Waveform Relaxation for Coupled Environmental Problems

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Contents

List of Publications

This report is based on the following publications:

I **Convergence Properties of Iteratively Coupled Surface-Subsurface Models**
V. Schüller, P. Birken, A. Dedner
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II **Quantifying Coupling Errors in Atmosphere-Ocean-Sea Ice Models: A Study of Iterative and Non-Iterative Approaches in the EC-Earth AOSCM**
V. Schüller, F. Lemarié, P. Birken, E. Blayo
Submitted to Geosci. Model Dev., under review.

III **Analysis of Bulk Interface Conditions for Atmosphere-Ice-Ocean Coupling**
V. Schüller, P. Birken, H. Kjellson
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Author Contributions

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I: Convergence Properties of Iteratively Coupled Surface-Subsurface Models

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II: Quantifying Coupling Errors in Atmosphere-Ocean-Sea Ice Models: A Study of Iterative and Non-Iterative Approaches in the EC-Earth AOSCM

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III: Analysis of Bulk Interface Conditions for Atmosphere-Ice-Ocean Coupling

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Waveform Relaxation for Coupled Environmental Problems

1 Introduction

The interaction of different components in the Earth system is at the heart of many open research questions in environmental and climate science. In these disciplines, simulations are a central tool to improve understanding and guide decision-making. We consider two exemplary applications, namely surface-subsurface flow for hydrological simulations and atmosphere-ice-ocean coupling in climate models.

The underlying physical processes in these applications are typically modeled with nonlinear, time-dependent partial differential equations (PDEs). It is common to use separate codes for distinctly modeled physics components, which are *coupled* to determine the evolution of the full system.

This thesis project aims to analyze the mathematical properties of currently used coupling algorithms and how they affect the numerical solutions produced by the resulting codes. Ultimately, the goal is to develop new algorithms that reduce numerical errors while being energy-efficient.

The starting point for the analysis is the framework of domain decomposition. We assume that the system state is governed by a set of PDEs

$$\begin{aligned} \partial_t U(t,\boldsymbol{x}) &= \mathcal{L}U(t,\boldsymbol{x}) \quad \text{on } (0,\mathcal{T}] \times \Omega, \\ \mathcal{B}U(t,\boldsymbol{x}) &= g(t,\boldsymbol{x}) \quad \text{on } (0,\mathcal{T}] \times \partial\Omega, \\ U(0,\boldsymbol{x}) &= \varphi(\boldsymbol{x}) \quad \text{on } \Omega, \end{aligned} \tag{1}$$

where $U(t,\boldsymbol{x})$ is a set of prognostic variables, $\mathcal{L}, \mathcal{B}$ are differential operators acting on the interior and boundary of the domain, and g, φ describe the boundary and initial conditions.

Instead of solving this problem on the full spatial domain Ω, one instead considers disjoint subdomains Ω_1, Ω_2, with $\Omega_1 \cup \Omega_2 = \Omega$. The subdomains are coupled at the lower-dimensional interface Γ; see Figure 1a for a depiction of this setup. One can now solve (1) with an iterative method: Starting with an initial guess U_2^0, solve in each step $k = 1, 2, \ldots$

$$
\begin{aligned}
\partial_t U_1^k &= \mathcal{L}_1 U_1^k \quad \text{on } (0, \mathcal{T}] \times \Omega_1, \\
\mathcal{B}_1 U_1^k(t, \boldsymbol{x}) &= g_1(t, \boldsymbol{x}) \quad \text{on } (0, \mathcal{T}] \times \partial\Omega_1 \setminus \Gamma, \\
U_1^k(0, \boldsymbol{x}) &= \varphi_1(\boldsymbol{x}) \quad \text{on } \Omega_1, \\
\mathcal{C}_{11} U_1^k(t, \boldsymbol{x}) &= \mathcal{C}_{12} U_2^{k-1}(t, \boldsymbol{x}) \quad \text{on } (0, \mathcal{T}] \times \Gamma,
\end{aligned}
\tag{2a}
$$

followed by

$$
\begin{aligned}
\partial_t U_2^k &= \mathcal{L}_2 U_2^k \quad \text{on } (0, \mathcal{T}] \times \Omega_2, \\
\mathcal{B}_2 U_2^k(t, \boldsymbol{x}) &= g_2(t, \boldsymbol{x}) \quad \text{on } (0, \mathcal{T}] \times \partial\Omega_2 \setminus \Gamma, \\
U_2^k(0, \boldsymbol{x}) &= \varphi_2(\boldsymbol{x}) \quad \text{on } \Omega_2, \\
\mathcal{C}_{22} U_2^k(t, \boldsymbol{x}) &= \mathcal{C}_{21} U_1^k(t, \boldsymbol{x}) \quad \text{on } (0, \mathcal{T}] \times \Gamma.
\end{aligned}
\tag{2b}
$$

