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Integrated solutions and distributed models' linkage procedures for food-energy-water-environmental NEXUS security modeling and management

T.Y. Ermolieva[1], A.G. Zagorodny[2,3,4], V.L. Bogdanov[3,4,5], P. Havlik[1], E. Rovenskaja[1], N. Komendantova[1], P.S. Knopov[6]

[1]International Institute for Applied Systems Analysis, Laxenburg, Austria
[2]National Academy of Sciences of Ukraine, Kyiv, Ukraine
[3]Bogolyubov Institute for Theoretical Physics of NAS of Ukraine, Kyiv, Ukraine
[4]State Institution "Center for evaluation of activity of research institutions and scientific support of regional development of Ukraine NAS of Ukraine", Kyiv, Ukraine
[5]S.P. Timoshenko Institute of Mechanics of NAS of Ukraine, Kyiv, Ukraine
[6]Institute of Cybernetics, NAS of Ukraine, Kyiv, Ukraine

Corresponding author: Tatiana Y. Ermolieva, ermol@iiasa.ac.at

Abstract

This paper discusses a new modelling approach enabling the linkage of distributed individual food, energy, water optimization models under joint (e.g., water, land) resource constraints, uncertainty, and asymmetric information. The approach is based on an iterative stochastic quasigradeint (SQG) solution procedure of, in general, nonsmooth nondifferentiable optimization. The SQG procedure organizes an iterative computerized negotiation between individual FEW systems (models) representing Intelligent Agents. The convergence of the procedure to the socially optimal solution is based on the results of nondifferentiable optimization providing a new type of machine learning algorithms. The linkage problem can be viewed as a general endogenous reinforced learning problem. The models act as "agents" that communicate with a "central hub" (a regulator) and take decisions in order to maximize the "cumulative reward". In this way, they continue to be the same individual models and different modeling teams do not need to exchange information about their models – instead, they only need to harmonize the inputs and outputs that are part of the joint resource constraints. In this way, the agents link their models into an integrated model under asymmetric information. The convergence of the solution of the linked models to the solution of the hard-integrated model is discussed. Application of the approach is illustrated with a case study linking distributed agricultural, water and energy sector models. The approach can be effectively used for decentralized deregulated planning of interdependent agricultural, energy, water systems.

Key words: Food-energy-water nexus, distributed models, uncertainty and asymmetric information, integrated modeling, models' linkage, SQG solution procedure, non-smooth optimization, subgradient, integrated modeling, food-energy-water-environmental nexus.

1.1. Introduction

The increasing interdependencies among food-energy-water-environmental (FEWE) sectors require integrated coherent planning and coordinated policies for sustainable development and nexus security. The sectors become more interconnected because they utilize common, often rather limited, resources, both natural (e.g., land, water, air quality) and socio-economic (e.g., investments, labor force). For example, land and water are needed not only for agricultural production, but also for hydropower generation, coal mining and processing, power plants cooling, renewable energy, and hydrogen production.

Detailed sectoral and regional models have traditionally been used to anticipate and plan desirable developments of respective sectors and regions. These models operate with a set of feasible decisions and aim to select a solution optimizing a sector- or region-specific objective function. When interdependencies between sectors and regions are increasing, such an independent analysis without accounting for interconnections can become misleading and even dangerous. Hence, it is necessary to link together the sectoral (regional) models to derive truly integrated solutions. Interdependent Food-Energy-Water-Environmental (FEWE) security goals contribute immensely to signifying the nexus security between sectors and regions (Zagorodny, Ermoliev, Bogdanov *et al*. 2020; Ermolieva *et al*. 2021; Zagorodny, Bogdanov *et al*. 2024; Zagorodny, Bogdanov, Zaporozhets 2024).

In this paper we consider the problem of linking individual sectoral and/or regional linear programming (LP) models into a cross-sectoral integrated model (IM) in the presence of joint constraints when "private" information about the models is not available or it cannot be shared by modeling teams (sectoral agencies), i.e., under asymmetric information (ASI). The approach provides a means of decentralized cross-sectoral coordination and enables to investigate policies in interdependent systems in a "decentralized" fashion. This enables more stable and resilient systems' performance and resource allocation as compared to the independent policies designed by separate models without accounting for interdependencies.

Limited resources can be allocated between systems (sectors/regions) in many ways. For example, Böhringer and Rutherford (2009) consider integrating mathematical programming models of the energy system into a general equilibrium (GE) model of the overall economy. Unfortunately, the convergence of the iterative procedure integrating the models could not be proven. For resource and production allocation with the generalized Nash equilibrium (GNE) approach, the existence, uniqueness, and stability of the GNE, and a realistic large-scale implementation of this concept, cannot be guaranteed. Ermoliev and von Winterfeldt (2012) demonstrate the complexity of the game-theoretic approaches, e.g., the Stackelberg leadership model, emerging due to quite unrealistic assumptions that each player (sector/region) possesses the knowledge about other players.

