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Integrated simulation-optimization modeling framework of resilient design and planning of supply chain networks

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Abstract: Optimal control is a convenient way to develop both supply chain process optimization models and describe the dynamics of process fulfillment. A rich diversity of knowledge has been developed for the integration of optimization and simulation methods with applications to supply chain management at conceptual, informational, and computational levels. At the same time, model-algorithmic integration and alignment frameworks have received less attention. The importance of this level should not be underestimated since synthesis and analysis problems in supply chains imply tight intersections between and within the models (e.g., objective functions and constraint systems). This paper seeks to bring the discussion forward by carefully elaborating on the issues of optimization and simulation model and algorithm integration and providing implementation guidance. Conventionally, optimization has pre-dominantly been used at the planning level while dynamic system control was frequently investigated using simulation models. This study develops an integrated optimization-simulation framework at the model-algorithmic level for the given domain. We offer insights on how to describe planning and control in a unified model-algorithmic complex with consideration of uncertainty factors which are anticipated at the planning and confronted at the control stages. The developed theoretical framework was exemplified by a combined optimization-simulation modelling of the SC design and planning problem with disruption risks consideration in anyLogistix.

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1. INTRODUCTION

Optimization and simulation approaches are most popular in supply chain (SC) design and planning with uncertainty and risk considerations analysis (Klibi and Martel 2012, Ivanov and Sokolov 2020). It is commonly known that simulation modeling is a preferable analysis tool in the following cases (Schmitt et al. 2017, Macdonald et al. 2018, Ivanov et al. 2020a, Ghadge et al. 2021): a closed form mathematical problem does not exist or cannot be solved analytically, analytical methods exist, but their computational complexity prevents the finding of a feasible solution in a reasonable time, while simulation provide an efficient and simple solution procedure and can be used with the existing qualification of decision-makers in the firms; forecast or monitoring of a system or object behavior in time is needed. At the same time, some limitations of “pure” simulation applications need to be ad-dressed, such as the nature of heuristic solutions due to fixed structural elements, behavior algorithms and parameters, as well as subjectivity in model development and result interpretation. We refer to the works by Snyder et al. (2016), Dolgui et al. (2018) and Hosseini et al. (2019) for more recent state-of-the-art reviews. Even if SC design with the help of mathematical optimization provides powerful decision-making support, it does not take into account some important dynamic restrictions such as inventory control or shipment policies for which simulation is considered to be a useful tool (Bottani and Montanari 2010, Ivanov 2017a, Schmitt et al. 2017, Ivanov and Rozhkov 2020). Therefore, modern commercial software for SC simulation and optimization such as anyLogistix apply a multi-method technology that combines optimization and simulation (Burgos and Ivanov 2021).

The purpose of the present study is to contribute to existing works by integration of planning and control decisions within a unified modelling-algorithmic framework. The combination of optimization and simulation was seen as a logical way of increasing the quality of the SC decision-support system (DSS), and different forms of such combinations have been developed (Gao and Chen 2016, Frazzon et al. 2018). These combinations resulted in the SC DSS that contained simulation models, analytical models, a database (which is presently evolving into a knowledge base with artificial intelligence roots), and an integration system for alignment of data, analytical models, simulation models, and decision-making needs leading to development of digital SC twins (Ivanov and Dolgui 2021b). In such a complex DSS, the integration and
alignment of simulation and optimization models plays a crucial role. Such integration and alignment are multidimensional and contain four levels, i.e., conceptual, model-algorithmic, informational, and computational (Pedrielli et al., 2015, Gao and Chen 2017). The literature developed a rich diversity of knowledge at the conceptual, informational, and computational levels. At the same time, model-algorithmic integration and alignment frameworks have received less attention. The importance of this level should not be underestimated. The synthesis and analysis problems in complex systems imply tight intersections between and within the models (e.g., objective functions and constraint systems).