The partial differential operators $\mathcal{C}_{ij}, i, j \in \{1, 2\}$ specify the interface boundary conditions to couple the two subdomains. For time-dependent systems, this iterative solution approach is referred to as (Schwarz) waveform relaxation (WR).

Splitting the problem into subdomains can simplify modeling (e.g., if material properties change significantly on Ω), algorithm development (e.g., if one solves problems on complex geometries), and parallel efficiency. For the coupled problems we study, the boundaries between subdomains align with changes in physical modeling; $\mathcal{L}_1$ and $\mathcal{L}_2$ differ due to distinct material properties, physical and chemical processes, and modeling assumptions.

The thesis project has so far resulted in three publications. This report positions these articles relative to the overall research aims, but also relative to each other. It is structured around the main pillars of our methodological approach: Considering how the applications fit into the domain decomposition and WR framework in Section 2, we develop and analyze simplified models which capture the dominating processes of the corresponding coupling iteration (Section 3). The analysis is not considered in isolation, but in relation to numerical results obtained with nonlinear, production(-like) codes, presented in Section 4. These three sections treat the two applications separately and point to the relevant sections of Papers I–III. The report concludes with a brief overview of three subprojects planned for the second half of the thesis project.

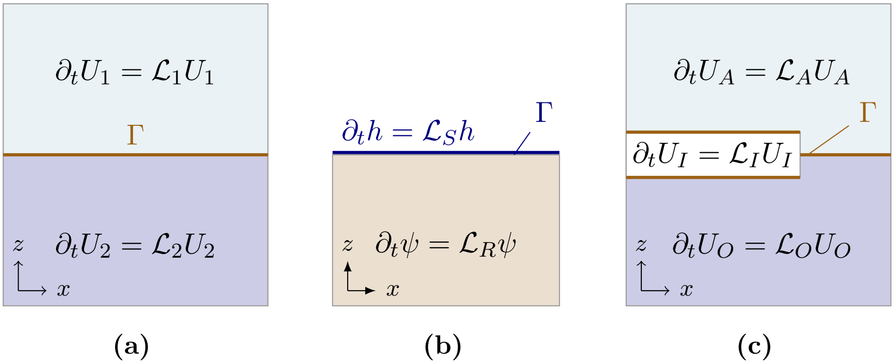

Figure 1: We consider surface-subsurface hydrology (b) and atmosphere-ice-ocean coupling (c) as special cases of the general domain decomposition setting (a).

2 Application Overview

This section gives a short introduction into the two applications under study, surface-subsurface hydrology and atmosphere-ice-ocean coupling. The aim is to illustrate how they, from a modeling and algorithmic perspective, fit into the (abstract) domain decomposition and WR framework from the introduction.

2.1 Surface-Subsurface Hydrology

We begin with simulations of the terrestrial water cycle, water management, and flooding, which are based on the dynamics of surface-subsurface flow. A typical coupled model for these combines two sets of nonlinear PDEs: the d-dimensional Richards equation and the $d-1$-dimensional shallow water equations (SWE). The former describes flow in a variably saturated porous medium (the soil) and the latter model a hydrostatic fluid moving on the upper surface of the domain. Figure 1b shows this as an example of a domain decomposition problem.

We consider the case where one uses separate solvers with potentially different discretizations for the two components, cf. [6, 17]. They interact by prescribing boundary conditions for each other: The SWE supply the water height $h(t)$ as a Dirichlet condition for the capillary head $\psi(t, \boldsymbol{x})$, and the Richards equation provides a surface flux which acts as a source term in the SWE. This exchange is performed in an iterative manner each solver time step.

