FINAM - is not a model (v1.0): a new Python-based model coupling framework

Sebastian Müller[1,*], Martin Lange[1,*], Thomas Fischer[1], Sara König[1], Matthias Kelbling[1], Jeisson Javier Leal Rojas[1], and Stephan Thober[1]

[1]Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany
[*]These authors contributed equally to this work.

Correspondence: Sebastian Müller (sebastian.mueller@ufz.de)

Abstract.

In this study, we present a new coupling framework named FINAM (short for "FINAM Is Not A Model"). FINAM is designed to facilitate the coupling of independently developed source codes and enable seamless model extensions by wrapping existing models into components with well-specified interfaces. Positioned between a coupling library and a full-fledged framework, FINAM allows users to couple preexisting wrapped models or to build models from scratch using its components. The primary goal of FINAM is to leverage the power of Python, facilitating rapid prototyping and ease of use for complex workflows while offloading computationally intensive parts to native models. FINAM supports bidirectional coupling of spatial models, enabling fast in-memory data exchange, and provides a consistent interface for flexible coupling. The main assumption for a successful coupling is that every model operates with a time loop at its core. This design of FINAM allows for straightforward model extensions written in Python without altering the original model source code. Python's robust interoperability features further enhance FINAM's capabilities, allowing interfaces with various programming languages including Fortran, C, C++, Rust, and others. This paper describes the main principles and modules of FINAM and presents example workflows to demonstrate its features. These examples range from simple toy models to well-established models like OpenGeoSys and Bodium covering features like bidirectional dependencies, complex model coupling, and spatio-temporal regridding.

1 Introduction

Environmental models represent specific systems or parts of the environment like the water cycle, the carbon cycle, or species distribution. They are usually developed to investigate specific research questions and phenomena such as hydrological droughts or reduced plant productivity. However, some phenomena are the result of processes that are interlinked and often occur at the same time. To study these complex phenomena, it is necessary to combine independently developed models.

Coupling models means that data is exchanged between them, which can be established at several levels (Brandmeyer and Karimi, 2000). There are three main approaches to exchange data between independently developed models: (i) using files, (ii) using external coupling libraries, and (iii) using modeling frameworks.

File-based coupling means that output files from one model are used as input for another model and each model is run separately for the entire simulation period. The advantage of this approach is that the two models can be executed asynchronously and that there are no modifications of the models required. However, this gets infeasible if the data to exchange is large, for example, if the models work with a high spatial resolution and intermediate results and states have to be saved unnecessarily for the entire simulation period. The even greater disadvantage of a file-based coupling is that dynamic feedbacks between models require overly complex workflows to correctly manage the huge amount of data I/O. It is an infeasible approach for complex systems with a large volume of data that needs to be exchanged. To overcome these issues, other approaches have been developed.

Coupling libraries enable data exchange between independently developed models. This is achieved by adding data exchange calls to the code base of each model. The coupling library then handles the data conversion and regridding. An example of a widely used coupling library is OASIS (short for "Ocean Atmosphere Sea Ice Soil"), particularly its latest version OASIS3-MCT together with the Model Coupling Toolkit (MCT) (Craig et al., 2017). It is a powerful library designed for climate modeling, known for its efficient parallel communication and its ability to handle high-resolution grids (Shrestha et al., 2014). Also Yet Another Coupler (YAC), a general-purpose coupling library, excels in efficient parallel communication and time synchronization, written in C with bindings to Fortran and Python supporting diverse applications (Hanke et al., 2016; Hohenegger et al., 2023). A disadvantage of these libraries is that the coupling needs to be configured explicitly. In other words, the coupler needs to be configured correctly and, for example, does not derive data conversion from metadata of the exchanged variables. This is an error-prone approach. The maintenance of the data exchange calls in each model creates additional work for model developers because they are not used in the "offline" model version.

The last approach to be mentioned is the integration of different model concepts within one larger model framework, resulting in large and complex model systems, such as earth system models that represent atmospheric, terrestrial, and marine compartments. The idea is to encapsulate processes of models in components provided by the coupling framework to have a unified data exchange mechanism. Model coupling frameworks provide a platform for researchers and practitioners to combine different models with different scales, time horizons, and disciplinary perspectives to capture complex interactions and feedback mechanisms between different components of a system. A well-known example for such a framework is the Earth System Modeling Framework (ESMF), which is widely used for its high-performance capabilities and standardized data structures, making it suitable for large-scale climate and weather simulations (Collins et al., 2005; Molod et al., 2015). The disadvantage of this approach is that it is not applicable for independently developed models with existing code bases because the framework is used to build model systems from scratch.

Here, we aim to overcome the mentioned disadvantages of the existing couplers by developing a new coupling framework framework named FINAM (short for "FINAM Is Not A Model"). FINAM allows us to couple independently developed codes and enable seamless model extensions by wrapping existing models in components with a well-specified interface. In the context of the coupling options described above, FINAM is located in the middle between a coupling library and a coupling framework. The user can build models with components from scratch, but they can also couple existing wrapped models. The primary goal of FINAM is to leverage the power of Python, which facilitates rapid prototyping and ease of use for fast

couplings while offloading computationally intensive parts to native models. FINAM allows for the bidirectional coupling of spatial models in an easy and flexible manner, enabling fast exchange of data in memory. It provides a consistent interface that supports flexible coupling based on the common assumption that every model operates with a time loop at its core. This allows for straightforward model extensions written in Python, enabling rapid prototyping without the need to alter the original model source code. Python's reputation as a "glue" language is well established, a characteristic that stems from its robust interoperability features. This compatibility is based on a suite of libraries such as Cython (Behnel et al., 2011), scikit-build (Fillion-Robin et al., 2018), f2py (Harris et al., 2020), pybind11 (Jakob et al., 2017), pyo3[1], ctypes[2], swig[3], and cffi[4], all of which facilitate the development of wrappers to integrate models regardless of their native programming languages.

Within the following, we first describe the main principles and modules of FINAM, and then give examples for workflows to show some of the features of FINAM including bidirectional coupling, complex model coupling, and spatio-temporal regridding. We further discuss future extensions and possible applications.

2 Design

2.1 Principles

The core idea for FINAM is that existing models are wrapped in components with a well-specified interface to get and set data and to update the respective model by one internal time step. Multiple *Components* that are linked to each other, potentially using *Adapters*, are called a *Composition* in FINAM. A composition can be executed, and automatically manages updates of the coupled models and the exchange of data between them.

This concept makes it easy for developers to wrap existing models (see Section 3.2), and for users to set up and run compositions. Consequently, components can be developed in isolation without detailed knowledge of the potential coupling partner models. Models can have their own temporal and spatial resolution, whereby FINAM mediates between them without user interaction.

There are multiple ways to couple models, like merging their code bases, rewriting them using a specific framework like ESMF, modifying source code with getters and setters from a native coupler like OASIS or YAC, or by exchanging files.

Compared to these approaches, FINAM does not require framework-specific code in the models except for some very basic, generally useful functionality (see Section 2.2). In addition, end-users need only minimal knowledge about coupled models, while the specifics are all managed automatically. Finally, using Python as the common glue language allows for coupling of models in virtually any programming language.

As a guiding light, we will use a simple but fully functional FINAM composition shown in Fig. 1. In this example, a model is coupled with a NetCDF reader to get the input data necessary to estimate the potential evapotranspiration (PET) using the Hargreaves-Samani method (H. Hargreaves and A. Samani, 1985), and with a NetCDF writer to store the results. The actual

---

[1] https://github.com/PyO3/pyo3
[2] https://docs.python.org/3/library/ctypes
[3] https://www.swig.org
[4] https://github.com/python-cffi/cffi