Traditional integrated deterministic optimization modeling incorporates goals, constraints, and data of all models into a single code (hard integration), which can be considered as a multi-criteria optimization problem (Ogryczak 2000). In the case of separate distributed models' and ASI, the linkage requires (see section 1.2.2-1.2.4) specific nonsmooth optimization methods. Problems under ASI are addressed with the agency theory (Gaivoronski and Werner 2012), in particular, on how to motivate information exchange. In this paper we consider, in a sense, the opposite, we minimize the necessity to exchange information.

Our approach for linking separate optimization models under ASI is based on the parallel solving of equivalent nonsmooth optimization models by an iterative stochastic quasigradient (SQG) procedure (Ermoliev 1976; Ermoliev 2009) based on subgradients or generalised gradients (Ermoliev 1976; Rockafeller 1981; Ermoliev and Norkin 1997) converging to an optimal welfare maximizing linkage solution, i.e., to the solution of a "hard-integrated" model (Ermoliev *et al.* 2022). The approach does not require to share details about models' specification. We can assume, there is a network of distributed computers connecting individual computer models with the computer of a "social planner" (decision-makers or regulatory agencies), who attempts to achieve the best result for all sectors/regions (parties) involved. The linkage procedure can be interpreted as a kind of a "decentralized market system" (Ermoliev and Ermolieva *et al.* 2015 and references therein). According to this procedure, the optimization of sectoral/regional goals under individual constraints is performed independently and in parallel, without considering joint constraints. Joint constraints can be imposed on total production, natural and financial resource use, emissions, pollution, joint food-energy-water-environmental (FEWE) security targets. The constraints can establish supply-demand relationships between the systems enabling to estimate optimal production, resource use, and emission quotas for each system. The balance between the total energy (including biofuels) production and demand defines energy security; agricultural production and consumption reflect food security; total emissions and pollution constraints correspond to environmental security. The joint FEWE constraints satisfaction establishes the FEWE security nexus (Zagorodny and Ermoliev 2013; Ermolieva and Havlik *et al.* 2016, 2021; Zagorodny *et al.* 2020, 2024). After the independent optimization using initial approximations of various (e.g., production, resource use, emission) quotas, the sectors/regions provide social planner with the information on their actual production, resource use, and respective shadow prices. The planner checks if the joint constraints are fulfilled. If not, i.e., there is "excess demand" or "excess supply" (i.e., total resource use, production, emissions by all systems are higher/lower than required), the planner revises the individual systems' quotas via shifting their current approximation in the direction defined by the corresponding dual variables. Thus, shadow prices signal systems to adjust their activities accordingly. Formally, the procedure is described in sections 1.2.3 - 1.2.5.

In this way, the linkage allows to avoid "hard linking" of the models in a single code, which is not possible because the systems (agencies) may not want to share the information or because the individual models are too detailed and complex to be "hard-linked". The approach saves reprogramming efforts and enables parallel distributed (decentralized) computations of sectoral models instead of a large-scale integrated (centralized) model. This also preserves the original models in their initial state for other linkages. The use of detailed sectoral and regional models instead of their aggregated simplified versions enables also to account for critically important local details. Similar computerized decentralized "negotiation" processes between distributed models (agents) have been developed for the design of robust carbon trading markets (e.g. (Ermoliev and Ermolieva *et al.* 2015 and references therein). The linkage procedure can be considered as a new machine learning algorithm, namely, as a general endogenous reinforced learning problem of how software agents (models) take decisions in order to maximize the cumulative reward (total welfare) (Ermolieva and Ermoliev *et al.* 2021)

The paper is organized as follows. Section 1.2 discusses the problem of models' linkage under joint constraints. Section 1.2.1 presents a short overview and main shortfalls of several existing approaches, section 1.2.2 formulates the problem of distributed LP models' linkage in the presence of joint resource constraints and ASI, sections 1.2.3-1.2.5 outline the details and the main properties of the linkage solution procedure based on the parallel solving of equivalent nonsmooth optimization model following a simple iterative subgradient algorithm. Section 1.3 illustrates the application of the methodology to link detailed energy and agricultural production planning models under joint constraints on water and land use. In addition, the joint constraints can impose restrictions on total energy production by energy sector (electricity, gas, diesel, etc.) and land use sector (biodiesel, methanol); total energy use by energy and agricultural sectors; total agricultural production by distributed farmers/regions. Section 1.4 concludes and outlines potential further extensions of the approach, for example, to include more details of energy and natural resources dynamics in general.

