Project deliverable

Project Number:	Project Acronym:	Project Title:
611281	DYMASOS	Dynamic Management of Physically Coupled Systems of Systems

Instrument:	Thematic Priority:
Collaborative Project	ICT

Title:

D2.1 Report on iterative constraint imposing coordination strategies for the management of systems of systems with physical couplings

Contractual Delivery Date:	Actual Delivery Date:
Month 18	Month 18

Start Date of Project:	Duration:
October 1st, 2013	36 months

Organization name of lead contractor for this deliverable:	Document version:
TUDO	V1.3

Dissemination level (Project co-funded by the European Commission within the Seventh Framework Programme):		
PU	Public	**X**
PP	Restricted to other programme participants (including the Commission)	
RE	Restricted to a group defined by the consortium (including the Commission)	
CO	Confidential, only for members of the consortium (including the Commission)	

This project has received funding from the European Union's Seventh Programme for research, technological development and demonstration under grant agreement No 611281.

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Abstract:

This document provides a report on coordination strategies studied and developed in the Workpackage (WP) 2 of the DYMASOS project. We present a subset of problems arising typically in processing industries, related to the case studies defined in the WP 5 of the project. We briefly review the approaches, present in the literature, for negotiation of active constraints that steer the behavior of the constituent systems of a system of systems to fulfill a common goal under present coupling in the form of shared resources. We select a method from the literature that mimics the negotiation process among different subsystems that perform an optimization of their operation and that share certain resources (e.g. raw materials, intermediates, energy). We extend this method to achieve a better performance and a reliable algorithm that can be seamlessly implemented in the simulation platform that is developed in WP 4 of the project. We provide a few small-scale examples to illustrate the basic features of the method and give an outlook of the application of this method for the case studies of DYMASOS.

Keywords:

Dynamic management, Systems of systems, Constraints negotiation, Production optimization.

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Revision History

Revision	Date	Description	Author (Organization)
V1.0	February 2015	Creation	Radoslav PAULEN (TUDO)
V1.1	March 2015	Contributions	Radoslav PAULEN (TUDO), Seyed-Amirreza SHAHIDI (TUDO), Goran STOJANOVSKI (TUDO), Lukas MAXEINER (TUDO), Shahbaz ALI (TUDO)
V1.2	March 2015	Review & Revision	Sergio GRAMMATICO (ETH), Radoslav PAULEN (TUDO)
V1.3	March 2015	Review & Revision	Sebastian ENGELL (TUDO), Radoslav PAULEN (TUDO)

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The DYMASOS Project

The well-being of the citizens in Europe depends on the reliable and efficient functioning of large interconnected systems, such as electric power systems, air traffic control, railway systems, large industrial production plants, etc. Such large systems consist of many interacting components. The sub-systems are usually managed locally and independently, according to different policies and priorities. The dynamic interaction of the locally managed components gives rise to complex behaviour and can lead to large-scale disruptions as e.g. black-outs in the electric grid.

Large interconnected systems with autonomously acting sub-units are called systems of systems. DYMASOS addresses systems of systems where the elements of the overall system are coupled by flows of physical quantities, e.g. electric power, steam or hot water, etc.

Within the project, new methods for the distributed management of large physically connected systems with local management and global coordination will be developed.

The **DYMASOS Consortium** consists of:

Participant No.	Participant Organisation Name	Participant Short Name	Country
1	Technische Universität Dortmund	TUDO	Germany
2	BASF SE	BASF	Germany
3	HEP-Operator distribucijskog sustava d.o.o	HEP	Croatia
4	INEOS Köln GmbH	INEOS	Germany
5	University of Seville	USE	Spain
6	University of Zagreb Faculty of Electrical Engineering and Computing	UNIZG-FER	Croatia
7	ETH Zürich	ETH	Switzerland
8	RWTH Aachen University	RWTH	Germany
9	inno TSD	inno	France
10	Optimizacion Orientada a la Sostenibilidad SL	IDENER	Spain
11	euTeXoo GmbH	TEX	Germany
12	Ayesa Advanced Technologies SA	Ayesa AT	Spain

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1. Introduction

Decomposition strategies are key components of many methods that look for the solution of large-scale optimization problems where subsystems that share some resources can be identified. The decomposition is applied to divide the original problem in subproblems whose solutions depend on some coordination variables (such as prices or multipliers) that are available as an information to each subsystem and computed in the upper coordination layer in order to satisfy the global constraints and to achieve desired optimal performance of the system.