The fully continuous iteration (2) takes the following form for this application: Given an initial guess for the water height $h^0(t)$ of the surface flow, in each iteration $k = 1, 2, \ldots$ solve the Richards equation in 2D

$$\begin{aligned} c(\psi^k)\partial_t\psi^k + \nabla \cdot \underbrace{\left(-K(\psi^k)\nabla(\psi^k + z)\right)}_{=:\boldsymbol{v}(\psi^k)} &= 0 \quad \text{on } (0, \mathcal{T}] \times \Omega, \\ \psi^k(0, \boldsymbol{x}) &= \psi_0(\boldsymbol{x}) \quad \text{on } \Omega, \\ \boldsymbol{v}(\psi^k(t, \boldsymbol{x})) \cdot \boldsymbol{n} &= 0 \quad \text{on } [0, \mathcal{T}] \times \partial\Omega \setminus \Gamma, \\ \psi^k(t, \boldsymbol{x}) &= h^{k-1}(t, x) \quad \text{on } [0, \mathcal{T}] \times \Gamma, \end{aligned} \tag{3a}$$

followed by the SWE on $\Gamma = [0, L_x]$

$$\begin{aligned} \partial_t h^k + \partial_x \left(h^k u(h^k)\right) &= r(t, x) + \left(\boldsymbol{v}(\psi^k) \cdot \boldsymbol{n}\right)\Big|_\Gamma \quad \text{on } (0, \mathcal{T}] \times \Gamma, \\ h^k(0, x) &= h_0(x) \quad \text{on } \Gamma, \\ \partial_x h^k(t, 0) = \partial_x h^k(t, L_x) &= 0 \quad \text{on } [0, \mathcal{T}], \end{aligned} \tag{3b}$$

with initial conditions ψ_0, h_0 and homogeneous Neumann conditions on the outer boundary $\partial\Omega \setminus \Gamma$. The hydraulic capacity c and conductivity K in the Richards equation depend on ψ via empirical, highly nonlinear, constitutive relations.

For the SWE we give a reduced form here, stating only the PDE for the water height $h(t, x)$. The flow speed u is either found from a separate PDE (standard SWE) or via Manning's equation (kinematic wave approximation). In both cases, it depends on h. Source terms entering the SWE are the inflow r from above due to rainfall and the surface volumetric flux $\boldsymbol{v}(\psi) \cdot \boldsymbol{n}$ from the Richards equation, where $\boldsymbol{n}$ is the outward pointing unit normal vector.

2.2 Atmosphere-Ice-Ocean Coupling

Earth system models (ESMs) are a prime example of a coupled problem solved using separate codes: We particularly consider the atmosphere-ice-ocean system as a coupled problem with three components, solving different nonlinear systems of PDEs. Atmosphere and ocean codes discretize the so-called primitive equations, which describe the flow of a shallow fluid on a rotating sphere. Modeling assumptions, computational grids, and numerical algorithms differ significantly, which is why one uses separate codes. They are coupled at the sea surface using nonlinear boundary conditions. Sea ice enters this coupled system by covering a fraction of the sea surface and thus affecting the boundary conditions for the atmosphere and ocean components; cf. Figure 1c.

To make long-term climate simulations with ESMs feasible, the governing equations are generally discretized on coarse grids with large time step sizes. In fact, the low resolution affects the modeling assumptions themselves: Physical processes on scales finer than the computational grid are not resolved, but their effect on large-scale flow is approximated using empirical *physics parameterization schemes*. In particular, the interface boundary condition operators $\mathcal{C}_{ij}$ in atmosphere-ocean coupling are part of the purely vertical turbulence and radiation schemes which differ between ESMs. In Paper II (§2), we provided a thorough overview of the coupling boundary conditions for the single column version of the EC-Earth General Circulation Model (GCM) [4], the EC-Earth AOSCM [9]. The AOSCM uses the same coupling setup and physics parameterizations as the EC-Earth GCM, while being computationally cheap to run.

State-of-the-art ESM coupling algorithms are WR procedures, stopped after one iteration [14] to save computational resources. Not iterating further introduces a numerical coupling error in time. Component models exchange data at coupling time steps which are typically 1 h to 1 d long. In between, they can take smaller model time steps, referred to as a multirate setting [13]. The coupling data exchanged at a coupling time step is then time-averaged over the model time steps.