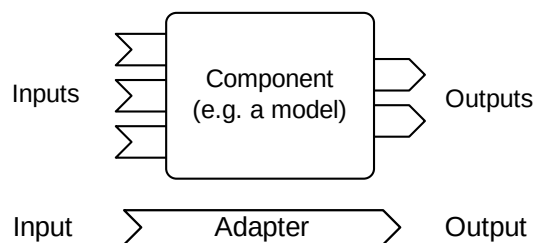
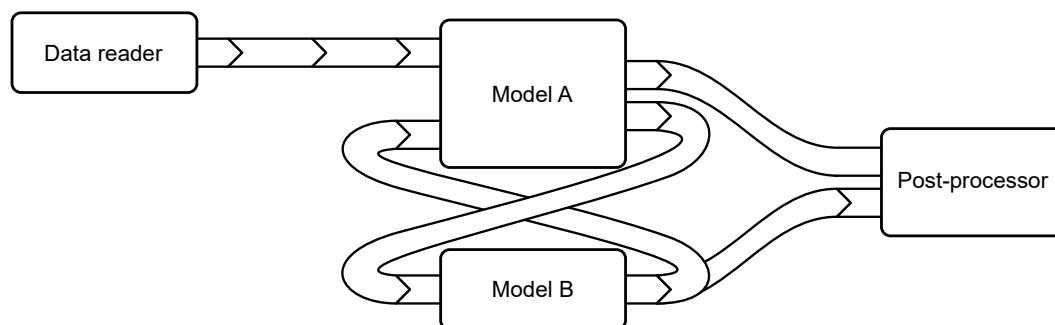
source code for this example can be found at https://git.ufz.de/FINAM/finam-examples under the *01_Hargreaves-Samani* folder.

```python
1   import datetime as dt
2   import finam as fm
3   import finam_netcdf as fm_nc
4   from component import PET
5   # config
6   start_time = dt.datetime(1990, 1, 1)
7   end_time = dt.datetime(1991, 1, 1)
8   day = dt.timedelta(days=1)
9   # components
10  pet = PET(start_time=start_time, step=day)
11  reader = fm_nc.NetCdfReader("data/temp.nc")
12  writer = fm_nc.NetCdfTimedWriter(
13      "results/pet.nc", inputs=["PET"], step=day)
14  # composition
15  composition = fm.Composition([pet, reader, writer])
16  composition.initialize()
17  # connections
18  reader.outputs["tmin"] >> pet.inputs["Tmin"]
19  reader.outputs["tmax"] >> pet.inputs["Tmax"]
20  reader.outputs["lat"] >> pet.inputs["lat"]
21  pet.outputs["PET"] >> writer.inputs["PET"]
22  # execution
23  composition.run(end_time=end_time)
```

Figure 1. A simple but fully working FINAM model consisting of three components: a `reader` providing data from a NetCDF file, a `writer` storing results in a NetCDF file, and a `pet` (potential evapotranspiration) calculator. The model calculates PET from the minimum and maximum daily air temperature and latitude values using the Hargreaves–Samani method (H. Hargreaves and A. Samani, 1985). First, the components are created, then the composition is defined, then the data connections are established, and finally the composition is executed.

2.1.1 Components and adapters

Components are the main building blocks of a FINAM *Composition*. Each component encapsulates a self-contained piece of logic. Typically, a component represents a simulation model that is prepared for FINAM by providing the required interface like `pet` in Fig. 1. But other types of components are also possible, such as I/O components to read and write files (like `reader` and `writer` in Fig. 1), real-time visualizations, or statistical models.

As indicated in Fig. 2, components can have an arbitrary number of inputs handled by *input slots* and outputs handled by *output slots*. In addition, components can have an internal time step, but do not have to. Examples of components with a time step are simulation models and components for reading time series data. Examples of components without a time step are statistical models, static data providers, or analytical models. Components without a time step can be push-based or pull-based. This means that they are executed when receiving input or when an output is requested, respectively.

2202

```
1    class PET(finam.TimeComponent):
2        @property
3        def next_time(self): ...
4        def _initialize(self): ...
5        def _connect(self): ...
6        def _update(self): ...
```

Figure 4. Pseudo code for implementing the PET component from the example above in FINAM. The `_initialize` method configures the model, `_connect` prepares I/O slots and sets initial data, and `_update` executes a single time step of the model. The `next_time` property returns the predicted simulation time of the next data pull.

2.1.2 Linking components

Components are linked through their input and output slots, with or without one or more adapters in between. The code example in Fig. 5 shows how two models are linked via a regridding adapter. Note that adapters, such as regridding or time interpolation, can be chained in place for minimal coding effort and readability. In Fig. 1 the `reader`, `writer` and `pet` component are linked in lines 18-21.

```
1    hydro["runoff"] >> RegridLinear() >> stream["runoff"]
```

Figure 5. Data connections are denoted by the overloaded bit shift operator "»" (for visual reasons).

Data exchange between linked components and adapters takes place purely in memory, and no files are used here. During the initialization process, the compatibility of the coupled slots is checked (see Data and metadata), and an error is raised in case of incompatibility.

2.1.3 Data and metadata

For all data exchanged, FINAM uses NumPy arrays(Harris et al., 2020), wrapped in `pint`[5] quantities for unit handling. This means that any exchanged data always has units, which can, however, be `dimensionless`.

Each coupling slot has associated metadata and a time stamp if it is not static data. Obligatory metadata are grid specification and units. Grid specification types provided by FINAM allow for spatial and non-spatial data. Spatial data can be defined on structured and unstructured grids (i.e. meshes) in up to three dimensions. In addition to a grid specification and units, each coupling slot can have arbitrary custom metadata fields. All metadata follows the NetCDF Climate and Forecast (CF) metadata conventions (Hassell et al., 2017).

---

[5]https://pint.readthedocs.io

```
1  def _initialize(self):
2      self.inputs.add(
3          name="tmin", time=self.time,
4          grid=None, units="degC")
5      ...
```

Figure 6. Excerpt from the `_initialize` method of the PET component from the example above. An input `"tmin"` for minimum temperature is created with metadata like units. The associated grid specification is undetermined at this point and will be inferred from the metadata of the connected output in the connect phase.

During the connection phase, the compatibility of linked slots is checked with respect to their grid specifications and units. When units are not equivalent, like $\mathrm{mm/m^2}$ and L, but compatible, like K and $°\mathrm{C}$, they are converted automatically. If slots are not compatible regarding grids or units, an error is raised. However, adapters can be used for transformations between different grids.

2.1.4 Scheduling algorithm

Component updates are scheduled by a central algorithm that decides which components will be updated next. An example of a component update method is given in Fig. 7. Updating a model involves at least three steps: (i) advance the internal time step to the next one, (ii) retrieve the input data for the current time step, and (iii) calculate the outputs for the current time step and push them to notify downstream components. In particular, the algorithm ensures that the required data for a component's next time step is available. For that sake, all time components must be able to report their current simulation time, as well as the (latest) expected time after the next update, as this is the latest target time for the inputs of the component. An example of an estimated next time stamp is given in Fig. 8.

```
1   def _update(self):
2       # Increment model time
3       self.time = self.next_time
4       # Retrieve inputs
5       data = {inp: self[inp].pull_data(self.time)
6               for inp in self.inputs}
7       # calculate PET for the current time step
8       pet = self._calc_pet(data)
9       # Push model state to outputs
10      self.outputs["PET"].push_data(pet, self.time)
```

Figure 7. The `_update` method of the PET component from the example above. First, the component time is update and the current required input is pulled. Then, PET is calculated and pushed to the output.

In each iteration, the scheduler starts with the component with the earliest current time and recursively analyzes its dependencies. The upstream components (the "provider") are then updated before the downstream components (the "consumer"). This ensures that the data required for the forthcoming time step is available, instead of, e.g. outdated data from the time step before.

```
1  @property
2  def next_time(self):
3      return self.time + self.step
```

Figure 8. The `next_time` property of the PET component from the example above. Since this component uses a fix time step, we simply advance the current model time by this step.

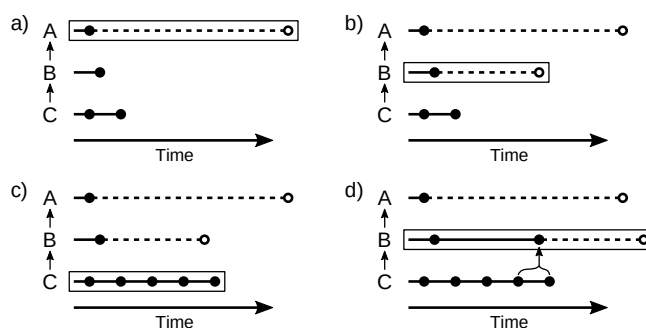



Figure 9. Illustration of the FINAM scheduling. Snapshots of a simulation featuring three components A, B and C with different time steps are shown. Component A depends on B, and B depends on C. Solid lines and dots denote already simulated model steps. The right-most solid dot of each component shows it's current simulation time. Dashed lines and hollow dots show the predicted next pull time of a component. The box denotes the active component.

145   Fig. 9 illustrates the scheduling algorithm with three components in FINAM. In panel a), A is selected as the active component because it is most back in time. The next pull time is determined, denoted by the hollow dot. A depends on B, which is not yet at A's next time, and thus becomes the active component. In panel b), B is the active component. Its next pull time is determined, again denoted by the hollow dot. B depends on C, which is not yet at B's next time, and thus becomes the active component. In panel c), C is the active component. It has no dependencies and can thus be updated. Steps a) to c) are

150 repeated until C catches up with B's next time. In panel d), all dependencies of B (i.e. C) have sufficiently advanced in time for B to update. As illustrated by the curly braces, it is guaranteed that the input data for B is available. Any kind of interpolation between adjacent source component time steps can be applied to derive the input date. This is a responsibility of the adapters. Particularly for components with large time steps, it is also possible to integrate over multiple source component time steps. For example, component B could use the weighted average of the several steps C has performed since the last updates of B.