In the petrochemical industry, hierarchical management and automation structures have been implemented in many plants, ranging from the basic automation over the regulatory control layer (often MPC controllers) to real-time optimization and plant-wide production planning. While a fully integrated real-time optimization of the operating points of a large complex may be feasible in principle, the size of the problem, the vulnerability to missing or perturbed data and above all the management structures of the plants often favor a distributed solution.

A characteristic feature of processing plant complexes is that the units are coupled by networks of utilities, e.g. steam, electricity, cooling water or raw materials. In these complex networks, the units can act as consumers and producers of resources. The utilization of these shared resources has to be coordinated between the distributed structures in order to fulfill the global demand-supply constraints for each shared resource network.

An additional reason for decomposition of the original problem are the privacy issues. For example, different plants may be operated by different business units of a company or even by different companies in a chemical park which do not want to make all the details of their operational constraints, costs and profits to be transparent. In such a situation, local optimizers (or managers supported by optimization algorithms) should be responsible for the optimization of the individual units, and the global coordination has to be achieved by suitable mechanisms that modify cost functions or constraints of the local optimization problems, possessing only limited information (”local” details) about the plants.

This deliverable deals with distributed optimization problems that arise in the management of physically-coupled systems-of-systems. In the context of processing industries, the distributed optimization problem represents the site-wide optimization problem where the local subsystems (production or business units, plants) solve their own local management problems, i.e. they perform local optimization. The subsystems have their individual objective functions and also local constraints, but they share together some common constraints which represent the shared resources and intermediates being consumed and produced at the site.

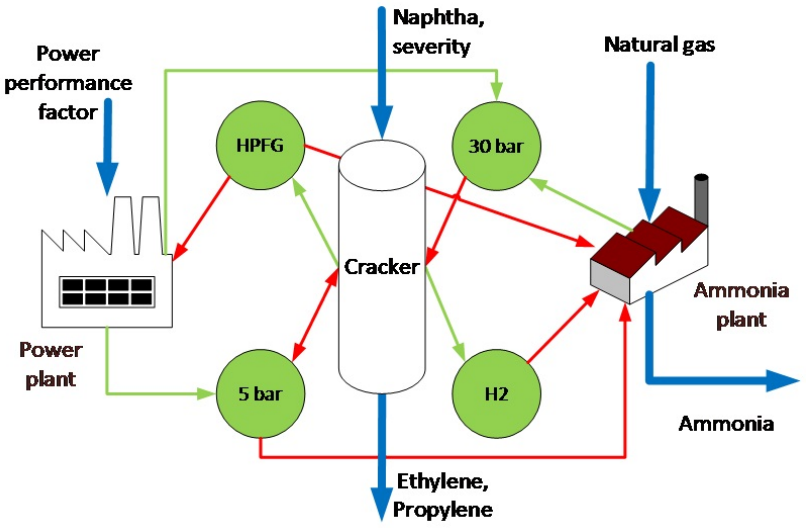

Figure 1: A part of the production site extracted from INEOS case study.

For instance, consider a problem of site-wide optimization as studied in the DYMASOS case study provided by partner INEOS. A part of the site involving cracker, ammonia and power plant is depicted in Fig. 1. This problem was studied in [2]. A global (overall) objective function is given that optimizes the profit of the site that is composed of the profits

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of individual units such that

$$J(\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3) = J_1(\boldsymbol{u}_1) + J_2(\boldsymbol{u}_2) + J_3(\boldsymbol{u}_3), \tag{1.1}$$

where three separable objectives represent the production profit of the three plants and the decision variables $\boldsymbol{u}_i$ stand for the operational degrees of freedom of the plants. It is quite common that, in practice, the optimization of plants' (local) objectives is done in distributed fashion, i.e. the local objectives are optimized by separate entities (business unit coordinators, agents) separately since the local degrees of freedom can only be adjusted locally. There exists then a central coordination authority which ensures that the networks of shared resources (raw materials, energy, intermediates) are balanced and that the demand does not surpass the supply. For the INEOS case study, this represents achievement of the balance of steam networks (5 bar and 30 bar), fuel gas (HPFG) and hydrogen (H2) depicted in Fig. 1.