3 Convergence Analysis of Simplified Models

A natural question to ask about a coupling iteration (2) is whether, and how quickly, the solution in iteration k

$$U^k(t, \boldsymbol{x}) = \begin{cases} U_1^k(t, \boldsymbol{x}), & \text{on } (0, \mathcal{T}] \times \Omega_1, \\ U_2^k(t, \boldsymbol{x}), & \text{on } (0, \mathcal{T}] \times \Omega_2, \end{cases}$$

approaches the solution of the underlying problem (1), i.e., $U(t, \boldsymbol{x})$. In other words, one is interested in the *coupling error*

$$e^k(t, \boldsymbol{x}) := \left| U^k - U \right|, \tag{4}$$

and the *convergence factor*

$$\varrho^k(t) := \frac{\|e^k(t, \boldsymbol{x})\|}{\|e^{k-1}(t, \boldsymbol{x})\|}. \tag{5}$$

To analyze these for the nonlinear applications, we use simplified models which capture the essence of the coupling iteration. The dominating coupling mechanism in both examples can, under simplifying assumptions, be considered as one-dimensional coupled heat equations with discontinuous material parameters. This link is explained in Paper I (§4) and Paper III.

There is an existing body of literature on coupled heat equations, with analysis techniques for fully continuous [7], discrete in time [10], discrete in space [12],

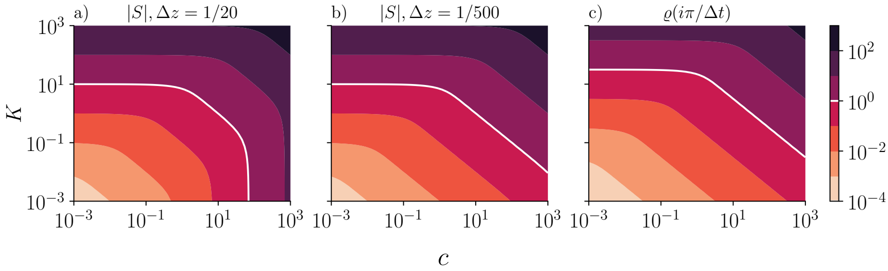

Figure 2: Linear analysis results for $\Delta t = 10^{-1}$ and varying material parameters. The discrete convergence factor $|S|$ is given for two different grid sizes Δz.

or fully discrete [18] WR. These allow to obtain analytical estimates for the convergence factor of the nonlinear higher-dimensional coupling iterations. Results depend on the material parameters and, in the (semi-)discrete cases, on the chosen discretization. It turns out that both applications yield non-standard versions of coupled heat equation problems studied previously. This lead to new analysis results, briefly summarized in this section.

3.1 Surface-Subsurface Hydrology

We consider a single column of the coupled system, assuming that the convergence behavior of the iterations is driven by vertical processes. In Paper I (§4), we introduce a linearized, one-dimensional model to study the coupling iteration (3). It reduces to a one-dimensional heat equation, coupled to an ordinary differential equation. We use techniques from [7, 18] to obtain convergence factors for the continuous and fully discretized version of this idealized model.

The continuous analysis we provide assumes $\mathcal{T} \to \infty$ and uses the Laplace transform to obtain a linear, iteration-independent convergence factor $\varrho(\tau)$ that depends on the Laplace variable $\tau \in \mathbb{C}$. For the fully discrete analysis, we used linear finite elements in space and the implicit Euler method in time. One obtains a linear iteration for the unknowns at the interface Γ at time $t^n = n\Delta t$ and iteration k. This reduces to a scalar equation with a fully discrete convergence factor $|S|$; cf. Eq. (30) in the paper. We validate in the paper that the discrete factor correctly captures the convergence behavior in a numerical implementation of the same model.

Figure 2 compares the analysis results for varying material parameters c, K and two different grid sizes Δz. The expression we obtain from the fully continuous analysis, Eq. (20) in the paper, is simpler to interpret and, as expected, represents a qualitative limit of $|S|$ for $\Delta z \to 0$. For coarse discretizations, the continuous result is a worse estimate.

3.2 Atmosphere-Ice-Ocean Coupling

In its simplest form, the atmosphere-ice-ocean problem reduces to two one-dimensional coupled heat equations with discontinuous material parameters [2]. However, the coarse resolution of ESMs directly affects the underlying modeling assumptions and yields nonstandard boundary conditions, so-called bulk interface conditions [5]: One requires (a) that the flux across the air-sea interface is continuous, to guarantee energy conservation, and (b) that the magnitude of the flux is proportional to the difference in (near-)surface temperatures. The temperature discontinuity is due to the fact that the turbulent surface layers at the interface are unresolved in ESMs. Another result of the low resolution is that one models the horizontal extent of sea ice with a *virtual* ice area fraction which affects the interface boundary conditions seen by the atmosphere and ocean.