155   The update scheme explained so far only works if there are no cycles in the dependencies. In the case of circular or bidirectional coupling, one of the involved components must use data from the past or extrapolate in time. FINAM provides dedicated adapters that resolve circular dependencies through delayed data usage or time extrapolation. This gives users full control over how circular dependencies are resolved.

    As mentioned earlier, there are also components without an internal time step. These can be updated either on pull by another
160 component, or on push. This allows for components like push-based file output or visualizations, or pull-based parametric data generators.

2.1.5   Iterative initialization

The initialization of the components may depend on other components. Possible examples are: (i) components depending on grid specification from a data source (an I/O component), (ii) deduction of the regridding transformation from input and output
165 grid specifications, or (iii) transfer of units of measurements from or to components that perform generic operations.

```python
1  def _initialize(self):
2      ...
3      self.outputs.add(name="PET")
4      self.create_connector(
5          pull_data=self.inputs.names,
6          out_info_rules={"PET": [
7              FromInput("tmin", ["grid", "time"]),
8              FromValue("units", "mm/day")]})
```

Figure 10. Another excerpt from the `_initialize` method of the PET component from the example above. An output `"PET"` is created along with a connector that is configured with rules to determine metadata for this output from given inputs (grid and time specification from `"tmin"`) or hard coded values (units set to `"mm/day"`).

    All of these examples require the exchange of metadata between components (and adapters), potentially in both directions. To make this possible in an automated way and without requiring a user to manually set all metadata, FINAM uses an iterative initialization process (Fig. 10). In this way, metadata can be exchanged downstream and upstream, regardless of complex dependencies, as long as they can be resolved.

170   Implementation-wise, this metadata exchange is realized by calling the `connect` method of components multiple times (see Fig. 11 for an example). Each time the method is called, the component can try to send or obtain metadata to/from its slots. Components indicate their connect progress (ready, something exchanged, or nothing exchanged) to the scheduler, which can thereby detect unresolvable dependency cycles. In this process, initial data exchange before the first time step is also handled. The procedure is largely automated through a helper class `ConnectHelper` to minimize the effort required by component
175 developers. An example of the setup of such a connector is given in Fig. 10. FINAM users who just write coupling scripts do not need to deal with the connect phase at all.

```
1  def _connect(self, start_time):
2      push_data = {}
3      if (self.connector.all_data_pulled
4      and self.connector.data_required["PET"]):
5          push_data["PET"] = self._calc_pet(
6              self.connector.in_data)
7      self.try_connect(
8          start_time=start_time,
9          push_data=push_data)
```

Figure 11. The `_connect` method of the PET component from the example above. The initial value for `"PET"` is calculated as soon as all required inputs are available.

2.2 Wrapping models

Wrapping an existing model requires (i) providing Python bindings for it and (ii) implementing FINAM's `Component` interface. Python bindings for an existing model need at least three features: (i) update the model by one time step, (ii) access state variables desired as outputs, and (iii) alter state variables desired as inputs.

Using Python bindings, the actual wrapper implementing the `Component` interface can be written with as few as 50 lines of code for a simple use case similar to the implementations of the PET example above, where the interaction with the wrapped model would be analogous to line 8 in Fig. 7. FINAM's extensive documentation[6] provides a detailed guide and examples for this task.

2.3 Modules

Following Python's "batteries included" philosophy, the FINAM core package, along with its external packages, provides a wide array of components and adapters designed to simplify common tasks in environmental modeling. This modular approach ensures that users can install only the components they need, avoiding unnecessary dependencies and keeping their environment clean and efficient.

FINAM includes regridding adapters based on robust libraries such as SciPy (core module) and ESMF (proved as separate package `finam_regrid`), facilitating spatial data transformation between different grids. Temporal interpolation and integration adapters align data from models operating at different time resolutions, ensuring coherent temporal data integration.

The framework supports file input/output (I/O) for commonly used formats in environmental modeling, such as NetCDF, VTK, and CSV, simplifying data exchange and storage. Live plotting capabilities enable real-time visualization of time series and spatial data, which is useful for monitoring ongoing simulations and making immediate adjustments. Additionally, live visualizations for scheduling and coupling composition provide an intuitive understanding of model interactions.

---

[6]https://finam.pages.ufz.de/finam/finam-book/development/components

To address dependency cycles, where components rely on each other's data, FINAM includes adapters designed to break these cycles, ensuring that one component uses past data to maintain simulation integrity. For rapid prototyping and testing, FINAM offers components like noise generators and generic transformations, allowing simulation of various scenarios and validation of model behavior without altering the core source code.

By integrating these components, FINAM enhances its utility and flexibility, making it a powerful tool for environmental modelers. The modular design simplifies installation and configuration, supporting the development and execution of complex simulations with greater ease and efficiency. This comprehensive suite of tools underscores the commitment of FINAM to providing a user-friendly and adaptable framework for the environmental modeling community.

3 Coupling examples

In the following, we describe three workflows to demonstrate different features and fundamental concepts of FINAM. It should be noted that the focus is not on the scientific outcome of these coupling examples but rather on the technical realization.

3.1 Bidirectional toy model

FINAM allows to create circular couplings, enabling compositions where the output of one component serves as the input for another, and vice versa. There, iterative data exchange allows the development of complex and interconnected networks of components. This section presents this concept and provides an illustrative example of the bidirectional coupling features in FINAM using simple toy models.

We couple a toy model that simulates the leaf area index (LAI) of the plant canopy with a toy model that calculates soil moisture (SM) based on precipitation data. The toy models represent simplified first-order effects, where LAI decreases for a dry soil, and new plant biomass can only be created with sufficient soil moisture. For soil moisture, it is a simple water balance with precipitation as a source term and transpiration, represented as a linear function of LAI, as a sink term. These models are set up purely for demonstration purposes and the coupling is illustrated in Fig. 12. To demonstrate why a bidirectional coupling is beneficial in this case, a second scenario was built, where SM is calculated using a fixed LAI value for the entire simulation period (see Fig. A1).

The two toy models are defined by the following equations for SM (1) and LAI (2):

$$sm(t) = sm(t-1) + B \cdot pre(t) - C \cdot lai(t) \tag{1}$$

$$lai(t) = A \cdot lai(t-1) + (1-A) \cdot f(sm(t)), \tag{2}$$

where t is the time step index, $sm[-]$ is the soil moisture, $lai[-]$ is the leaf area index, $pre\,[mm/d]$ the precipitation, A is a parameter to account for the relationship between LAI and SM, $B[-]$ and $C[-]$ are parameters to control the impact of precipitation and vegetation characteristics on the evolution of soil moisture. The term $f(sm(t))$ represents the effect of soil moisture on LAI as a piecewise linear function. For a completely dry soil (that is, sm of zero), it is zero, increasing to a

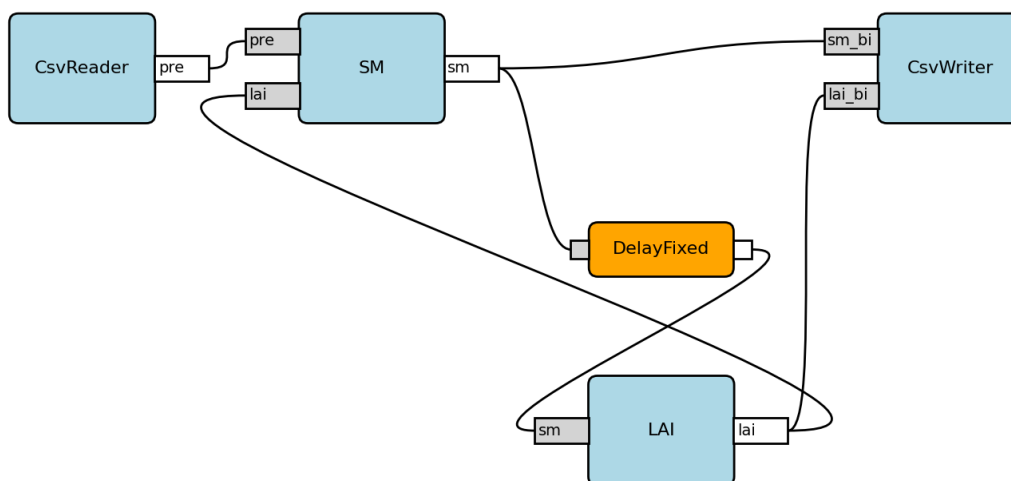



Figure 12. FINAM coupling diagram of a bidirectional model between LAI and SM.

maximum of five at sm of 0.6, and decreasing to three for completely saturated soil. Soil moisture is bounded to be between zero and one.