1.2. Linking distributed optimization models under joint resource constraints

1.2.1. *Social equilibrium game*

In the absence of coordination between systems (sectors, regions), they can act selfishly and aim at maximizing their own objective function. They attempt to secure as high resource quotas as possible. Such situation can be modeled using the non-cooperative game-theoretic framework. For example, social equilibrium games (Harker 1991) have been formulated to include joint constraints. The generalized Nash equilibrium (GNE) solution, if it exists, allocates production and resources among systems (sectors/regions) fulfilling the joint constraint. However, the decisions are made independently and collective efforts for managing common resources are ignored. Important, that the existence, uniqueness, and stability of the GNE, as well as a realistic large-scale implementation of this concept, cannot be guaranteed as emphasized by Harker (1991). Moreover, in Harker (1991) it is highlighted that the

GNE solutions set is rarely connected. Hence, a complete analysis of equilibriums in this case is a complex task, requiring additional assumptions.

The analysis can become even more complex if the joint constraints are based on the equilibrium (optimality) conditions arising from the problem formulated in the form of a principal-agent game or a leader-follower Stackelberg game (Ermoliev and von Winterfeldt 2012). For example, in the case of nonsmooth goal functions required for linking systems under ASI (distributed models' optimization), the use of optimality conditions would require implicit sets of generalized gradients. Due to the computational complexity, heuristic methods are often used, however, they are lacking a rigorous convergence proof.

Linking bottom-up mathematical programming models of the energy system into a top-down general equilibrium model of the overall economy is discussed by Böhringer and Rutherford (2009). The paper shows, that the formulation of market equilibrium conditions by using complementarity equations permit integration of models, but the convergence of the iterative procedure integrating the models cannot be guaranteed. In specific cases, models of general equilibrium are reduced to optimization problems (Norkin 1999).

Ermoliev and von Winterfeldt (2012) demonstrate that the complexity of the game-theoretic approaches is due to quite unrealistic assumptions that each player (sector/region) is in the possession of the knowledge on exact and unique responses of other players. Therefore, even in the simplest linear cases, this assumption leads to extremely complex discontinuous problems. More realistic assumptions of uncertain response functions in combination with a concept of robust decisions results in stable large-scale solutions.

There exists a vast literature on important problems and methods for distributed systems' optimization (Yang *et al.* 2019) under joint constraints, e.g., optimal control and economic dispatch in smart grids (Prakash and Nygard 2017), agricultural production planning for the multi-farmer systems (Alemany et al. 2021), network optimization (Liang et al. 2019), optimal transportation problems (Dean and Cortés 2015; Galichon 2016). Yet, these approaches consider optimization of a total objective function representing a sum of individual objective functions of the involved systems. Thus, the problems assume full information is available to a social planner about the systems. They are formulated similarly to the traditional integrated "centralized" optimization modeling combining goals, constraints, and data of all models into a single code.

Our problem is more complex as it deals with the coordination of decentralized systems' models in the presence of joint constraints and ASI. In this case, the approach is based on a specific iterative nonsmooth optimization procedure (see section 1.2.3-1.2.5). As we noted, integrated solution of separate LP models under ASI cannot be accomplished by LP methods. In section 1.2.2 we formulate the problem of distributed systems optimization in the presence of joint resource constraint under ASI and in sections 1.2.3-1.2.5 we discuss the models' linkage algorithm and its convergence characteristics.

1.2.2. *LP models under joint constraints*

The basic problem of distributed individual sectoral (or regional) LP models optimization under joint resource constraint can be formulated as follows. Assume that there are K systems' models formulated in the following LP form:

$$\langle c^{(k)}, x^{(k)} \rangle \to max, \tag{1.1}$$

$$x^{(k)} \geq 0, \tag{1.2}$$

$$A^{(k)} x^{(k)} \leq b^{(k)} \tag{1.3}$$

where components of vector $x^{(k)}$ are unknown variables, vector $b^{(k)}$ defines system-specific demand or resource constraints, and vector $c^{(k)}$ corresponds to net unit profits, $k = 1,2, \dots, K$. The common resource constraint [1.4] connects the systems through a common unknown (linkage) variable $y^{(k)}$

$$B^{(k)} x^{(k)} \leq y^{(k)}, \tag{1.4}$$

where $y^{(k)}$ defines resource quota allocated to system k. In this formulation, equation [1.3] defines individual systems' constraints and formula [1.4] establishes systemic supply-demand relationships among systems by distributing resources $y^{(k)}$. If matrix $D^{(k)}$ defines the marginal resource use by system k and d is the total available resource, $d \geq 0$, then the quotas $y^{(k)}$ fulfil the joint resource constraint on the common resources use

$$\sum_{k=1}^{K} D^{(k)} y^{(k)} \leq d. \tag{1.5}$$

Thus, the overall problem is to maximize the individual objective function (1) for each system k by choosing $x^{(k)}$ and $y^{(k)}$ from the feasible set defined by (2), (3), so that (4) and (5) are also fulfilled.

In the presence of full information about systems, the problem of models' linkage can be formulated and solved by a central planner (regulator) as a total net profit maximization

$$\sum_{k=1}^{K} \langle c^{(k)}, x^{(k)} \rangle \to \max \tag{1.6}$$

s.t. to constraints [1.2-1.5], $k = 1,2, \dots, K$. The net profits can be defined as total profit net of production costs, possible taxes and other expenses.

