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Coupling stochastic optimization with agent-based simulation: A framework for efficient power expansion planning under uncertainty

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ABSTRACT

Policymakers today face many, interrelated uncertainties. In addition, they have to strike a balance between efficiency, cost-effectiveness, and overarching social objectives. Addressing these problems requires a coupling of several approaches. Thus, we model the power generation expansion planning (PGEP) problem as a combined simulation-optimization problem. Since agent-based simulations (ABM) are able to effectively represent markets, we formulate the PGEP as a multi-stage multi-scale mixed-integer linear optimization problem, where the results of the ABM are integrated into a stochastic optimization model using affine cuts. First, we propose a double decomposition framework combining Benders decomposition and stochastic dual dynamic programming (SDDP) algorithms to solve the PGEP problem. Second, we couple the stochastic optimization model with an agent-based electricity market simulation (AMIRIS) to evaluate power portfolio decisions from a market perspective. We discuss the process of extracting dual values from agent-based simulations with the goal of calculating optimality cuts for the Benders decomposition, to incorporate the simulation results into the optimization model. In particular, we investigate three coupling strategies connecting the optimization and AMIRIS models. Our results show that integrated simulation-optimization approaches yield superior portfolio decisions using both centralized and decentralized operations. Furthermore, they combine recourse and wait-and-see solutions, enhancing resilience against uncertainties.

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1. Introduction

Renewable energy sources are an essential component of most power systems and have been thoroughly assessed for long-term power expansion planning. Studies have analyzed integrating renewable technologies by using energy storage systems and for complementing them with conventional technologies (Parker et al., 2019). With the rising penetration of renewable sources, the need for expansion planning models with high temporal and spatial resolutions and long-term planning horizons has increased significantly. Such models are typically of massive size, posing challenges in solving these models. However, many uncertainties, e.g., due to price changes and weather-dependent production, have to be integrated into modeling. Given the inherent computational burden from discrete characteristics and high time-resolution requirements, the stochastic nature of the PGEP increases computational complexity. Using advanced decomposition algorithms is one solution used in this paper and elsewhere to handle these computational complexities.

Yet, the profit-maximizing behavior of actors also has to be considered. Agent-based simulations are a particularly effective tools for that, analyzing the effects of different market designs. Furthermore, their computational performance can be considered a competitive advantage for large-scale problems. There is some research in the literature focusing on the coupling of several short-term and long-term decisions, including the use of optimization models within agent-based simulations (Tao et al., 2021). This paper couples a stochastic optimization model with an ABM to be able to address both the uncertainties of expansion planning and market-oriented behavior of actors at the electricity markets. Combining modeling approaches addresses structural weaknesses inherent in relying solely on a single modeling method. However, integrating models is challenging for several reasons: First, different models often operate on distinct spatial and temporal scales. Second, the underlying assumptions of the approaches differ. Third, ensuring convergence to a stable system state poses a significant challenge. Even with meticulous calibration, coupled models may diverge into incompatible system states. Given these problems, we design a framework for model coupling ensuring convergence. In addition, we examine coupling strategies to determine long-term power portfolio decisions. We are

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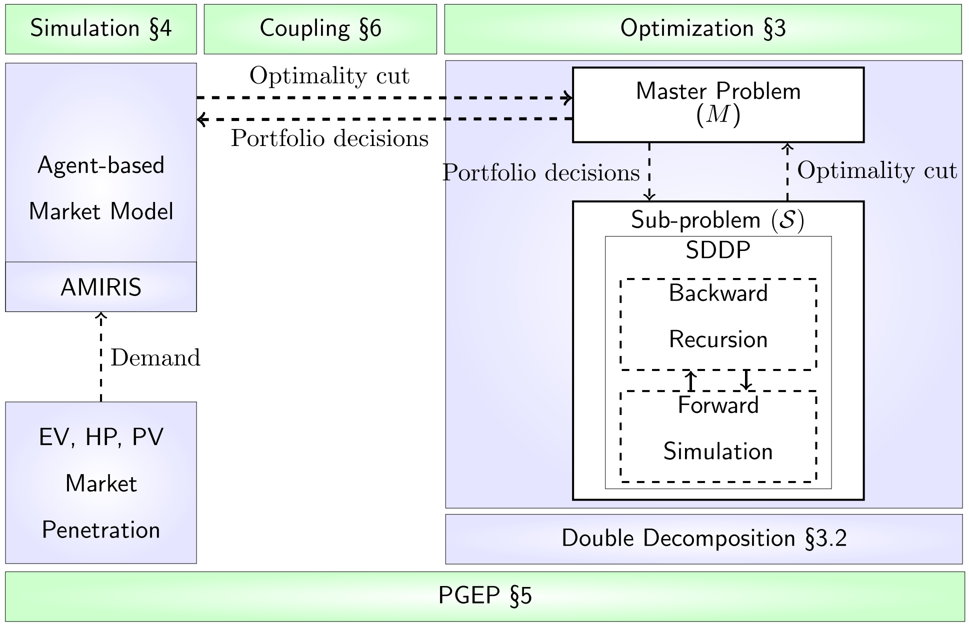


Figure 1. A framework for power expansion planning.

not aware of any research that couples decomposition algorithms with agent-based simulations for PGEP problems.

The primary research question in this study is focused on the PGEP framework for the development of conventional and renewable power plant capacities under multiple uncertainties. Evaluating both centralized and market-based frameworks enables policymakers to establish a balance between efficiency, cost-effectiveness, and social objectives when planning long-term power expansion. While a market-based structure can increase efficiency through competition, a centralized structure is required to achieve greater social goals (e.g., power sustainability). Thus, we address the effects of uncertainties, the long planning horizon with an hourly time resolution, the centralized economic dispatch decisions and market clearing operations, all of which result in complicated interactions for power portfolio decisions. This paper addresses multiple uncertainties, with a particular focus on political, economic, and socio-economic uncertainties in the context of our case study. These include fuel and CO_2 prices, influenced by political and economic factors, as well as demand, shaped by the market penetration of emerging technologies, as discussed in Section 7. Given such multiple uncertainties and operational constraints, our aim is to determine a long-term power expansion planning by minimizing total costs, including investment and operational costs. Thus, we model a dynamic PGEP problem under multiple uncertainties, taking both optimization and simulation into account (Figure 1). Importantly, since dual values are not generated directly from the agent-based simulation, this study demonstrates how to extract dual information from a non-LP-based simulation model and incorporate them through affine cuts. In this way, we couple the optimization model with an agent-based electricity market simulation (AMIRIS) to solve the PGEP problem by evaluating power portfolio decisions through both centralized and electricity market operations, and to employ both recourse and wait-and-see approaches for addressing uncertainty.

The unique contributions of this paper are:

1. We model the PGEP problem under uncertainty as a combined simulation-optimization problem with a long planning horizon and an hourly time resolution to evaluate both centralized and market-based frameworks. In particular, we explain the process of obtaining dual values from an agent-based simulation to be used in the coupling process.
2. For the optimization approach, we propose a double decomposition framework to combine Benders decomposition and Stochastic Dual Dynamic Programming (SDDP). To connect the optimization and simulation models, we examine three strategies that incorporate the results of the agent-based simulation into the optimization model by using affine cuts.
3. We present a case study of the German power system, discussing the performance of coupling strategies. This integration of models yields accurate, plausible and robust results, allowing policymakers to analyze both centralized and market-based factors in future energy systems while considering multiple uncertainties.

The remainder of the paper is organized as follows: In the next section, we review the related literature. In Section 3, we introduce the standard problem formulation and the double decomposition framework. In Section 4, we discuss AMIRIS. We outline the coupling of the optimization model with AMIRIS in Section 5. The coupling strategies are presented in Section 6. The case study of the German power system is presented in Section 7. Lastly, Section 8 emphasizes key directions and concludes the paper.

2. Literature review

The power expansion planning is a core problem in power systems optimization that has been extensively researched; a substantial and increasing body of literature exists. We evaluate the literature on four key research streams that are important for our context: power expansion planning, decomposition methods, agent-based simulation and model coupling.

Starting in the 1990s, operational and system limitations have appeared in PGEP problem formulations; environmental constraints (Ishfaq et al., 2016; Rebennack, 2014), the utilization of renewable sources (Zhan & Zheng, 2018), incorporating unit commitment and economic dispatch problems (Lara et al., 2018) have been commonly studied in the literature. It is now necessary to address operational constraints in PGEP problems. To consider operational constraints, many studies in the literature utilize an hourly resolution; however, they generally apply it to representative time periods rather than throughout the complete planning horizon (Kaya et al., 2026). Thus, representative time periods (Lara et al., 2018; Yagi & Sioshansi, 2024) are typically used to simplify the computational process. However, Merrick (2016) investigated how representations can disregard technological capabilities in PGEP models. It is worth mentioning that the full hourly time resolution allows for capturing system dynamics, while representative time periods can only capture certain aspects. In this paper, we model hourly time resolution across a full planning horizon to consider all system dynamics. On the other hand, the objective function of the PGEP problem switched from cost minimization to profit maximization with the shift from a centralized to a decentralized power market structure. Thus, the market clearing mechanism has been considered in the PGEP problem (Lohmann & Rebennack, 2017). Equilibrium problems with equilibrium constraints (EPEC) and mathematical program with equilibrium constraints (MPEC) have been employed to solve the market-based PGEP problem (Baringo & Conejo, 2012).

