Energy 284 (2023) 129320

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Efficient coordination of top-down and bottom-up models for energy system design: An algorithmic approach

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ARTICLE INFO

Keywords:
Model linking
Coordination algorithm
Energy system modeling
Economic modeling

ABSTRACT

To account for endogeneity effects in, e.g., energy demand, modern bottom-up energy system models are often linked to a top-down model describing the macroeconomic system. Solving such linked models involves iteratively passing solutions from one model to the other and vice versa until convergence is reached, which can be computationally demanding. This paper proposes a coordination algorithm that speeds up convergence for the linkage of the two models in case the bottom-up model is a linear program and the top-down model is a mixed-complementarity problem. The coordination algorithm uses duality theory to select optimal bases from previous iterations to predict the solution of the bottom-up model. If the predicted solution is correct, which is shown to be equivalent to the predicted solution vector being non-negative, the bottom-up problem need not be solved in that iteration, resulting in a time gain. Numerical experiments on an energy system design problem illustrate that our coordination algorithm correctly predicts the bottom-up solution in most iterations, resulting in a significant reduction in overall computation time.

1. Introduction

Decarbonization ambitions pose important challenges to the way society produces, distributes, and consumes energy. Transitioning to a low-carbon system involves broad changes at national and continental scales, with effects extending well beyond the boundaries of the energy system. For instance, changes in the availability of fossil fuels and gradual increase of CO_2 prices will influence the price of substitute commodities and resources, such as electricity and biofuels, and might also influence the production costs of several industries, in particular the energy-intensive ones. This will reflect changes in demand for commodities and services, including energy commodities.

The interplay between the energy system and the wider economy is a prominent topic of current research and discussion among academics and policymakers. In a broad sense, the energy system can be defined as a combined set of energy processes. These processes, which cover all sectors, involve the production, conversion, or utilization of energy. They are interconnected through their inputs and outputs and ultimately supply end-use energy services. In contrast, the general economy considers a wider set of commodities and services. Currently, energy policy studies tend to factor in effects from the wider macroeconomic system, as well as provide feedback to it.

Typically, these studies combine a bottom-up (BU) energy system model with a top-down (TD) economic model. In our context, BU models focus on the detailed representation of specific technologies, processes, and practices within the energy system. These models are often represented as optimization models that determine the least-cost way to meet a particular energy demand or policy target. BU models can assist in planning for energy infrastructure needs under specific policy measures on technology adoption and energy use. In contrast, TD models focus on the broader economic system and represent the energy system in a more aggregated manner. These models capture the interactions between the energy system and the rest of the economy, providing information about the evolution of energy prices, GDP, employment, and other macroeconomic variables. TD models may incorporate behavioral aspects, such as consumer preferences and producer behavior, that go beyond simple cost-minimization.

While BU models provide detailed descriptions of the energy system, they struggle to account for the impacts of changes in the energy system on the wider economy, such as changes in demand patterns. By combining a BU model with a TD model that captures the broader economy, one can account for such endogeneities and gain insights into the interplay between the energy system and the economy as a whole. The most popular way to combine these two classes of models is by *linking* them, which means that the models are solved in an alternating fashion, with each model providing input to the other model, until the solutions converge to an equilibrium [1].

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https://doi.org/10.1016/j.energy.2023.129320
Received 31 May 2023; Received in revised form 4 September 2023; Accepted 7 October 2023
Available online 10 October 2023

Nomenclature

Acronyms

BU	bottom-up
CGE	computable general equilibrium
KKT	Karush–Kuhn–Tucker
LP	linear program
MCP	mixed-complementarity program
TD	top-down
TDM	top-down master

Functions

$\mathcal{M}(y)$	mapping of elements of the basic solution into the solution vector
$\mathcal{Q}(x)$	outer approximation of $Q(x)$
$F(x, y)$	mapping defining the top-down problem
$Q(x)$	optimal value of the bottom-up problem at top-down solution x

Parameters

α_K, α_L	scaling factor of the capital and labor parameter, respectively, in the top-down model in the numerical experiments
A	constraint coefficient matrix in bottom-up model
$b(x)$	constraint right-hand side vector in bottom-up model
B_k	kth dual feasible basis matrix in the bottom-up model
c	cost vector in bottom-up model
n	algorithm iteration counter

Sets

$\mathcal{K}$	index set of all dual feasible bases
K	index set of all optimal bases found in previous iterations

Variables

η	decision vector in dual to the predicting problem
θ	Auxiliary decision variable in predicting problem
u	decision vector in dual formulation of bottom-up model
x	decision vector in top-down model
$y, \hat{y}$	decision vector in bottom-up model and the predicted bottom-up solution, respectively

The current iterative approaches for solving linked TD and BU models can be time-consuming. Many iterations may be needed to reach convergence, and in every iteration, both the TD and the BU models need to be solved. Usually, the BU model is quite large and takes up the main share of the computational time. Additionally, a practical challenge arises when the TD and BU models are managed by different institutions. Each iteration requires an exchange of results, which necessitates communicating, processing, and translating results from one institution's model to the other. All of these steps can be labor and time-consuming and add to the burden of solving the linked TD-BU model. Methods that could bypass some of these iterations could potentially drastically reduce the computational burden of solving linked TD and BU models.

This paper uses concepts drawn from parametric linear optimization [2] and duality theory [3] to develop a coordination algorithm designed to expedite the process of solving linked TD and BU models. Our coordination algorithm is tailored to the typical setting where the TD model is a mixed-complementarity model (MCP) [4] and the BU model is a linear program (LP). The main idea is to *predict* the solution of the BU model using a list of basis matrices that were optimal in previous solutions of the BU model. Duality theory is used to determine which of the previously optimal basis matrices produces the "best" prediction. The algorithm assigns a cut to each new basis provided by the BU problem. It then predicts the correct basis to use by observing which cut is active when solving the TD problem augmented with these additional cuts. If the predicted solution is correct (which is the case if and only if it is non-negative), one can skip solving the BU model and hence, greatly reduce the computation time in the corresponding iteration. If the prediction is incorrect, the BU problem is solved anew and a new optimal basis is added to the list.

Interestingly, the procedure that predicts the BU solution can be incorporated into the TD problem. Predicting the BU solution is equivalent to solving a small-scale LP. The Karush–Kuhn–Tucker conditions of this LP yield complementarity conditions that can be incorporated directly into the TD problem. The resulting *TD master problem* (TDM) simultaneously finds a solution to the TD problem and predicts a basis for the BU problem. As will be shown, computing the BU solution corresponding to this predicted basis and checking its optimality can be performed very efficiently: it is a matter of a single matrix multiplication and checking whether a vector is non-negative.

The numerical performance of the coordination algorithm is illustrated using the linked TD and BU models taken from [1], in which the TD model is a computable general equilibrium (CGE) model and the BU model is an energy system model. Compared to an uncoordinated iterative scheme, our coordination approach bypasses on average 89% of the BU models by correctly predicting their solution. This leads to an average time gain of 75% compared to an uncoordinated approach that simply iterates between the BU and TD model. Moreover, the coordination algorithm performs significantly better than a procedure using warm starts in the form of an advanced basis, which speeds up computation times by only 12% on average. These results illustrate the potential of our approach for significantly speeding up computations.

The remainder of the paper is structured as follows. Section 2 reviews the relevant literature. Section 3 outlines the coordination algorithm in detail. Section 4 provides a numerical application of our algorithm on an energy system design problem. Finally, Section 5 concludes the paper.

2. Literature review

Top-down macroeconomic models provide a holistic view of the economy but lack sector-specific details. On the other hand, bottom-up energy system models offer detailed insights into a specific sector. To leverage the overlap in the energy sector, a loop can be established where information is exchanged iteratively between the two models until convergence is achieved. This process is known as model *linking*.