The described problem can be considered as three subproblems with local objectives $J_1(\boldsymbol{u}_1)$, $J_2(\boldsymbol{u}_2)$ and $J_3(\boldsymbol{u}_3)$, each of which may have its local constraint functions. The global problem is also subject to some global constraint functions ($\boldsymbol{g}(\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3) \leq 0$) that couple the variables of the local problems.

1.1 Problem Definition

The formulation of the studied problem, defined in mathematical terms, is to find a vector $\boldsymbol{U} := (\boldsymbol{u}_1^T, \ldots, \boldsymbol{u}_n^T)^T$ that solves the optimization problem

$$\min_{\boldsymbol{U}} J(\boldsymbol{U}) := \min_{\boldsymbol{U}} \sum_{i=1}^{n} J_i(\boldsymbol{u}_i), \tag{1.2a}$$

with possibly nonconvex functions J_i (for any $i \in \{1, \ldots, n\}$) subject to individual (local) constraints

$$\boldsymbol{f}_i(\boldsymbol{u}_i) \leq 0, \qquad i \in \{1, \ldots, n\}, \tag{1.2b}$$

and global (joint) constraints

$$\sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i) \leq 0. \tag{1.2c}$$

We assume that the functions J_i, $\boldsymbol{f}_i$ and $\boldsymbol{g}_i$ are differentiable sufficiently many times.

In order to characterize the solution of the problem (1.2), we may formulate the conditions for optimality using the Lagrangian function

$$L(\boldsymbol{U}, \boldsymbol{\nu}, \boldsymbol{\lambda}) = \sum_{i=1}^{n} J_i(\boldsymbol{u}_i) + \sum_{i=1}^{n} \boldsymbol{\nu}_i^T \boldsymbol{f}_i(\boldsymbol{u}_i) + \boldsymbol{\lambda}^T \sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i), \tag{1.3}$$

where $\boldsymbol{\nu} \geq 0$ and $\boldsymbol{\lambda} \geq 0$ represent the vectors of Lagrange multipliers associated with local and global constraints respectively. The first-order Karush-Kuhn-Tucker conditions for optimality are given by

$$0 = \nabla_{\boldsymbol{u}_i} L = \nabla_{\boldsymbol{u}_i} J_i(\boldsymbol{u}_i) + (\nabla_{\boldsymbol{u}_i} \boldsymbol{f}_i(\boldsymbol{u}_i))^T \boldsymbol{\nu}_i + (\nabla_{\boldsymbol{u}_i} \boldsymbol{g}_i(\boldsymbol{u}_i))^T \boldsymbol{\lambda}, \qquad \forall i \in \{1, \ldots, n\}, \tag{1.4}$$

$$0 = \nu_{ij} f_{ij}(\boldsymbol{u}_i), \qquad \forall i, j \in \{1, \ldots, n\}, \tag{1.5}$$

$$0 = \lambda_j \sum_{i=1}^{n} g_{ij}(\boldsymbol{u}_i), \qquad \forall j \in \{1, \ldots, n\}, \tag{1.6}$$

together with (1.2b) and (1.2c).

We will assume in this study that the local constraints are satisfied with strict inequalities (i.e. optimal $\nu_{ij} = 0$, $\forall i, j \in \{1, \ldots, n\}$) and only the global constraints determine the global optimum, i.e. $\sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i) = 0$ at the optimum.

The optimization problem (1.2) can be decomposed into n local optimization problems. We will refer to each subproblem as a local problem of subsystem S_i ($i \in \{1, \ldots, n\}$). The optimality conditions for the subsystem S_i can be

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now written as

$$0 = \nabla_{\boldsymbol{u}_i} J_i(\boldsymbol{u}_i) + (\nabla_{\boldsymbol{u}_i} \boldsymbol{g}_i(\boldsymbol{u}_i))^T \boldsymbol{\lambda}_i, \qquad \forall i \in \{1, \dots, n\}, \tag{1.7}$$

$$0 = \lambda_{ij} \sum_{i=1}^{n} g_{ij}(\boldsymbol{u}_i), \qquad \forall j \in \{1, \dots, n\}. \tag{1.8}$$

Here $\boldsymbol{\lambda}_i$ refers to the vector of local Lagrange multipliers of the ith subsystem.

