



Workshop National Strategy Earth System Modelling 14/15 June 2021, online

<u>Extended Steering Group</u>: Jochem Marotzke (Chair), Sabine Attinger, Joachim Biercamp, Georg Feulner, Sarah Jones, Thomas Jung, Stefan Kollet, Roland Potthast, Markus Rapp, Hauke Schmidt, Michael Schulz, Ina Tegen

Working Document

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Day 1:

Clarifying questions, any topic, such as:

Purpose of software clear and relevant for ESM?

Established or potential range of users and applications clear?

Ownership and institutional support clear?

Software sufficiently mature to be considered for the development of the strategy?

Sufficient level of institutional/developing activity?

Day 2:

Is the software compatible with the criteria agreed upon at the 2019 workshop, or does it show promise to become compatible with reasonable effort in a reasonable time?

Criteria for an ESM system

Our ambition is to create a world-leading, multiscale, seamless Earth system modelling system, usable in research, operational applications, training, and education

That has the following properties:

- Well-defined interfaces between Earth system components
- Allows simulations from global to local
- Exascale-ready
- Scalable work flows
- Portability
- Modularity
- Data assimilation capacity
- Diagnostic capacity
- User friendly and well documented
- Traceability, reproducibility and version control
- Standardization
- Open source

The modelling system considers German expertise, does not exclude international components but avoids dependencies, and has a fit-for-purpose transparent governance structure.





Breakout Groups

The discussions will be held in five breakout groups. The software to be discussed along the guiding questions is assigned as follows.

Please note that some software, marked in red, has a twofold assignment. In this case, please coordinate with your colleagues beforehand to make sure to delegate one person to each group (if possible).

1. Atmosphere; Coupler

Facilitator: Jochem Marotzke Support: Markus Rapp

Name of software to be discussed:

- HAMMOZ (Hamburg Aerosol Module MOZART chemistry model)
- ICON Generalized Interface (GI3)
- ICON (ICOsahedral Nonhydrostatic Modeling Framework)
- ICON-CLM
- MESSy Modular Earth Submodel System
- PALM
- REMO
- Terrestrial Systems Modeling Platform

2. Land surface including vegetation

Facilitator: Stefan Kollet Support: NN

Name of software to be discussed:

- CPlantBox, DuMux-ROSI
- Fastscape
- Golem, Lynx, DwarfElephant
- HD Model (Hydrological Discharge Modell)
- ICON (ICOsahedral Nonhydrostatic Modeling Framework)
- ParFlow
- Terrestrial Systems Modeling Platform

3. Ocean & Cryosphere; Marine Biology and Biochemistry

Facilitator: Sarah Jones Support: Michael Schulz

Name of software to be discussed:

COSIPY





- ECOSMO
- FESOM (Finite-Element/volumE Sea ice-Ocean Model)
- IceSheetModelling
- ICON (ICOsahedral Nonhydrostatic Modeling Framework)
- NEMO (Nucleus for European Modelling of the Ocean)
- REcoM2 (Regulated Ecosystem Model 2)
- SCHISM
- VILMA (Viscoelastic Lithosphere and Mantle Model)
- Wave Model WAM, Cycle 6

4. Infrastructure, Data Assimilation, Diagnostics, Workflows

Facilitator: Hauke Schmidt Support: Joachim Biercamp

Name of software to be discussed:

- DACE (Data Assimilation Coding Environment)
- DKRZsw
- ESMTools
- ESMValTool (Earth System Model Evaluation Tool)
- HeAT
- PDAF (Parallel Data Assimilation Framework)
- SAD wavelets
- Xarray-simlab

5. Impact of climate change and hydrometeorological extremes on different landscape systems

Facilitator: Sabine Attinger Support: NN

Name of software to be discussed:

- Fastscape
- FORMIND/GRASSMIND
- GLUES (Global Land Use and Technological Evolution Simulator)
- HD Model (Hydrological Discharge Modell)
- LPJmL
- mHM mesoscale Hydrologic Model
- MONICA (The Model for Nitrogen and Carbon in Agro-ecosystems)
- OpenGeoSys
- PALM
- RFM (Regional Flood Model)
- SIMPLACE
- SWIM (Soil and Water Integrated Model)
- WaterGAP
- Wave Model WAM, Cycle 6