If the information about parameters $b^{(k)}$, $c^{(k)}$, $A^{(k)}$, $B^{(k)}$, $x^{(k)}$ of systems k is not available to the planner, the integrated LP model [1.2-1.6] under ASI cannot be solved by LP method due to the lack of common information about submodels.

In this situation, the consistent approach for linking distributed optimization models is based on the parallel solving of equivalent nonsmooth optimization model following a simple iterative subgradient algorithm. The convergence and other properties of the algorithm are presented in section 1.2.4. The proposed linkage approach does not require to know full information about models' specification, and it can be seen as an endogenous reinforced learning algorithm describing how distributed agents (models) can take decisions to maximize the "cumulative reward". Sections 1.2.3-1.2.5 outline various aspects of the algorithm.

1.2.3. *Nonsmooth model and linking algorithm*

A core part of the algorithm is a central hub computer that recalculates the resource quotas y by shifting their current approximation in the direction defined by the corresponding vectors of dual variables (shadow prices of resources) from the primal optimization problems. These quotas are received by sectorial/regional computers enabling parallel computations of solutions and fast adjustments of vector y. Ermoliev (1980) initially introduced the idea of this algorithm and current computer capacities enable its implementation to large-scale models used to support decisions.

Consider the main implicit maximization problem. For a given vector $y = (y^{(1)}, \dots, y^{(K)})$ let us denote the optimal value of function [1.6] under constraints [1.2-1.4] by $F(y)$, in other words, in this function $x^{(k)}(y)$ are optimal solutions to [1.1] under [1.2-1.4] ignoring joint constraints [1.5]. Therefore,

$$F(y) = \sum_{k=1}^{K} f^{(k)}(y),$$

where $f^{(k)}(y) = c^{(k)}, x^{(k)}(y))$ are concave non-differentiable (continuously) or non-smooth functions.

The following algorithm defines a rule for adjusting y towards an optimal y^* that maximizes function $F(y)$ under the joint constraints [1.5] defining the feasible set Y.

Consider an arbitrary feasible solution $y^s = (y^{s(1)}, \dots, y^{s(K)})$ for iteration $s = 1,2, \ldots$ of the algorithm. For given quotas $y^s = \left(y^{s(1)}, \ldots, y^{s(K)}\right)$, independently and in parallel, computers of sectors/regions solve primal models [1.1-1.4] and obtain primal solutions $x^{s(k)} = x^{s(k)}(y^s)$ together with the corresponding shadow prices of resources, that is, solutions $(u^{s(k)}, v^{s(k)})$ of the dual problems

$$\langle b^{(k)}, u^{(k)} \rangle + \langle y^{(k)}, v^{(k)} \rangle \to min, \qquad [1.7]$$

$$A^{(k)}u^{(k)} + B^{(k)}v^{(k)} \geq w_k c^{(k)}, \quad [1.8]$$

$$u^{(k)} \geq 0, v^{(k)} \geq 0, \quad [1.9]$$

$k = 1,2,\ldots$, where vectors $v^{s(k)}$ are the driving force of algorithm [1.10].

The next approximation of quotas $y^{s+1} = \left(y^{s+1(1)}, \ldots, y^{s+1(K)}\right)$ is derived by the computer of the central hub by shifting y^s in the direction of vector $v^s = (v^{s(1)}, \ldots, v^{s(K)})$, that is, optimal dual variables (shadow prices) corresponding to constraints [1.4]. Hence, we have iterative procedure defining in a sence the artificial "intellect" of the designed solution system:

$$y^{s+1} = \pi_Y(y^s + \rho_s v^s), = 1,2,\ldots, \quad [1.10]$$

where ρ_s is an iteration-dependent multiplier, which is a method's parameter, and $\pi_Y(\cdot)$ is the orthogonal projection operator onto set Y (see, e.g., Ermoliev 1976; Ermoliev 1980; Ermoliev 2009). The orthogonal projection y^{s+1} of vector $\bar{y}^s = y^s + \rho_s v^s$ onto Y is calculated by minimizing the quadratic function $\|y^s + \rho_s v^s - y\|^2$ subject to joint constraints [1.5]. This minimization is very fast due to $\rho_s v^s \to 0$, as vectors v^s are bounded optimal dual solutions and if y^s is used as an initial approximation for y^{s+1}.

Vector v^s defines sub-gradient of the continuously non-differentiable function $F(x)$. This and the convergence of solutions y^s to an optimal solution of the linkage problem [1.2-1.6] as $s \to \infty$ is analyzed in 1.2.4. The step-size ρ_s is chosen from rather general and natural requirements: $\rho_s \geq 0$, $\sum_{s=1}^{\infty} \rho_s = \infty$, because generalized gradients are not the increasing directions of functions.

