Baby steps in conducting complex simulations across HPC infrastructures

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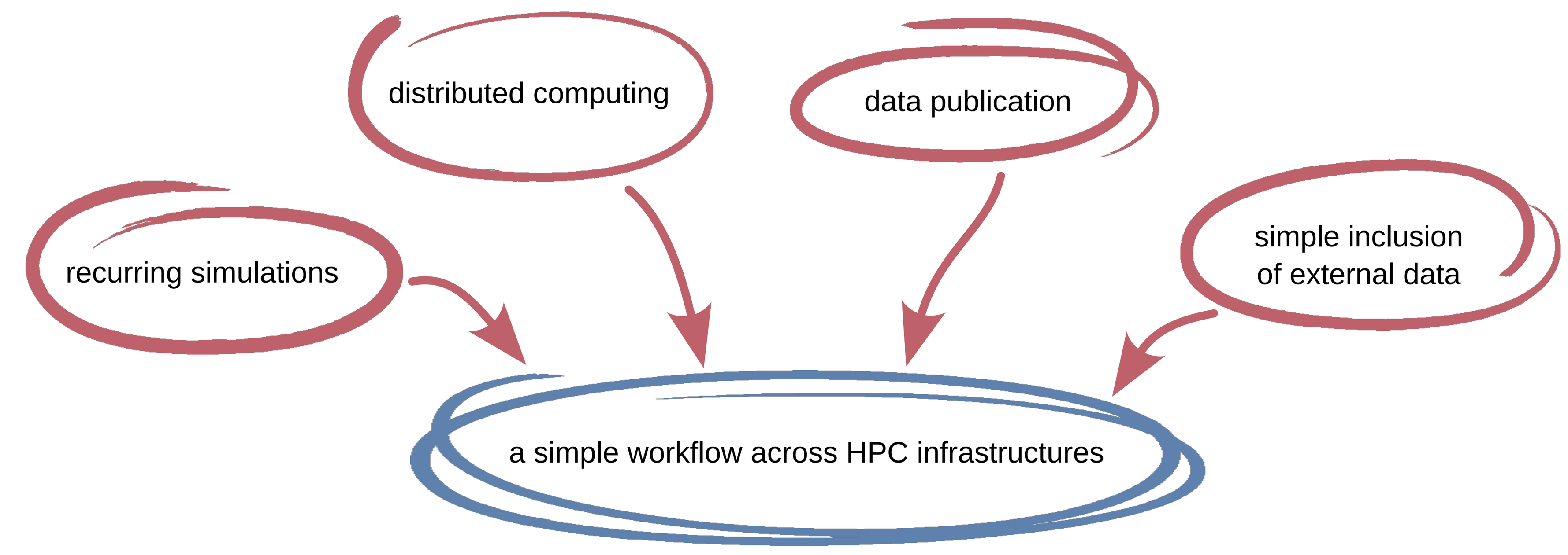


Complex simulations, such as ice sheet modeling, do not just require computations on a HPC infrastructure to solve the ice sheet model itself. Rather, an ice sheet model relies on forcing data, which is often the output of other models, such as atmospheric data from climate models. This project aims to develop a workflow across different HPC infrastructures that allows for efficient data ingestion, a user-friendly framework, and the possibility of data publication. While the current focus is on ice sheet modeling, the developed workflow will be designed to be applicable to other model setups.

The Distributed Aspect of Ice Sheet Modeling

Ice sheet simulations rely on the output of other models. Just as the cryosphere is only one part of the climate system, an ice sheet model is only one part of a climate model. Output from atmospheric models is needed to evaluate the temperature and surface mass balance of an ice sheet. The moving front module of an ice sheet model requires remote sensing data. In this sense, ice sheet modeling already follows a distributed approach.