This paper seeks to bring the discussion forward by carefully elaborating on the issues of optimization and simulation model and algorithm integration described above and providing some ideas and implementation guidance on how to think in relation to these challenges. The purpose of the present study is to contribute to existing works by arguing that, rather than simulation and optimization opposing each other, the consideration of these perspectives can be done within an integrated framework to enhance the quality of SC DSS. More specifically, we focus on the integration of planning and control decisions. Conventionally, optimization has predominantly been used at the planning level while dynamic system control was frequently investigated in the simulation models (Namdar et al. 2021, Pavlov et al. 2019, 2020). The objectives of developing the integrated optimization-simulation framework at the model-algorithmic level are to obtain insights on how to describe SC planning and control in a unified model-algorithmic complex with consideration of structural dynamics and disruptions which are anticipated at the planning and confronted at the control stages.

2. INTEGRATION OF SIMULATION AND OPTIMIZATION APPROACHES

Simulation and optimization combination depends on the modeling objective and can differ regarding conceptual and algorithmic alignment. Three major combinations can be distinguished as follows (Fig. 1):

- Optimization inside the simulation, e.g., for searching the exogenous variable ranges,
- Simulation inside the optimization, e.g., for making the relaxed solutions obtained analytically more precise, and
- Hybrid simulation-optimization techniques, e.g., simulation-based optimization.

The first two combinations variants (Figs 1a and 1b) are usually used for modeling a high frequency of numerical realizations for relatively small-dimensional problems. These combinations are widely automated due to standardized procedures and do not require decision-maker or modeler involvement. Examples of hybrid combinations can be found in (Ivanov et al. 2014a, 2015, 2016a,b, Frazzon et al. 2018). The analysis allows for the preliminary conclusion that integration and alignment of simulation and optimization is comprised of multiple dimensions, i.e., conceptual, model-algorithmic, informational, and computational levels. While the conceptual, informational, and computational levels have attracted considerable research attention, the model-algorithmic combination and simulation has mostly been considered within particular software, whereby a human interaction for interpretation of results of one model and transforming these results into the input of another model was presumed. The synergetic effects and the model-algorithmic integration and alignment frameworks have received less attention. Notwithstanding the application software package, the importance of this level should not be underestimated. Synthesis and analysis problems in complex systems imply tight intersections between and within the models (e.g., objective functions and constraint systems). As such, simulation and optimization combination problems in the SC need to be studied further with regards to building more sophisticated SC DSS.

3. GENERALIZED FRAMEWORK OF INTEGRATED SIMULATION-OPTIMIZATION MODELLING

Optimal control is a convenient way to develop both supply chain process optimization models and describe the dynamics of process fulfilment (Dolgui et al. 2019, Ivanov et al. 2021). Consider a generalized form of an objective function of a SC design or planning problem (1):

$$f(x) \rightarrow \text{extr } x \in \Delta_0,$$

where $\vec{x} = (x_1, x_2, \ldots, x_n)^T$ is a vector of SC design or planning parameters (e.g., locations, capacities, and costs) and $\Delta_0$ is a set of feasible values in $\vec{x}$ (e.g., minimum and maximum capacities). Since $\vec{x}$ is a large scale vector, instead of $f(\vec{x})$ a number of objective functions can be introduced and distributed between $m$ different models (Eq. 2).

$$f_i(\vec{x}^{(i)}) \rightarrow \text{extr } x^{(i)} \in \Delta_0^{(i)},$$

Where $\vec{x} = \| \vec{x}^{(1)} \| \cdots \| \vec{x}^{(m)} \|$, $\vec{\bar{x}} = \| \vec{x}_1^{(i)} \bar{x}_2^{(i)} \cdots \bar{x}_n^{(i)} \|$. For the decomposition, $m<<n$, each $\vec{x}^{(i)}$ is sub-vector of $\vec{x}$, and the number of components in $\vec{x}^{(i)}$ is much less as in $\vec{x}$. It is assumed, that the extremum is reached in one of the Pareto set points as a result of the combined solution of the sub-models. Then, the solution of (1) can be replaced by solution of (3)-(4) as follows.

$$f(\vec{x}(\bar{a})) \rightarrow \text{extr } a \in \Delta_0, (\bar{a}),$$

$$f(\vec{x}(\bar{a})) \rightarrow \text{extr } a \in \Delta_0,$$
\[
\sum_{i=1}^{\alpha} f_i(x^{(\alpha)}) \rightarrow \text{extr}, \quad \alpha_i \geq 0; \quad \sum_{i=1}^{\alpha} \alpha_i = 1; \quad \hat{\alpha} = \|\alpha_1, \ldots, \alpha_{\alpha}\|.
\] (4)

The vector \(\hat{\alpha}\) is fixed in an optimization model in (2) to find \(\tilde{x} = \tilde{x}(\hat{\alpha})\). \(\hat{\alpha}\) is a small-dimensional vector for which direct numerical experiments can be run in a simulation model. The values of \(\tilde{x}(\hat{\alpha})\) are obtained in the optimization model for fixed \(\hat{\alpha}\), and direct simulation experiments allow finding \(\tilde{\alpha}_{\text{optimum}}\). \(\hat{\alpha}\) plays the role of parametric alignment. Its values are obtained in the optimization model and used as input into the simulation model.