Although the standard sub-gradient projection method converges without condition $\sum_{s=1}^{\infty} \rho_s^2 < \infty$, the proposed linkage algorithm for problems under asymmetric information (10) requires this additional condition to enable the convergence of not only function $F(y^s)$, but also solutions y^s. This allows us to propose a simple stopping criterion enabling the independent optimization of interdependent sectors by [1.10].

1.2.4. *Convergence of the linking algorithm (stopping criterion)*

Assume there exist solutions $x^{(k)}(y)$ of all K sectoral/regional models for feasible y satisfying constraints [1.5]. Then:

a). Functions $f^{(k)}(y) = (c^{(k)}, x^{(k)}(y))$, $F(y) = \sum_{k=1}^{K} f^{(k)}(x^{(k)})$ are concave continuously non-differentiable functions for all k;

b). The dual problem (7)-(9) has a solution $(u^{(k)}(y), v^{(k)}(y))$ for all k, and these solutions satisfy the stopping criterion of the linkage algorithm:

$$f^{(k)}(y) = (c^{(k)}, x \quad (y)) = (b^{(k)}, u \quad (y)) + (y, v \quad (y)).$$

This proposition leads to the following important fact (Ermoliev 1976; Ermoliev 1980; Ermoliev 2009), which is fundamental for solving the linkage problem through maximizing non-differentiable function $F(y)$ by algorithm [1.10]:

c). For any feasible solution z and y, $f^{(k)}(y) - f^{(k)}(z) \geq (v^{(k)}(y), y - z)$, that is, $v^{(k)}(y)$ is a subgradient of the concave non-differentiable function $f^{(k)}(y)$. Vector $v(y) = (v^{(1)}(y), \dots, v^{(K)}(y))$ is a subgradient of function $F(y) = \sum_{k=1}^{K} f^{(k)}(y)$, $F_y(y) = v(y)$, that is, $F(y) - F(z) \geq (v(y), y - z)$.

Therefore, the procedure [1.10] is a specific subgradient algorithm for maximizing the (continuously) non-differentiable concave function $F(y)$.

The following proposition shows that y^s converges (non-monotonic convergence) to an optimal linking vector y^*, maximizing $F(y)$ subject to joint constraints [1.5]. Let us denote this feasible set by Y: Assume that

(1). The feasible set Y is bounded;

(2). Step size ρ_s satisfies the conditions: $\rho_s \geq 0$, $\sum_{s=1}^{\infty} \rho_s = \infty$, $\sum_{s=1}^{\infty} \rho_s^2 < \infty$, say $p_s = 1/s$.

Then $lim\, y^s \in Y^*$ for $s \to \infty$.

The following sequence of ρ_s satisfies the conditions of the theorem:$\rho_s = \gamma_s / s$, $0 \leq \underline{\gamma} \leq \gamma_s \leq \overline{\gamma} < \infty$ for some positive constants $\underline{\gamma}$ and $\overline{\gamma}$.

Joint constraints (5) may have the following form:

$$\sum_{k=1}^{K} M^{(k)} x^{(k)} + \sum_{k=1}^{K} D^{(k)} y^{(k)} \leq \delta \qquad [1.11]$$

with some matrices $M^{(k)}$. Yet, problem (1)-(4) s.t. (11) can be reformulated similar to problem [1.1-1.5]. Let us define vectors $y^{(K+k)}$ such that $M^{(k)} x^{(k)} = y^{(K+k)}$, $k = 1, \dots, K$. Now it is possible to rewrite (11) as $\sum_{k=1}^{K} D^{(k)} y^{(k)} \leq \delta - \sum_{k=k+1}^{2K} y^{(k)}$ and after some renotation derive the problem in the form [1.1-1.5].

1.2.5. *Distributed computation*

The linkage algorithm can be summarized as follows. Imagine, there is a network of distributed computers connecting submodels, say sectors, with a computer of a social planner. At the initial step, sectors k, $k = 1, \dots, K$, use arbitrary chosen vectors $y^{0(k)}$ of resource quotas. They submit the information on $y^{0(k)}$ to the central computer. The computer updates quotas $y^0 = (y^{0(1)}, \dots, y^{0(K)})$ by projecting them onto the set Y defining a first feasible approximation $y^1 = (y^{1(1)}, \dots, y^{1(K)})$. All sectors independently solve models [1.1-1.4] with resource quotas y^1, calculate shadow prices $v^{1(k)}$ of common resources (constraint (4)) and submit to the central computer. The central computer calculates $y^1 + \rho_1 v^1$ with a step-size ρ_1 such that the product $\rho_1 v^1$ corresponds to the scale of y^1. Vector $y^1 + \rho_1 v^1$ is projected onto Y to derive quotas y^2. At the iteration $s+1$, the algorithm derives the next approximation of quotas $y^{s+1} = (y^{s+1(1)}, \dots, y^{s+1(K)})$ by shifting y^s in the direction of vector $v^s = (v^{s(1)}, \dots, v^{s(K)})$, according to procedure [1.10].