Integrating discrete decision and uncertainties into power generation expansion planning coupled with an hourly time resolutions results in gigantic stochastic mixed-integer (linear) optimization models. For practical applications, such models cannot be solved monolithically by the current state-of-the-art MI(L)P solvers. To account for the uncertainty in power expansion planning, stochastic dynamic programming (Mo et al., 1991), bundle methods (Sagastizábal & Solodov, 2012), robust optimization (Dehghan et al., 2014), fuzzy logic (Aghaei et al., 2012) and multi-stage adaptive robust optimization (Abdin et al., 2022) have been used. Decomposition algorithms were mainly utilized in the literature for solving power expansion planning problems, where Benders decomposition is a natural choice. It separates the original problem into a master problem and a sub-problem (Sudermann-Merx et al., 2021). The master problem represents the investment problem, whereas the sub-problem refers to the operational decisions used to assess trial investment decisions. In addition to the standard Benders decomposition (Benders, 1962), several extensions have been proposed for multi-stage problems such as nested Benders decomposition (Birge, 1985) and nonconvex nested Benders decomposition (Füllner & Rebennack, 2022). Nested Benders Decomposition (NBD), presented by Birge (1985), iteratively applies Benders decomposition on nested two-stage problems. NBD carefully generates optimality and feasibility cuts to ensure a finite convergence to an optimal solution, if the algorithmic strategy is chosen carefully, especially with respect to the feasibility cuts. Stochasticity is considered through its deterministic equivalent. As such, NBD faces a "curse-of-dimensionality". In an effort to overcome this curse, Pereira and Pinto (1991) proposed a sampling-based version of NBD, namely the Stochastic Dual Dynamic Programming (SDDP) algorithm. In SDDP, sample path(s) of the scenario tree are sampled independently to generate the optimization problem to be solved with NBD. Through the update of the sampled path(s) within the algorithm, a statistical convergence can be achieved. The stochastic dual dynamic integer program (SDDiP), which was developed to handle integer recourse decisions (Zou et al., 2019), has been applied to solve a power expansion planning problem (Lara et al., 2020). Benders decomposition was used in Gorenstin et al. (1993) to solve a two-stage stochastic planning problem. Sub-problems were tackled using an earlier SDDP methodology. In Rebennack (2014), Benders decomposition is employed to address the hydrothermal expansion planning problem. The sub-problems are multi-stage stochastic linear optimization problems handled using SDDP. In this study, we combine Benders decomposition with SDDP as a double decomposition method, like in Rebennack (2014). However, an important aspect of this paper is coupling the optimization model with a non-LP-based simulation model using the decomposition technique. In particular, we explain how to extract dual information from a non-LP-based simulation model and apply coupling strategies. Here, we integrate the feedback of AMIRIS through affine cuts, interpreting the results of the simulation as an additional value function for the double decomposition algorithm. Thus, we evaluate power portfolio decisions from a policymaker's perspective using both centralized and market-based operations.

When examining electricity markets, factors such as market power, renewable technologies, and market regulations need to be taken into account. Agent-based modeling is particularly well suited to analyze the heterogeneous preferences of actors (Frey et al., 2020) and to check optimization models for the realizability of solutions in an economic sense. Particularly, the question is answered whether actors are really able to refinance themselves, given optimal system solutions. Agent-based modeling is also able to host various modeling paradigms (Klein et al., 2019) and is thus well suited for coupling (Axelrod, 2006). A number of agent-based models have been proposed in the literature to evaluate short-term power market operations and investment decisions such as PowerACE (Genoese et al., 2005), EMCAS (Botterud et al., 2007) and AMIRIS. We use AMIRIS (acronym for Agent-Based Market Model for the Investigation of Renewable and Integrated Energy Systems) as a simulation tool for electricity markets (Deissenroth et al., 2017; Schimeczek et al., 2023) to inform the optimization model of our PGEP problem. Its code base is openly available (Schimeczek et al., 2023). There have been several studies on power expansion planning that integrate agent-based simulation with optimization models. Genoese et al. (2005) utilize a linear program in an investment agent to determine expansion decisions. Tao et al. (2021) employ an optimization model as part of the simulation to obtain the price projection.

3. Optimization model

This section explains the optimization model using a standard and compact formulation. We also present a double decomposition framework to solve the proposed model. Note that the results of an agent-based simulation are integrated into this formulation in Section 5.

3.1. Problem formulation

We model power portfolio decisions through integer variables and the operational decisions through continuous variables. Since we also consider stochastic uncertainty, this yields a multi-stage stochastic mixed-integer linear optimization problem of the following form:

$$(P) z^* := \min \quad \sum_{t=1}^{T}\sum_{i=1}^{I} C_{it}^{\top} x_{it} + \mathbb{E}\left[\sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} G_{iht}^{\top} y_{iht}\right] \tag{1}$$

$$\text{s.t.} \quad \sum_{i=1}^{I} y_{iht} - \sum_{i=1}^{I} e_{iht} + \sum_{i=1}^{I} f_{iht} = D_{ht} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \tag{2}$$

$$b_{i(h-1)t} + A_{iht} e_{iht} - B_{iht} f_{iht} = b_{iht} \quad \forall t \in \mathcal{T}, \forall h \in \mathcal{H} : h > 1, \forall i \in \mathbb{I}, \tag{3}$$

$$b_{iH(t-1)} + A_{i1t} e_{i1t} - B_{i1t} f_{i1t} = b_{i1t} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I}, \tag{4}$$

$$T_{it} x_{it} + W_{iht} y_{iht} \leq H_{iht} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \tag{5}$$

$$U_{it} x_{it} \leq M_{it} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I}, \tag{6}$$

$$y_{iht}, b_{iht}, e_{iht}, f_{iht} \geq 0 \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \tag{7}$$

$$x_{it} \in \mathbb{Z}^{n_t^x} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I}, \tag{8}$$

with non-negative integer power portfolio decisions x_{it} and non-negative continuous operational decisions y_{iht}, b_{iht}, e_{iht} as well as f_{iht}. Let there be I investment projects $i \in \mathbb{I} = \{1, ..., I\}$, and there are T stages, $t \in \mathcal{T} = \{1, ..., T\}$, and H hours, $h \in \mathcal{H} = \{1, ..., H\}$. Vectors $C_{it} \in \mathbb{R}^{n_t^C}$, $M_{it} \in \mathbb{R}^{m_t^M}$ and matrices $U_{it} \in \mathbb{R}^{n_t^U} \times \mathbb{R}^{m_t^U}$, $T_{it} \in \mathbb{R}^{n_t^T} \times \mathbb{R}^{m_t^T}$ are deterministic along with the decision variables $x_{it} \in \mathbb{Z}^{n_t^x}$ for $t \in \mathcal{T}$ and $i \in \mathbb{I}$.

Let (Ω, Σ, P) be a random space and let ξ be a random vector on Ω. Vectors $D_{ht} = D_{ht}(\xi_t) \in \mathbb{R}^{m_t^D}$ for $t \in \mathcal{T}$, $h \in \mathcal{H}$, and $G_{iht} = G_{iht}(\xi_t) \in \mathbb{R}^{n_t^G}$, $H_{iht} = H_{iht}(\xi_t) \in \mathbb{R}^{m_t^H}$ for $t \in \mathcal{T}$, $h \in \mathcal{H}$, $i \in \mathbb{I}$, and matrices $A_{iht} = A_{iht}(\xi_t) \in \mathbb{R}^{n_t^A} \times \mathbb{R}^{m_t^A}$, $B_{iht} = B_{iht}(\xi_t) \in \mathbb{R}^{n_t^B} \times \mathbb{R}^{m_t^B}$, $W_{iht} = W_{iht}(\xi_t) \in \mathbb{R}^{n_t^W} \times \mathbb{R}^{m_t^W}$ for $t \in \mathcal{T}$, $h \in \mathcal{H}$, $i \in \mathbb{I}$ are functions of random process $\xi_1, ..., \xi_T$. The decision vectors $y_{iht} = y_{iht}(\xi_t) \in \mathbb{R}^{n_t^y}$, $b_{iht} = b_{iht}(\xi_t) \in \mathbb{R}^{n_t^b}$, $e_{iht} = e_{iht}(\xi_t) \in \mathbb{R}^{n_t^e}$ and $f_{iht} = f_{iht}(\xi_t) \in \mathbb{R}^{n_t^f}$ are determined after uncertain realization in stage $t \in \mathcal{T}$. Problem (P) incorporates both expansion and operational problems. Power portfolio decisions (x_{it}) are scenario independent and hedge against uncertainty in the operational problem, which is a multi-stage stochastic optimization problem. Based on portfolio decisions, the operational problem is optimized for each short time step $(h \in \mathcal{H})$ given the uncertain realizations at each stage $t \in \mathcal{T}$. Please refer to Section 3.2 for details. Operational decision variables $(y_{iht}, b_{iht}, e_{iht}, f_{iht})$ typically represent generation output, storage state of charge, and charging/discharging quantities, respectively. Constraints (2)–(4) capture operational limitations that are not impacted by power portfolio decisions. Constraints (5) ensure alignment between power portfolio decisions and operational decisions. Constraints (6) impose restrictions on power portfolio decisions. We now make the following assumptions.

(A1) Problem (P) has a finite number of realizations of ξ_t for all $t = 2, ..., T$. The complete path of realizations over all stages is defined as scenarios, indexed by $s \in \mathcal{S} = \{1, ..., S\}$.

(A2) The random data process is stage-wise independent, i.e. random vector ξ_{t+1} is independent of ξ_t for $t = 1, ..., T$.

Assumptions *(A1)* and *(A2)* imply that the distribution of ξ_t has a finite support with respective probabilities $p_{ts}, s = 1, ..., S, t = 2, ..., T$ and $\sum_{s=1}^{S} p_{ts} = 1$, for each $t = 2, ..., T$.