In a generalized form, the combined problem (5) needs to be solved.

\[
f_0(\tilde{x}) \rightarrow \text{extr}, \quad \tilde{x}(\hat{\alpha}), \quad \Delta = \{\tilde{x} | f_i^{(\text{opt})}(\tilde{x}) \leq 0, i \in I; \quad \phi_j^{(\text{Sim})}(\tilde{x}) \leq 0, j \in J\},
\] (5)

where \(\tilde{x} = (x_1, \ldots, x_{y})\) is a parametric vector of SC design; \(f_0\) is an objective function (or a set of objective functions in a multi-criteria optimization); \(f_i^{(\text{opt})}(\tilde{x})\) are analytical constraints; \(\phi_j^{(\text{Sim})}(\tilde{x})\) are algorithmic constraints (e.g., inventory control policy) that are considered via simulation. Such a procedure is implemented in modern commercial software for SC optimization and simulation, e.g., in anyLogistix (Dolgui et al. 2020, Ivanov 2020c, Singh et al. 2021).

In this case, the objective function description and the constraint system settings can form a number of possible combinations of analytical and simulation methods. Consider a simple example. A general simulation model can be described by \(N\) simulation sub-models and are described with the help of isochronal operators

\[
y(t) = S\tilde{x}(t),
\] (6)

where \(y = (y_1, y_{11}, \ldots, y_{N})\), \(\tilde{x} = (\tilde{x}_1, \tilde{x}_{11}, \ldots, \tilde{x}_{N})\) are vectors of endogenous and exogenous variables of the general simulation models, respectively; \(S\) is the operator of algorithmic approximation of the link between \(\tilde{y}(t)\) and \(\tilde{x}(t)\); \(\tilde{y}(t)\) and \(\tilde{x}(t)\) are subject to the links \(\tilde{x}(t) \in D_x(\tilde{y}(t))\), which differ from the links \(y_j(t) = s_{ij}\tilde{x}_j(t)\). Then \(N\) models are aligned with the help of the isochronal operator so that \(\tilde{x}(t) = S_0\tilde{y}(t)\) if \(\tilde{x}(t) \in D_0\) is the given Euclid space and there is an aligned solution \((\tilde{x}(t), \tilde{y}(t))\)

\[
y(t) = S_0\tilde{y}(t) \quad \text{or} \quad \tilde{x}(t) = S_0S\tilde{x}(t).
\] (7)

The model and result consistency should meet the functional homomorphism conditions (Ivanov and Sokolov 2012).

4. EXAMPLE OF INTEGRATED SIMULATION-OPTIMIZATION MODELLING IN anyLogistix

This section demonstrates an integrated optimization-simulation decision-support system for SC design and planning with consideration of disruption risks. In particular, the SC design and material flow plans in the SC need to be computed to suggest ways for reconfiguration of product flows in the event of disruptions. More specifically, three problems need to be solved. The first problem is to find the aggregate product flows to be moved in some periods through the SC network subject to demand from the customer and minimizing total SC cost. The second problem consists of a detailed dynamic analysis of ordering, production, inventory and sourcing control policies within the periods. The third problem is the parametrical synthesis of a resilient SC design, e.g., to find the optimal capacities of the firms in the SC design.

Following this structure, an integrated optimization-simulation decision-support system for SC design and planning with consideration of disruption risks has been developed in multi-method software anyLogistix (Fig. 2).