To enable a bidirectional coupling, we use a time delay adapter provided by FINAM as seen in Fig. 12. Since the components
230 implement the equations (1) and (2), where both variables need the other already calculated for the current time step, we need to provide one model with past data to break the dependency cycle. We offset the SM input of the LAI component by one time step, which means that it uses the soil moisture of the previous day. A five-year precipitation time series (1989 - 1993) was taken from the test domain of the mesoscale hydrological model (mHM) (Samaniego et al., 2010; Kumar et al., 2013), by extracting data from a single coordinate in space. This data was stored as a CSV file for reading by the FINAM `CsvReader`
235 component.

The results of both models (unidirectional and bidirectional) are shown in Fig. 13. The upper panel shows the precipitation data used as input for the SM component in both models, while the lower panel showcases the two model results as time series of LAI (dashed) and SM (solid).

A key observation is the deviation from the bidirectional model (blue) and the unidirectional model (orange), especially in
240 1992. A dry period results in a dryer soil that effectively reduces LAI. This then results in less transpiration and a steeper

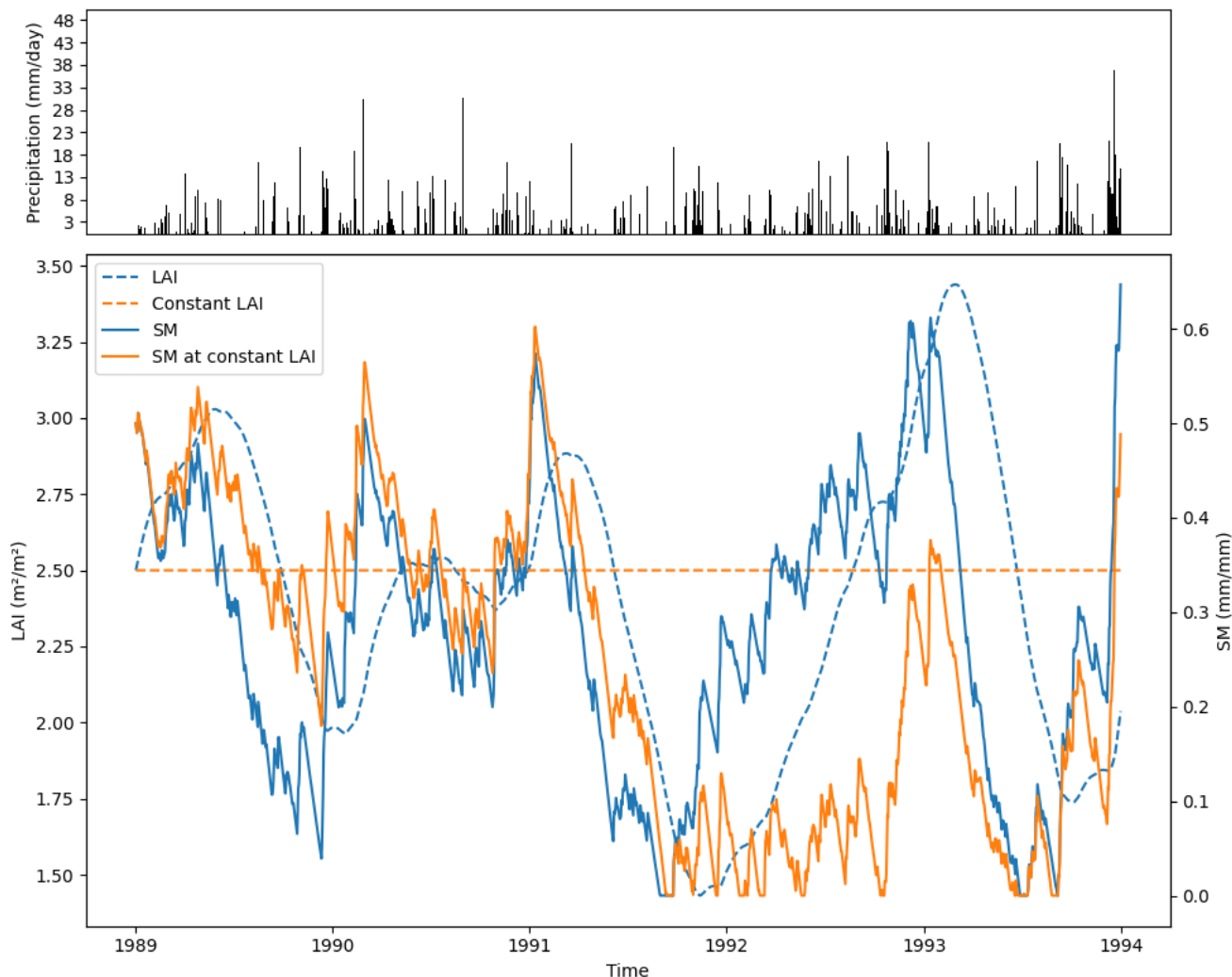



Figure 13. Precipitation (top figure), LAI (dashed lines), and SM (solid lines) time series for a FINAM uni- (orange) and bi- (blue) directional model coupling (bottom figure). Ticks mark the beginning of the year.

increase in SM afterwards compared to the constant LAI case. This reflects the bidirectional interaction of the two toy models. One should note that the cyclic coupling of the two components only needed two lines of code in the composition script.

Implementing bidirectional couplings in FINAM is notably straightforward due to its modular design and Python-based architecture. FINAM manages the complexities of time-stepping, data exchange, and synchronization, allowing users to focus
245   on model development rather than integration logistics. This ease of use contrasts sharply with traditional frameworks, which often require significant effort to configure and manage bidirectional interactions. In comparison to unidirectional coupling, where the data flow is one-way only and feedback loops are ignored, the difference in implementing bidirectional coupling

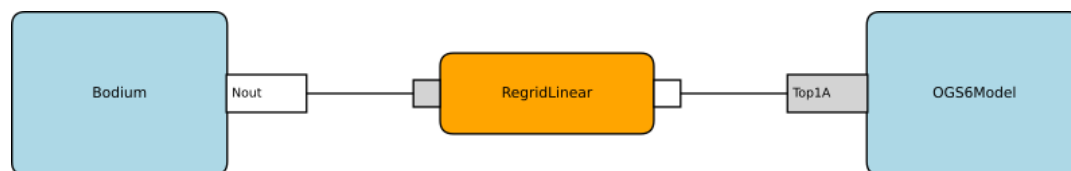



Figure 14. FINAM coupling diagram of BODIUM and OGS

with FINAM is minimal. Adjusting the data flow from a LAI generator to the LAI component, for instance, involves only a few additional lines of code.

3.2 Coupling complex wrapped models

One major application of FINAM is the coupling of complex models to answer scientific research questions where a single model alone reaches its limits in terms of system boundaries or implemented processes. To demonstrate the applicability of FINAM for such tasks, in this section we present a unidirectional coupling of the systemic soil model BODIUM (König et al., 2023) and the component transport process implemented in OpenGeoSys (OGS) (Kolditz et al., 2012). BODIUM simulates the most important processes in soil and at the plant-soil interface on the field scale, including plant growth, and is developed for agricultural systems. The lower boundary is the rooting layer or a few centimeters below. This is the spatial boundary where a coupling to OGS is of interest. OGS is an open-source simulation software for thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media. The partial differential equations used for modeling are solved numerically using the finite element method.

Reducing the pollution of water bodies with nitrate from agricultural sources is an important challenge. To understand the fate and transport of nitrate from its application as a fertilizer to its entry into groundwater and rivers, model simulations are a powerful tool. In this coupling example, we use BODIUM to simulate two hypothetical agricultural fields in different locations managed with a winterwheat monoculture and different levels of nitrogen fertilization (170 kg/ha/a and 340 kg/ha/a, respectively). The simulated nitrate leachate from each time step is passed through FINAM to OGS, where the transport within groundwater and to a nearby river is simulated.

BODIUM and OGS operate on the same temporal scale (daily time step) but on different spatial scales. While BODIUM is a 1D model simulating on the field scale, OGS simulates on irregular grids on the catchment scale. However, the exchange variable in this specific coupling example is given in mass per area and thus is independent of the exact spatial distribution. Thus, we can apply a simple linear regridding within FINAM to overcome the spatial differences between the coupled models with BODIUM simulating two different instances for the two agricultural field sites. The basic diagram in Fig. 14 shows the components involved (colored blue) and the linear regridding adapter (colored orange). The connection lines between the components and adapters indicate data exchange controlled by FINAM, from white outputs to gray inputs.