Although it is sometimes possible to integrate the two models into a single model, there are advantages to considering them as separate entities. One crucial benefit, as demonstrated in [5], is improved computational efficiency when the models are solved separately as linked models. This is particularly relevant due to the large size of energy system models. Linking methods explored thus far involve the mutual exchange of data between models, either manually (soft-linking) or through automated computer programs (hard-linking) [1]. The following sections provide an overview of well-known examples of soft- and hard-linking in the literature to emphasize their significance. Afterwards, the advantages of our contribution compared to the current approach are discussed.

2.1. Examples of soft-linking

The first example of soft-linking energy and economy models is reported in [6], which combines an econometric and a process analysis model to evaluate the impact of energy research, development, and demonstration policies in combination with tax and tariff policies to reduce imports of energy resources. After this first example, several other linking exercises have been carried out, where the transfer of information between models was directly controlled by the user, such as the example from [7]. Most of the early cases were focused on the linkage between a single sector without automating the transfer of data between models; for instance, [8] linked ETEM and GEM-E3 via residentials, while [9] link MARKAL and EPPA via the transport sector.

The best-known examples of soft-linking between economy and energy models are the cases of MESSAGE-MACRO [10], where the energy system model MESSAGE supplies energy costs/prices to MACRO, which in turn provides sectoral demand for energy commodities. Another notable example is the connection between MARKAL and EPPA [9], with the transport sector in the CGE model EPPA modified to mimic the behavior from the modal split in MARKAL. The modification involves the transport sector inputs and the related elasticity of substitution. MARKAL, in turn, receives data related to the change in fuel prices and transport demand. A third example of soft-linking is the one between MARKAL and MSG [11], which was used to investigate the energy demand in the Norwegian residential sector, while [12] used the same link to analyze the effects on Norway of a national CO2 tax and international CO2 quota prices. Yet another example of soft linking is the one between EMEC, a static CGE model, and the TIMES energy system model [13]. A last example of soft-linking multi-sector bottom-up (BU) and CGE models is the one presented by [14] where the authors compare the outcomes of three scenarios for the Portuguese energy and climate policy. An example of combining models via integration of the optimality conditions of the BU into the TD is introduced by [15], and extended by [16]. The macroeconomic model receives input for the energy mix and provides the change in energy demand to the energy system model.

2.2. Examples of hard-linking

Some examples of hard-linking between economic and energy system models are the ETA–MACRO model [17], MESSAGE–MACRO [18], which automates the soft-linking that was developed in [10], and MARKAL–MACRO, initially developed in [19] to stress the potential of linking procedures in facilitating the communication between policy-makers. The models all exchange electrical and other energy demands on one side and the structure of the cost functions on the other side. MARKAL and MACRO are hard-linked, with MACRO supplying energy demand and MARKAL providing supply costs. A multi-regional version of MARKAL–MACRO was employed in [20] to study the effects of emission reductions on international trade. MARKAL–MACRO has been applied to analyze energy policies in China [21], Italy [22], and the United Kingdom to study the long-term effects of a reduction in emissions [23], and to model the effects of energy policy [24].

Another notable case of hard linking is the one between TIAM and GEMINI-E3 [25]. GEMINI-E3 provides information about the key macroeconomic indicators, which are used to define the energy demand function which, in turn, feeds the TIAM energy system model. TIAM responds by providing the energy mix, investment costs, and technical progress on energy back to GEMINI-E3.

A more recent example of hard-linking is the one between IMACLIM–R, a CGE model for investigating climate and energy policies, and TIMES/POLES, two bottom-up energy system models used to study the effects of climate agreements and the impact of electric vehicle penetration in EU28 [26]. In this case, the BU model feeds the CGE model with energy import prices, primary energy output, energy intensities of non-energy productions, the energy consumption of households, capital intensity of energy suppliers and end-users, and energy exports while the CGE provides the BU model with GDP level, sectoral drivers and relative prices for capital and labor [26].

A final example of hard-linking is that between SAGE and SATIM in [27]. The CGE model SAGE provides electricity demand and fossil fuel prices to the energy system model SATIM, while SATIM provides the generation mix, the final electricity price, and the construction investment costs.

2.3. Positioning of this paper

In the studies above, the linked TD and BU models are solved by straightforwardly iterating between the TD and BU models until convergence is reached. However, this approach can be time-consuming, particularly when dealing with large BU models. In this paper, we propose a coordination algorithm that significantly reduces computation time for hard-linked TD and BU models. Instead of "naively" iterating between the TD and BU model, our algorithm utilizes previous optimal bases of the BU model to predict the optimal basis for the next iteration. If successful, this prediction allows us to skip the subsequent run of the BU model. Our contribution represents the first instance of a coordination algorithm for linked TD and BU models, offering a novel approach to tackle the computational challenges mentioned above.

3. Coordination algorithm

Consider a linked TD-BU model, in which the TD model is a mixed-complementarity problem (MCP) of the form

$$[\mathrm{TD}(y)] \qquad 0 \leq F(x,y) \perp x \geq 0, \tag{1}$$

typically representing the broad economy, and the BU model is a linear program (LP) of the form

$$[\mathrm{BU}(x)] \qquad \min_{y \in \mathbb{R}^n_+} \left\{ c^T y \mid Ay = b(x) \right\}, \tag{2}$$

typically representing a specific sector of the economy, e.g., the energy system in power generation and transmission expansion problems [15]. Traditionally, these BU models are solved stand-alone, taking macroeconomic data such as energy demand as exogenous parameters to the BU model. However, in reality, the solution to the BU model (e.g., decisions on the energy transmission network) affects these macroeconomic data. Hence, the parameters are *endogenous*. To explicitly account for this endogeneity, one can link the BU model to a TD model describing the full economy. A popular choice for the TD model are CGE models, which can be written in MCP form [28]. The resulting linked TD-BU model solves the BU model while taking the effects of the resulting TD solution into account.

When solving a linked TD-BU model, the aim is to find an equilibrium solution pair (x^*, y^*) that solves both models simultaneously. Typically, this is achieved by solving the TD and BU in an alternating fashion [29]. Given some starting value for x provided by the TD model, the BU model is solved, yielding a solution y. This solution is fed into the TD model, yielding a new solution x, which is fed into the BU model again. The process is repeated until some measure of convergence is satisfied, typically when the $\mathcal{L}_\infty$ norm of the difference between data passed from one model to another in two subsequent iterations falls below a given threshold. As mentioned in the introduction, this iterative process can be slow, especially when the BU model is large.

The remainder of this section presents our coordination algorithm for linked TD-BU models, aimed at expediting the solving process. The main idea, explained in Section 3.1, is to predict the BU solution using previously visited basis matrices. Section 3.2 describes how the prediction procedure can be incorporated into the TD problem. Finally, Section 3.3 outlines the coordination algorithm.

3.1. Main idea

To understand the main idea underlying our coordination algorithm, consider the BU model at a given solution $\bar{x}$ to the TD model:

$$\min_{y\in\mathbb{R}^n_+}\{c^T y \mid Ay = b(\bar{x})\}. \tag{3}$$

Assuming that the BU model has an optimal solution, it always has a basic optimal solution. That is, there exists a basis B (a submatrix of A) such that y with $y_B = B^{-1}b(\bar{x})$ and $y_N = 0$, is optimal, with subscript B and N referring to the basic and non-basic variables, respectively. Now, as one iterates with the TD problem, the value of $\bar{x}$ will change. Since the TD problems in subsequent iterations are typically similar, it is reasonable to expect that $\bar{x}$ will be close to its value in the previous iteration. If the right-hand side $b(\bar{x})$ is well-behaved (e.g., Lipschitz continuous in $\bar{x}$), one expects $b(\bar{x})$ to be close to its previous value, too. Hence, by a sensitivity argument, a reasonable prediction for the new BU solution $\bar{y}$ is given by $\bar{y}$, defined by $\tilde{y}_B = B^{-1}b(\bar{x})$ and $\tilde{y}_N = 0$. That is, the prediction states the optimal basis for the BU problem with $x = \bar{x}$ is the same as for the old value for x. This is the main idea underlying our coordination algorithm: *it uses an optimal basis from a previous iteration to predict the optimal basis in the current iteration and thus, the optimal solution to the current BU problem.*