**Fig. 2.** Integrated simulation-optimization modelling of resilient SC in anyLogistix

anyLogistix is a multi-method software for SC simulation and optimization. It contains a CPLEX solver for network optimization and a simulation engine based in the well-known AnyLogic simulation software (Burgos and Ivanov 2021). According to Fig. 2, the first step is setting and solving a multi-period, multi-stage network optimization problem. The second step is the setting and experimental running of the simulations to investigate the dynamics of the aggregate flows found in step 1. The third, and final step is the optimization of the SC design parameters (i.e., capacities) subject to the insights gained via simulation and using the inverse optimization model.

To illustrate, we consider a multi-stage SC in line with the study by Ivanov et al. (2013) that is comprised of production plants (nodes 1 and 6) that deliver a single product to a central distribution hub (node 4) via two intermediate terminals (nodes 2 and 3). From node 4, the product is shipped to the customer (node 5) directly or via an outsourcing terminal (node 7) (see Fig. 3). The objective is to find the optimal plan of material flow in the SC that minimizes total costs and satisfies customer demand. The network throughput is limited by maximum node capacities and arc throughputs (cf. Fig. 3). The multi-criteria modifications of this model have been shown in (Ivanov et al. 2013, 2014a, 2016b). Disruptions may change the SC design shown in Fig. 3 for some period of time. This is why the planning horizon is divided in some periods, i.e., so-called intervals of structural constancy (cf. Ivanov et al. 2014a, 2016b).
The event of transition to the next period is a change in the SC design, i.e., either a disruption or recovery. These events are fixed in the form of a disruption scenario. Within the intervals of structural constancy, the SC design remains unchanged. Suppliers deliver certain order quantities to nodes 1 and 6 at the beginning of each period. Inventory from previous periods may be used in the following periods. Procurement and production and transportation (if $\Delta_{t}$); and problem B: variation of $\xi_{t}$, $\Delta_{t}$ is a SC state vector such as produced and shipped quantities in the SC; $\Delta_{t}$ is a SC control vector that represents the SC plan or schedule; $\xi_{t}$ is a vector of impulse stochastic disturbances subject to some disruption scenario; $\xi_{t}$ is a set of node numbers for the nodes receiving products from $A_{xi}$ at time interval $k$. $N_{ix}$ is the set of node numbers for the nodes receiving products from $A_{xi}$ at time interval $k$.

Consider an integrated simulation-optimization model of SC design with disruption considerations (Eqs 8-11).

\[ J_{G}(\bar{x}(t), \bar{u}(t), \bar{\beta}, \xi(t), t) \rightarrow \text{extr } \bar{u}(t) \in \Delta, \]

\[ \Delta = \left\{ \bar{u}(t) \mid \bar{x}(t) = \phi(\theta_{0}, \bar{x}(t_{0}), \bar{u}(t), \bar{\beta}, \xi(t), t) \right\}, \]

\[ \bar{f}(\bar{x}(t), \bar{u}(t), \bar{\beta}, \xi(t), t) = \left[ J^{(o)}(t) \right], \]

\[ J_{G} = \sum_{a=1}^{h} \lambda_{a} J_{a}, \lambda_{a} \geq 0, \sum_{a=1}^{h} \lambda_{a} = 1. \]

The solution of problem (8)-(9) towards the optimization of (11) can be implemented by decomposition into two subproblems, i.e., problem A: variation of $\xi_{t}$ for a fixed SC parameter vector $\bar{\beta}$; and problem B: variation of $\bar{\beta}$ for $\xi_{t}$.

The integrated simulation-optimization model for problem A is shown in Eq. (12)

\[ f(\theta_{0}(\xi), \bar{\beta}_{v}) \rightarrow \min_{\bar{\beta}_{v} \in \Omega} \]

where $\theta_{0}(\xi)$ is an analytical-simulation description of parametric connections of optimization and simulation models, and $\Omega$ is a set of possible values of SC design parameters described by vector $\bar{\beta}_{v}$, e.g., production and transportation capacity limits.

The integrated simulation-optimization model for problem A is shown in Eq. (13)

\[ f(\theta_{0}(\xi), \bar{\beta}_{v}) \rightarrow \min_{\xi_{t} \in Z} \xi_{t}, \]

where $Z$ is a set of possible values of disturbance vector, e.g., levels of production capacity degradation.

