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Towards Foundations for Open Interfaces for Scientific Computing

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Algorithms and models realized by established software packages can be hard to exchange, compose or interconnect in the context of complex modeling or simulation workflows.

In this contribution we will present our work towards developing and establishing open interface standards with a core API toolkit.

These open interfaces will improve the reusability of numerical models and facilitate their recombination in complex simulation workflows. By enabling researchers to reuse existing realizations of numerical models, significant development time can be saved, while collaboration between experts in different fields of scientific computing is fostered. Moreover, interface standards for numerical models improve the comparability of numerical methods by facilitating computations with competing algorithms for the same model.

We will showcase a prototype C-language based API toolkit that allows accessing interfaces implemented with the toolkit by loading the other software component as a shared library plugin. Language bindings for this toolkit are implemented for C, C++, Julia and Python.

Our efforts are part of the scientific computing task area in the Mathematical Research Data Initiative (MaRDI), a consortium in the German National Research Data Infrastructure (NFDI).

Hauptautor: FRITZE, René

Co-Autoren: OHLBERGER, Mario; RAVE, Stephan

Vortragende(r): FRITZE, René

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