One can do a better job at predicting, though, by making use of *all* previously encountered optimal bases and picking the *best* basis to construct a prediction. To understand how to find the best one, consider the dual of the BU problem (3) at the current TD solution $\bar{x}$, given by

$$\max_{u\in\mathbb{R}^m_+}\{u^T b(\bar{x}) \mid u^T A \le c^T\}. \tag{4}$$

Let B_k, $k \in \mathcal{K}$ be the collection of all dual feasible bases, i.e., the set of all bases for which the corresponding dual solution $u_k^T := c_{B_k}^T B_k^{-1}$ is feasible. Then the dual problem (4) can be written as

$$\max_{k\in\mathcal{K}}\{u_k^T b(\bar{x})\}. \tag{5}$$

Now suppose only a subset $K \subseteq \mathcal{K}$ of the dual feasible bases is available. In particular, suppose that K is the index set of all optimal bases found in previous iterations. Then, clearly, our best prediction among these bases is the basis that maximizes

$$\max_{k\in K}\{u_k^T b(\bar{x})\}. \tag{6}$$

Let k^* denote the optimal argument in (6). Then, define the best prediction to the BU problem as $\hat{y}$ with $\hat{y}_{B_{k^*}} = B_{k^*}^{-1}b(\bar{x})$ and $\hat{y}_{N_{k^*}} = 0$.

An important question is whether this prediction $\hat{y}$ is correct. It turns out that checking the correctness of our prediction boils down to the simple check that the vector $\hat{y}$ is non-negative.

Theorem 1. *Consider the BU problem (3) with $x = \bar{x}$ and let $\hat{y}$ be the primal solution corresponding to the dual feasible basis B_k, i.e., $\hat{y}_{B_k} = B_k^{-1}b(\bar{x})$ and $\hat{y}_{N_k} = 0$, where the index $k \in \mathcal{K}$ is given arbitrarily. Then, $\hat{y}$ is an optimal solution to the BU problem if and only if $\hat{y} \ge 0$.*

Proof. If any element of $\hat{y}$ is negative, then $\hat{y}$ is infeasible and hence, not optimal. It remains to prove that $\hat{y}$ is optimal if $\hat{y} \ge 0$. Suppose that $\hat{y} \ge 0$ holds true. Then, $\hat{y}$ is feasible, as it satisfies both the non-negativity constraints and, by construction, the constraint $A\hat{y} = b(\bar{x})$. Next, consider the dual solution $\hat{u} := c_{B_k}^T B_k^{-1}$. By definition of $k \in \mathcal{K}$, it follows that $\hat{u}$ is a dual feasible solution. Hence, $(\hat{y}, \hat{u})$ is a feasible primal/dual solution pair. Comparing the primal and dual objective at $\hat{y}$ and $\hat{u}$, respectively,

$$c^T\hat{y} = c_{B_k}^T\hat{y}_{B_k} + c_{N_k}^T 0 \tag{7}$$

$$= c_{B_k}^T B_k^{-1} b(\bar{x}) \tag{8}$$

$$= \hat{u}^T b(\bar{x}), \tag{9}$$

i.e., the primal and dual objective values are equal. By weak LP duality, it follows that $\hat{y}$ and $\hat{u}$ are optimal in the primal and dual problem, respectively. □

3.2. Incorporating predictions into the top-down problem

Interestingly, the predicting problem (6) can be incorporated into the TD problem. First, recognize that (6) can be written as an LP, whose optimal solution is characterized by the Karush–Kuhn–Tucker (KKT) conditions. Second, observe that these KKT conditions form an MCP. Combining this MCP with the MCP that constitutes the TD problem, a large MCP can be formed, called the *top-down master* (TDM) problem. The TDM problem simultaneously solves the TD problem and finds a prediction for the BU problem. This eliminates the need for solving the predicting problem (6) separately.

To specify this integration in more detail, first reformulate the predicting problem (6) as a linear program:

$$\min_\theta\{\theta \mid \theta \ge u_k^T b(\bar{x}),\ \forall k \in K\}. \tag{10}$$

The dual is given by

$$\max_{\eta\ge 0}\left\{\sum_{k\in K}\eta_k u_k^T b(\bar{x}) \mid \sum_{k\in K}\eta_k = 1\right\}. \tag{11}$$

The KKT conditions of this primal/dual pair, which are necessary and sufficient, are given by the MCP

$$\begin{cases} 0 \le \eta_k \perp \theta - u_k^T b(\bar{x}) \ge 0,\ \forall k \in K, \\ \sum_{k\in K}\eta_k = 1. \end{cases} \tag{12}$$

Integrating these KKT conditions into the TD problem yields our TDM problem at the current BU solution $\bar{y}$:

$$[\mathrm{TDM}_K(\bar{y})] \quad \begin{cases} 0 \le F(x,\bar{y}) \perp x \ge 0, \\ 0 \le \eta_k \perp \theta - u_k^T b(x) \ge 0,\ \forall k \in K, \\ \sum_{k\in K}\eta_k = 1. \end{cases} \tag{13}$$

Any positive η_k in a solution to this problem corresponds to a best-guess basis B_k. In the non-degenerate case, $\eta_k = 1$ for a single $k \in K$.

3.3. Algorithm outline

The stage has now been set to outline the full coordination algorithm. Pseudocode is provided in Algorithm 1. Initialize with an initial TD solution x_0 and an empty index set $K = \emptyset$ for previously visited bases. Next, the *outer loop* starts. In each outer iteration n, the BU problem is solved explicitly, yielding primal/dual solutions (y, u) and a corresponding optimal basis B_n that are added to the list indexed by K. The $TDM_K(\bar{y})$ problem is assumed to automatically incorporate the new dual solution.

Next, an *inner loop* is started. In each inner iteration, the TDM problem is solved, yielding a new TD solution x, which is used to update $\bar{x}$, and a solution η, indicating the active basis. If convergence is reached, the algorithm is stopped and the current TD-BU solution $(\bar{x}, \bar{y})$ is output. If not, the algorithm continues by computing the next BU prediction $\hat{y}$. If the prediction is correct (i.e., if $\hat{y} \ge 0$), a new inner iteration is started. Otherwise, jump out of the inner loop and start a new outer iteration. We denote by $\mathcal{M}(\hat{y}_{B_k})$ the mapping reallocating the elements of the basic solution into the vector of the overall solution $\hat{y}$.

3.4. Extension: endogenous cost vector

In our definition of the BU model in (2), the TD solution x is linked to the BU model through the endogenous right-hand-side vector $b(x)$ in the BU model. However, our coordination approach can be extended to a setting where instead the *cost vector* c of the BU model is endogenous, i.e., to BU models of the form

$$[\mathrm{BU}(x)] \qquad \min_{y\in\mathbb{R}^n_+}\{c(x)^T y \mid Ay = b\}. \tag{14}$$

The main idea is that by taking the dual of this BU problem, one obtains a dual problem that depends on x through its right-hand side vector:

$$\max_u\{u^T b \mid u^T A \le c(x)^T\}. \tag{15}$$

Algorithm 1: TD-BU Coordination Algorithm

$n \leftarrow 0$
$K \leftarrow \emptyset$
$\bar{x} \leftarrow x_0$
while true do // outer loop
  $n \leftarrow n + 1$
  Solve $\text{BU}(\bar{x}) \rightarrow (y; B; u)$
  $\bar{y} \leftarrow y$, $B_n \leftarrow B$, $u_n \leftarrow u$, $K \leftarrow K \cup \{n\}$
  while true do // inner loop
    Solve $\text{TDM}_K(\bar{y}) \rightarrow (x, \eta)$
    $\bar{x} \leftarrow x$
    if *convergence reached* **then**
      terminate. Output $(\bar{x}, \bar{y})$.
    end
    $k \leftarrow \text{argmax}_{k \in K} \eta_k$ // get active basis
    $\hat{y} \leftarrow \mathcal{M}(B_k^{-1} b(\bar{x}))$ // BU prediction
    if $\hat{y} \geq 0$ **then**
      $\bar{y} \leftarrow \hat{y}$ // prediction correct
    else
      break // back to outer loop
    end
  end
end

Introducing slack variables z, "splitting" the dual variables u into their positive and negative part, and changing the maximization to minimization, this can be reformulated as

$$\min_{\substack{u^+, u^- \\ z \geq 0}} \left\{ (u^- - u^+)^T b \mid (u^+ - u^-)^T A + z^T = c(x)^T \right\}, \tag{16}$$

which has the same structure as (2). Hence, the coordination algorithm can be applied to this reformulated BU problem.