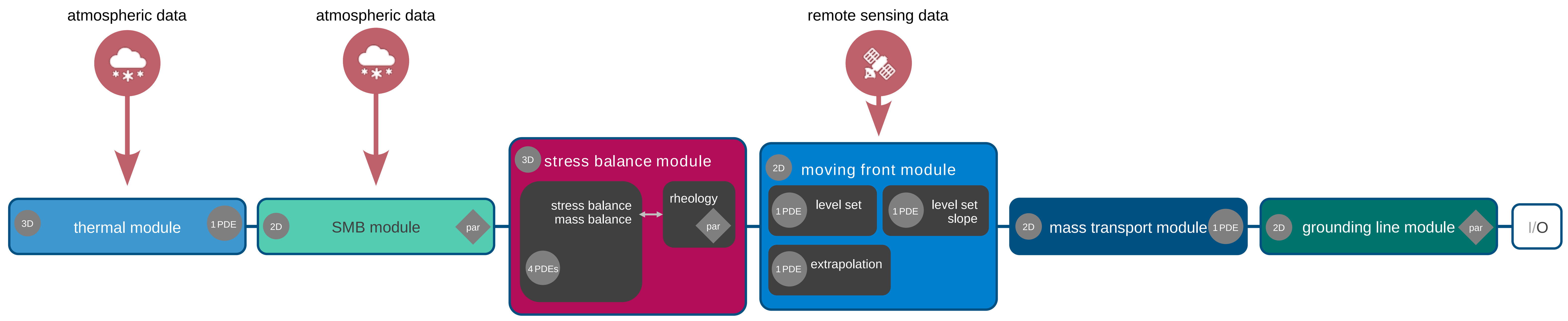


Fig. 1: Schematic showing one time step of a typical ice sheet model. The thermal module, which solves the enthalpy field, relies on atmospheric forcing data. The same is true for the surface mass balance module, which describes mass accumulation and ablation processes at the ice sheet surface. The stress balance module, solves the stress and mass balance of continuum mechanics to evaluate the velocity field. The moving front module, which describes the advance and retreat of the ice sheet's lateral margins, can benefit from additional data derived from satellite remote sensing. The mass transport module describes the evolution of the ice sheet geometry. The grounding line module tracks the position of the grounding line. At the end of the time step, the model output is written.

Using Additional Data in Ice Sheet Modeling

Easy integration of external data is crucial for ice sheet modeling. For example, prescribing the calving front position of floating glacier tongues using satellite remote sensing data products allows the development of new calving laws and the adjustment of existing ones. This can be achieved using inverse modeling and data assimilation techniques. The workflow developed in this project will allow the user to easily integrate data from external sources into the ice sheet model.