Since bulk interface conditions are specific to ESMs, there are fewer results. In terms of convergence analysis for this problem, Clément [2, §6.B] studied a simplified, discrete-in-space atmosphere-ocean model, focusing on vertical momentum transfer. Lozano [15] derived the convergence factor of a coupling iteration for an atmosphere–sea ice toy model. However, neither of these models reflects the partial sea ice cover typical in climate models.

We recently contributed to this area with Paper III, wherein we propose a simplified model for thermodynamic atmosphere-ice-ocean coupling. We use a Fourier-based analysis technique, similar to the continuous analysis in Paper I, to obtain convergence factor estimates. These differ from results obtained for standard conjugate heat transfer problems.

We compare our analysis results to a numerical implementation of the *simplified* model using an open-source coupling software for climate applications, ClimaCoupler.jl. As we show in the paper, much of the numerically observed convergence behavior can be explained from the continuous estimate. However, the continuous factor tends to overestimate numerically observed convergence factors, most striking for ice-free conditions. The difference gets smaller for smaller time steps and grid sizes $\Delta t, \Delta z \to 0$, suggesting that it is related to the coarse discretization typical in climate models.

4 Realistic Nonlinear Models

Ultimately, it is the aim of this research to link the linear analysis results from the previous section to the original, nonlinear problems and "real-world" codes introduced in Section 2. This joint consideration allows reaching conclusions that are directly interpretable for model developers. Furthermore, it is the basis for developing novel, useful, energy-efficient algorithms which reduce numerical errors. This section illustrates how Papers I and II contribute here.

4.1 Surface-Subsurface Hydrology

In Paper I, we investigated how well the discrete analysis result explains the numerical convergence behavior of the 2D-1D nonlinear coupling iteration (3). To this end, we worked with a partitioned code base solving the discrete nonlinear problem given in §3 of the paper: the Richards equation is discretized with linear finite elements and the SWE with the finite volume method. Both solvers use the implicit Euler method in time and are coupled every time step. We used the PDE software framework DUNE-FEM [3] for the subsolvers and the preCICE library [1] for coupling.

Numerical experiments for realistic materials confirm that iteration convergence is indeed mainly driven by vertical processes and resolution in the Richards equation, as we assumed in the linear analysis. The analysis result naturally fails to represent processes which are not part of the linear model (e.g., the effect of external source terms); cf. Figure 3. There were also some unexpected differences in the dependence of the observed convergence factor on time step and vertical grid size.

The observed convergence factors in the nonlinear code did not exceed 10^{-3} for typical simulation parameters. The linear analysis is able to explain the fast convergence, as well as how dynamically changing material properties during a simulation affect the speed of convergence. Overall, our research here shows why the iteration (3) terminates quickly when coupling surface-subsurface hydrology codes every model time step.

4.2 Atmosphere-Ice-Ocean Coupling

While partitioned surface-subsurface hydrology codes already use multiple iteration steps to solve the underlying coupled problem, this is not the case in climate models. Since it is uncommon to test multiple iterations during code development, it is not even clear that the coupling iteration (2) would converge for a given ESM. If it does converge, one can use WR to estimate the error that is introduced with standard algorithms. Thus, there is a place for WR studies in the climate model development context: (a) to test whether physics parameterizations in the model components are "compatible" [8], and (b) to investigate the coupling error (4) of standard coupling algorithms [16].

In Paper II, we contribute to both aspects with an in-depth study of the EC-Earth AOSCM. We implemented a non-intrusive WR method in this model, tested whether WR converges in ice-free and ice-covered conditions, and estimated the numerical coupling error of multi-day simulations.