It should be noted that our approach does not apply if the TD solution x is linked to the BU model through the right-hand-side vector b and the cost vector c *simultaneously*. The reason is that the dual feasible region of the BU model should remain the same for every x. This cannot be achieved if both b and c depend on x. Moreover, linking through the constraint matrix D is not possible either, since this would change the bases themselves.

3.5. Benders interpretation and graphical illustration

This section is concluded with an interpretation of our algorithm in terms of an analog of Benders' decomposition [3] of the combined TD-BU model (1)–(2). This interpretation has two benefits. First, it facilitates understanding of our coordination algorithm by framing it in terms of a well-known algorithm from the literature. Second, it allows us to illustrate the progression of our algorithm graphically, which is especially useful for understanding patterns of progression expressed in our numerical experiments. First, a short summary of Benders decomposition for linear programs is provided, followed by an explanation of how the coordination algorithm fits in this framework.

Benders' decomposition [3] was developed as a solution algorithm for linear programs. The outline of the algorithm is as follows. First, split the decision variables into two vectors, say, x and y. Let $Q(x)$ denote the optimal value of the subproblem in y if x is fixed. The main idea in Benders' decomposition is to iteratively construct an *outer approximation* $\mathcal{Q}$ of the function Q, by means of so-called *optimality cuts*. That is, $\mathcal{Q}$ is the maximum of a finite number of affine functions in x, each of which corresponds to an optimality cut. In every iteration, an optimality cut is generated by solving the dual of the subproblem in y at the current candidate solution of x. The *master problem* then consists of solving the original linear program but with the role of y replaced by the outer approximation $\mathcal{Q}(x)$ of $Q(x)$. Whenever $\mathcal{Q}(\bar{x})$ and $Q(\bar{x})$ coincide at a solution $\bar{x}$ to the master problem, the outer approximation $\mathcal{Q}$ of Q is "good enough" and convergence is reached: an optimal solution to the original linear program has been found.

Our coordination algorithm can be interpreted as an extension of Benders' decomposition to linked TD-BU models. To see this, start out with the combined TD-BU model (1)–(2). Denote by $Q(x)$ the optimal value of the "subproblem" BU(x), i.e.,

$$Q(x) = \min_{y \in \mathbb{R}^n_+} \left\{ c^T y \mid Ay = b(x) \right\}. \tag{17}$$

By the analysis in Section 3.1, it follows that

$$Q(x) = \max_{k \in \mathcal{K}} \left\{ u_k^T b(x) \right\}. \tag{18}$$

The prediction step in our coordination algorithm replaces this by the outer approximation

$$\mathcal{Q}(x) := \max_{k \in K} \left\{ u_k^T b(x) \right\}, \tag{19}$$

where the index set K corresponds to all previously visited bases. This outer approximation is the maximum over all "optimality cuts", which are represented by the functions $u_k^T b(x)$[1] in x, and which are iteratively generated by solving the dual of the subproblem $\text{BU}(\bar{x})$ if the predicted BU solution at a candidate TD solution $x = \bar{x}$ is incorrect.

One major difference between our coordination algorithm and traditional Benders' decomposition is that while traditional Benders' decomposition *minimizes* over the outer approximation $\mathcal{Q}(x)$ (jointly with the direct costs associated with x), the coordination algorithm merely uses $\mathcal{Q}(x)$ to predict the BU solution y. That is, it *evaluates* $\mathcal{Q}(x)$ at the current TD solution $\bar{x}$ and uses the resulting optimal index $k^* \in K$ in (19) to generate the prediction $\hat{y} := B_{k^*}^{-1} b(\bar{x})$ for the BU solution.

The interpretation above allows us to illustrate our coordination algorithm in terms of $Q(x)$ and $\mathcal{Q}(x)$. Fig. 1 illustrates two runs of the coordination algorithm with different convergence patterns. In the upper figure, the first iteration starts with some initial value x_1. The BU model $\text{BU}(x_1)$ is solved, yielding a BU solution y_1 and an optimal basis, which is added to the list. This optimal basis is represented in the figure by the downward-sloping dashed line. Solving $\text{TD}(y_1)$ yields a second TD solution x_2. In the second iteration, the algorithm predicts the solution to $\text{BU}(x_2)$ using the previously found basis. The prediction is incorrect, as is illustrated by the red dot and the fact that this dot is below the true value of $Q(x_2)$. Thus, $\text{BU}(x_2)$ is solved explicitly, yielding a solution y_2 and a new basis, illustrated by the upward-sloping dashed line. Solving $\text{TD}(y_2)$ yields a new TD solution x_3. In the third iteration, the prediction to $\text{BU}(x_3)$ is based on the best basis out of the two that have previously been visited. This best guess is the basis that corresponds to the dashed line that achieves the maximum at x_3. As can be seen from the green dot in the figure, the prediction is correct and $\text{BU}(x_3)$ need not be solved explicitly. The algorithm continues in this manner until convergence has been reached.

Note that the convergence pattern in the top image in Fig. 1 is "monotone", i.e., subsequent candidate solutions for x move in the same direction. This pattern guarantees that in every iteration, either the most recently visited basis is optimal or a new basis must be computed. In contrast, the lower figure shows an "oscillating" convergence pattern, in which case not only the most recent basis but also previously visited bases can be optimal. A priori, it cannot be excluded that an oscillating convergence pattern will arise. This is corroborated by Helgesen et al. [1], who indeed observe oscillating convergence patterns in some instances. This is also the reason why, in our algorithm, all previously visited basis matrices are stored, rather than only the most recent one.

[1] In our coordination algorithm, these functions need not be affine, in contrast with traditional Benders' decomposition for linear programs.

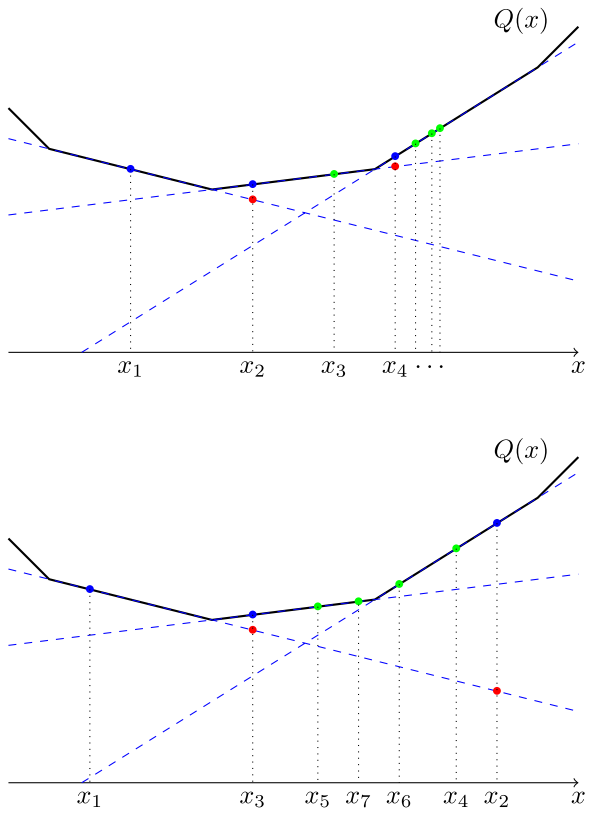

Fig. 1. An illustration of two runs of our coordination algorithm, with a monotone (top) and an oscillating (bottom) convergence pattern. Green dots represent points at which the predicted value of $Q(x)$ (and thus, the predicted BU solution) is correct; red dots represent incorrect predictions; blue dots represent points at which a new basis B_k is generated, corresponding to the optimality cut $u_k^T b(x)$ represented by the corresponding dashed blue line.

