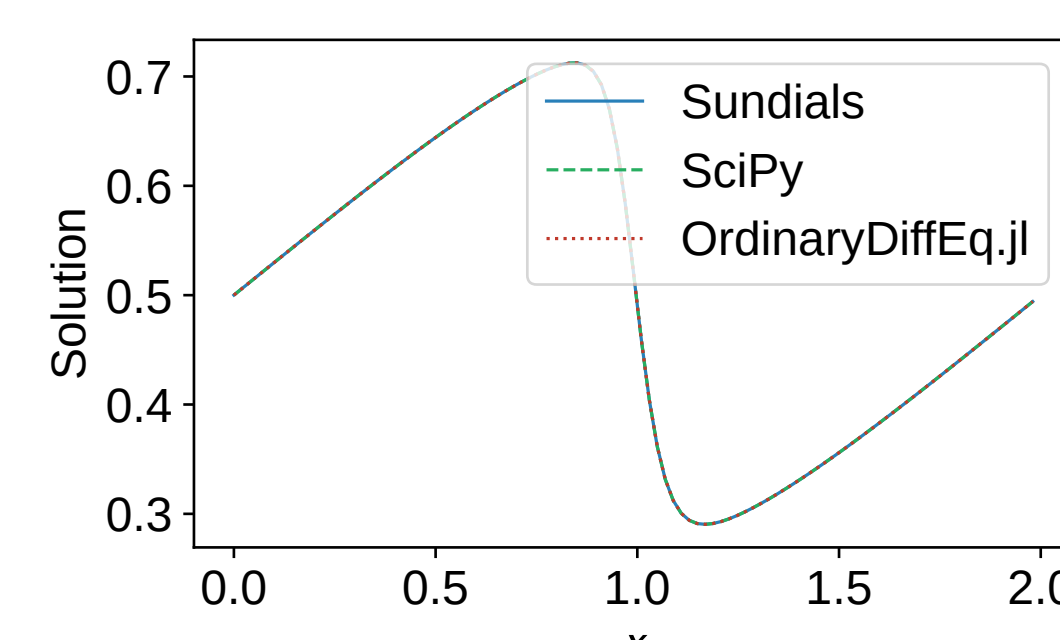


Figure 2: Solution of the Burgers' problem using open interface IVP with three implementations: SUNDIALS CVODE, SciPy (Virtanen et al., 2020), and ORDINARYDIFFEQ.JL (Rackauckas and Nie, 2017).

## User code in Python:

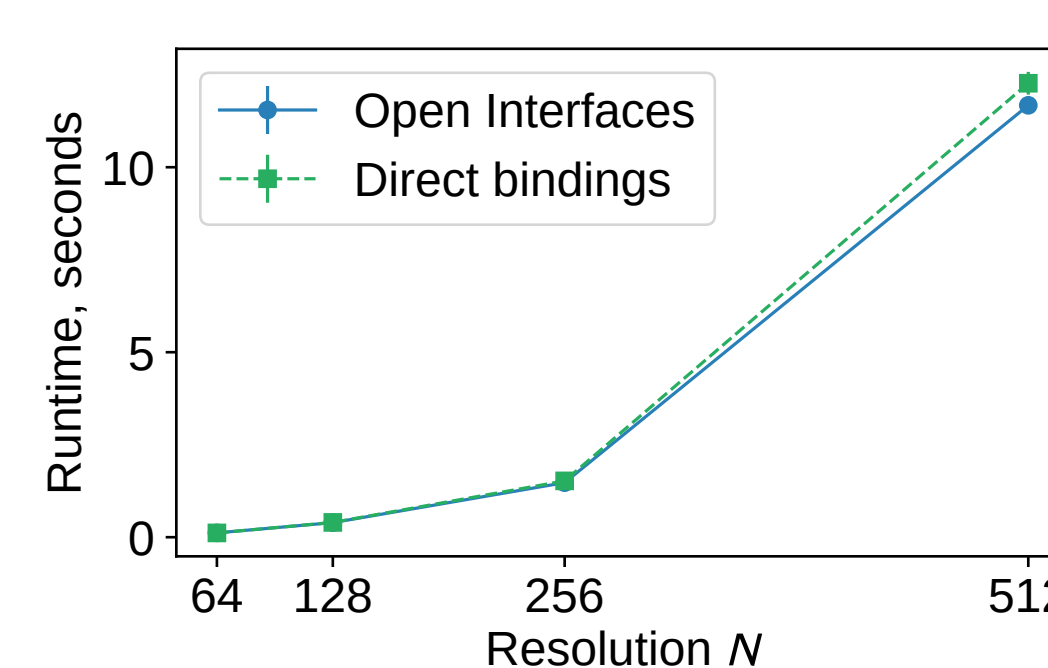
```
from oif.interfaces.iver import IVP
...

# `BurgersEquationProblem` is a utility user class.
impl = "scipy_ode" # or "sundials_cvode", or "jl_diffeq"
problem = BurgersEquationProblem(N=1001)
s = IVP(impl)
s.set_initial_value(problem.y0, problem.t0)
s.set_rhs_fn(problem.compute_rhs)

times = np.linspace(problem.t0, problem.tfinal, num=11)

soln = [y0]
for t in times[1:]:
    s.integrate(t)
    soln.append(s.y)
```

## Performance study



Do we sacrifice high-performance computing? No. Integration of a 2D Gray–Scott reaction–diffusion system using MARDI OPEN INTERFACES and SUNDIALS CVODE solver and using the same solver via direct bindings (from Python) takes virtually the same time.

Figure 3: Comparison of runtimes, averaged over 30 runs, between using the same solver via MARDI OPEN INTERFACES and directly.

## Conclusions

We demonstrated how MARDI OPEN INTERFACES can be used to improve interoperability in Scientific Computing. Using this software package, computational scientists can connect numerical solvers written in different languages, without explicitly writing bindings to these solvers, enabling complex experiment workflows.

Besides, the library allows switching between different implementations of a numerical algorithm without extensive modifications of user's code, which facilitates benchmarking numerical software in terms of performance and correctness.

## References

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