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Mission

September 2019

The challenges currently posed by global change require a step change in our capability to simulate, predict, and understand the Earth system and its impact on society. Advances in Earth-system modelling (ESM) are fundamentally challenged by the uncertain prospects of future high-performance computing architectures. The German ESM community must establish a new level of sustainable, institutional cooperation to develop the next-generation ESM system, bundling national resources such that scientific and technological developments are accelerated and shared.

Document from January 2019

Towards a National ESM Strategy—Working Groups (Steering Group: Jochem Marotzke, Sarah Jones, Thomas Jung, Michael Schulz, Ina Tegen)

Background

The push toward establishing a national ESM strategy arose as a bottom-up initiative from the research community, in consultation with BMBF/PT-DLR. Germany has a strong and diverse ESM community, with several major ESM developments going on right now (e.g., ICON mainly at DWD and MPI-M, Advanced ESM Capacity within HGF). All ESM efforts worldwide are fundamentally challenged by the uncertain prospects of future HPC architectures. It is hence imperative to bundle resources such that technical developments are shared to the extent possible, while maintaining the scientific and strategic independence of the individual institutions in Germany that are engaged in ESM development and use, each according to its own mission. At the same, Earth system modelling has become a complex endeavour, with world leading expertise for different Earth system model components lying in different institutes and research organisations. In order to provide advanced Earth system modelling capacity ("bringing it all together"), it is imperative that ongoing and planned activities are coordinated.

Again in consultation with BMBF/PT-DLR, a steering committee was formed to provide the stewardship of the process toward an intended national (German) strategy on Earth system modelling (see author list above). There was general agreement that the Deutsches Klima-Konsortium (DKK), of which most institutions active in ESM development are members, should be asked to organise the process. An initial workshop in September 2018, with around 75 participants representing the entire German ESM community, established that working groups should be formed to prepare a second workshop in September 2019. The working groups will be tasked to formulate options in critical areas (see below). This document provides guidance for this (second) phase toward an ESM strategy, by detailing what types of options for which requirements should be developed, and also by suggesting how each working group should be composed.





Guiding principles of an ESM strategy

The strategy must be ESVP:

- 1. **Enabling** the motivation for gathering behind it is built by making life easier through the strategy.
- 2. **Sustainable** the required long-term stewardship of model systems (in the broadest sense) and its sub-systems can be secured only if the steward's legitimate self-interest is aligned with the community task or service expected of the steward.
- 3. **Verifiable** it must be possible to diagnose, after a reasonable time, whether the strategy has succeeded or failed.
- 4. **Pragmatic** whatever is agreed upon must be usable and efficient. Moreover, code options, while offering enhanced flexibility, can create substantial overhead especially when code must be ported to a new architecture, and can hence severely curtail efficiency. Sometimes clear choices must be made, to be re-assessed later.

Working Groups

There was wide agreement among the participants of the kick-off workshop (17./18.9.2018) that three working groups need to be formed that will be tasked to address important open issues in three key areas:

- ESM components and configurations
- Shared modelling infrastructure
- Governance

The working groups are expected to be formed early in 2019 and to meet, separately, during spring 2019. During the meeting each working group should develop options in its area; these options will form the basis for the second plenary workshop in September 2019.