4. Numerical illustration

To illustrate the potential of the coordination algorithm from Section 3, this section applies it on a hard-linked TD-BU model from the literature. First, a short description of the model is given, followed by the numerical results. All data and code used in the work is publicly available in [30].

4.1. Model description

Consider the numerical example taken from the TD-BU model in Helgesen et al. [1] used to study the energy system impacts and economic impacts of reducing greenhouse gas emissions from transport. A concise description of the models is provided here; for more details, see Appendix.

The BU model considered here is an adaptation from [31] of the TIMES model in [32]. TIMES (The Integrated Markal Efom System) [33] is a techno-economic model generator for energy systems that describes the energy system considering resources, technologies, energy carriers, demand sources, and demand for energy services from both production sectors and consumption. The model is formulated as a linear program and aims to supply energy services at minimum total cost by making equipment decisions, as well as operating, primary energy supply, and energy trade decisions.

The TD model is a CGE model of the wider economy, featuring a simple nesting structure for the production functions. Capital and labor are aggregated according to a constant elasticity of substitution function and the result is further aggregated with intermediate goods according to a Leontief nest. In this context, it functions to describe

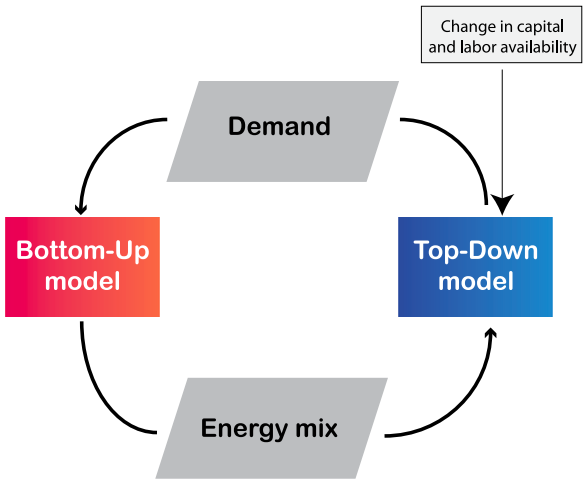

Fig. 2. Schematic overview of the linked models. The initial shock is defined as a change in the availability of capital and labor in the Top-Down CGE model. This shock leads to the computation of new demand projections for energy commodities, which are passed to the Bottom-Up energy system model which, in turn, will use this information to compute a new projection for the energy mix.

the effects of changes in the energy system on the demand for energy commodities.

The TD and BU models are hard-linked through the equations described in [1] and reported in Appendix. The energy mix from the BU solution is translated into Leontief coefficients for energy production factors in the TD model, while the TD solution provides input for the BU model in the form of projected demand for energy services. See Fig. 2 for an illustration of the linking.

The reason for using the TD-BU model from [1] to test our coordination algorithm is that it provides a known, published case study as a direct benchmark to our results. Moreover, the authors present the explicit formulas used to hard-link the TD and BU models to each other; these formulas are needed in order to be able to implement our coordination algorithm. Thus, testing our coordination algorithm on this TD-BU model yields an interesting proof-of-concept that can show the potential of our coordination algorithm.

4.2. Experiments

The coordination algorithm is tested on various instances of the linked TD-BU model described above. Instances are created by varying two parameters in the TD model: K and L. The parameter K represents the amount of capital present in the economy, while L represents the amount of labor. The values used in [1], indicated by K_0 and L_0, are used as a benchmark and these are varied using the formula $K = \alpha_K K_0$ and $L = \alpha_L L_0$. All combinations of the scaling values $\alpha_K, \alpha_L \in \{1.0, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3\}$ are used, i.e., in total, there are $7 \times 7 = 49$ experiments. (Values of α_K, α_L smaller than one are not considered to avoid feasibility issues.)

To test our coordination algorithm, it is compared with a "naive" benchmark algorithm that simply iterates between the TD and BU problem. Moreover, a version of this naive algorithm is included that uses a warm start in the BU model in the form of an advanced basis from the previous BU iteration. For each algorithm run, the following results are stored: (1) the optimal value of the final BU model, (2) the number of full TD models solved, (3) the number of TD (master) models solved, and (4) the computation time.

4.3. Results

This section discusses the results of the numerical experiments. It subsequently discusses initial sensibility checks, the algorithm's performance, and the algorithm's convergence behavior.

Table 1
Comparison of computational performance of the naive approach ("Naive"), the naive approach with warm starts in the BU model ("WS"), and the coordination algorithm ("Coord."). Columns with header "Impr." represent the improvement (in %) of the previous column with respect to the corresponding "Naive" column. Positive percentages indicate improvements; negative percentages represent deteriorations.

α_K	α_L	# BU models solved			Runtime (s)				
		Naive	Coord.	Impr.	Naive	WS	Impr.	Coord.	Impr.
1	1	27	1	96%	5.86	6.05	−3%	1.20	80%
1	1.05	24	1	96%	5.26	7.75	−47%	1.25	76%
1	1.1	21	1	95%	4.83	4.73	2%	0.98	80%
1	1.15	18	1	94%	4.75	3.97	16%	0.86	82%
1	1.2	16	2	88%	3.52	3.62	−3%	0.98	72%
1	1.25	15	2	87%	3.42	3.56	−4%	0.97	72%
1	1.3	13	2	85%	2.87	2.90	−1%	0.87	70%
1.05	1	25	2	92%	5.62	5.53	2%	1.30	77%
1.05	1.05	22	2	91%	4.88	4.87	0%	1.22	75%
1.05	1.1	18	1	94%	4.06	4.07	0%	0.89	78%
1.05	1.15	16	1	94%	3.64	3.54	3%	0.82	78%
1.05	1.2	15	2	87%	3.38	3.42	−1%	0.97	71%
1.05	1.25	14	2	86%	4.06	3.35	18%	0.92	77%
1.05	1.3	13	2	85%	2.97	3.04	−2%	0.90	70%
1.1	1	24	1	96%	5.26	5.33	−1%	1.07	80%
1.1	1.05	19	1	95%	4.72	4.23	10%	0.92	81%
1.1	1.1	17	1	94%	5.40	3.86	28%	0.82	85%
1.1	1.15	15	3	80%	4.83	3.37	30%	1.27	74%
1.1	1.2	14	2	86%	3.15	3.15	0%	0.91	71%
1.1	1.25	13	2	85%	2.92	2.95	−1%	0.88	70%
1.1	1.3	12	1	92%	2.71	2.71	0%	0.69	74%
1.15	1	22	2	91%	5.81	4.80	17%	1.20	79%
1.15	1.05	17	1	94%	5.81	3.74	36%	0.85	85%
1.15	1.1	16	3	81%	5.92	3.55	40%	1.19	80%
1.15	1.15	14	2	86%	3.59	3.05	15%	0.96	73%
1.15	1.2	13	1	92%	2.89	2.97	−3%	0.69	76%
1.15	1.25	12	1	92%	2.82	2.68	5%	0.66	77%
1.15	1.3	12	1	92%	2.67	2.72	−2%	0.67	75%
1.2	1	20	2	90%	4.43	4.73	−7%	1.16	74%
1.2	1.05	16	2	88%	3.69	3.94	−7%	0.98	74%
1.2	1.1	15	3	80%	3.51	3.65	−4%	1.14	67%
1.2	1.15	14	1	93%	4.50	3.47	23%	0.86	81%
1.2	1.2	13	1	92%	4.77	3.32	30%	0.69	86%
1.2	1.25	12	2	83%	4.37	2.92	33%	0.99	77%
1.2	1.3	11	1	91%	3.91	2.62	33%	0.61	84%
1.25	1	18	3	83%	6.60	4.34	34%	1.54	77%
1.25	1.05	15	3	80%	5.38	3.63	32%	1.26	77%
1.25	1.1	14	2	86%	5.52	3.36	39%	0.94	83%
1.25	1.15	13	2	85%	5.03	3.10	38%	0.89	82%
1.25	1.2	12	2	83%	3.05	2.95	3%	0.88	71%
1.25	1.25	12	1	92%	2.69	2.85	−6%	0.68	75%
1.25	1.3	11	2	82%	2.42	2.64	−9%	0.82	66%
1.3	1	18	18	0%	4.07	4.20	−3%	4.06	0%
1.3	1.05	14	2	86%	3.95	3.31	16%	0.97	75%
1.3	1.1	13	1	92%	4.98	3.13	37%	0.76	85%
1.3	1.15	12	1	92%	4.70	2.78	41%	0.85	82%
1.3	1.2	12	1	92%	5.32	2.93	45%	0.68	87%
1.3	1.25	11	1	91%	4.09	2.60	36%	0.64	84%
Average		**15.59**	**1.96**	**87%**	**4.26**	**3.65**	**12%**	**1.00**	**76%**