The solution of the problem (12)-(13) is based on an iterative procedure. At iteration $v = 0$, initial values for $\xi^{(v)} = \xi^{(0)}$ need to be given, e.g., a SC disruption profile. The iterative search terminates when the difference between functionals $|f(\theta_{0}(\xi^{(v+1)}), \bar{\beta}) - f(\theta_{0}(\xi^{(v)}), \bar{\beta})| < \varepsilon$, where $\varepsilon$ is a given error value.

Step 1. An initial SC structural dynamics control policy $\bar{u}_{g}(t) \in t \in [t_{0}, t_{f}]$ is determined via simulation.

Step 2. Main equation system $\hat{\bar{\beta}} = \bar{f}(\hat{\bar{x}}, \bar{u}, t)$ is integrated with the boundary condition $\bar{u} = \bar{u}_{g}(t)$ which results in a vec-
tor function $\tilde{x}_L(t)$. At the end of integration, $J_C$ and transversality conditions are computed.

Step 3. At $t = t_f$ until $t = t_0$ with $\tilde{u} = \tilde{u}_L(t)$, the integration with adjoint equation system is performed as shown in Eqs (14) and (15).

$$\psi_l = \frac{-\partial H}{\partial x_l} + \sum_{p=1}^l \eta_{lp}(t) \frac{\partial q^p_l(\bar{x}(t),\bar{u}(t))}{\partial x_l} + \sum_{r=1}^l \rho_{lr}(t) \frac{\partial q^r_l(\bar{x}(t),\bar{u}(t))}{\partial x_l}, \quad l = 1, \ldots, n, \quad (14)$$

$$\quad \text{subject to} \quad \text{grad}_l H(\bar{x}(t),\bar{u}(t),\psi_l(t)) = \frac{\partial}{\partial x_l} \left[ \sum_{p=1}^l \eta_{lp}(t) \frac{\partial q^p_l(\bar{x}(t),\bar{u}(t))}{\partial x_l} + \sum_{r=1}^l \rho_{lr}(t) \frac{\partial q^r_l(\bar{x}(t),\bar{u}(t))}{\partial x_l} \right], \quad (15)$$

where $H = \psi^T(t) \bar{\psi}(t)$ is Hamiltonian function, $\eta_{lp}(t)$ and $\rho_{lr}(t)$ are Lagrange multipliers, $\bar{\psi}(t)$ is vector of adjoint equation system, $q^p_l(\bar{x}(t),\bar{u}(t))$ and $q^r_l(\bar{x}(t),\bar{u}(t))$ are components of the constraint system. At $t = t_0$, the first approximation of $\bar{\psi}_l(t_0)$ is obtained. The Iteration $r = 0$ is completed.

Step 4. Steps 2 and 3 are repeated until $|J_G^{(r+1)} - J_G^{(r)}| \leq \varepsilon$ is reached: termination of the algorithm.

The solution results in the vector of dynamic coefficients $\tilde{\zeta}(t) = \zeta(\psi(t_0))$ which are connected with the adjoint equation system via Hamiltonian and represent the SC structural dynamics control plan with disruption considerations. The optimality of the gained solution has been discussed in (Ivanov et al. 2016b).

The optimization-simulation model of flow reconfiguration in the SC according to structural dynamics can now be written in line with Ivanov et al. (2014a) as balance equations (16)-(17) and capacity constraints (18-19):

$$\dot{x}_{z,ip}(t) = x_{z,ip}(t) + y_{z,ip}(t) + z_{z,ip}(t), \quad i \in N_z = \{1,2,\ldots,n_z\}, \quad (16)$$

$$\dot{y}_{z,ip}(t) = \psi_{z,ip}(t) + \sum_{j=1}^{n_z} e_{z,ip}(t) \cdot \omega_{z,ip}(t) \cdot w_{z,ip}(t), \quad i \in N_z, \quad \quad (17)$$

$$\dot{z}_{z,ip}(t) = \varphi_{z,ip}(t) \cdot \theta_{z,ip}(t) + \sum_{j=1}^{n_z} e_{z,ip}(t) \cdot \omega_{z,ip}(t) \cdot w_{z,ip}(t), \quad i \in N_z, \quad \quad (18)$$

$$0 \leq x_{z,ip} \leq \omega_{z,ip} \cdot (t_k - t_{k-1}), \quad 0 \leq \sum_{j=1}^{n_z} y_{z,ip} \leq V_{z,ip} \quad \quad (19)$$