3.2. Double decomposition method

We present a double decomposition method, introduced (Kaya et al., 2024; Rebennack, 2014) as a state-of-the-art solution method, to combine Benders decomposition and SDDP. As presented in Figure 1, this approach involves leveraging both the two-stage nature of the problem—one master problem (M) and one sub-problem (S)—along with the multi-stage structure—the sub-problem (S) is a multi-stage stochastic linear optimization problem—to solve the multi-stage, multi-scale stochastic mixed-integer linear optimization problem (P).

3.2.1. Benders decomposition

Benders decomposition separates the optimization problem (P) into a master and a sub-problem. In our application, the master problem is a deterministic investment and decommissioning problem, while the sub-problem is a stochastic operational problem. The master problem can now obtain optimality cuts based on the sub-problem's response to trial investment and decommissioning decisions $\hat{x}_{i1}, ..., \hat{x}_{iT}$. If all possible optimality cuts are added—there are finitely many—the master problem is equivalent to (P). The (restricted) master problem then reads as follows

$$(M) \quad \underline{z} := \quad \min \qquad \sum_{t=1}^{T}\sum_{i=1}^{I} C_{it}^{\top} x_{it} + \eta \tag{9}$$

$$\text{s.t.}\quad \eta \geq \lambda_k^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I}(\lambda_{ihtk}^{\text{var}})^\top x_{it} \qquad \forall k \in K, \tag{10}$$

$$U_{it}x_{it} \leq M_{it} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I}, \tag{11}$$

$$x_{it} \in \mathbb{Z}^{n_t^x} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I}, \tag{12}$$

where $k \in K$ is the cut (and iteration) index and K is a subset of all cuts. For cut $k \in K$, λ_k^{const} represents the cut constant and $\lambda_{ihtk}^{\text{var}}$ is the cut variable at time $t \in \mathcal{T}$. We derive the formulas for λ_k^{const} and $\lambda_{ihtk}^{\text{var}}$ below. Because (M) considers only a subset of all cuts, it is a relaxation of (P) implying that its objective function value is a lower bound on z^*. Note that η is an unrestricted continuous decision variable of dimension 1. Thus, problem (M) is a deterministic mixed-integer linear optimization problem. Given the trial decisions $\hat{x}_{i1}, \ldots, \hat{x}_{iT}$ from the master problem, the sub-problem is formulated as follow

$$(S) z_{(S)}(\hat{x}_{i1}, \ldots, \hat{x}_{iT}) := \min \mathbb{E}\left[\sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} G_{iht}^\top y_{iht}\right] \tag{13}$$

$$\text{s.t.}\quad \sum_{i=1}^{I} y_{iht} - \sum_{i=1}^{I} e_{iht} + \sum_{i=1}^{I} f_{iht} = D_{ht} \forall t \in \mathcal{T}, \quad \forall h \in \mathcal{H} : \vartheta_{ihtk}^1 \tag{14}$$

$$b_{i(h-1)t} + A_{iht}e_{iht} - B_{iht}f_{iht} = b_{iht} \quad \forall t \in \mathcal{T}, \forall h \in \mathcal{H} : h > 1, \forall i \in \mathbb{I} : \vartheta_{ihtk}^2 \tag{15}$$

$$b_{iH(t-1)} + A_{i1t}e_{i1t} - B_{i1t}f_{i1t} = b_{i1t} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I} : \vartheta_{ihtk}^3 \tag{16}$$

$$W_{iht}y_{iht} \leq H_{iht} - T_{it}\hat{x}_{it} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I} : \vartheta_{ihtk}^4 \tag{17}$$

$$y_{iht}, b_{iht}, e_{iht}, f_{ht} \geq 0 \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}. \tag{18}$$

Sub-problem (S) evaluates the operational costs associated with trial decisions $\hat{x}_{i1}, \ldots, \hat{x}_{iT}$. This problem (S) is a linear program. Hence, $z(x)$ is a piece-wise linear and convex function in all state variables $x = (x_{i1}^\top, \ldots, x_{iT}^\top)^\top$. This implies that the value function $z(x)$ can be linearly approximated for any $x_{i1}, \ldots, x_{iT}$. The dual value vectors ϑ_{ihtk}^1, ϑ_{ihtk}^2, ϑ_{ihtk}^3 and ϑ_{ihtk}^4 correspond to the constraints (14), (15), (16) and (17), respectively. Duality theory yields the following cut coefficients, which are iteratively integrated into the master problem,

$$\lambda_{ihtk}^{\text{var}} := -(\vartheta_{ihtk}^4)^\top T_{it} \quad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \forall k \in K, \tag{19}$$

$$\lambda_k^{\text{const}} := z(\hat{x}_{i1}, \ldots, \hat{x}_{iT}) - \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I}(\lambda_{ihtk}^{\text{var}})^\top \hat{x}_{it} \quad \forall k \in K. \tag{20}$$

Thus, the Benders sub-problem (S) serves two purposes: (1) it generates optimality cuts for the master problem (M) and (2) it provides the optimal value function value $z(\hat{x}_{i1}, \ldots, \hat{x}_{iT})$. Please note that the constructed optimality cut underestimates $z(x)$ and is tight for the trial decisions $\hat{x}_{i1}, \ldots, \hat{x}_{iT}$ (Rebennack, 2016).

3.2.2. Stochastic dual dynamic program (SDDP)

The sub-problem (S) is the operational problem. It's multi-stage nature makes the stochastic sub-problem (S) of large-scale. Representing uncertainty with a scenario tree can result in an exponentially large number of potential realizations in the number of stages T; a curse-of-dimensionality. This curse makes the sub-problem intractable to be solved by a monolithic method or even nested Benders decomposition. With the help of SDDP, we can break this curse-of-dimensionality and obtain a solution algorithm for our sub-problem (S). Sampling is here the key ingredient. While this leads to a tractable algorithm, its convergence to an optimal policy is no longer guaranteed in finite time. For an in-depth introduction into SDDP, we refer to Füllner and Rebennack (2025).

Sub-problem (S) is a T-stage problem. This nested formulation can be broken apart into one-stage problems which are connected among each other through value functions and associated state variables. Therefore, let $\phi_t(\cdot, \cdot)$ represent the expected t-stage cost-to-go function corresponding to the trial power portfolio decisions $(\hat{x}_{it}, \ldots, \hat{x}_{iT})$, the trial state variables $(\hat{b}_{iH(t-1)})$, and uncertain realization. For $t \in \mathcal{T}$, the t-stage problem (S_t) is then given by

$$(S_t) \quad \phi_t(\hat{x}_{it}, \ldots, \hat{x}_{iT}, \hat{b}_{iH(t-1)}) := \min \sum_{h=1}^{H}\sum_{i=1}^{I} G_{iht}^\top y_{iht} + \mathbb{E}\left[\phi_{t+1}(\hat{x}_{it+1}, \ldots, \hat{x}_{iT}, b_{i1t})\right] \tag{21}$$

$$\text{s.t.}\quad \sum_{i=1}^{I} y_{iht} - \sum_{i=1}^{I} e_{iht} + \sum_{i=1}^{I} f_{iht} = D_{ht} \qquad \forall h \in \mathcal{H}, \tag{22}$$

$$b_{i(h-1)t} + A_{iht}e_{iht} - B_{iht}f_{iht} = b_{iht} \qquad \forall h \in \mathcal{H} : h > 1, \forall i \in \mathbb{I}, \tag{23}$$

$$\hat{b}_{iH(t-1)} + A_{i1t}e_{i1t} - B_{i1t}f_{i1t} = b_{i1t} \qquad \forall i \in \mathbb{I}, \tag{24}$$

$$W_{iht}y_{iht} \leq H_{iht} - T_{it}\hat{x}_{it} \qquad \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \tag{25}$$

$$y_{iht}, b_{iht}, e_{iht}, f_{iht} \geq 0 \qquad \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \tag{26}$$

with $\hat{b}_{iH0} \equiv 0$, $\hat{x}_{iT+1} \equiv 0$ and $\phi_{T+1}(\cdot, \cdot) \equiv 0$. By construction, $(S) = (S_1)$ and $z(\hat{x}_{i1}, \ldots, \hat{x}_{iT}) = \phi_1(\hat{x}_{i1}, \ldots, \hat{x}_{iT}, \hat{b}_{iH0})$.

We make the next assumption to avoid feasibility cuts:

(A3) We assume that problem (P) has relative complete recourse, i.e., sub-problem (S_t) is feasible for any x_t satisfying (6) & (8) and b_{t-1} satisfying (15)–(16) for $t \in \mathcal{T}$.

Next, we look into the details of the sampling, forward pass, backwards pass and the approximate cut calculation.

3.2.2.1. Sampling. The complete scenario tree contains S scenarios as a result of assumption $(A1)$. We build a sub-tree of the entire scenario tree for the problem (P) during the sampling process. In particular, $M \ll S$ different sample scenarios are selected from the set of scenarios S by using a Monte Carlo technique. These sampled scenarios are indexed by m, representing the random process realizations, and occur with probability p_m with $\sum_{m=1}^{M} p_m = 1$.