4.3.1. Sensibility checks

In all tested instances, the naive approach (with and without warm starts) and the coordination algorithm consistently converge and achieve the same BU optimal objective values. Additionally, the number of TD (master) problems is identical across algorithms in each instance. These observations confirm that all algorithms yield the same sequence of converging solutions. The distinction lies in the method of computing the BU solutions: solving the BU model from scratch, solving with a warm start, or predicting the BU solution in the inner loop.

4.3.2. Performance

Results on the computational performance of the different algorithms are presented in Table 1. The approaches compared are the naive approach of iteratively solving the TD and BU model, the naive approach with warm starts in the BU model, and the coordination algorithm.

Using the naive approach, the linked TD-BU model needs to solve 15.59 BU models on average until convergence is reached. The idea behind our coordination approach is that it can speed up computation by skipping some of these runs by correctly predicting the BU solution using previous optimal bases. Indeed, observe that on average, our coordination algorithm only needs to solve 1.96 BU models to reach convergence. In fact, in many instances merely *one* BU model is needed. Hence, in the vast majority of iterations, the optimal basis for the BU model was already observed before, and the coordination algorithm is able to skip many of the computations. On average, in the 16 iterations needed to reach convergence on average, only 2 different optimal bases are used. Thus, using the coordination algorithm allows us to eliminate 87% of the BU runs.

In terms of computation times, the effects are also significantly noticeable. Using the naive approach, the average computation time is 4.26 s. Our coordination algorithm outperforms this approach in all instances. On average, it solves an instance in 1.00 s, with an average time gain of 76% compared to the naive approach. Hence, the fact that the coordination algorithm can skip most of the BU runs indeed

drastically reduces computation times. This shows the effectiveness of our approach.

Next, the performance of a naive approach using warm starts in the BU runs is analyzed. On average, this warm-start approach yields computation times of 3.65 s. Compared with the naive approach without warm starts, this constitutes an average time gain of 12%. Our coordination algorithm is more than three times faster on average than the warm-start approach, though. This can be explained by the fact that the coordination algorithm does not simply leverage the optimal BU basis of the previous iteration to warm start the BU problem in the next iteration but uses it to provide an exact solution of the BU model without actually summoning the BU model. Moreover, providing an advanced basis is not always helpful as the pre-solving algorithms of many solvers may cause the advanced basis to be ignored [34]. This latter point is confirmed in a number of our test instances, in which warm starts actually increase the computation time (e.g., $\alpha_K = \alpha_L = 1$). Thus, while the idea underlying our coordination algorithm is close to that of using a warm start, the coordination algorithm performs significantly better.

It must be noted that it cannot be guaranteed that the coordination algorithm always outperforms the naive approach. In particular, one instance has been observed ($\alpha_K = 1.3, \alpha_L = 1$) where every iteration, a new basis is optimal in the BU model. Hence, the coordination approach is not able to yield any computational gains in this instance. However, this behavior has only been observed in a single instance; all other instances showed significant improvement in performance. Moreover, the computational burden imposed by the prediction step in our coordination algorithm is typically negligible, as is confirmed by the equal computation times of the naive approach and the coordination algorithm in the instance mentioned above. So even if one is unlucky and the coordination algorithm does not yield any performance gains, it is not expected to negatively affect computation times.

4.3.3. Coordination algorithm behavior

Finally, the behavior of the coordination algorithm is investigated in more detail. For this purpose, some (representative) runs of the algorithm are illustrated in Fig. 3. In the figure, the red bars denote iterations in which the BU model is solved to compute an optimal basis, whereas the green bars denote iterations in which the optimal basis is computed within the inner loop (i.e., using the prediction formula).

The top graph denotes Case 0, which corresponds to a typical run of the naive algorithm: every iteration, the BU model is solved from scratch, regardless of whether the optimal basis has been observed before or not. The coordination algorithm improves upon this by skipping some (hopefully many) of these iterations using the prediction formula. A typical case can be seen in Case 3, where only a single basis is computed in the first iteration, which remains optimal during all subsequent iterations. This happens in 23 out of the 49 instances considered in our experiments.

Next, consider instances in which the coordination algorithm uses more than one basis. From Table 2 observe that in such instances, the second basis is found after 2.58 iterations of the inner loop on average. In instances with at least three bases stored, the average number of inner iterations until the third basis is found is 3.67. The largest number of inner iterations observed until all bases were added is merely six. These results show that the coordination algorithm typically needs only a few iterations to find a set of bases that contains an optimal one. The remainder of the algorithm merely iterates between the TD model and the BU prediction formula.

Second, it was observed that for all instances, in all iterations in which the predicted BU solution is correct, the optimal basis is the *most recently added* basis. That is, it has not been observed that the coordination algorithm picks up an "old" basis. The reason for this "monotone" behavior is likely due to the fact that the solutions in subsequent iterations of the algorithm move more or less "monotonically" in a certain direction, as illustrated in the top image in Fig. 1. It is suspected that a different algorithmic behavior might be observed in problems that converge to their solution in a less "monotone" way, but exhibit an "oscillating" pattern, as illustrated in the bottom image in Fig. 1.

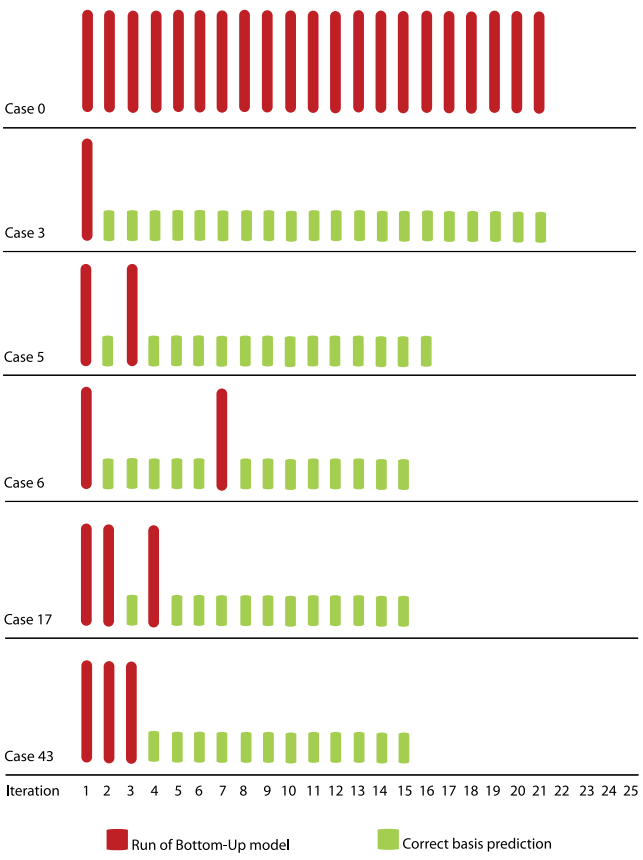

Fig. 3. Behavior of the algorithm for a selection of the cases in Table 1. The red bars represent the computation of a solution of the BU model, while the green bars represent the usage of a previously visited basis.