The surface of the model domain with x-extent of 1830 m, y-extent of 830 m, and z-extent of 48 m is given by a topography extracted from SRTM data. In the bottom panel of Fig. 15, the domain is exaggerated five times and the two agriculture sites

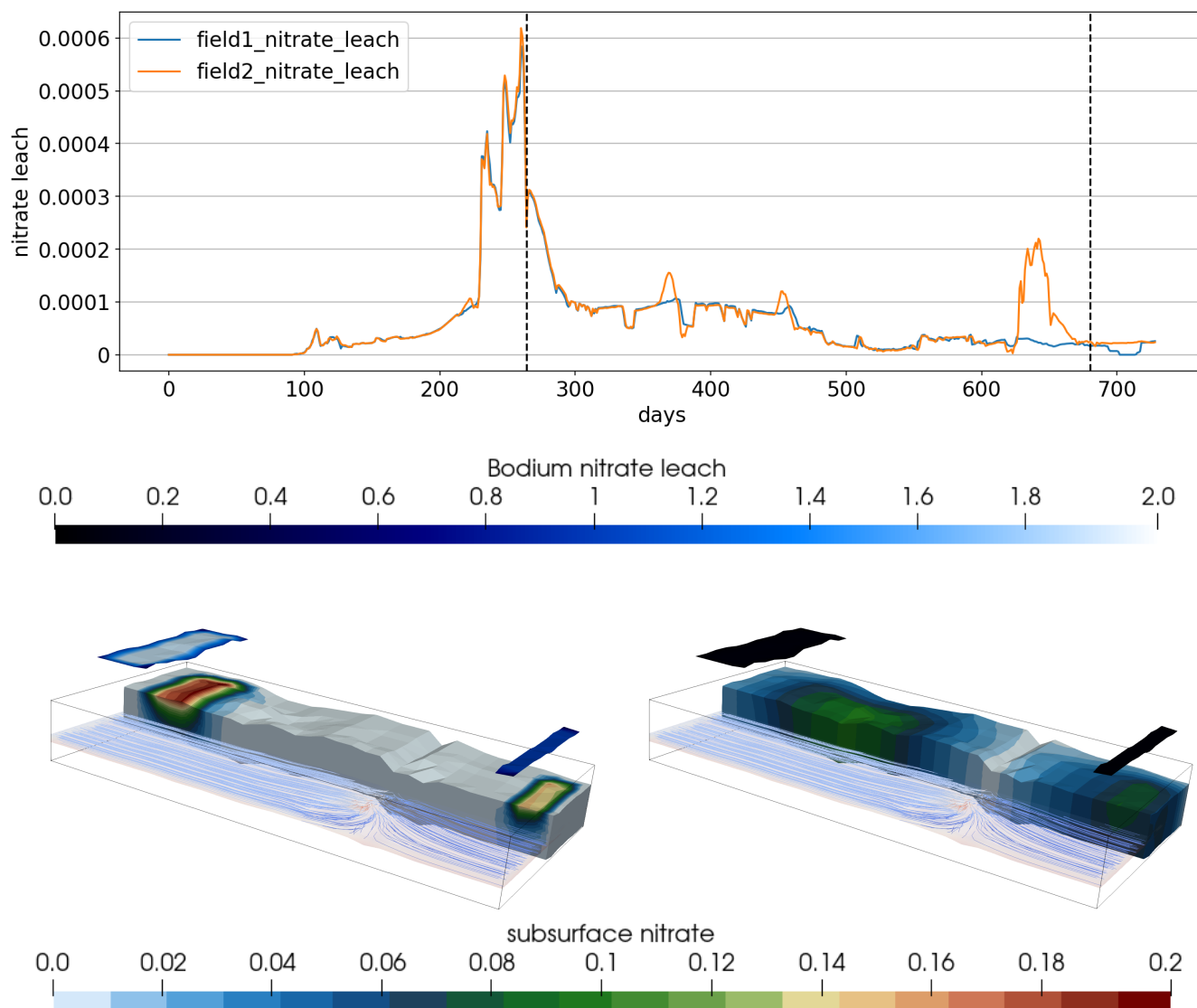



Figure 15. Top panel: nitrate leachate computed by BODIUM for the two different fields (field1 and field2); bottom: subsurface domain outline and (for visualization purposes translated as 'clouds') boundary patches above coloured by BODIUM nitrate leachate; in the background (exaggerated 5 times) nitrate concentration computed by OGS: left: after 264 days, right: after 680 days, in the front groundwater flow paths coloured by velocity

275 are delineated by the two stripes, which move up a little bit for visualization purposes. In the upper panel of Fig. 15 the nitrate leachate is plotted over time.

For each agricultural site, a different BODIUM instance simulates nitrate leachate, which is passed to OGS at the specific field locations via the FINAM linear regridding adapter. At all other parts of the simulation domain, nitrate leachate passed to OGS is set to zero (assuming neglectable nitrate leaching in non-agricultural fields). The amount of nitrate leached into groundwater depends on the time of fertilizer application, precipitation, and nitrogen uptake by plants, resulting in temporal peaks of nitrate passing from BODIUM to OGS (top panel of Fig. 15). After the nitrate has reached the subsurface, it is transported along the groundwater flow field. The subsurface nitrate distribution is shown after $264\,\mathrm{days}$ in the left part and after $680\,\mathrm{days}$ in the right part of Fig. 15. In order to create a more dynamic behavior, both fields have slightly different time series of nitrate leach.

This example demonstrates how established complex models can be easily coupled via FINAM. However, note that both models had to be prepared for model coupling with existing python bindings and a FINAM wrapper, i.e. the interface shown in Fig. 4 has to be implemented. In addition, to apply this coupling for advanced research questions, further extensions of the coupling would be of interest, such as a bidirectional coupling by passing the hydraulic head from OGS to BODIUM.

3.3 Spatio-temporal regridding

Spatio-temporal regridding is a fundamental concept in the field of spatial data analysis and processing. It involves the transformation of data from one spatio-temporal grid or coordinate system to another. This regridding process plays a crucial role in various disciplines such as atmospheric research, climate modeling, remote sensing, and environmental research. Regridding algorithms are a big part of the mentioned coupling frameworks and libraries ESMF, YAC or OASIS.

```
1  import finam as fm
2  import finam_regrid as fm_rg
3  ...
4  # Adapters
5  method = fm_rg.RegridMethod.CONSERVE
6  regrid = fm_rg.Regrid(regrid_method=method)
7  mean = fm.adapters.AvgOverTime(step=0)
8  ...
9  # Connections
10 reader["pre"] >> regrid >> mean >> writer["pre"]
```

Figure 16. FINAM composition excerpt to regrid and average precipitation over time. The reader and writer modules specify the spatial and temporal resolutions of the source and target precipitation data. The writer is pre-configured with a regular mesh and a writing frequency of 30 days. This implies that the `regrid` and `mean` adapters do not need further information about the data specification, as it is determined from the connected components. The regridding method is set to `CONSERVE` in order to preserve the total amount of precipitation and the averaging adapter is configured to interpret the data to be valid for the time span right before the time stamp (`step=0`).

FINAM provides built-in regridding adapters for linear and nearest-neighbor interpolation designed to easily transform data from one model to another. For advanced regridding operations, we provide a dedicated package `finam-regrid`, which wraps the regridding algorithms of ESMF (Collins et al., 2005), covering a wide range of regridding methods, grid types, and

coordinate systems. For details, we refer to the documentation of `finam-regrid`[7]. These adapters are designed to translate data between different grid formats - structured or unstructured - and adjust resolutions to ensure compatibility between models. Incorporating regridding capabilities directly within the framework significantly reduces the workload on model developers and

300 users. Performing as a dynamic adapter, it automatically detects the specifications of the source and target grids and derives the required transformation. Despite the underlying complexity of this task, we have engineered the tool to be user-friendly, ensuring that its advanced capabilities are accessible without the need for detailed knowledge about regridding of the involved grid specifications.

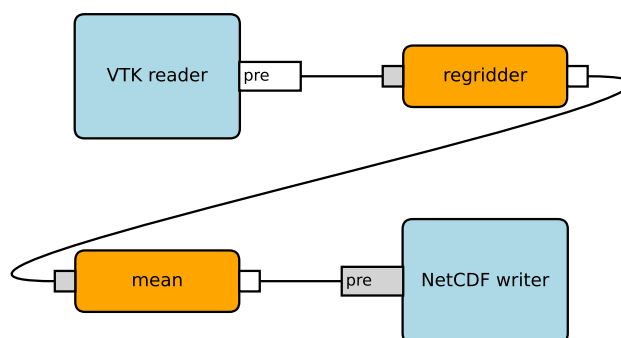



Figure 17. FINAM coupling diagram of the spatio-temporal regridding of precipitation.