and objective function (20):

$$J_G = \sum_{z=1}^{n_z} \sum_{i=1}^{n_z} \sum_{j=1}^{n_z} \left[ \omega_{z,ip}(t) \cdot w_{z,ip}(t) + \sum_{j=1}^{n_z} k_{z,ip}(t) \cdot y_{z,ip}(t) + \sum_{j=1}^{n_z} \sum_{k=1}^{n_z} \sum_{j=1}^{n_z} \sum_{k=1}^{n_z} \sum_{l=1}^{n_z} z_{z,ip}(t) \cdot \theta_{z,ip}(t) \cdot \theta_{z,ip}(t) \right]$$

The model (16)-(20) details the analytical part of the integrated simulation-optimization model presented in Sect. 3. Eqs (16)-(18) describe the SC flow dynamics. Note that $\psi_{z,ip}(t)$, $\omega_{z,ip}(t)$, $\varphi_{z,ip}(t)$ are known for intervals of structural constancy, and $e_{z,ip}(t)$ reflects the SC structural dynamics according to the disruption scenario $S_{c,ip}$. Eq. (19) sets inventory constraints subject to maximal warehouse capacity as well as flow dynamics constraints on processing and delivery. $V_{z,ip}(t)$ is maximal warehouse capacity at $A_{z,ip}$; $x_{z,ip}$ is flow $\rho_i$ transmitted from $A_{z,ip}$ to $A_{z,ip}$ and received at $A_{z,ip}$; $y_{z,ip}$ is flow $\rho_i$ to be stored at $A_{z,ip}$; $z_{z,ip}$ is flow $\rho_i$ to be delivered from $A_{z,ip}$; $z_{z,ip}$ is flow $\rho_i$ to be returned from $A_{z,ip}$ if maximum storage capacity is exceeded. Functions $y_{z,ip}(t)$, $z_{z,ip}(t)$, $u_{z,ip}(t)$, $\varphi_{z,ip}(t)$, $\omega_{z,ip}(t)$ are unknown, and controls $u_{z,ip}(t)$, $\varphi_{z,ip}(t)$ uniquely define $z_{z,ip}(t)$ and $y_{z,ip}(t)$. Therefore, the pairs $y_{z,ip}(t)$, $z_{z,ip}(t)$ can be considered as SC dynamic structural states. In the objective function (20), the following notations are used, $c_{z,ip}(t)$ are transportation costs for $\rho_i$ from $A_{z,ip}$ to $A_{z,ip}$, $h_{z,ip}(t)$ are inventory costs for $\rho_i$ at $A_{z,ip}$, $\pi_{z,ip}(t)$ are processing costs for $\rho_i$ at $A_{z,ip}$, and $r_{z,ip}(t)$ are return costs for $\rho_i$ at $A_{z,ip}$.

5. CONCLUSIONS

The purpose of the present study is to contribute to existing works by arguing that, rather than simulation and optimization opposing each other, the consideration of these perspectives can be done within an integrated framework to enhance the quality of supply chain decision-support systems. Conventionally, optimization has predominantly been used at the SC design level while dynamic system control (i.e., inventory and shipment control) was investigated in simulation models.

This study develops an integrated optimization-simulation framework at the model-algorithmic level for the given domain. This provides insights on how to describe planning and control in a unified model-algorithmic complex with consideration of uncertainty factors which are anticipated at the planning and confronted at the control stages. Using the unified formal language of the dynamic control system analysis, SC design and control problems have been described in unified model-algorithmic complex with uncertainty factor considerations. This is a difference to typical approaches which either separately solve SC design problems with optimization and SC control problems with simulation or achieve some level of integration numerically. Moreover, the developed theoretical framework was exemplified by a combined optimization-simulation modeling of the SC design and planning problem with disruption risks consideration in anyLogistix.

The results gained provide evidence that the modeling needs to be based on a combined methodology to achieve the adequacy, precision, and validity of models accuracy, closeness, and consistency of results. The formalized model integration allows description of how the ad-va ntages of some methods can compensate for the limitations of other methods (Ivanov 2009). Moreover, the synergetic effects from the combined usage of different methods can be achieved resulting in new
knowledge generation about the system and its dynamic behavior (Dolgui et al. 2018, Ivanov and Dolgui 2020).

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