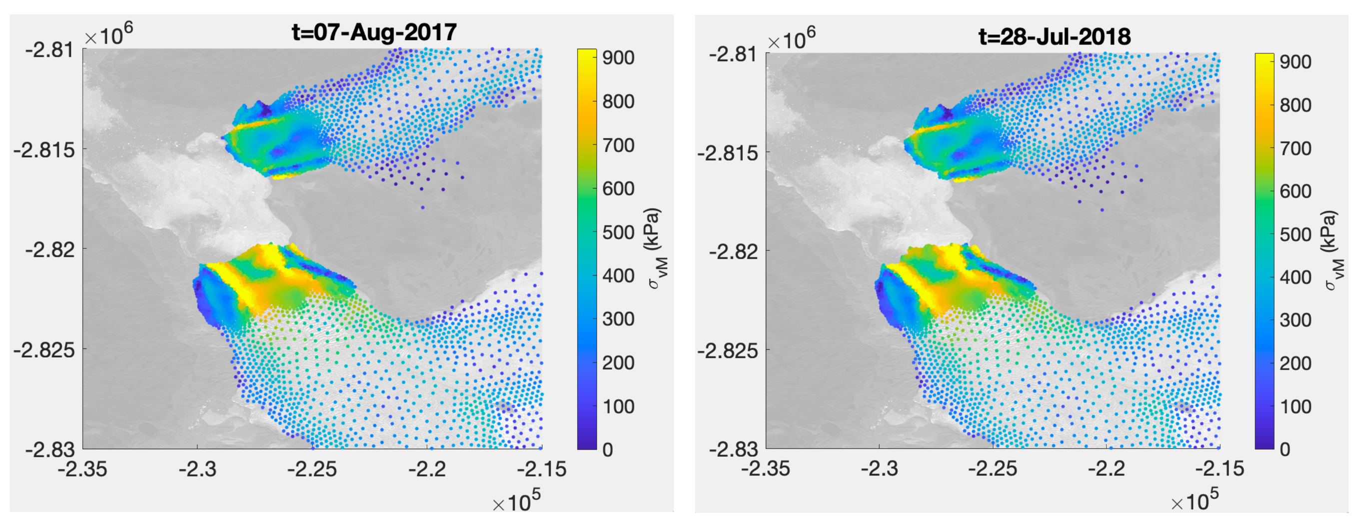


Fig. 2: Prescribing the geometry of floating glacier tongues in Greenland with calving front positions derived from satellite remote sensing allows the calculation of the equivalent von Mises stress, color coded in the figure. Equivalent von Mises stress values are consistent with corresponding calving laws.

Recurring Simulations

As in many other simulations, ice sheet modeling sometimes requires the computation of similar model setups where only minor aspects are changed. This is the case, for example, when calculating model spinups. Here, recurring simulations are performed with different computational grids and different model settings. However, the model input is not changed. A good workflow should allow the user to easily perform recurring simulations.