3.2.2.2. Forward pass. In the forward pass, the constructed sub-problems are solved for the M sampled scenarios. This way, the existing cuts are utilized to calculate a feasible policy for (S), an approximate upper bound on $z(\hat{x}_{i1}, ..., \hat{x}_{iT})$ and new trial values used in the backward pass. Specifically, we solve the optimization problems $(\underline{S}_t)$ for $m = 1, ..., M$ and $t = 1, ..., T$. Linear optimization problem $(\underline{S}_t)$ approximates (S_t) by using affine cuts, exploiting that the cost-to-go functions $\phi_t(\hat{x}_{it}, ..., \hat{x}_{iT}, \hat{b}_{iH(t-1)})$ are piecewise linear and convex in the state variables $\hat{b}_{iH(t-1)}$. With the iteration index l in SDDP, the LP then reads

$$(\underline{S}_t) \quad \underline{z}_{(S)t}(\hat{x}_t, ..., \hat{x}_T, \hat{b}_{iH(t-1)m}) := \min \sum_{h=1}^{H} \sum_{i=1}^{I} G_{iht}^{\top} y_{iht} + \phi_{t+1} \tag{27}$$

$$\text{s.t.} \quad \phi_{t+1} \geq \pi_{(t+1)lm}^{\text{const}} + \sum_{i=1}^{I} (\pi_{i(t+1)lm}^{\text{var}})^{\top} b_{i1t} \quad \forall l, \ \forall m \in M, \tag{28}$$

$$\sum_{i=1}^{I} y_{iht} - \sum_{i=1}^{I} e_{iht} + \sum_{i=1}^{I} f_{iht} = D_{ht} \qquad \forall h \in \mathcal{H}, \tag{29}$$

$$b_{iht} = b_{i(h-1)t} + A_{iht} e_{iht} - B_{iht} f_{iht} \quad \forall h \in \mathcal{H} : h > 1, \forall i \in \mathbb{I}, \tag{30}$$

$$b_{i1t} = \hat{b}_{iH(t-1)m} + A_{i1t} e_{i1t} - B_{i1t} f_{i1t} \qquad : \mu_{itlm}^{2} \forall i \in \mathbb{I}, \tag{31}$$

$$W_{it} y_{iht} \leq H_{iht} - T_{it} \hat{x}_{it} \qquad \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \tag{32}$$

$$y_{iht}, b_{iht}, e_{iht}, f_{iht} \geq 0 \qquad \forall h \in \mathcal{H}, \forall i \in \mathbb{I}. \tag{33}$$

Note that we omit the scenario index m for the decision variables and stochastic data to enhance readability. We store the trial values of state variable vectors $(b_{i1tm} = b_{i1tm}^{*})$, along with optimal solutions y_{ihtm}^{*}, e_{ihtm}^{*}, f_{ihtm}^{*}. For each sample with index m, the objective function is assessed

$$Z_m := \sum_{t=1}^{T} \sum_{h=1}^{H} \sum_{i=1}^{I} G_{ihtm}^{\top} y_{ihtm}^{*}. \tag{34}$$

The approximate upper bound is then given through the sample mean

$$\hat{Z} := \sum_{m=1}^{M} p_m Z_m. \tag{35}$$

3.2.2.3. Backward pass. The forward pass provides the trial state variables vectors $(\hat{b}_{iH(t-1)m})$ associated with the M samples drawn during sampling. This allows us to solve problem $(\underline{S}_t)$ in a backwards manner—i.e., for $t = T, ..., 1$—for those trial variable vectors. We do so for each $m = 1, ..., M$. This backwards pass further allows us to compute the coefficients of the Benders optimality cut (28) as follow

$$\pi_{itlm}^{\text{var}} := (\mu_{itlm}^{2})^{\top} \tag{36}$$

$$\pi_{tlm}^{\text{const}} := \underline{z}_t(\hat{x}_t, ..., \hat{x}_T, \hat{b}_{iH(t-1)m}) - \sum_{i=1}^{I} (\pi_{itlm}^{\text{var}})^{\top} \hat{b}_{iH(t-1)m} \tag{37}$$

3.2.2.4. Approximate cut calculation. SDDP approximately solves the sub-problem (S); since we evaluate each calculated policy only at the M sample paths drawn, the upper bound is only an approximation; the lower bound is valid, though. Next to the approximate upper bound, we also obtain the dual solution vectors only for those M scenarios drawn in the final iteration of SDDP. However, by setting up the double decomposition like we do, we both need a valid upper bound and all optimal dual variables associate with the entire scenario tree to obtain a valid cut for the master problem (M). As we do not have these, we work with their approximations. In particular, given the M independent scenarios from the last iteration of SDDP, the corresponding dual solution vectors ϑ_{ihtmk}^{1}, ϑ_{ihtmk}^{2}, ϑ_{ihtmk}^{3}, ϑ_{ihtmk}^{4} and the upper bound $\hat{Z}$—all obtained from the final forward pass—we can compute approximate cut coefficients as follows

$$\lambda_{ihtk}^{\text{var}} \approx \sum_{m=1}^{M} p_{tm} (-\vartheta_{ihtk}^{4})^{\top} T_{it} \tag{38}$$

$$\lambda_{k}^{\text{const}} \approx \hat{Z} - \sum_{t=1}^{T} \sum_{h=1}^{H} \sum_{i=1}^{I} (\lambda_{ihtk}^{\text{var}})^{\top} \hat{x}_{it} \tag{39}$$

3.2.2.5. Discussion. The resulting double decomposition algorithm provides an approximately optimal policy of (P). The reason why we cannot guarantee optimality is the large size of the scenario tree. So, if we can solve the sub-problem (S) to optimality (in finite time)—for example with NBD—then the resulting double decomposition will also yield a proven optimal solution. However, for the purpose of this research, an exact algorithm seems not immediately necessary, as we also incorporate the simulation results. This integration also comes at the cost of loosing exactness.

4. Agent-based electricity market simulation (AMIRIS)

AMIRIS is designed to study the integration of renewables into electricity markets. It simulates the behavior of individual market participants under various conditions, such as changes in power generation portfolio and policy regulations. Unlike optimization models, which operate with a central objective function to find optimal solutions, AMIRIS models a decentralized system where individual agents make independent decisions. This agent-based approach enables a more flexible and realistic representation of market behavior, capturing diverse strategies and interactions. Thus, the model focuses on agents within the electricity system, each with their own goals and decision-making processes (Nitsch et al., 2021). AMIRIS (Schimeczek et al., 2023) is based on the day-ahead electricity market, which facilitates clearing of the hourly market with uniform pricing. AMIRIS, with all of its agents and their relationships in terms of information, energy and revenue streams, is shown in the online supplement. Traders submit bids to the market, informed by key data including fuel prices, CO_2 prices, and marginal costs obtained from power plant operators. Traders may incorporate markups and markdowns to accommodate non-convex expenses. Integration of neighboring markets is realized through time series of imports and exports.

The agent-based simulation AMIRIS enables the examination of how energy policy tools influence the economic outcomes of power plant operators and marketers. It operates on an hourly basis, generating wholesale electricity prices internally by simulating the strategic bidding strategies of various market participants. These strategies not only account for marginal pricing but also incorporate the impact of support mechanisms such as market premiums. Bidding decisions are based on electricity prices and generation forecasts. AMIRIS emphasizes understanding the perspectives, interactions, and competitive dynamics among actors in the energy system. It accommodates uncertainties inherent in these actors' decisions, such as variations in market premiums or renewable energy feed-in, shaping their strategies accordingly. Each agent pursues its own objectives and adheres to different decision-making protocols; for example, traders seek profit maximization. Actors with different strategies can be modeled on different time scales. Some agents fulfill specific roles within the simulations, like an energy exchange agent facilitating energy market clearing on the day ahead market. This granular approach allows for a detailed simulation of the energy system, dissecting its components and stakeholders. In particular, AMIRIS lacks a predefined overarching objective function; instead, it derives simulation outcomes from the collective actions of individual agents operating under specified regulatory conditions. It enables users to model in detail short- to mid-term dispatch decisions. The validation of the day-ahead spot market model spanning the years 2015–2019 for Germany and 2019 for Austria (Nienhaus et al., 2024) ensures the reliability of assertions regarding electricity price trends.

Executing AMIRIS on a typical laptop computer for one year requires less than one minute, providing day-ahead prices, power plant dispatch, market values, emissions, and system costs for an entire year with hourly precision. In AMIRIS, the electricity markets are modeled and fine-tuned using a fundamental approach for the merit-order model, drawing upon empirical data. While the optimization model determines the capacities of power generation, storage, and transmission technologies, AMIRIS evaluates these results each year, determining whether the optimized scenarios are, in fact, economically viable for the actors.

Given the emphasis on model coupling in this paper, it is essential to highlight the key features of both models: the optimization model and AMIRIS. Both models are evaluated from the policymakers perspective. In the optimization model, the objective is to minimize the total system cost while taking into account the centralized economic dispatch problem. The merit-order market clearing mechanism implemented in AMIRIS maximizes social welfare implicitly. Given inflexible demand, the objective of AMIRIS becomes the minimization of generation costs, which aligns with the optimization model. This is accomplished through the energy exchange agent, calculating the intersection of demand and supply curves. Market bids to the energy exchange agent are submitted by both conventional and renewable traders, each seeking to maximize their profits. Additionally, storage, as a flexible agent, plays a crucial role in the market by submitting bids to the operator. There are two primary strategies for the storage agent: minimizing the total costs and maximizing its profits. For both strategies, forecasted market clearing prices from the forecaster agent is used to determine submitted bids. Here, dynamic programming is employed in the storage agent to apply a strategy of minimizing the total costs. As a result, in AMIRIS, the market clearing price serves as the pivotal factor influencing the decisions of the storage agent.

5. Coupling AMIRIS to the optimization model: the power generation expansion planning (PGEP) problem

In this section, we discuss the coupling of the optimization model (P) with AMIRIS to yield our PGEP problem framework. The key idea here is that we utilize the already existing double decomposition framework for problem (P). This allows us to incorporate additional information into the master problem (M). Our proposed approach treats AMIRIS as a gray-box simulation model, which allows the extraction of information through affine cuts. These cuts can then be readily integrated into our master problem (P). Specifically, among the many components in AMIRIS, we utilize its hourly electricity market clearing mechanism. Given the merit order model in AMIRIS, we explain the process of extracting dual values from the agent-based simulation—AMIRIS—even though AMIRIS does not have a single objective function which is taken into account; see Section 4.