Table 2
Computational results related to the addition of new bases in the coordination algorithm. The first row indicates the number of instances with the indicated number of bases added in the coordination algorithm. The other columns indicate the average iteration in which the first, second, or third basis was added, if applicable.

# bases	≥ 1	≥ 2	≥ 3
# instances	49	26	6
avg. iteration added	1	2.58	3.67

5. Conclusion

This paper proposes a coordination algorithm for linked TD-BU models. The main idea behind the approach is to *predict* BU solutions by making use of optimal basis matrices found in previous iterations. The prediction procedure can be written in terms of an MCP and can be incorporated into the TD model. Checking if the prediction is correct is very easy: it is equivalent to checking if the predicted BU solution is non-negative. If the prediction is correct, one can skip solving the BU model and hence, greatly reduce the computation time in the corresponding iteration.

The coordination algorithm is tested using a numerical illustration of an energy system design problem. The results show that the coordination algorithm reduces the number of times the BU problem needs to be solved by 87% on average while reducing the computation time by

76% on average. Moreover, our algorithm significantly outperforms a procedure using warm starts in the form of an advanced basis, which speeds up computation times by only 12% on average. These results illustrate the potential of the coordination algorithm to significantly speed up the time needed to solve linked TD-BU models.

Our coordination algorithm may open the door to solving larger-scale linked TD-BU models that have thus far been computationally intractable. Future research may be aimed at numerically testing this claim numerically by applying our coordination algorithm on larger-scale linked TD-BU models. An interesting question in this regard is whether the relative time gain resulting from using the coordination algorithm tends to become more or less significant as the size of the problem increases.

Another direction for future research would be to investigate how the performance of our coordination algorithm depends on the convergence pattern observed in the TD-BU model at hand. In particular, it would be interesting to investigate whether the "monotone" behavior of our coordination algorithm described in Section 4.3.3 carries over to problems that do not converge as "monotonically" as the problem considered in our experiments.

Finally, future research may extend our coordination algorithm to TD-BU models with more general linking structures. Currently, our approach is only applicable if the TD solution x is linked to the BU model through either the right-hand side b or the cost vector c, but not both simultaneously. Using new algorithmic ideas, it might be possible to extend our approach to handle simultaneously linked b and c, or a linked coefficient matrix A. In the same vein, extensions may be possible to settings where the BU is not a linear program, but a mixed-integer linear program or a quadratic program, for instance.

CRediT authorship contribution statement

Paolo Pisciella: Conceptualization, Methodology, Software, Writing – original draft. **E. Ruben van Beesten:** Software, Formal analysis, Writing – original draft. **Asgeir Tomasgard:** Funding acquisition, Writing – review & editing.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Paolo Pisciella reports financial support was provided by Research Council of Norway.

Data availability

The data and code are freely available on Github [30]. The link to the GitHub page has been referenced in the article.

Acknowledgments

We are grateful to the Research Council of Norway for funding this work through the project "Norwegian Energy Roadmap" (Grant number: 255100). We thank Per-Ivar Helgesen for sharing the code for the linked TD-BU model from [1], which we used in our numerical analyses.

Appendix. Model formulation

This appendix provides the mathematical formulation of the TD and BU models used in Section 4. The models are taken from Helgesen et al. [1]. Below, the BU and TD models are first described in some detail, followed by a description of how they are linked.

A.1. Bottom-up model

Sets

T	Time periods in BU model, indexed by t and τ.
P	Processes in BU model, indexed by p.
$P_{\text{prod}} \subseteq P$	Production processes (as opposed to supply and demand processes).
$P_c^{\text{in}} \subseteq P$	Processes with commodity c as input
$P_c^{\text{out}} \subseteq P$	Processes with commodity c as output.
C	Commodities in BU model, indexed by c.
$C_{\text{sup}} \subseteq C$	Naturally supplied commodities.
$C_{\text{prod}} \subseteq C$	Produced commodities.

Parameters

$C_{t,p}^{\text{cap}}$	Capacity investment cost for process p in year t.
$C_{t,p}^{\text{fom}}$	Fixed operating and maintenance cost for process p in year t.
$C_{t,p}^{\text{act}}$	Activity cost in year t for process p.
$C_{t,c}^{\text{prd}}$	Production cost for commodity c in year t.
A_p^f	Availability factor for process p.
α_p^{capact}	Capacity factor in process p.
$\phi_{p,c,c'}$	Flow conversion factor in process p from commodity c to c'.
$D_{t,c}$	Demand in year t for commodity c.
$I_{t_0,p}^{\text{cap}}$	Existing capacity in base year (t_0) for process p.
$U_{t,p}^{\text{cap}}$	Upper bound on capacity investment for process p in year t.
$S_{t,p}$	Salvage value in horizon year (t_{end}) from investment in process p in year t.
L_p	Technical lifetime (number of years) on investment in process p.
$\rho_{t,p}$	Remaining share of capacity from base year ($I_{t_0,p}^{\text{cap}}$) in year t of process p.

Variables

$i_{t,p}^{\text{cap}}$	Capacity investment in year t in process p.
$x_{t,p}^{\text{act}}$	Activity in year t in process p.
$x_{t,c}^{\text{prd}}$	Production of commodity p in year t.

The BU model is formulated as a linear program and aims to supply energy services at minimum total cost by making equipment decisions, as well as operating, primary energy supply, and energy trade decisions. The model considers the production of electricity either from hydropower or from gas to cover the demand of a single region using a yearly time slice. The mathematical formulation of the bottom-up model is given by

$$\min_{i_{t,p}^{\text{cap}}, x_{t,p}^{\text{act}}, x_{t,c}^{\text{prd}}} \sum_{t=t_0}^{t_{\text{end}}} \sum_{p \in P} \Bigg[\sum_{\tau=t}^{\min(t_{\text{end}}, t+L_p-1)} C_{\tau,p}^{\text{fom}} i_{t,p}^{\text{cap}} + C_{t,p}^{\text{act}} x_{t,p}^{\text{act}} + (1 - S_{t,p}) C_{t,p}^{\text{cap}} i_{t,p}^{\text{cap}} \Bigg] + \sum_{t=t_0}^{t_{\text{end}}} \sum_{c \in C} C_{t,c}^{\text{prd}} x_{t,c}^{\text{prd}} \tag{20}$$

subject to

$$x_{t,p}^{\text{act}} \leq \sum_{\tau=\max(t_0, t-L_p+1)}^{t} A_p^f \alpha_p^{\text{capact}} i_{\tau,p}^{\text{cap}} + A_p^f \alpha_p^{\text{capact}} \rho_{t,p} I_{t_0,p}^{\text{cap}}, \qquad t \in T,\ p \in P_{\text{prod}}, \tag{21}$$

$$D_{t,c} + \sum_{\substack{p \in P_c^{\text{in}} \\ c' \in C}} \frac{x_{t,p}^{\text{act}}}{\phi_{p,c,c'}} \leq \sum_{p \in P_c^{\text{out}}} x_{t,p}^{\text{act}}, \quad t \in T,\ c \in C \setminus C_{\text{sup}}, \tag{22}$$

$$x_{t,c}^{\text{prd}} = \sum_{P_c^{\text{out}}} x_{t,p}^{\text{act}}, \qquad t \in T,\ c \in C, \tag{23}$$

$$i_{t,p}^{\text{cap}} \le U_{t,p}^{\text{cap}}, \qquad t \in T,\ p \in P. \tag{24}$$

$$i_{t,p}^{\text{cap}}, x_{t,p}^{\text{act}}, x_{t,c}^{\text{prd}} \ge 0 \tag{25}$$

The objective function (20) expresses the minimization of the total system costs, also considering the residual value of the plant after the planning horizon has been passed. Constraints (21) require that the activity level of a process p does not exceed its capacity; constraints (22) ensure the coverage of the final and intermediate demand for each commodity c; constraints (23) require that the total production level of each commodity c coincides with the sum of the process activities used to produce such commodity; constraints (24) define the upper bounds on expansion capacity. For a more detailed discussion of the BU model, see [1].