Our goal is to solve the site-wide optimization problem (i.e. to drive the subsystems to a global optimum) while performing limited communication among the subsystems. Referring to Eq. (1.2c) as a global or joint constraint, it is obvious that each subproblem should have an access to some (partial) information on it. The termination of the coordination procedure is reached when the optimality conditions (1.7) are satisfied which in turn means that the Lagrange multipliers associated with joint constraints become equal $\boldsymbol{\lambda}_1 = \boldsymbol{\lambda}_2 = \cdots = \boldsymbol{\lambda}_n$.

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2. Literature review

The technological growth motivates the development of more and more complex process plants. This usually results in complex interconnected systems of interacting entities [3]. Such systems can be difficult to manage and to control in a centralized fashion so the distributed and hierarchical solutions are often favored by engineers and managers.

There are several reasons for this. One is the complexity of the resulting centralized problem. When dealing with complex systems that consist of several units with a large number of manipulated and state variables, feasible solutions may be difficult to compute in real-time or on required time scale using a centralized approach. Another reason is that all subsystems must have coherent software solutions in order to construct a centralized problem formulation and implement the result of centralized optimization, which often is not the case in industry. The third reason that arises from the centralized approach is the necessity of data availability. In order to optimize or control a complex system, a centralized solution requires to access all the data across the system. In practice, this is hindered by three issues. The first issue is the size of the data, which might be very big and therefore its transfer is either practically infeasible or not desired due to reliability and robustness of their transfer. Secondly, in complex systems, some local data might be confidential or vulnerable within the subsystems and therefore should not be shared with the central management or other subsystems. The third issue is the lack of flexibility. Distributed solutions can easier handle structural changes in the complex systems, e.g. replacement of one plant with another or a shutdown of a certain part of the system. This means that, using a distributed approach, the complex system organization can be made modular such that the reconfiguration of subsystems can be performed seamless.

To get these advantages of distributed solutions, a proper coordination mechanism is required in order to make the overall system converge to the system-wide optimum.

Distributed optimization problems have attracted the attention of researchers in the recent past. A generally accepted idea to solve large-scale optimization problems is to decompose the main (centralized) system into smaller subsystems. The coupling (joint or global) constraints must be identified and enforced in some way via some kind of iterative negotiation process. As the structure of Eqs. (1.7) suggest, there is either:

1. relaxation of the global constraints performed and the Lagrange multipliers are (common) parameters that are adjusted to reach the satisfaction of the global constraints—we refer to this class of approaches as price-based or market-based approaches—or

2. relaxation of the equality between the Lagrange multipliers and application of an iterative procedure on allocating different quantities of the shared resources to the different systems is carried out until the equality of Lagrange multipliers is enforced—we refer to this class as constraint-negotiation approaches.

Price-based coordination algorithms are based on the general micro-economic theory, where a market is defined as a population of agents—producers and consumers of goods and services [4]. A consumer's demand of a particular good depends on how useful this good is to him and it decreases when the price increases. The goal of price coordination is to determine the equilibrium prices of all goods that will result in market clearing (no agent can further increase its profit at the equilibrium price). In the following we will review the possibilities to implement market-based mechanisms that iteratively update the prices of the shared resources in order to reach equilibrium prices. Here we provide only a brief review of price-based approaches, but we refer the interested reader to Deliverables 3.1 and 3.3 of the HYCON2 project [5, 6].

Some recent studies of application of price-based coordination can be found in [7, 8, 9, 10]. To solve the optimization problem (1.2) by price-based coordination methods, a Lagrangian relaxation of the coupling constraints is performed. Hence, the problem can be decomposed into n subproblems of the form of (2.1) each corresponding to one of the subsystems.

$$\min_{\boldsymbol{u}_i} J_i(\boldsymbol{u}_i) + \boldsymbol{\lambda}^T \boldsymbol{g}_i(\boldsymbol{u}_i) \tag{2.1}$$

$$\text{s.t. } \boldsymbol{f}_i(\boldsymbol{u}_i) \leq 0. \tag{2.2}$$

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The Lagrangian multipliers for the different shared resources are added to the local economic objective functions in order to account for production and/or consumption. The Lagrange multipliers can also be interpreted as marginal prices for strengthening/relaxing of the shared-resource constraints.