5.1. Benders decomposition

The Benders decomposition breaks problem (P) into a master problem and a sub-problem. The master problem (M) is a deterministic investment problem while the sub-problem (S) is an operational problem (as explained in Section 3.2.1). To couple AMIRIS to this framework, we add another sub-problem, the market clearing problem. Since the energy exchange agent is responsible for market clearing and resource allocation in AMIRIS, we utilize a standard market clearing problem (Tanaka et al., 2022) to represent the energy exchange agent and its process. This additional sub-problem (A) for trial power portfolio decisions $\hat{x}_{i1},...,\hat{x}_{iT}$ is then given by

$$(A) \qquad z_{(A)}(\hat{x}_{i1},...,\hat{x}_{iT}) := \min \sum_{s=1}^{S} p_s \left[\sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} G_{ihts}^{\top} y_{ihts} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{j=1}^{J} B_{jhts}^{\top} e_{jhts} \right] \quad (40)$$

$$\text{s.t.} \sum_{i=1}^{I} y_{ihts} + \sum_{j=1}^{J} e_{jhts} = \sum_{j=1}^{J} D_{jhts} : \lambda_{hts} \quad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall s \in \mathcal{S}, \quad (41)$$

$$y_{ihts} \le \hat{x}_{it} \quad : \mu_{ihts} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \forall s \in \mathcal{S}, \quad (42)$$

$$e_{jhts} \ge 0 \quad : \alpha_{jhts} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall j \in \mathcal{J}, \forall s \in \mathcal{S}, \quad (43)$$

$$y_{ihts} \ge 0 \quad : \beta_{ihts} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \forall s \in \mathcal{S}, \quad (44)$$

$$y_{ihts} \in \mathbb{R}^{n_i^y}, e_{jhts} \in \mathbb{R}^{n_i^e} \qquad \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall i \in \mathbb{I}, \forall j \in \mathcal{J}, \forall s \in \mathcal{S} \quad (45)$$

with continuous operational decisions y_{ihts} and e_{jhts}. We note that the sets $\mathcal{T}$, $\mathcal{H}$ and $\mathbb{I}$ are identical to the ones in model (P) as explained in Section 3.1. The uncertainty is again modeled through the same scenario tree as in formulation (P), where these scenarios are hidden in the expectation operation in the objective function. The number of scenarios S grows exponentially in the number of time periods T. Given the market context, we also assume that there are J customers $j \in \mathcal{J} = \{1,...,J\}$ to allow a description of the AMIRIS process. Because supply and demand agents (as well as their interactions) play an essential role in the market clearing, constraints (41) assure supply-demand balance, while constraints (42) & (44) and (43) apply supply and demand bounds, respectively. Thus, the sub-problem (A) is a market clearing problem. The dual values λ_{hts} of the balance constraints (41) represent the market clearing price.

Linear optimization problem (A) decomposes with the scenarios, hours and stages. The reason lies in AMIRIS and the market clearing procedure. The agents' behaviors and interactions in AMIRIS are followed by predefined rules without any uncertainty. That is, AMIRIS is considered as a deterministic agent-based simulation. In order to consider uncertainty and calculate the expected value function, a wait-and-see approach is utilized. As a market clearing problem, (A) has no hourly coupling; hence, there is also no stage coupling. Algorithm 1 exploits this separability in solving (A). Note that $r \in R$ is an iteration index of the Benders decomposition algorithm, calling the subproblem (A).

Algorithm 1 Wait-and-see solution process for the market clearing problem

Input: Trial value vectors $\hat{x}_1,...,\hat{x}_T$; iteration index r
Output: Duals μ_{ihtsr} on the capacity constraint
for $s = 1, \ldots, S$ **do**
for $t = 1, \ldots, T$ **do**
for $h = 1, \ldots, H$ **do**;
solve problem (A_{hts}) and store (μ_{ihtsr})

$$(A_{hts}) \quad z_{(A)hts}(\hat{x}_t) := \min \sum_{i=1}^{I} G_{ihts} y_{ihts} + \sum_{j=1}^{J} B_{jhts} e_{jhts} \quad (46)$$

$$\text{s.t.} \sum_{i=1}^{I} y_{ihts} + \sum_{j=1}^{J} e_{jhts} = \sum_{j=1}^{J} D_{jhts} \quad (47)$$

$$y_{ihts} \le \hat{x}_{it} : \mu_{ihtsr} \qquad \forall i \in \mathbb{I} \quad (48)$$

$$e_{jhts} \ge 0 \qquad \forall j \in \mathcal{J} \quad (49)$$

$$y_{ihts} \ge 0 \qquad \forall i \in \mathbb{I} \quad (50)$$

end for
end for
end for

The idea is now to approximate the subproblem (A) through affine cuts. These cuts are then integrated into the master problem (M) of Section 3.2.1. We discuss three different strategies for this incorporation in Section 6. In a multi-cut version, we obtain one cut for each scenario and this cut reads

$$\eta_s \ge \theta_{rs}^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\theta_{ihtsr}^{\text{var}})^{\top} x_{it} \qquad \forall r \in R, \forall s \in \mathcal{S} \quad (51)$$

with scenario-dependent free variable η_s which is to be minimized. With the solution of (A), we can compute its cut coefficients

$$\theta_{ihtsr}^{\text{var}} := \mu_{ihtsr} \forall i \in \mathbb{I}, \quad \forall h \in \mathcal{H}, \forall t \in \mathcal{T}, \forall s \in \mathcal{S}, \forall r \in R \quad (52)$$

$$\theta_{sr}^{\text{const}} := \sum_{t=1}^{T}\sum_{h=1}^{H} z_{hts}(\hat{x}_t) - \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{\mathbb{I}} (\theta_{ihtsr}^{\text{var}})^{\top} \hat{x}_{it} \quad \forall s \in \mathcal{S}, \forall r \in R \quad (53)$$

When inspecting problem (A), we encounter a similar challenge as in problem (S) in that the number of scenarios might be too large to allow for an efficient solution. Even though problem (A) decomposes with the scenarios, there might just be too many sub-problems to be solved. Therefore, we utilize again sampling and consider only $N \ll S$ different sample scenarios. These sampled scenarios, indexed by n, occur with probability p_n satisfying $\sum_{n=1}^{N} p_n = 1$.

5.2. Efficiently solving the market clearing model

Linear optimization problems (A_{hts}) are continuous knapsack problems with an upper bound on the decision variables y_{ihts}. As such, (A_{hts}) can be solved very efficiently. An optimal solution can be iteratively computed by selecting the variable with the lowest objective function value coefficient and by choosing this variable as large as possible, while respecting constraints (47)–(48). This process is repeated until the supply-demand balance constraint (47) is satisfied. This boils down to sorting the objective function coefficients in increasing order. As such, problems (A_{hts}) can be solved in a worst-case running time of $O((I+J)\log(I+J))$ (Lohmann & Rebennack, 2017).

When executing this sorting algorithm, we obtain the values y_{ihts}^*, e_{jhts}^* and $z_{hts}(\hat{x}_t)$. However, for the affine cut (51), we also require the dual values μ_{ihtsr}, which are not obtained directly from AMIRIS. The Lagrangian function incorporates both the objective function and the constraints, using dual variables. Since the primal market clearing model (46)–(50) is separable for each scenario, year, and hour, the Lagrangian function is formulated for each scenario, year, and hour as follows:

$$\left\{\mathcal{L}_{hts} = \left(\sum_{i=1}^{I} G_{ihts}^{\top} y_{ihts} + \sum_{j=1}^{J} B_{jhts}^{\top} e_{jhts}\right) - \lambda_{hts}\left(\sum_{i=1}^{I} y_{ihts} + \sum_{j=1}^{J} e_{jhts} - \sum_{j=1}^{J} D_{jhts}\right) - \sum_{i=1}^{I}\mu_{ihts}(\hat{x}_{it} - y_{ihts}) - \sum_{i=1}^{I}\beta_{ihts} y_{ihts} - \sum_{j=1}^{J}\alpha_{jhts} e_{jhts}\right\} \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall s \in \mathcal{S}, \tag{54}$$

where the KKT conditions imply that

$$\mu_{ihts} = \lambda_{hts} - G_{ihts}, \quad \text{if } y_{ihts} > 0, \qquad \forall i \in \mathbb{I}, \forall t \in \mathcal{T}, \forall h \in \mathcal{H}, \forall s \in \mathcal{S} \tag{55}$$

We provide a formal proof in the online supplement.

Here we can use the interpretation of dual variables. If the right-hand-side, $\hat{x}_{it}$ increases by $+1$, then the objective function value does not decrease, if $y_{ihts}^* < \hat{x}_{it}$, *i.e.*, the additional capacity does not help to reduce the objective function value. With other words, since the generator i is not used in stage t, hour h and scenario s at its full capacity, additional capacity does not help. Now, if $y_{ihts}^* = \hat{x}_{it}$, then the objective function value decreases by $\lambda_{hts} - G_{ihts} \geq 0$, where λ_{hts} is the largest objective function value among all non-zero decision variables. This is true as the largest cost generator is replaced by a cheaper generator with the additional capacity. Notice that λ_{hts} is the market clearing price.

Thus, for iteration index r, we obtain

$$\mu_{ihtsr}^* = \begin{cases} 0, & \text{if } y_{ihts}^* < \hat{x}_{it} \\ \lambda_{hts} - G_{ihts}, & \text{o/w} \end{cases} \forall i \in \mathbb{I}, \forall h \in \mathcal{H}, \forall t \in \mathcal{T}, \forall s \in \mathcal{S} \tag{56}$$

As mentioned before, AMIRIS does not solve optimization problems but is rather built on decision rules. As such, AMIRIS uses an algorithm based on the merit-order curve as described above to solve the market clearing problems. With the help of formula (56), we can then compute the affine cut (51) to be included in our master problem (M). We discuss possible coupling strategies next.