Working group "ESM components and configurations" (Chairs: Georg Feulner, Hauke Schmidt)

Terms of Reference:

- Characterise required components and configurations, guided by concrete ideas of possible overarching applications and classes of experiments.
 - Experience such as the consortium "Millennium" project (Jungclaus et al., *Clim. Past.*, 6, 723-737) has shown that concrete experiments can very effectively guide model development, by focusing on what is required for carrying out the experiment (there: closing the global carbon budget).
- Characterise options for both standard configurations and configurations for frontier simulations
- Develop suggestions for standard configurations:
 - Screening and identification of ESM standard configurations for the global scale (e.g., NWP, CMIP, PMIP, seasonal and decadal prediction including data assimilation) and regional systems including impact models
 - Future development potential (horizon screening) including potential ESM components (e.g., link to "solid" Earth and interface to human dimension)



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- Opportunities to develop novel ESM modules: Assess ongoing and planned model development and identify models/components for further development (e.g., clouds, land surface, ice sheets, hydrology, hydrogeology, air quality, and anthroposphere)
- Which level of model diversity is desirable?
- \circ $\;$ Check practical feasibility for implementation of suggested configurations
- o Potential contributions to European ESM research
- Explore options for ensuring innovation and consolidation cycles in model development
- Develop an overview of candidates of components for standard configurations of ESM (including comparison of components and their pros and cons).
- Suggest an initial starting setup (nucleus), develop a timeline for extensions
- Define and specify performance indicators

Participants

- Core team with fewer than 10 people, plus further members with additional expertise, community needs to be fully represented
- Model developers, persons with technical background (interface/hardware), validation experts, users that need easy access

Working group "Shared modelling infrastructure" (Chairs: Joachim Biercamp, Stefan Kollet)

Terms of Reference:

- Identify technical options for modelling infrastructures that deal efficiently with the expected heterogeneity of HPC infrastructures (e.g., accelerators)
 - For example: DSL, IO, parallelization, pre- and post-processing, scalability, workflow, online diagnostics, visualization
 - Check feasibility of technical options
 - o Maintain focus on adaptability to possible future HPC architechtures
- Explore concepts of modularity
 - Modularity and flexibility vs. performance
 - Flexible interfaces for model components
- Identify requirements for:
 - Choice of programming languages and coding standards
 - Efficiency, stability, flexibility, portability, maintainability, readability and extensibility of ESM code
 - o Software repositories, e.g. git, github, perforce
 - Technical support of standard configurations
 - Module development and incorporation
 - o Infrastructure development and maintenance
 - o User interfaces (including their usability in education and training)
 - Long-term technical user support
 - Model evaluation and benchmarking
 - o Data assimilation, re-analysis and re-forecasts for ESM
- Identify hardware requirements
 - HPC requirements
 - Challenges and risks associated with expected developments



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- Options for embedding the national modelling strategy in the national HPC landscape (including dedicated HPC for ESM vs. multi-purpose HPC systems)
- Data storage and sharing
- Software engineering and numerics

Participation:

- Core team with fewer than 10 people, plus further members with additional expertise
- "Hands-on-people" who do the work, computer scientists, model developers, some people who control budgets

Working group "Governance" (Chairs: Detlev Majewski, Markus Rapp)

Terms of Reference:

- Screen governance of existing model consortia (COSMO, CESM, CLM, EMAC, NEMO, ...)
- Identify governance requirements
 - o Balance between centralized and decentralized decision making
 - Which roles and responsibilities need to be defined?
 - Ensuring quality control
 - Decisions on standard configurations
 - Which components make it into the modelling system?
- Develop governance options
 - How could it be structured (steering committee, SAB, representation of operational agencies, lab directors, funding agencies, ...?)
 - Who needs to be involved and at which level? For example: Key users, BMBF, science organizations (MPG, HGF, Leibniz, DFG), federal states, BMVI, BMWi, BMU, universities)
 - Which commitments are necessary to enable a sustainable structure (e.g. with regard to [tentative] financial and personnel resources)
 - Options to ensure freedom to pursue model developments (e.g. at institutional level) without interfering with other groups (branch/fork strategies)
 - Consider code ownership and IPRs of national ESM
 - Consider licensing of national ESM for different purposes, e.g. non-commercial research, official duty, commercial activities

Participation:

- Core team with fewer than 10 people, plus further members with additional expertise
- Propositions bottom-up, from those who will be governed; they should suggest a structure that would serve them best
- Propositions top-down, from those who decide on how much base funding goes into which activity; they should suggest a structure that would serve them best
- At a later stage: Include high-level stakeholders from funding bodies