A.2. Top-down model

The TD model describes a static closed economy. Structurally, it is a CGE featuring a simple nesting structure for the production functions, where capital and labor are aggregated according to a constant elasticity of substitution (CES) function, and the result is further aggregated with intermediate goods according to a Leontief nest.

The considered economy consists of four sectors, each producing a single good, and a representative household. The exchanged goods are gas, electricity (ele), manufacturing (man), and non-manufacturing (non). Capital and labor are the two resources provided by the households to the production sectors. The income received from lending capital and labor to the production sectors is used to purchase the produced goods according to a utility maximization approach. Namely, a Stone–Geary utility function is used to model the purchase behavior of the households, which is translated into a linear expenditure system (as described in Goldberger and Gamalestos [35]). The social accounting matrix (SAM) in Table 3 is used as data describing the monetary exchanges in the base year.

The TD model is formulated by considering three groups of conditions: a zero-profit condition, requiring no activity from the production sectors when there are losses, a market clearing condition requiring that a positive price provides a balance between demand and supply of each commodity, and an income balance condition requiring that the income obtained by lending the resources to the production sectors is spent for consumption. The notation is given below.

Sets

I	Economic sectors; $I = \{\text{gas, ele, man, non}\}$

Parameters

KS	Capital endowment (given in the SAM).
LS	Labor endowment (given in the SAM).
$io_{i,j}$	Amount of good i to produce one unit of output j.
σ_i^F	Elasticity of substitution between capital and labor in sector i.
γ_i^F	Cost share for capital in sector i.
a_i^F	Efficiency parameter CES production function for sector i.
α_i^h	Household percent share of budget allocated to consumption of good i.
μ_i^h	Household subsistence level of good i.

Variables

p_l	Price of labor (wage rate).
p_k	Price of capital (return to capital).
p_i	Price of good i.
x_i	Production good i.
h	Household income.
L_i	Demand for labor from sector i.
K_i	Demand for capital from sector i.

Table 3
Social accounting matrix (SAM).

	gas	ele	man	non	L	K	hou	*Tot*
gas		4	2	3			1	10
ele	1	1	7	8			5	22
man	1	3	6	26			2	38
non	5	10	10	30			92	147
L	1	1	5	53				60
K	2	3	8	27				40
hou					60	40		100
Tot	10	22	38	147	60	40	100	

The mathematical formulation of the top-down model is as follows. The zero profit condition is given by

$$0 \le p_l \cdot L_i + p_k \cdot K_i + \sum_{j \in I} p_j io_{j,i} x_i - p_i \cdot x_i \perp x_i \ge 0, \quad i \in I. \tag{26}$$

The market clearing conditions for goods are given by

$$0 \le x_i - \mu_i^h - \frac{\alpha_i^h}{p_i}\left(h - \sum_{j \in I} p_j \mu_j^h\right) - \sum_{j \in I} io_{i,j} x_j \perp p_i \ge 0, \quad i \in I. \tag{27}$$

The market clearing condition for labor is given by

$$0 \le LS - \sum_{i \in I} L_i \perp p_l \ge 0, \tag{28}$$

where, for every $i \in I$,

$$L_i = \frac{x_i}{a_i^F}\left(\frac{1-\gamma_i^F}{p_l}\right)^{\sigma_i^F} \tag{29}$$

$$\times \left(\gamma^{G\sigma_i^F} \cdot p_k^{1-\sigma_i^F} (1-\gamma^{G\sigma_i^F})^{\sigma_i^F} \cdot p_l^{1-\sigma_i^F}\right)^{\left(\frac{\sigma_i^F}{1-\sigma_i^F}\right)}. \tag{30}$$

The market clearing condition for capital is given by

$$0 \le KS - \sum_{i \in I} K_i \perp p_k \ge 0, \tag{31}$$

where, for every $i \in I$, K_i equals

$$K_i = \frac{x_i}{a_i^F}\left(\frac{\gamma_i^F}{p_k}\right)^{\sigma_i^F} \tag{32}$$

$$\times \left(\gamma^{G\sigma_i^F} \cdot p_k^{1-\sigma_i^F} (1-\gamma^{G\sigma_i^F})^{\sigma_i^F} \cdot p_l^{1-\sigma_i^F}\right)^{\left(\frac{\sigma_i^F}{1-\sigma_i^F}\right)}. \tag{33}$$

Finally, the income balance condition is given by

$$h = p_k \cdot KS + p_l \cdot LS, \tag{34}$$

with associated dual variable h.

Condition (26) states that a positive production from sector $i \in I$ is possible only if all the production factors are compensated. Condition (27) states that a positive price will ensure that the supply of goods is equal to their demand, while a zero price will be considered in case of excess supply. Similar conditions are established for the demand and supply of labor and capital in (28) and (31). Finally, condition (34) states that the total budget used for consumption is formed as compensation for the lending of capital and labor to the production sectors.

The system is homogeneous of degree one in prices, which means that there is an infinite number of solutions, each differing by a multiplicative scalar for prices. As a consequence, prices are only relevant in terms of their relative value compared to a numéraire. The wage rate p_l is defined as numéraire and its value is fixed to 1. The model assumes no savings, exogenously fixed endowments of capital and labor, no government, and is defined as static. This last feature implies that, in this simple model, the state of the economy at the end of the planning horizon is projected by setting capital and labor force at the values that are expected to be found in that last period and computing the resulting equilibrium. For a more detailed discussion of the TD model, see [1].

A.3. Linking the top-downand bottom-up model

The energy mix from the BU solution is translated into Leontief coefficients for energy production factors in the TD model, while the TD solution provides input for the BU model in the form of projected demand for energy services. See Fig. 2 for an illustration of the linking.

Specifically, the formula for the Leontief coefficient $io_{\text{gas,ele}}$ in the TD model is

$$io_{\text{gas,ele}} = \frac{x^{\text{act}}_{t_{\text{end}},\text{gaspower}}}{x^{\text{act}}_{t_{\text{end}},\text{electricitydemand}}}, \tag{35}$$

where $x^{\text{act}}_{t_{\text{end}},\text{gaspower}}$ and $x^{\text{act}}_{t_{\text{end}},\text{electricitydemand}}$ are the activity levels of producing electricity using gas and of electricity demand, respectively, in the BU model solution.

Moreover, the formula for the projected demand for energy services $D_{t,c}$ in the BU model is

$$D_{t,c} = D_{t_0,c} + D_{t_0,c} \cdot \frac{x_{\text{gas}} + x_{\text{ele}} - x^0_{\text{gas}} - x^0_{\text{ele}}}{x^0_{\text{gas}} + x^0_{\text{ele}}} \cdot \frac{t - t_0}{t_{\text{end}} - t_0}, \tag{36}$$

for every $t \in T,\ c \in C$, where x_{gas} and x_{ele} are the projected demand of gas and electricity, respectively, at the end of the modeling horizon in the TD model, and x^0_{gas} and x^0_{ele} are the corresponding initial values. In our framework $\left[x_{\text{gas}}, x_{\text{ele}}\right]$ corresponds to x in the algorithm, while $\left[x^{\text{act}}_{t_{\text{end}},\text{gaspower}}, x^{\text{act}}_{t_{\text{end}},\text{electricitydemand}}\right]$ corresponds to y in the algorithm.

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