In the absence of sea ice, WR convergence is robust and coupling errors for atmospheric variables can be substantial. When sea ice is present, WR lead to large-amplitude oscillations in old versions of the AOSCM, making coupling

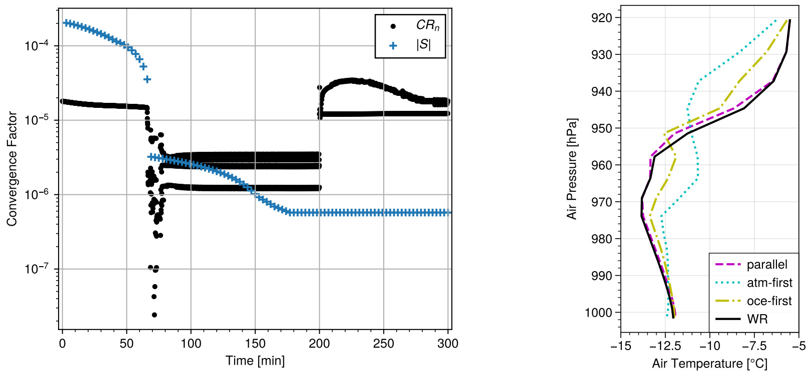

Figure 3: Left: Observed vs. predicted convergence factors for surface-subsurface hydrology simulations (cf. Paper I, Fig. 10). Right: Standard ESM coupling methods vs. WR in the EC-Earth AOSCM at $\mathcal{T} = 48\,\mathrm{h}$ (cf. Paper II, Fig. 12).

error estimation impossible. This was improved in the latest version of the EC-Earth AOSCM; here we find that coupling errors in sea ice surface and atmospheric boundary layer temperature are often large, cf. Figure 3. Generally, we found that abrupt transitions between distinct physical regimes in certain parameterizations can lead to substantial coupling errors and even non-convergence of the iteration. Particularly, we were able to attribute discontinuities in the computation of atmospheric vertical turbulence and sea ice albedo as sources for these problems.

5 Planned Work

The large coupling errors we observed in the EC-Earth AOSCM in Paper II suggest that there is a need for energy-efficient coupling algorithm improvement in atmosphere-ice-ocean coupling. The remainder of the PhD builds on this topic in three subprojects, briefly introduced below.

5.1 Reliable WR Convergence Rate Estimates

We have done some foundational work to define a continuous coupling iteration for thermodynamical atmosphere-ice-ocean coupling which we analyzed and compared to an implementation in `ClimaCoupler.jl` in Paper III. A first set of experiments with the EC-Earth AOSCM has shown that the convergence factor seen in practice is lower and seems to vary in different physical conditions. In this project, we aim to refine the model and our analysis in order to find a reliable estimator for the convergence rate seen in EC-Earth. Missing pieces in the existing analysis are, in particular, the impact of the specific numerical setup used in ESMs: coarse discretization in time and space, as well as exchanging time-*averaged* coupling variables. Furthermore, the toy model from Paper III neglects some physical processes in sea ice which might affect results (e.g., albedo feedback, lateral ice growth, and nonlinear vertical gradients).

5.2 Non-Invasive Coupling Error Reduction in EC-Earth

We want to use our WR implementation in the EC-Earth AOSCM to improve the coupling setup in the EC-Earth GCM in an energy-efficient manner. Potential solutions here will be: (a) running two iterations with a single relaxation step, (b) adding a correction step based on past interface data, or (c) changing the boundary conditions used in the model components. The project will include the following aspects for these methods:

1. evaluation of what is feasible to implement in practice;
2. evaluation of the potential coupling error reduction, using the model and code from Paper III;
3. implementation tests with the EC-Earth AOSCM from Paper II;
4. suitable numerical experiments with the EC-Earth GCM to prove relevance of our methods, while being energy-aware (e.g., picking sufficient resolution, simulation time, and precision).

5.3 An Energy Efficiency Perspective on Coupled Models

There has been a push for energy awareness in high performance computing (HPC) and numerical method development [11]. This requires users to know about power consumption of their codes and how they can affect it without compromising on accurate results. Climate simulations are energy-intensive coupled simulations, affected by static and dynamic load imbalances both *in* and *between* the components [19]. In this project, we particularly investigate whether dynamic frequency and voltage scaling (DVFS) is a viable method to reduce energy use for coupled simulations with dynamic load imbalance.

We plan to run small-scale simulations solving the Laplace equation on the Karolina cluster. The aim is to systematically study how energy efficiency can be affected with MERIC [20], which allows changing CPU frequency and voltage at runtime. We will furthermore use energy measurements in subproject 2 above to understand energy use and dynamic load imbalances in EC-Earth simulations. This will allow us to estimate whether DVFS is a suitable tool for real-world HPC use cases.

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