6. Coupling strategies

We examine three coupling strategies connecting the optimization and simulation models. In particular, when coupling AMIRIS to the optimization model (P), we discuss the sequence for applying the double decomposition method and the affine cuts generated from each sub-problem through AMIRIS.

6.1. Coupling strategy 1 (baseline simulation (market) approach)

The first strategy involves coupling AMIRIS as the only sub-problem with the master problem (M). AMIRIS, which represents the electricity market operation, is thus considered as the only sub-problem of the PGEP problem. That is, power portfolio decisions are decided based on the extracted affine cuts from AMIRIS, without taking the sub-problem (S) into account. In particular, SDDP is not involved in this strategy. Given the cut coefficients (52)–(53) from problem (A), the master problem for coupling strategy 1 reads

$$(M_1) \quad \underline{z} := \min \quad \sum_{t=1}^{T}\sum_{i=1}^{I} c_{it}^{\top} x_{it} + \sum_{s=1}^{S} p_s \eta_s^{AMIRIS} \tag{57}$$

$$\text{s.t.} \quad \eta_s^{AMIRIS} \geq \theta_{sr}^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\theta_{ihtsr}^{\text{var}})^{\top} x_{it} \quad \forall r \in R, \forall s \in \mathcal{S} \tag{58}$$

$$U_{it} x_{it} \leq M_{it} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I} \tag{59}$$

$$x_{it} \in \mathbb{R}^{n_t^x} \qquad \forall t \in \mathcal{T}, \forall i \in \mathbb{I} \tag{60}$$

As such, coupling strategy 1 extends AMIRIS to an expansion planning problem which is itself a significant contribution.

6.2. Coupling strategy 2 (robust approach)

In the second strategy, a double decomposition framework is used to solve the PGEP model before it is connected to AMIRIS. Then, AMIRIS receives initial power portfolio decisions based on the double decomposition and generates market outputs required to calculate dual values and optimality cuts. All generated cuts are kept throughout the process.

Given the cut coefficients (52)–(53) from problem (A) and (38)–(39) from problem (S), the master problem for coupling strategy 2 reads as follow:

$$(M_2) \quad \underline{z} := \quad \min \quad \sum_{t=1}^{T}\sum_{i=1}^{I} C_{it}^{\top} x_{it} + \eta \tag{61}$$

$$\text{s.t.} \quad \eta^{SDDP} \geq \lambda_k^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\lambda_{ihtk}^{\text{var}})^{\top} x_{it} \qquad \forall k \in K, \tag{62}$$

$$\eta_s^{AMIRIS} \geq \theta_{sr}^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\theta_{ihtsr}^{\text{var}})^{\top} x_{it} \quad \forall r \in R, \forall s \in S, \tag{63}$$

$$\eta \geq \max\{\eta^{SDDP}, \sum_{s=1}^{S} p_s \eta_s^{AMIRIS}\} \tag{64}$$

$$U_{it} x_{it} \leq M_{it} \qquad \forall t \in T, \forall i \in I, \tag{65}$$

$$x_{it} \in \mathbb{Z}^{n_t^x} \qquad \forall t \in T, \forall i \in I, \tag{66}$$

Master problem (M_2) considers affine cuts, from both sub-problems (S) and (A) by selecting the maximal ones among the two groups, *i.e.*, the largest cost associated with the chosen expansion decision x_{it} among both (S) and (A). This makes coupling strategy 2 a robust approach in the sense that it chooses the worst cost predictions among the two models (S) and (A). Different strategies here also exist on when exactly in the algorithm the cuts are calculated. Instead of solving the master problem (M_2) until convergence taking first the cuts from (S) into account, one could also alternate between the cuts from (S) and (A), or first take the cuts from (A) into account. All these strategies would lead to the same optimal objective function value if the cuts are valid and tight—which they are not in our case.

6.3. Coupling strategy 3 (multi-objective approach)

In the last coupling strategy, we acknowledge that AMIRIS and the subproblem (S) look at the same operational problem from different perspectives, leading to different cost predictions. As both approaches have their merits, we want to incorporate both approaches through a multi-objective approach. Each sub-problem (S) and (A) contribute their own objective function to be minimized.

To resolve the multiple objectives, we choose the weighted sum approach. In particular, we assign weight $w_{(S)} > 0$ to the expected value function of SDDP and weight $w_{(A)} > 0$ to the expected value function of AMIRIS. Both weights should sum to one, *i.e.*, $w_{(S)} + w_{(A)} = 1$. This yields the master problem of our PGEP model for coupling strategy 3 as

$$(M_3) \quad \underline{z} := \quad \min \sum_{t=1}^{T}\sum_{i=1}^{I} C_{it}^{\top} x_{it} + w_{(S)}\eta^{SDDP} + w_{(A)}\eta^{AMIRIS} \tag{67}$$

$$\text{s.t.} \quad \eta^{SDDP} \geq \lambda_k^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\lambda_{ihtk}^{\text{var}})^{\top} x_{it} \qquad \forall k \in K, \tag{68}$$

$$\eta_s^{AMIRIS} \geq \theta_{sk}^{\text{const}} + \sum_{t=1}^{T}\sum_{h=1}^{H}\sum_{i=1}^{I} (\theta_{ihtsk}^{\text{var}})^{\top} x_{it} \quad \forall k \in K, \forall s \in S, \tag{69}$$

$$\eta^{AMIRIS} = \sum_{s=1}^{S} p_s \eta_s^{AMIRIS} \tag{70}$$

$$U_{it} x_{it} \leq M_{it} \qquad \forall t \in T, \forall i \in I, \tag{71}$$

$$x_{it} \in \mathbb{Z}^{n_t^x} \qquad \forall t \in T, \forall i \in I, \tag{72}$$

where η^{SDDP} and η^{AMIRIS} represent the expected value function of SDDP and AMIRIS, respectively. The iteration index is $k \in K$; it is the same for both the SDDP and the AMIRIS sub-problems as we solve both sub-problems (S) and (A) per iteration.

In the above formulation, we use fixed weights for each expected value function. As an improvement, we adjust weights based on the performance of each sub-problem over a given number of iterations. The process includes three steps: (i) We start with equal weights for both expected value functions, *i.e.*, $w_S^1 = w_A^1 = 0.5$. The weights carry now the additional iteration index k. (ii) After each Benders iteration k, the absolute optimality gap of each value function and its approximation is calculated through

$$\begin{aligned} \epsilon_{(A)}^k &:= |z_{(A)}(x_1^*, \ldots, x_T^*) - \eta^{AMIRIS,*}| \\ \text{and } \epsilon_{(S)}^k &:= |z_{(S)}(x_1^*, \ldots, x_T^*) - \eta^{SDDP,*}|. \end{aligned} \tag{73}$$

(iii) We increase the weight of the value function that has a smaller optimality gap and decrease the other weight accordingly, as

$$\begin{aligned} w_{(A)}^{k+1} &= \psi w_{(A)}^k + (1-\psi)\frac{\epsilon_{(A)}^k}{\epsilon_{(A)}^k + \epsilon_{(S)}^k} \qquad \text{and} \\ w_{(S)}^{k+1} &= 1 - w_{(A)}^{k+1}, \end{aligned} \tag{74}$$

with adjustment factor $\psi \in [0,1]$ to avoid high fluctuations. Based on real-time feedback from each iteration, these weight adjustments will continue until the solution converges.

7. Case study for Germany

7.1. Case study description

We develop a PGEP model of the German power system using data from 2020 following the ARIADNE REMIND reference scenario (Luderer et al., 2021). We examine all existing technologies, including coal, natural gas, nuclear, oil, bio-energy, geothermal, hydro, solar photovoltaic (PV), wind and storage. Throughout the planning horizon, annual decommissioning of all existing technologies is allowed. A maximum of 40% of the existing capacity for each technology may be decommissioned annually. In addition to existing technologies, annual investment opportunities are considered throughout the planning horizon with investment projects. These projects contain five technologies: wind, solar photovoltaic (PV), natural gas, coal and nuclear. Due to construction limitations, we assume that the total invested capacity cannot exceed 15 GW per year. The PGEP model combines a 10-year planning horizon (with 2020 as the starting year) with hourly resolution, representing the temporal characteristics of a large-scale power system.

For the case study, Germany is subdivided into 16 multiple zones, each sharing common characteristics such as geography and climate. This regional division simplifies the problem and provides an efficient representation of generators in the planning process by assigning a single node to each technology for each region. Hence, the PGEP model considers 113 existing and 19 potential generation nodes across 16 zones. Furthermore, it is assumed that all generators are centrally located within each respective region.

Conventional generators of the same technology have uniform parameters regardless of their location. Each solar and wind technology has different hourly capacity factors based on their location. We aggregated weather data for the years 2018–2020 to generate a representative year. In particular, as a representative year, we synthesized the hourly capacity factors for each hour and day to determine their capacity factors for each zone. Hydro and bio-energy technologies, like wind and solar, exhibit hourly capacity factors, however these factors are not location-dependent. The capacity factors are considered to remain constant across the planning horizon (please see the online supplement for more details).