At each iteration, all sectors independently calculate stopping criteria $\varepsilon_k(s) = (b^{(k)}, u^{s(k)}(y^s)) + (y^{s(k)}, v^{s(k)}(y^s)) - w_k(c^{(k)}, x^{s(k)}(y^s))$ and submit values $\varepsilon_k(s)$ to the central computer. If $\sum_k \varepsilon_k(s) \le \varepsilon \ge 0$, where ε is an admissible accuracy, then the algorithm stops. Otherwise, it continues further. The convergence of the parallel independent optimization (linkage) of sectoral/regional models according to this algorithm without revealing sectoral/reginal information is possible due to the additional requirement $\sum_s \rho_s^2 < \infty$. This allows to prove the convergence of solutions (linkages) y^s rather than the convergence of objective function $F(y^s)$. The convergence of the proposed linkage algorithm under ASI is based on the theory of (continuously) non-differentiable optimization (more details see in Ermoliev 1980).

1.3. Linking energy and agricultural models for food-energy-water nexus

The proposed iterative algorithm has been applied for linking energy and agricultural sectoral models under joint constraints on water and land use. Both models can be used for optimal energy and agricultural production and allocation planning. In the following, we only briefly outline the models. Further details can be found for example in (Havlik *et al.* 2011; Ermolieva and Havlik *et al.* 2016; Gao *et al.* 2018; Ermolieva and Havlik *et al.* 2021; Ermoliev *et al.* 2022; Golodnikov *et al.* 2024; Pepelyaev et al. 2023, 2024; Zagorodny et al. 2024). The models are spatially explicit, which allows to link the models across locations and thus control local drivers having significant implications on the overall results of models' integration.

The energy model (Ermoliev *et al*. 2023) incorporates main stages of energy flows from resources to demands: energy extraction from energy resources, primary energy conversion into secondary energy forms, transport and distribution of energy to the point of end, conversion into products for end users to fulfill specific demands. The structure of the model is such that it can incorporate various energy resources as, e.g., coal, gas, crude oil, renewables. Primary energy sources include coal, crude oil, gas, solar, wind, etc.; secondary energy sources are fuel oil, methanol, hydrogen, electricity, ammonia, etc.; final energy products are coal, fuel oil, gas, hydrogen, ammonia, methanol, electricity, etc. Demands for useful energy products come from main sectors of the economy: industrial, residential, transport, agricultural, water, energy. Each technology is characterized by unite costs, efficiency, lifetime, emissions, etc. Additional sectoral (and cross-sectoral joint) constraints are imposed to capture the requirements and the limitations on the natural resource use and availability, and investments. The model can include the existing technologies, as well as the new zero-carbon green technologies, at the beginning of implementation or even in the research stage, e.g., various renewable and carbon capturing technologies.

The agricultural model (Havlik *et al.* 2011; Ermolieva and Havlik *et al.* 2016, 2021) can include main crops and livestock production and management systems, characterized by systems-specific production costs, water and fertilizers requirements, emission factors, and other parameters. The supply of crops and livestock products need to cover food, feed, and biofuel demands and fulfill security constraints. The food security constraint requires that the energy and nutrients consumption from grain and livestock products is not less than the required kilocalories and nutrients needed to satisfy dietary requirements in cereals, vegetable and animal products (meat and dairy products). Livestock feeds fulfill the livestock dietary requirements in energy intake measured in megacalories. Biofuels production from crops (and agricultural residues) have to fulfill biofuel mandates. In the model, land uses comprise agricultural (crop and pasture) land, grass land, and natural land. Land use changes can be regulated by setting regulatory constraints on land expansion and conversion. Security constraints introduce competition for limited natural resources (land and water) among different land uses.

Energy and agricultural sectors compete for common land and water resources. Assume, that regional planners, decision makers, sectoral authorities pursue a goal to minimize costs and maximize profits from energy and agricultural production under various joint balance (supply-demand) and resource constraints to fulfill the energy and agricultural demands. Namely, the goal is to choose a portfolio of energy technologies to be installed and operated to produce, convert, and transfer energy products among locations; and a portfolio of agricultural technologies and management systems to produce and transfer among locations agricultural commodities fulfilling constraints on natural resources, environmental pollution, end-products demands. The models include relevant risk-related systems performance criteria. These performance measures enable better understanding of how systems (individually and jointly) can perform in the uncertain environment, in the presence of climate change, weather variability, market uncertainties, etc. Better understanding of how interdependent energy-water-agricultural systems can operate and how dangerous impacts of inappropriate decisions can be motivates regional and sectoral planners, experts, involved stakeholders to make cross-sectoral coherent and risk-adjusted robust decisions.

1.3.1. *Energy, water, and agricultural security nexus, case study in China*

In the case study in Shanxi province, China (Gao *et al.* 2018), the energy model was customized to include only coal-based industries and processes, i.e., mining, washing, chemical production, and power generation. The coal-based technologies consume vast amount of water, for example, for coal mining and washing, coal power plants cooling and steam production.