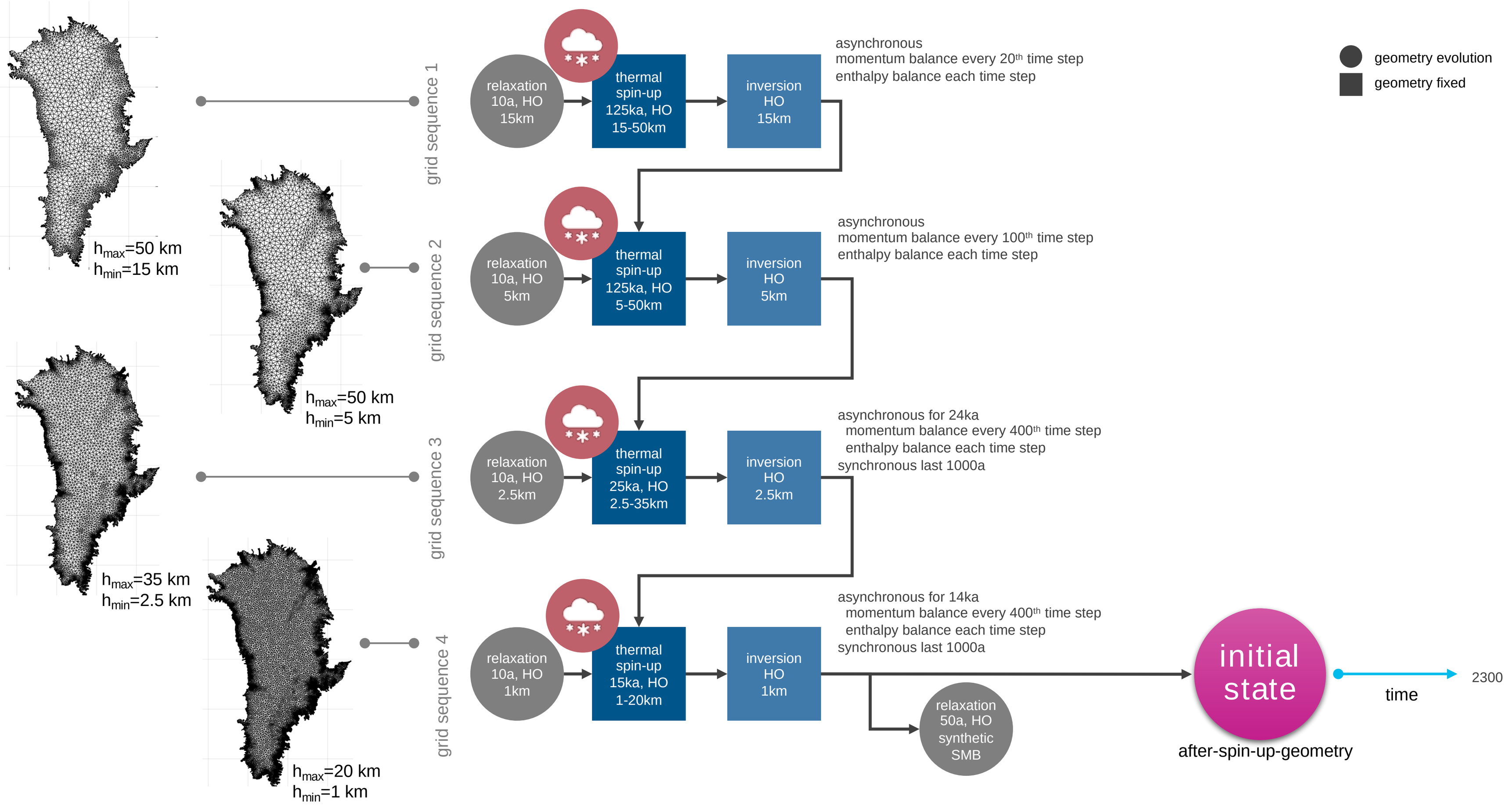
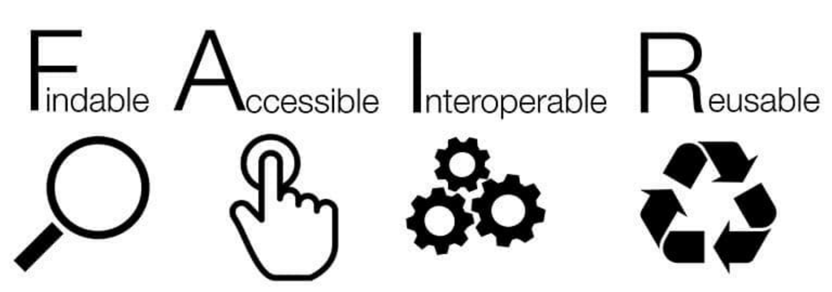


Fig. 3: Illustration of the spinup process used by Rückamp et al. (2018) to generate an initial state for the simulation of the Greenland Ice Sheet. To generate a model of the ice sheet that is consistent with the current geometry and temperature field, several similar simulations have to be run. Here, four different sequences with different grids and different coupling between the evolution of the geometry and the evolution of the temperature field are used.

Data Publishing and Dissemination

An often overlooked aspect of modeling is the publication and dissemination of model results. According to the FAIR principles, research data should be findable, accessible, interoperable and reusable. The WDCC service provided by DKRZ is aligned with these principles. Our workflow includes the easy publication of data using the infrastructure provided by DKRZ.



Distributed Computing - The Workflow

Example of the distributed computing approach. Model development takes place at the AWI. A runtime script is sent to the terrabyte platform of the LRZ, where simulations are performed. Simulation data will be requested from partners like DKRZ, TU Dresden and DLR. The simulation results are then published at DKRZ.