In this example, we illustrate the spatio-temporal regridding capabilities of FINAM by converting daily precipitation data

305 from an unstructured grid, with a cell edge length of approximately 0.5 km, to a 30-day mean precipitation on a regular grid with 1 km cells, covering an area of five by four kilometers. To simplify the example, we utilize the finam-vtk package to read the unstructured data time series stored in the PVD format and then write the data using the finam-netcdf module. However, this workflow could also be integrated into a larger system in which meteorological data from an atmospheric model serves as input for a crop yield estimator that operates on monthly data.

310 Fig. 16 shows the important parts of the coupling setup script, which shows the ease of configuring the data flow, while Fig. 17 shows the overall coupling scheme. We employ a five-year time series of daily data and apply a rolling mean with a 30-day window after regridding the data to the structured target grid. Fig. 18 shows the averaging of an extracted time series from the top right grid cell. The time averaging adapter is capable of converting the data on the fly with almost no configuration. Input and output time stepping is purly derived from the connected components, where the input precipitation is pushed daily

315 by the reader component and the writer will request data every 30 days. This highlights the ease of creating data streams, where users do not need to worry about time-stepping compatibilities. Furthermore, Fig. 19 shows the results of the regridding for a single day on the unstructured grid and the average of one month on the target grid, which includes that day. To ensure that the total amount of precipitation is preserved, conservative regridding was used in this example. Again, the adapter for spatial

---

[7]https://finam.pages.ufz.de/finam-regrid

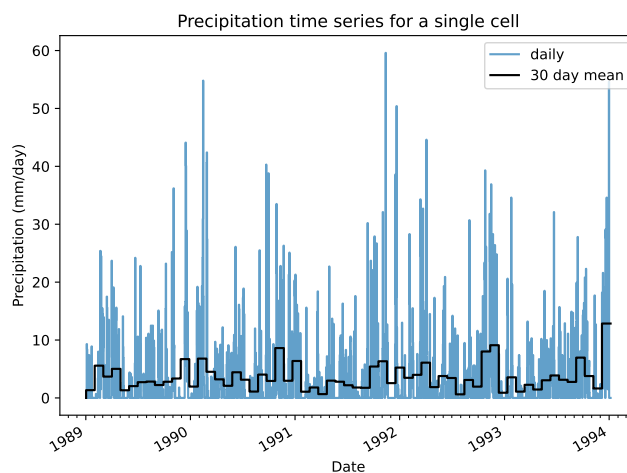



Figure 18. Temporal aggregation of precipitation data for a single grid cell. The five year input time series of daily data is shown in blue and the 30-day rolling average is shown in black.

regridding will determine its configuration entirely from the data specifications of the connected components, which avoids

320 sources of error. A more detailed overview of different regridding constellations is given in the Appendix in Fig. B1.

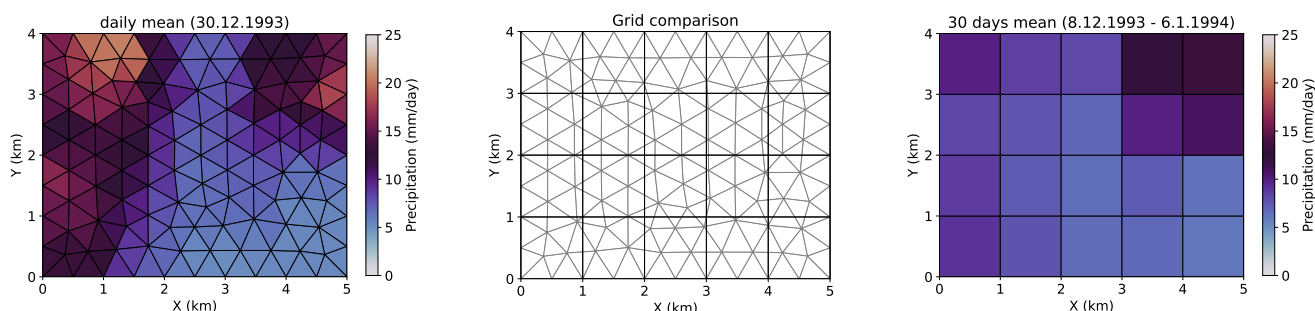



Figure 19. This figure illustrates the regridding process of precipitation data. The left panel shows the input unstructured grid for a single day, highlighting the original distribution and variability of the data on an irregular grid. The middle panel overlays the unstructured and resulting structured grids, without displaying data, to emphasize the differences in grid configurations and cell outlines. The right panel presents the resulting structured grid with time-averaged precipitation data over 30 days, including the single day from the left panel, demonstrating the transformation and smoothing effect achieved through regridding.

This workflow demonstrates the ease of creating data workflows that connect components operating on different spatio-temporal scales. By regridding daily precipitation data from an unstructured grid to a regular grid and aggregating it into 30-day means, it showcases the integration of various data formats and the seamless data flow configuration, highlighting the potential for coupling diverse data-driven models.

4 Discussion

In the development of the model coupling framework FINAM, our primary goal was to address the significant challenges inherent in coupling models written in diverse programming languages, operating on different time steps and grid systems. The selection of Python as the foundational language for this coupler was predicated on several of its intrinsic qualities that make it exceptionally suited for such a complex task.

Python's interoperability is enhanced by a variety of libraries that facilitate the development of wrappers for integrating models across different native programming languages like C, C++, Fortran, or Rust. Additionally, Python's extensive ecosystem and library support simplify the process of model creation and data processing, backed by a strong, global community of developers and researchers. This supportive environment, combined with the cross-platform nature of Python and the ability to rapidly prototype it, creates an optimal setting for the development and fast and easy testing of complex model couplings.

One fundamental idea of FINAM is the assumption that temporal models inherently contain a time loop within their code structure. The coupler makes use of this characteristic by requiring that each model needs to be able to perform a single time iteration. This should be controlled by interface routines provided in Python that also provide access to the internal states between these iterations. Such an approach allows for the seamless implementation of a FINAM component to wrap around any model, facilitating its integration into the coupling framework without necessitating direct further modifications to the model's source code, when Python-bindings are available.

Compared against a pure pull-based approach, where models are only executed if data is requested by downstream components, FINAM's scheduling provides several advantages. Firstly, a pure pull-based approach requires a single component that is the end point of the coupling, which drives the complete chain via pull. With FINAM's approach, this is not required and a coupling setup can have an arbitrary number of end points. Secondly, in a pull-based approach, it is not guaranteed that all components run over the entire simulation time frame. In FINAM, this is guaranteed.

In contrast, traditional coupling methods often involve the integration of routines in their supported languages directly into the model source code, enabling data exchange during runtime (Hanke et al., 2016; Craig et al., 2017). However, this method imposes a significant burden on modelers, who must ensure data compatibility with respect to units, grid definitions, and time references, often necessitating extensive modifications to the original model code. FINAM distinguishes itself by offering utilities to validate and process data on the fly, thereby simplifying the coupling process and minimizing the need for direct alterations to model code.

To further emphasize the practical advantages of the FINAM framework, it is essential to highlight the usability of the adapters provided within the system. These adapters enable smooth data exchange between models with varying data requirements and formats, without the need for explicit configuration. As an example, regridding adapters automatically determine their required transformation from the connected source and target components.

In addition, FINAM includes a variety of readers and writers designed to handle multiple file formats, such as NetCDF, VTK, or CSV. This versatility allows researchers to integrate models from different domains without the need for time-consuming conversions or extensive preprocessing. All data exchanged in FINAM is wrapped by `pint` to enable automatic unit conversion

and checking. This means that incompatible inputs and outputs can never be connected by mistake, and, if required, a unit
360   conversion is performed on the fly.

However, FINAM still has several limitations and potential for improvements and extensions. One of the main challenges
FINAM is currently facing is the issue of parallelization. Particularly, the integration of MPI (Message Passing Interface) for
parallel computing, to distribute models to different CPU cores, is work in progress. Other frameworks like YAC that are built
on top of MPI support this out of the box but follow a different approach of model coupling. Additionally, making a model
365   ready for FINAM can require a significant investment of time and resources. Although Python facilitates rapid prototyping and
development, preparing a model to comply with FINAM's requirements can be a demanding process, particularly for legacy
systems or highly complex models, depending on their internal structure. If the code base is well written and its functionality is
encapsulated in logical units, such as executing the time loop as a separate subroutine, the Python interface is reasonably easy
to implement.