In the context of coal-based energy production, the integrated energy-agricultural-water model is formulated as follows. The problem is to decide how much coal x_{ijlmt} of type $i, i = 1, \dots, I$, to extracted in location $j, j = 1, \dots, J$, transport to location m, $m = 1, \dots, M$, and converted by technology $t, t = 1, \dots, T$, to cover coal-based products (electricity, heating, cooling, pharmaceutical industry, etc.) demands.

Agricultural model decisions z_{kjm} concern agricultural commodities production, $k = 1, \dots, K$, in location j and transported to location m. The overall goal is to minimize the total costs of energy and agricultural production, transportation, and conversion.

Individual sectoral goal functions are formulated as follows

$$\sum_{i,j,k,m,t} \left[c_{ij}^{CP} + c_{ijm}^{CT} + c_{ijt}^{CC} \right] x_{ijmt} \to min \qquad [1.12]$$

and

$$\sum_{i,j,k,m,t} \left[c_{kj}^{AP} + c_{kj}^{AT} \right] z_{kjm} \to min \qquad [1.13]$$

for energy [1.12] and agricultural [1.13] sectors. Production costs c_{ij}^{CP} define all components of coal production costs, including extraction and washing, of a unit (tonne) coal of type i in location j, transportation costs c_{ijm}^{CT} represent all costs associated with transporting a unit coal i from location j to location m, c_{ijt}^{CC} define conversion costs of a unit coal i by technology t in location j, c_{kj}^{AP} denote agricultural production cost per unit (ton) agricultural commodity k in location j, and c_{kjm}^{AT} stand for transportation costs of a unit agricultural commodity k from j to m, $i = 1, \dots, I$, $j = 1, \dots, J, m = 1, \dots, M, t = 1, \dots, T, k = 1, \dots, K$.

The energy security constraints ensure that the demands for coal-based end products (electricity, heat, coke, gas, and oil) are fulfilled:

$$\sum_{ijt} \alpha^d_{imt} x_{ijmt} \geq D^d_m, \quad [1.14]$$

where α^d_{ijt} denotes the conversion coefficient of coal i in location j by technology t, D^d_j stands for the end product d demand.

Agricultural production fulfils food security constraints, which can be calculated according to nutrients and kilocalories norms for population by age groups:

$$\sum_j z_{kjm} \geq D^A_{km}, \quad [1.15]$$

where D^A_{km} is the demand for agricultural commodity k in location m to meet food security requirements.

Sectoral land use constraints

$$\sum_{i,m,t} x_{ijmt} (1 - r_{ij}) \ \Delta l_j S_{ij} + g \sum_{i,m,t} x_{ijmt} \leq L^C_j \quad [1.16]$$

and

$$\sum_{k,m} l_{kj} z_{kjm} \leq L^A_j \quad [1.17]$$

incorporate land demand by coal [1.16] and crop [1.17] production activities, where L^C_j and L^A_j are land use constraints for coal and agricultural sectors in location j, respectively. Parameter S_{ij} in [1.16] defines the area that may become unusable as a result of coal mining, Δl_j is a portion of agricultural land overlapping with a coal field in location j, parameter r_{ij} for coal i in location j defines plausible land reclamation rate, and g_{ij} is a parameter allowing to calculate the land under coal reject material. In equation [1.17], parameter l_{kj} defines the area required for a unit crop k production in location j. Equation [1.18] introduces the restriction on the total land use in location j by energy and agricultural sectors

$$\sum_{k,m} l_{kj} y_{kjm} + \sum_{i,m,t} x_{ijmt} (1 - r_{ij}) \ \Delta l_j l_{ij} + g_{ij} \sum_{i,m,t} x_{ijmt} \leq L_j. \quad [1.18]$$

Total available water W_j for both sectors and sectoral water quotas (W^E_j and W^A_j) significantly affect the choice of coal and crop (energy) production technologies through water utilization constraints:

$$\sum_{i,m,t} [w^P_{ij} + w^d_{ij}] x_{ijmt} \leq W^E_j \quad [1.19]$$

and

$$\sum_{k,m} w_{kj}^{c} z_{kmj} \leq W_j^A \quad [1.20]$$

where W_j^E and W_j^A are quotas on water use by coal and agricultural activities in location j, w_{ij}^P defines water requirement for a unit coal i production in location j, w_{ij}^d is water required for a unit coal i conversion in location j, w_{km}^c is water required for a unit crop k production in location j. Water use W_j^E for coal and W_j^A for agricultural production are constrained by total water W_j available in j:

$$W_j^E + W_j^A \leq W_j. \quad [1.21]$$

In the condition of ASI, the planner does not have full information about separate LP energy ([1.12], [1.14], [1.16], [1.19]) and agricultural ([1.13], [1.15], [1.17], [1.20]) submodels. To link the models under joint constraints [1.18] and [1.21] we implement procedure [1.10]. At the initial step of the procedure s=0, individual sectoral models are solved using initial sectoral land and water quotas $L_j^C(0)$, $L_j^A(0)$ and $W_j^C(0)$, $W_j^A(0)$. Resource quotas $y^s = (L_j^C(\mathrm{s}), L_j^A(\mathrm{s}), W_j^C(\mathrm{s}), W_j^A(\mathrm{s}))$ at step s are adjusted according to [1.10] using shadow prices (dual variables) of energy and agricultural sectors land and water resource constraints

$$\sum_{i,m,t} x_{ijmt} (1 - r_{ij}) \Delta l_j S_{ij} + g \sum_{i,m,t} x_{ijmt} \leq L_j^C(s-1) \quad [1.22]$$

$$\sum_{k,m} l_{kj} y_{kjm} \leq L_j^A(s-1) \quad [1.23]$$

$$\sum_{i,m,t} w_{ij}^P x_{imlt} + \sum_{i,m,t} w_{ij}^d x_{ijmt} \leq W_j^C(s-1) \quad [1.24]$$

$$\sum_{k,m} w_{kj}^c y_{kmj} \leq W_j^A(s-1) \quad [1.25]$$

and constraints [1.18], [1.21]

1.3.2. *Selected results*

Results were calculated and compared for 3 scenarios: 1. separately optimized energy and agricultural models; 2. hard-linked integrated model (one-code model); 3. separate models integrated via the linkage procedure [1.10]. In the first scenarios, the net profits can be higher than in other two scenarios because the sectors are not restricted by joint constraints. This result is misleading the resource allocation analysis. In scenario 3, the solution of the iterative linkage process converges rather quickly (only in 10 iteration steps) to the solutions of the hard-integrated model, scenario 2.

Figure illustrates the nonmonotonic convergence of the linkage algorithm for three different scenarios of initial y^0 quotas allocated to energy and agricultural sectors. The choice of the step-size ρ_s in [1.10] affects the convergence rate, the value of the product $\rho_s v^s$ must correspond to the value of solutions y^s.

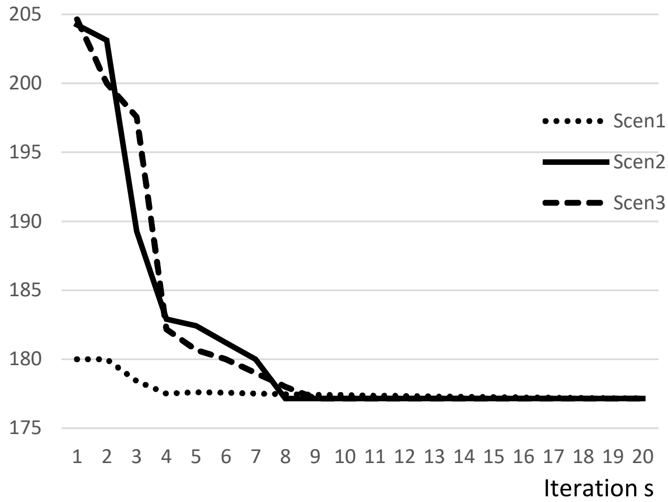

Figure 1.1. *Convergence of the iterative linking procedure in terms of the goal function values $F(y^s)$. Vertical axis displays net profits, the iteration step is marked on the horizontal axis. The three curves (Scen1, Scen2, Scen3) correspond to three different initial land and water quota scenarios at s = 0*

1.4. Conclusions

In the paper, we discuss the problem of linking distributed individual sectoral and/or regional optimization models into an inter-sectoral integrated model. The approach for linking models is based on an iterative stochastic quasigradient (SQG) procedure of, in general, nonsmooth nondifferentiable optimization converging to a socially optimal solution maximizing an implicit nested nondifferentiable social welfare function. The convergence of the algorithm relies on the duality theory and the nondifferentiable optimization. The iterative solution procedure can be used for robust estimation and machine learning problems, in particular, it can be viewed as an endogenous reinforced learning problem.

The iterative SQG-based methods and their stochastic versions are intended for robust optimization of deterministic and stochastic systems with large number of decision variables and scenarios of uncertainties due to the ability of these methods to link scenario-simulation and optimization procedures. The proposed linkage method will be further developed for linking stochastic models enabling integrated management of global systemic risks.

The linkage of models is, in a sense, opposite to decomposition methods. While in the decomposition (e.g., Dantzig and Wolfe 1960; Kim and Nazareth 1991) we split an existing integrated optimization model into a number of smaller sub-models, in the linkage we obtain an integrated model of the system by linking existing explicitly unknown sub-models. The proposed linkage procedure provides a flexibility enabling the simultaneous use of linkage and decomposition procedures, in other words, endogenously disaggregating models to make their further integration (linkage) more efficient.

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