Now the optimization task is split into two layers [11], where the upper layer will coordinate the actions of the local optimizers by iteratively updating the Lagrange multipliers of the coupling constraints [3].

At the kth step of the coordination, after the local optimization have been performed for a given set of multipliers $\boldsymbol{\lambda}$, the coordinator evaluates the network balance. If the shared resource networks are not balanced, the price is updated using a price-update rule, which, in its basic form, can be written as

$$\boldsymbol{\lambda}(k+1) = \boldsymbol{\lambda}(k) - \alpha(k) \sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i(k)), \tag{2.3}$$

where the prices are updated proportionally to the balance error (imbalance) by the factor $\alpha(k)$. Then, the updated price is communicated to the local subsystems and the local optimization is performed again. The goal is that in each iteration, the price moves closer towards the equilibrium price and the difference between demand and supply decreases until the market is cleared. The formulation of the subproblems (2.1) and the price update methods (2.3) vary depending on the implemented algorithm.

One of the first approaches of price-based coordination in the chemical industry was the one presented in [12]. Here the authors propose a slack resource auction as a method for decomposition of the centralized approach to obtain plant-wide profit maximization. They introduce slack resources and the prices of the resources are adjusted using auctions. The slack resource auction method overcomes the failure of Lagrangean procedure to converge for units with piecewise linear utility function. The authors extend their work in [13]. In this approach, the couplings of the subsystems are referred to as interprocess streams, which are seen as slack resources. The system is compared to a supply chain, where subsystems buy and sell slack resources between each other. To find the global optimum, slack auctions are used to determine the equilibrium prices of these slack resources.

In [14, 15], the authors propose a solution based on multi-agent systems for a distributed resource allocation in technical or industrial environments. They refer to a mathematical formulation of the resource allocation problem as an optimization problem and use this formulation to derive the local behavior and the interaction behavior of the agents. The novelty presented here is the combination of market-based mechanisms for resource allocation and process control in continuous production.

In [16], the authors present the mathematical conditions under which a system-level optimization of supply and demand scheduling can be implemented as a distributed optimization in which users and suppliers, as well as the load serving entities, are decision makers with well-defined partial objectives using price-based coordination. The requirements for convergence of the global objectives and the local/individual objectives are defined and novel algorithms for coordinating of the supply-demand problems on different time scales like day ahead horizon and real time adjustment are developed.

The distributed optimization methods are especially suitable for the application in model predictive control (MPC) of interconnected units [17] which is a problem that is structurally very similar to dynamic site-wide management and optimization. For a variety of challenging control tasks, MPC has already been adopted by industry, however, it is mostly used to control subsystems only. As with the site-wide optimization, the coordination is mostly done by the site managers. Distributed control via price-based mechanisms can be an easily understandable and accountable way to coordinate the local controllers to reach optimal plant or site performance [18]. This is currently researched on for the main fields of MPC application, i.e. chemical industry and electrical power systems [19, 20]. Further investigation of the applicability of the price-based techniques on the case studies investigated in DYMASOS will be a core part of Deliverable 2.4 of the project.

Distributed model predictive control concerning coupled constraints was proposed in [21] and [22]. Camponogara and coworkers propose an objective function and constraints to solve a centralized MPC problem in various decentralized (subsystems) fashion. They consider two scenarios for communication between the subsystems. The first case covers the subsystems that can exchange information without any limit and the second case deals with subsystems which can only exchange information while not performing an optimization task of finding the respective local

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optimum. In the first case, conditions have been studied under which performing multiple iterations of each subsystem results in the convergence of the shared variables to the same values for all subsystems. It has been shown that the solutions of the subsystems under these conditions will result in global optima of the main, centralized system.

Jia and Korgh [22] proposed distributed model predictive control with stability constraint (DMPC-SC) in which coordination between subsystems takes place by an exchange of predictions on future behavior of different subsystems. Subsystems are being solved locally with MPC. They introduce two conditions for exchange of information and prove that this method guarantees the stability of system.