370   Another technical limitation arises from the nature of Python itself. Preventing unnecessary data copying within the FINAM
framework can become complicated due to different data representations in different models. By default, numpy masked arrays
are used to exchange data, but these arrays could hold copies instead of views to the underlying data. Efficiently managing
data without unnecessary copying is crucial for maintaining performance, especially when dealing with large datasets or high-
frequency data exchanges. This challenge underscores the need for ongoing development within the FINAM framework to
375   enhance its efficiency and reduce overhead, ensuring that it remains a viable solution for complex model coupling scenarios.

A last area to mention is the handling of metadata and configuration. Although the basic infrastructure to track metadata
from components has been implemented, there is currently no best-practice guide on how to utilize this feature effectively.
Establishing such guidelines would help standardize metadata usage, making it easier for users to follow the *FAIR* data prin-
ciples (Barker et al., 2022). Together with metadata, there is the lack of a unified configuration system for compositions. This
380   can make it challenging to reuse compositions in complex computational workflows, potentially hindering the efficiency and
reproducibility of simulations. Developing a unified configuration approach would streamline the setup process and simplify
the sharing and replication of complex model compositions.

A unique feature of FINAM is its support for bidirectional coupling by temporal delaying circular input/output connections.
Using this method, we do not require models to save and reset states, a process that can be overly demanding for many models.
385   The gained flexibility is further enhanced by FINAM's approach to time representation. By assuming that valid time spans
for data are defined by timestamps, with the current timestamp indicating the end of the reference period that started from the
previous timestamp, FINAM standardizes time representation across models. This method clarifies the time frame for *extensive*
variables, like total precipitation of a day, and provides a precise reference for *intensive* variables, such as air temperature for
a specific point in time, without requiring direct modifications to the handling of time of the models.

390   Furthermore, FINAM includes time adapters designed to bridge models with differing time steps and spans through tech-
niques such as integration, summation, and temporal disaggregation. This capability not only enhances the framework's flexibil-
ity, but also significantly reduces the complexity involved in model integration, allowing researchers to focus on the substantial
aspects of their work without being encumbered by technical incompatibilities.

5   Summary and Outlook

395 In this study, we present FINAM, short for "FINAM Is Not A Model", which is a Python based coupling framework designed to connect models written in diverse programming languages. Models are wrapped in components with a well-specified interface that facilitates the exchange of data between them. Additionally, FINAM provides a set of tools to process data that includes functionality such as regridding and unit conversion, but also reading and writing different file formats (such as NetCDF, VTK, and CSV). FINAM handles data compatibility checks, unit conversion, and component scheduling, which makes the model

400 coupling process less error-prone. It provides a unique and intuitive mechanism to link components, which makes it easy to set up a coupled model. We presented three examples that highlight different features of FINAM. The first example consisted of two toy models, simulating soil moisture and LAI with cyclic dependencies on each other to demonstrate the capabilities of FINAM of handling dynamic feedbacks between components. The second example illustrates the usage of FINAMs to couple the separately developed models BODIUM and OGS to simulate the transport of nitrate leachate in groundwater. In a third

405 workflow, we demonstrated important features to spatio-temporal regrid data within a FINAM coupling. To do so, we remapped the daily precipitation data of an unstructured grid to a coarser structured grid and applied a rolling average of 30 days.

In summary, FINAM embodies a forward-thinking approach to model coupling, leveraging Python's unique features to facilitate the integration of diverse models. By minimizing the need for direct modifications to the model code and offering innovative solutions to handle time representation and data compatibility, FINAM represents a significant advancement in the

410 field of computational modeling.

Code availability.   The code of FINAM is developed at https://git.ufz.de/FINAM/finam and available via Zenodo at https://doi.org/10.5281/zenodo.7602944. It is distributed under the GNU LGPL v3.0 license. The documentation, which includes a quick start guide, a more in-depth hand book, and a complete overview of the API, can be accessed via https://finam.pages.ufz.de. All mentioned expansion modules and examples are hosted under https://git.ufz.de/FINAM.

415 *Author contributions.*   Martin Lange and Sebastian Müller are the main developers of FINAM and contributed both equally to all sections of the text. Sara König and Thomas Fischer wrote the section about coupling complex wrapped models and helped proofreading the text. Jeisson Javier Leal Rojas wrote the section on the bidirectional toy model. Stephan Thober wrote the introduction and the summary and supervised the project. Matthias Kelbling helped with implementation details and helped to improved the text.

Competing interests.   The authors declare that they have no conflict of interest.

420 *Acknowledgements.* Sara König was funded by the German Federal Ministry of Education and Research (BMBF) in the framework of the funding measure 'Soil as a Sustainable Resource for the Bioeconomy—BonaRes', project 'BonaRes (Module B): BonaRes Centre for Soil Research'. This work is a contribution to the LandTrans simulator initiative at the Helmholtz Centre for Environmental Research - UFZ.

Appendix A: Unidirectional coupling of LAI and SM

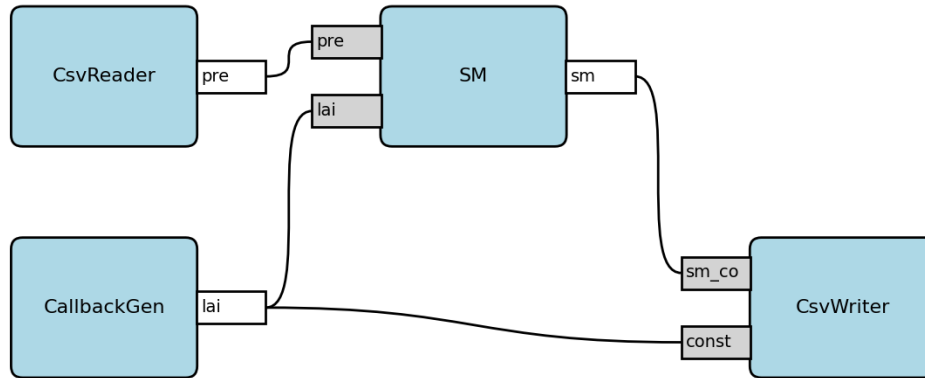



Figure A1. FINAM coupling diagram of a unidirectional model between LAI and SM.