Demand is an important driver for any future energy system. We use the specific demand time-series from the ARIADNE-project (Luderer et al., 2021). Within this project, the REMix-model calculated hourly electricity demand profiles from 2020 for every five years up to 2030. These time-series are thus calibrated exactly to the total electricity consumption of ARIADNE (model used: REMIND) that are used for starting the simulations in 2020. The diffusion of PV and storage systems and electric vehicles in AMIRIS is calculated with a diffusion model that is based on a representative survey of around 900 participants and a latent class analysis, 20 household types were identified. Three out of 20 types have a PV rooftop, 2 an electric vehicle. These prototypical households were fed into a BASS diffusion model, resulting in the estimated number of households for each year up to 2030. Heat pump diffusion is aligned with the political targets (BMWK., 2022) of 6 million heat pumps for 2030, and 11 million for 2040 (Sperber et al., 2020). These numbers were then used to parametrize AMIRIS and optimization model. From an economic perspective, natural gas and emission prices are considered as uncertain parameters. In order to address these uncertainties, we model them using a scenario tree approach. Due to page limits, we include all information regarding the scenario tree, model and data in the online supplement.

7.2. Computational results

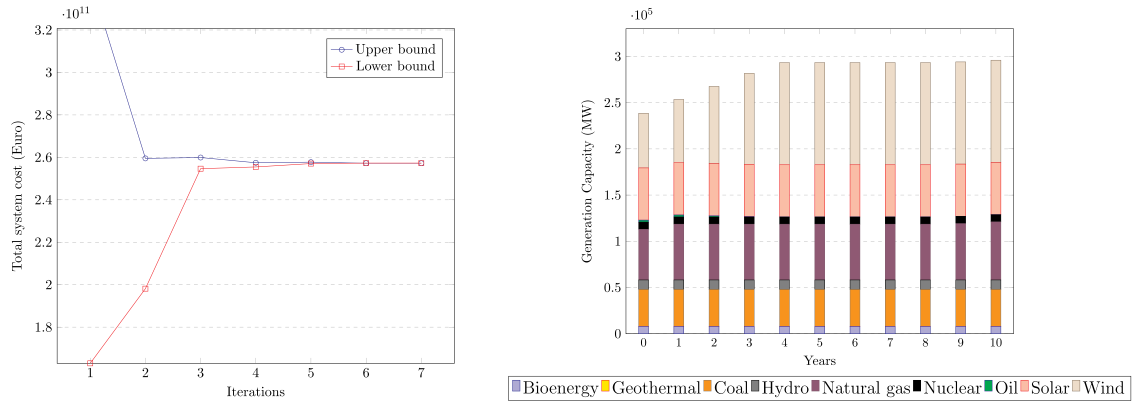
We utilize Julia-version 1.9.4 to implement the SDDP and Benders decomposition algorithms (Dowson & Kapelevich, 2021). The generated optimization problems are solved using Gurobi version 10.0.3. AMIRIS version 1.2.17 has been tested with Java Development Kit (JDK) versions 11–21. We execute the numerical tests on an AMD Ryzen Threadripper PRO 5955WX Prozessor with 4.0 GHz CPU for the Benders and SDDP algorithms and on an Intel Core I7 on a Dell Latitude 5431 for AMIRIS. Benders decomposition algorithm (for both double decomposition and coupling methods) is terminated if a relative gap of 0.1% is obtained, and the SDDP algorithm is stopped after six backward-forward iterations. Furthermore, in order to couple the optimization model and AMIRIS (Schimeczek et al., 2023), an automatic workflow had to be established. Each component of the workflow—i.e., preparing the data, running AMIRIS, transferring the results to the optimization model, running that model, converting the results into a format that can be used by AMIRIS—was programmed in Python to be executed on remote servers connected by the RCE software (RCE Environment, 2024).

7.2.1. Double decomposition method

As a benchmark for our simulation-optimization methods developed in this paper, we solve the PGEP problem without considering AMIRIS. The resulting model is solved through the double decomposition algorithm. To enhance computational performance, we incorporate the total power demand as a valid inequality in the master problem of the double decomposition algorithm. As an initial step, we compare the double decomposition method (BD-SDDP) with the existing method (BD-NBD), where the subproblem is solved using the nested Benders decomposition. We test these two methods on small- to mid-size cases with planning periods from 3 to 5 years and scenarios from 8 to 243. Each case is executed 10 times across the different scenarios. Table 1 reports their summary statistics (M), the size of the scenario (S), the total number of years (T) and hours (H), and computational results, including computational time (s), the number of Benders iterations, and the optimality gap (%). BD-NBD requires a considerable amount of time to compute the optimal value because it considers every possible scenario. In the first three cases, reaching a zero optimality gap demanded significant computational effort. Starting with

Table 1. Comparison of computational performance of BD-NBD and BD-SDDP

					BD-NBD			BD-SDDP		
No	T	H	S	M	Time (s)	Benders It (#)	Gap (%)	Time (s)	Benders It (#)	Gap (%)
				Min	2,524	3.0	0.00	522	3.0	0.00
1	3	26,280	8	Avg	2,745	3.1	0.00	615	3.1	0.23
				Max	3,663	4.0	0.00	822	4.0	1.03
				Min	13,703	3.0	0.00	586	2.0	0.00
2	3	26,280	27	Avg	14,733	3.1	0.00	997	3.4	0.11
				Max	20,571	4.0	0.00	2,019	7.0	0.19
				Min	9,352	3.0	0.00	1,132	3.0	0.01
3	4	35,040	16	Avg	12,094	3.9	0.00	1,245	3.3	0.12
				Max	13,048	4.0	0.00	1,570	4.0	0.36
				Min	77,251	5.0	0.00	2,263	4.0	0.01
4	5	43,800	32	Avg	84,204	6.1	0.06	2,627	4.5	0.18
				Max	86,400	7.0	0.44	2,963	5.0	0.58
				Min	86,400	1.0	53.62	4,896	4.0	0.03
5	5	43,800	243	Avg	86,400	1.0	57.73	5,950	4.8	0.12
				Max	86,400	1.0	59.86	6,354	5.0	0.18



(a) Computed upper and lower bound (b) Generation capacity (MW)

Figure 2. Results computed by double decomposition algorithm.

Case 4, the BD-NBD approach fails to achieve a zero optimality gap within a 24-hour time limit; therefore, the last achieved optimality gaps are shown in Table 1. A significant optimality gap is observed for Case 5. On the other hand, BD-SDDP attains a small optimality gap (<0.6%) with the best runtime efficiency for all cases.

Regarding the main case study, the results of the double decomposition method are shown in Figure 2. The double decomposition method requires 7 iterations to reach convergence in the Benders algorithm. Figure 2(a) illustrate the convergence of upper and lower bounds and the evolution of total system cost for the double decomposition solution. Figure 2(b) indicates yearly total generation capacity per technology. Oil is totally decommissioned, while wind and natural gas have 87% and 15% capacity increments, respectively.

7.2.2. Comparison of coupling strategies

Next, we compare the coupling strategies of Section 6 and the double decomposition method of Section 3. That is, we consider two baseline approaches: a double decomposition method—a stochastic optimization with centralized operations—and coupling strategy 1—agent-based simulation approach with a wait-and-see approach. Apart from the baseline approaches, the coupling strategies 2 and 3 are considered to address both stochastic optimization and agent-based simulation. The results of all coupling strategies are presented in Figure 3, illustrating the convergence, the total system cost and power portfolio decisions.

First, we compare the total system cost. While this seems a natural comparison, any conclusions can hardly be drawn since the four methods tested have different objective functions. The double decomposition method yields the lowest cost, while coupling strategy 1 results in the highest cost, with a difference of nearly 0.1% compared to the double decomposition method. Since investment costs and the associated constraints in the master problem dominate operational costs, they impose an unavoidable cost across all strategies. As a result, both the double decomposition method and the coupling strategies tend to converge toward similar values. The observed differences between the methods are relatively small. The main variation arises from the operation of storage units, which introduces slight differences in the resulting portfolios. The reason is that coupling strategy 1 uses only the agent-based simulation AMIRIS as a sub-problem. Although the market-clearing process by the energy exchange agent and power plant decisions are well aligned with the optimization model, note that agents are not optimized in the agent-based simulation, because its main aim is to examine the interactions and behaviors of agents rather than to achieve optimal results across a simulation. In particular, the storage agent places bids to the energy exchange agent based on forecasted market clearing prices, operating on a shorter horizon. Thus, it may be impacted from forecasted price fluctuations or be unable to utilize storage fully over the entire planning horizon. In the double decomposition method, the usage of storage is optimized over a planning horizon. This would lead to a balanced storage usage. Furthermore, coupling strategies 2 and 3 yield a total system cost that is between the double decomposition method and the coupling strategy 1.

Second, power portfolio decisions show a similar trend across all strategies; oil technology is decommissioned, while wind and natural gas technologies expand capacity by 81-87% and 15-18%, respectively. Specifically, for coupling strategy 1, Figure 3(d) shows that oil is completely decommissioned, while wind and natural gas increase their capacities by 81% and 18%, respectively. In addition to the decommissioning of oil, coupling strategy 2 has capacity increases of 82% for wind and 17% for natural gas *cf.* Figure 3(e). Coupling strategy 3 provides a capacity expansion of 84% for wind and 16% for natural gas *cf.* Figure 3(f). On the other hand, the double decomposition approach invests less in natural gas (15%) and more in wind technologies (87%). Overall, the total power portfolio capacity of all strategies in year 10 is around 293–295 GW.