Several possibilities to deal with different cooperative subsystems are available. For instance, consensus algorithms were developed in literature to solve similar cooperative problems (see e.g. [23]). Nedic and coworkers [24, 25, 26] studied distributed optimization of problems in the form of (1.2). They [25] solve control problems in which subsystems are only aware of their own local constraints. The effect of these constraints is underlined by solving a constrained consensus problem and projecting the consensus algorithm to be dealt according the local information. The global objective function of their study is subject to the intersection of the constraint sets of these individual systems. Two cases are studied; the first one is the case of the constraint sets being equal but communication among subsystems is time-varying and the second case is the problem with dissimilar constraint sets and time-invariant constant communication. The analysis of convergence and its rate also has been presented in their work. Uncertainty in communication of subsystems also has been investigated in another work by Nedic [26]. The approaches to cooperative control, however, are not directly adaptable for the type of the problems in question. On the other hand, they present a field where many research efforts were invested and thus, bearing in mind the distributed nature of the subsystems being in common scope, there is a possibility to adopt certain developments from the field.

Another promising way of solving distributed optimization (and control) problems is represented by studying the properties of Nash equilibria and application of dynamic and mean-field games for reaching the Nash equilibria [27]. Novel techniques in this direction are developed in WP 1 of the DYMASOS project.

A common algorithm for solving the management problems concerning systems of systems is a gossiping [24, 28, 29]. Gossiping refers to a form of shared computation, in which the mean value of a set of present measurements in a subsystem is calculated [28]. Subsystem i can decide upon the local scalar quantity u_i (gossip variable) that is updated through the time. Gossiping between the subsystems i and j takes place at time t if

$$u_i(t+1) = u_j(t+1) = \frac{(u_i(t) + u_j(t))}{2}.$$

If no gossiping happens for a subsystem, its state value remains unchanged. In this setup, subsystems are put in a network with non-directed edges and the main difference with other general consensus algorithms is that each subsystem is allowed to be in contact (gossip) with just one other subsystem. The termination of algorithm occurs when gossip variables reach a consensus when t goes towards the infinity. Lu and coworkers [29] employ the gossip algorithm to solve unconstrained problem by exchanging the values of the local cost functions.

As mentioned above, the price-based techniques are presently studied in the framework of DYMASOS project. These techniques are promising but possess an inherent downside, since they relax the constraints of the problem, they are of *infeasible-path* type. This means that the only feasible solution is the optimal one that is reached at the convergence of the price-based coordination. In order to perform a thorough investigation on the possibilities of coordination and dynamic management of systems of systems, DYMASOS also studies constraint negotiation algorithms that represent *feasible-path* solution approaches. Such type of algorithm was recently presented in [1] which was selected as a promising approach for dynamic management of systems of systems. In this report, we show an adaptation of this algorithm to the class of problems studied in DYMASOS. We present the extensions that were developed in DYMASOS on the constraint negotiation procedure and we illustrate the performance of the algorithm on academic problems.

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3. Proposed Methodology

In this section, we study and implement the *constraint negotiation* procedure that is adapted from [1]. The procedure represents a coordination algorithm that mimics a negotiation between multiple agents. It is assumed that each system knows its own dynamics, cost function and local constraints and actively contributes to the balance (fulfillment) of the global constraints.

3.1 Local Optimum vs. Global Optimum

The trivial solution of the global optimization problem that consists of different subproblems is the case where optimum value for each subproblem results in a feasible set of coupling constraints. Therefore, the optima of the global problem can be constructed through the set of optima of the individual subsystems.

The procedure of decoupling the problem takes place as follows. Consider the global objective function (3.23a). We can form the decomposed (local) optimization problems as follows. Suppose $i \in \{1, \dots, n\}$ and S_i reads as

$$\begin{aligned} \min_{\boldsymbol{u_i}} \quad & J_i(\boldsymbol{u}_i) \\ \text{s.t.} \quad & \boldsymbol{f}_i(\boldsymbol{u}_i) \leq 0, \quad \forall i \in \{0, \dots, n\}. \end{aligned} \tag{3.1}$$

Consider $u_i^\dagger$ to be the solution to this optimization problem. Additionally consider that the vector $\boldsymbol{U}^\dagger = \{\boldsymbol{u}_1^\dagger, \dots, \boldsymbol{u}_n^\dagger\}$ satisfies Eq. (1.2c)

$$\sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i^\dagger) \leq 0. \tag{3.2}$$

This means that we have found a set of variables which solve the local optimization problems and also satisfy the global coupling constraints. Therefore, the vector $\boldsymbol{U}^\dagger$ is clearly the solution to the global optimization problem (1.2).