Appendix B: Regridding of different resolutions

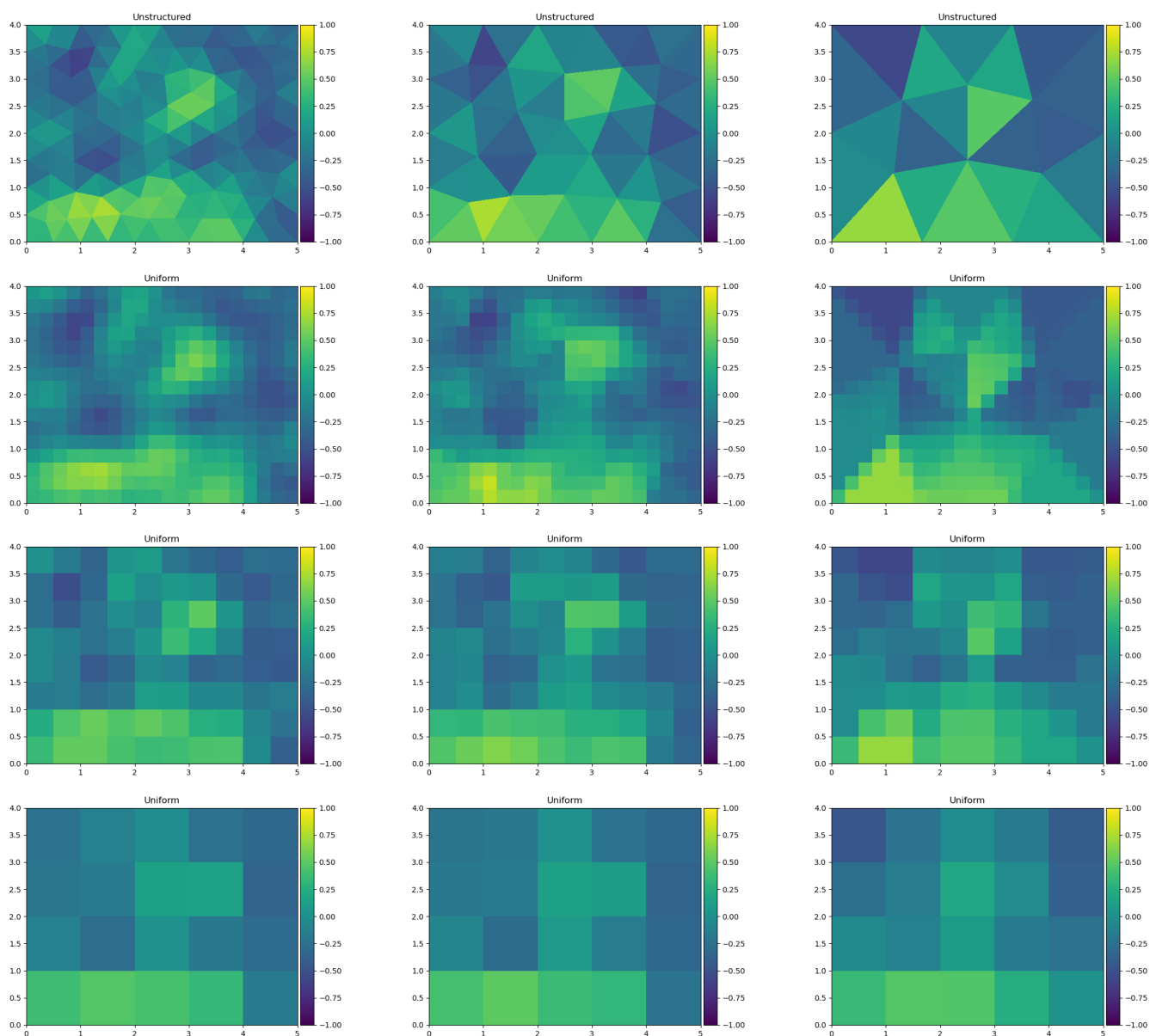



Figure B1. Regridding cell associated data from unstructured grids with different triangular edge lengths (top row, ~ 0.5, ~ 1.0, ~ 2.0 in columns 1-3) to uniform grids with different cell sizes (0.25, 0.5, 1.0, in rows 2-4) using conservative regridding provided by the ESMF library.

References

Barker, M., Chue Hong, N. P., Katz, D. S., Lamprecht, A.-L., Martinez-Ortiz, C., Psomopoulos, F., Harrow, J., Castro, L. J., Gruenpeter, M., Martinez, P. A., and Honeyman, T.: Introducing the FAIR Principles for research software, Scientific Data, 9, 622, https://doi.org/10.1038/s41597-022-01710-x, publisher: Nature Publishing Group, 2022.

Behnel, S., Bradshaw, R., Citro, C., Dalcin, L., Seljebotn, D. S., and Smith, K.: Cython: The Best of Both Worlds, Computing in Science Engineering, 13, 31–39, https://doi.org/10.1109/MCSE.2010.118, conference Name: Computing in Science Engineering, 2011.

Brandmeyer, J. E. and Karimi, H. A.: Coupling methodologies for environmental models, Environmental Modelling & Software, 15, 479–488, https://doi.org/10.1016/S1364-8152(00)00027-X, 2000.

Collins, N., Theurich, G., DeLuca, C., Suarez, M., Trayanov, A., Balaji, V., Li, P., Yang, W., Hill, C., and da Silva, A.: Design and Implementation of Components in the Earth System Modeling Framework, The International Journal of High Performance Computing Applications, 19, 341–350, https://doi.org/10.1177/1094342005056120, publisher: SAGE Publications Ltd STM, 2005.

Craig, A., Valcke, S., and Coquart, L.: Development and performance of a new version of the OASIS coupler, OASIS3-MCT_3.0, Geoscientific Model Development, 10, 3297–3308, https://doi.org/10.5194/gmd-10-3297-2017, publisher: Copernicus GmbH, 2017.

Fillion-Robin, J.-C., McCormick, M., Padron, O., Smolens, M., Grauer, M., and Sarahan, M.: jcfr/scipy_2018_scikit_build_talk: SciPy 2018 Talk | scikit-build: A Build System Generator for CPython C/C++/Fortran/Cython Extensions, https://doi.org/10.5281/zenodo.2565368, 2018.

H. Hargreaves, G. and A. Samani, Z.: Reference Crop Evapotranspiration from Temperature, Applied Engineering in Agriculture, 1, 96–99, https://doi.org/10.13031/2013.26773, place: St. Joseph, MI Publisher: ASAE, 1985.

Hanke, M., Redler, R., Holfeld, T., and Yastremsky, M.: YAC 1.2.0: new aspects for coupling software in Earth system modelling, Geoscientific Model Development, 9, 2755–2769, https://doi.org/10.5194/gmd-9-2755-2016, publisher: Copernicus GmbH, 2016.

Harris, C. R., Millman, K. J., van der Walt, S. J., Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., van Kerkwijk, M. H., Brett, M., Haldane, A., Fernández del Río, J., Wiebe, M., Peterson, P., Gérard-Marchant, P., Sheppard, K., Reddy, T., Weckesser, W., Abbasi, H., Gohlke, C., and Oliphant, T. E.: Array programming with NumPy, Nature, 585, 357–362, https://doi.org/10.1038/s41586-020-2649-2, 2020.

Hassell, D., Gregory, J., Blower, J., Lawrence, B. N., and Taylor, K. E.: A data model of the Climate and Forecast metadata conventions (CF-1.6) with a software implementation (cf-python v2.1), Geoscientific Model Development, 10, 4619–4646, https://doi.org/10.5194/gmd-10-4619-2017, publisher: Copernicus GmbH, 2017.

Hohenegger, C., Korn, P., Linardakis, L., Redler, R., Schnur, R., Adamidis, P., Bao, J., Bastin, S., Behravesh, M., Bergemann, M., Biercamp, J., Bockelmann, H., Brokopf, R., Brüggemann, N., Casaroli, L., Chegini, F., Datseris, G., Esch, M., George, G., Giorgetta, M., Gutjahr, O., Haak, H., Hanke, M., Ilyina, T., Jahns, T., Jungclaus, J., Kern, M., Klocke, D., Kluft, L., Kölling, T., Kornblueh, L., Kosukhin, S., Kroll, C., Lee, J., Mauritsen, T., Mehlmann, C., Mieslinger, T., Naumann, A. K., Paccini, L., Peinado, A., Praturi, D. S., Putrasahan, D., Rast, S., Riddick, T., Roeber, N., Schmidt, H., Schulzweida, U., Schütte, F., Segura, H., Shevchenko, R., Singh, V., Specht, M., Stephan, C. C., von Storch, J.-S., Vogel, R., Wengel, C., Winkler, M., Ziemen, F., Marotzke, J., and Stevens, B.: ICON-Sapphire: simulating the components of the Earth system and their interactions at kilometer and subkilometer scales, Geoscientific Model Development, 16, 779–811, https://doi.org/10.5194/gmd-16-779-2023, publisher: Copernicus GmbH, 2023.

Jakob, W., Rhinelander, J., and Moldovan, D.: pybind11 – Seamless operability between C++11 and Python, 2017.

Kolditz, O., Bauer, S., Bilke, L., Böttcher, N., Delfs, J.-O., Fischer, T., Görke, U. J., Kalbacher, T., Kosakowski, G., McDermott, C. I., Park, C. H., Radu, F., Rink, K., Shao, H., Shao, H. B., Sun, F., Sun, Y. Y., Singh, A. K., Taron, J., Walther, M., Wang, W., Watanabe, N., Wu, Y., Xie, M., Xu, W., and Zehner, B.: OpenGeoSys: An open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media, Environmental Earth Sciences, 67, 589–599, https://doi.org/10.1007/s12665-012-1546-x, 2012.

465 Kumar, R., Samaniego, L., and Attinger, S.: Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations, Water Resources Research, 49, 360–379, https://doi.org/10.1029/2012WR012195, 2013.

König, S., Weller, U., Betancur-Corredor, B., Lang, B., Reitz, T., Wiesmeier, M., Wollschläger, U., and Vogel, H.-J.: BODIUM—A systemic approach to model the dynamics of soil functions, European Journal of Soil Science, 74, e13 411, https://doi.org/10.1111/ejss.13411, 2023.

470 Molod, A., Takacs, L., Suarez, M., and Bacmeister, J.: Development of the GEOS-5 atmospheric general circulation model: evolution from MERRA to MERRA2, Geoscientific Model Development, 8, 1339–1356, https://doi.org/10.5194/gmd-8-1339-2015, publisher: Copernicus GmbH, 2015.

Samaniego, L., Kumar, R., and Attinger, S.: Multiscale parameter regionalization of a grid-based hydrologic model at the mesoscale, Water Resources Research, 46, https://doi.org/10.1029/2008WR007327, 2010.

475 Shrestha, P., Sulis, M., Masbou, M., Kollet, S., and Simmer, C.: A Scale-Consistent Terrestrial Systems Modeling Platform Based on COSMO, CLM, and ParFlow, Monthly Weather Review, 142, 3466–3483, https://doi.org/10.1175/MWR-D-14-00029.1, publisher: American Meteorological Society Section: Monthly Weather Review, 2014.