Last, in our context, the number of iterations in the Benders algorithm is directly related to how quickly each method converges to a solution. With respect to this, the double decomposition method requires 7 iterations to achieve convergence, whereas the coupling strategy 1 needs 8 iterations. As a robust approach, coupling strategy 2 needs 10 iterations due to sequential solving. Since coupling strategy 3 connects the PGEP model's master problem with

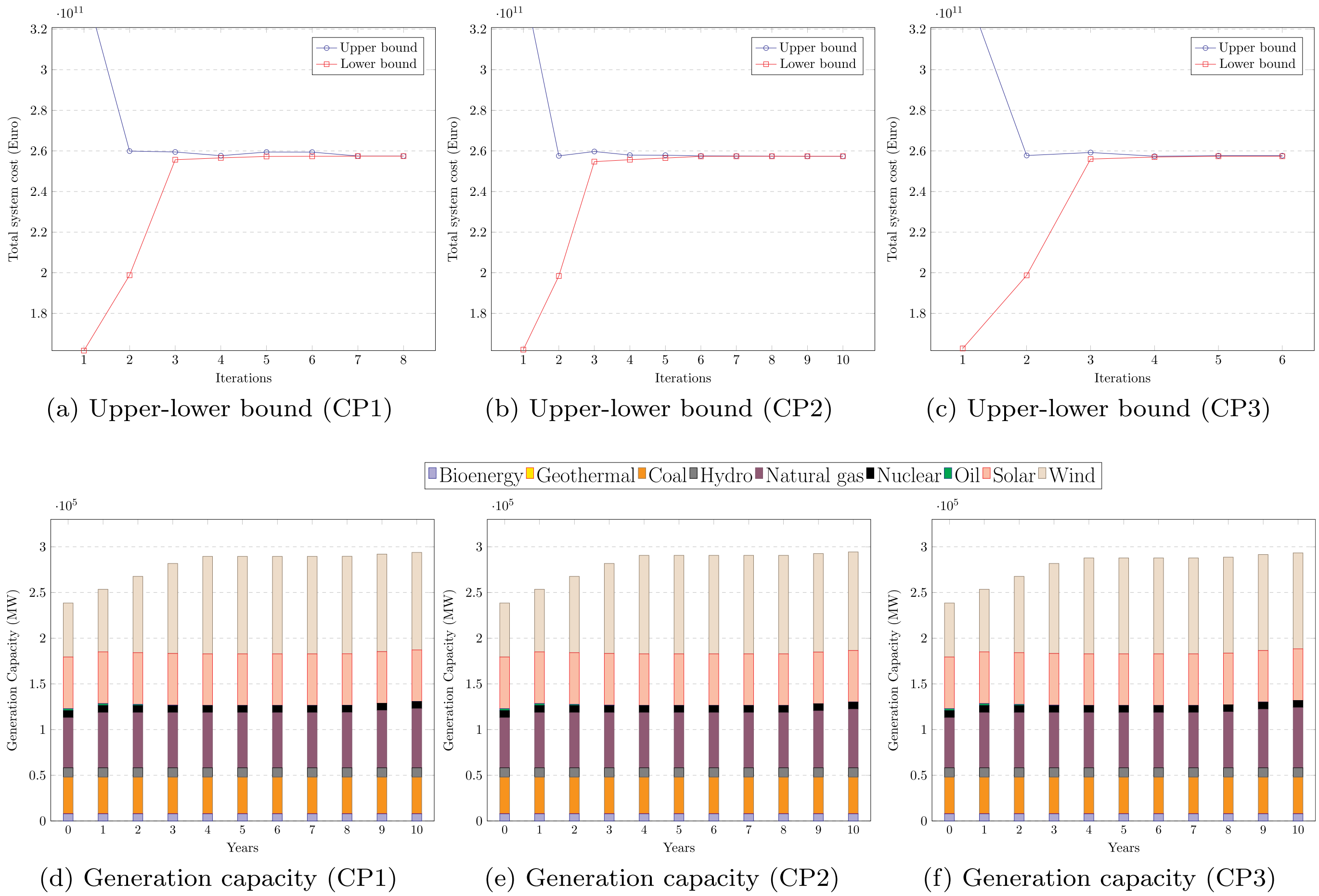


Figure 3. Results computed by coupling strategies.

Table 2. Computational performance of double decomposition and coupling strategies

	DD			CP1			CP2			CP3		
No	Time	It	Z (×1000€)	Time	It	Z (×1000€)	Time	It	Z (×1000€)	Time	It	Z (×1000€)
Min	22,277	5	256,881,423	20,666	5	257,079,770	32,169	8	257,199,208	22,787	5	257,125,543
Avg	26,726	6.2	257,175,816	27,571	6.8	257,353,139	40,505	10	257,358,123	25,691	5.6	257,312,998
Std	3,063	0.8	143,858	3,745	1.0	150,881	5,400	1.3	125,482	2,703	0.5	111,781
Max	31,041	7	257,307,653	32,169	8	257,595,371	49,214	12	257,571,069	28,148	6	257,484,078

AMIRIS and SDDP simultaneously using dynamic multi-objective optimization, it has an advantage in the solution process. Thus, it outperforms other strategies, reaching convergence in 6 iterations yielding also faster runtimes.

7.2.3. Sensitivity analysis and out-of-sample test

Next, we want to study the robustness of the obtained results and we give a first attempt to evaluate the additional benefits by the proposed simulation-optimization framework.

As a sensitivity analysis, we run all four strategies ten times to capture the range of possible outcomes. The resulting computational performance of all strategies is presented in Table 2. Again, the costs cannot be compared to each other, as the models have different objective functions. The reason that we obtain different results when re-running the algorithms is the sampling within the methods, implying that only an approximate solution is computed instead of a guaranteed optimum. We observe that coupling strategy 3 has the lowest spread among the four strategies. In addition, coupling strategy 3 achieves the fastest convergence with an average of less than 6 Benders iterations. As such, CP3 yields preferable computational performance in this comparison.

Next, we apply out-of-sample tests to evaluate the obtained portfolio decisions under both stochastic and AMIRIS frameworks, to finally yield some first attempt to compare the total costs obtained by the four methods. As an out-of-sample test, we evaluate the power portfolio decisions of each strategy under both stochastic and AMIRIS frameworks to analyze their performance. As we do not have a unique solutions, but there is a range of possible solutions—see above discussion and Table 2—we choose one solution randomly for the out-of-sample test. Regarding this evaluation, we fix the power portfolio decisions from each model (three strategies + double decomposition) and then solve their operational stages in both SDDP and AMIRIS separately. This provides comparable values. We consider a total

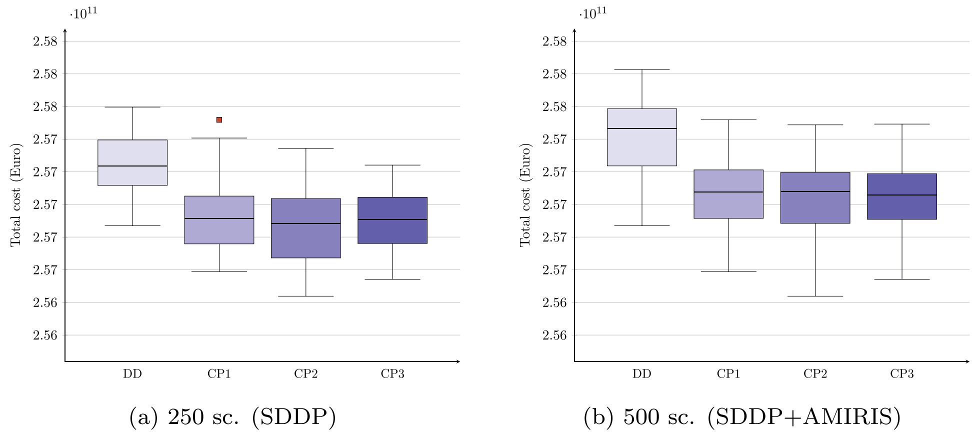


Figure 4. Out-of-sample test results.

of 500 scenarios—250 scenarios for SDDP and 250 scenarios for AMIRIS. Figure 4(a) presents the results of stochastic framework, while Figure 4(b) displays the outcomes for both frameworks (SDDP and AMIRIS).

Our key observations are as follows: (1) The results of Figure 4(a) seem to indicate that the optimization approach alone yields higher cost when evaluating the optimization model alone. This is counter-intuitive and can be explained by the particular solution analyzed. Our tests have shown that among the other 9 solutions, these results differ. (2) The three coupling strategies yield lower total system cost compared to the optimization model alone at a statistically significant level; see Figure 4(b). (3) Though the relative improvement of the three coupling strategies over the optimization method (DD) alone is rather small, the absolute difference is large, due to extremely high system cost. (4) Coupling strategy 3 (CP3) has the smallest standard deviation while achieving better computational performance. In summary, the three coupling strategies seem to yield better expansion decisions than the optimization model (DD) alone. The three coupling strategies have similar performance, while coupling strategy 3 seems to have the best statistical indicators. As such, CP3 seems to be the best method among the four strategies tested. Further tests are necessary to analyze and quantify the total cost savings.

8. Conclusions

This study describes a framework for power generation expansion planning. We model the PGEP problem under uncertainty as a combined simulation-optimization problem with a long planning horizon and an hourly time resolution. As a contribution, we couple the optimization model with an agent-based simulation through decomposition technique to assess electricity market operations. This integration enables us to analyze both centralized and market-based frameworks from a policymaker's perspective, as well as combining both recourse and wait-and-see solutions. First, we show the process of extracting dual values from AMIRIS, managed by if-then rules, in order to incorporate the results of an agent-based simulation using affine cuts. Second, we examine coupling strategies that include coupling sequences and approaches. In particular, coupling strategy 1 only considers agent-based electricity market simulation as a subproblem, whereas coupling strategies 2 and 3 include both stochastic optimization and agent-based electricity market simulation. Importantly, we discuss how the double decomposition framework can be integrated into the coupling mechanism via dynamic multi-objective optimization. The power portfolio decision across all strategies show a similar trend that oil is gradually being phased out and wind is the key driver of the capacity expansion. The three integrated simulation-optimization strategies outperform the pure optimization model. In particular, coupling strategy 3 seems to be the best strategy among the four tested, having superior statistical indicators.

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