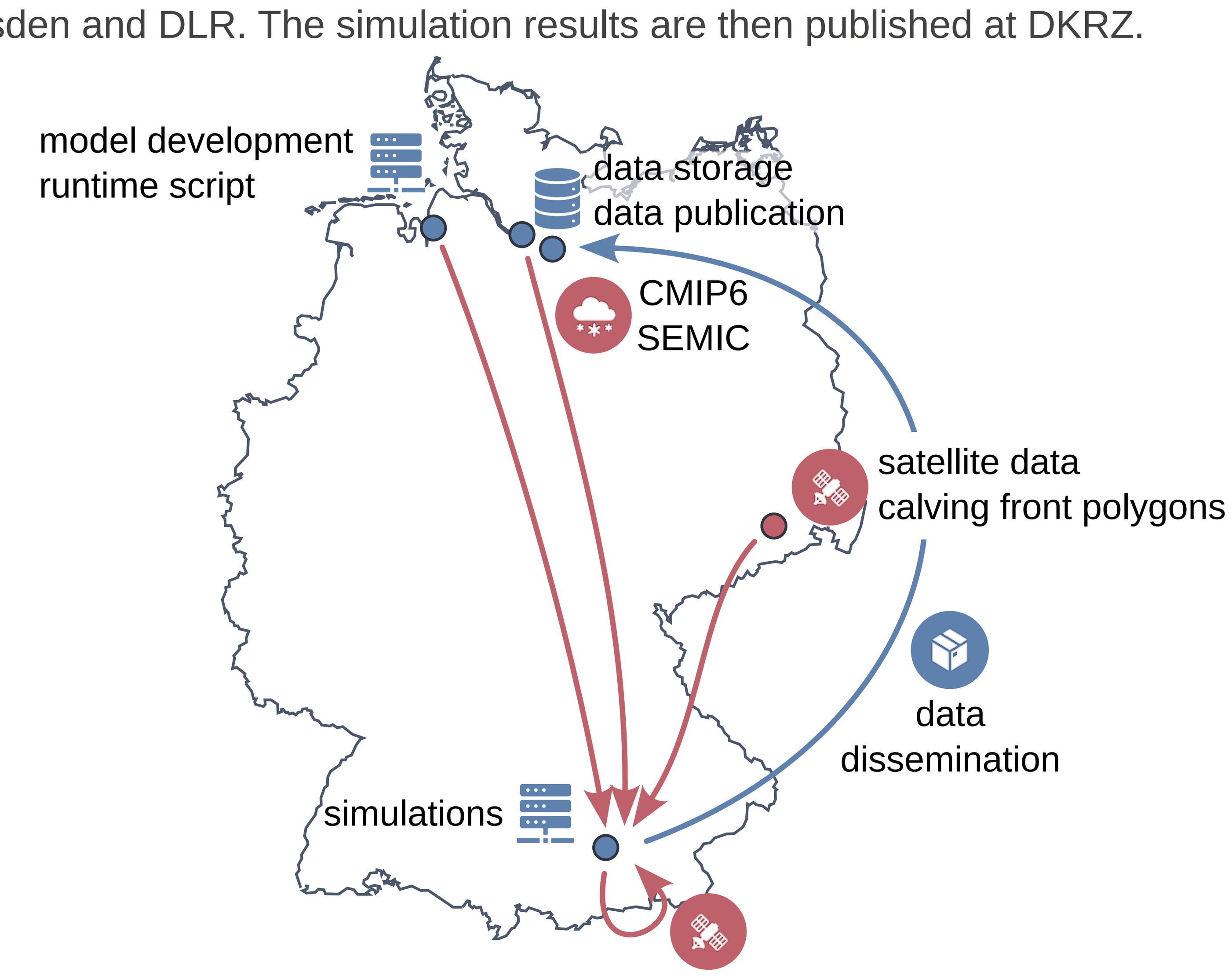


Fig. 4: Illustration of the planned workflow for the ice sheet modeling application. The workflow will be designed to be easily transferable to other applications.

Data Analytics Software Framework

For the implementation of our workflow we employ the Data Analytics Software Framework (Eggert et al. 2022).

Data Analytics Software Framework

- central message broker
- remote procedure calls
- messaging protocol language bindings for python and typescript
- example: Digitial Earth Flood Event Explorer (Eggert et al. 2022)

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