3.2 Coordinate Descent

The coordinate descent procedure, illustrated for $n = 2$ in Fig. 2, is applied in the case when

$$\sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i^\dagger) \not\leq 0, \tag{3.3}$$

i.e. where the optima for individual subsystems do not satisfy the global coupling constraint. We will consider a set of variables $\boldsymbol{U}^f = \{\boldsymbol{u}_1^f, \dots, \boldsymbol{u}_n^f\}$ which satisfy Eqs. (1.2b) and (1.2c) where superscript f denotes a feasibility of the point w.r.t. all constraints.

The following steps are followed:

1. Starting with system 1, compute $\boldsymbol{u}_1^{cd}$ such that

$$\boldsymbol{u}_1^{cd} = \operatorname*{argmin}_{\boldsymbol{u}_1} \quad J_1(\boldsymbol{u}_1) \tag{3.4}$$

$$\text{s.t.} \quad \boldsymbol{g}_1(\boldsymbol{u}_1) \leq -\sum_{i=2}^{n} \boldsymbol{g}_i(\boldsymbol{u}_i^f), \tag{3.5}$$

$$\boldsymbol{f}_1(\boldsymbol{u}_1) \leq 0. \tag{3.6}$$

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2. For $i \in \{2, \ldots, n-1\}$ compute $\boldsymbol{u}_i^{cd}$ such that

$$\boldsymbol{u}_i^{cd} = \underset{\boldsymbol{u}_i}{\text{argmin}} \quad J_i(\boldsymbol{u}_i) \tag{3.7}$$

$$\text{s.t.} \quad \boldsymbol{g}_i(\boldsymbol{u}_i) \leq -\sum_{j=i+1}^{n} \boldsymbol{g}_j(\boldsymbol{u}_j^f) - \sum_{j=1}^{i-1} \boldsymbol{g}_j(\boldsymbol{u}_j^{cd}), \tag{3.8}$$

$$\boldsymbol{f}_i(\boldsymbol{u}_i) \leq 0. \tag{3.9}$$

3. Compute $\boldsymbol{u}_n^{cd}$ such that

$$\boldsymbol{u}_n^{cd} = \underset{\boldsymbol{u}_n}{\text{argmin}} \quad J_n(\boldsymbol{u}_n) \tag{3.10}$$

$$\text{s.t.} \quad \boldsymbol{g}_n(\boldsymbol{u}_n) \leq -\sum_{j=1}^{n-1} \boldsymbol{g}_j(\boldsymbol{u}_j^{cd}), \tag{3.11}$$

$$\boldsymbol{f}_n(\boldsymbol{u}_n) \leq 0. \tag{3.12}$$

It is evident that the obtained set $\boldsymbol{U}^{cd} = (\boldsymbol{u}_1^{cd}, \ldots, \boldsymbol{u}_n^{cd})$ is both locally and globally feasible, i.e. it satisfies Eqs. (1.2c) and (1.2b). Besides, the following holds

$$J(\boldsymbol{u}_1^{cd}, \ldots, \boldsymbol{u}_n^{cd}) \leq J(\boldsymbol{u}_1^{f}, \ldots, \boldsymbol{u}_n^{f}), \tag{3.13}$$

where the equality holds just when two sets are equal $(U^{cd} = U^f)$.

To justify the relation (3.13), without a loss of generality, we consider the case with two subsystems (Eq. (1.1)). In this case $\boldsymbol{U}^f = (\boldsymbol{u}_1^f, \boldsymbol{u}_2^f)$. We can write

$$J(\boldsymbol{u}_1^f, \boldsymbol{u}_2^f) = J_1(\boldsymbol{u}_1^f) + J_2(\boldsymbol{u}_2^f), \tag{3.14}$$

and obviously, $\boldsymbol{g}_1(\boldsymbol{u}_1^f) + \boldsymbol{g}_2(\boldsymbol{u}_2^f) \leq 0$. If we solve the subsystem S_2 considering $\boldsymbol{u}_1 = \boldsymbol{u}_1^f$ we will end up with

$$\boldsymbol{u}_2^{cd} = \underset{\boldsymbol{u}_2}{\text{argmin}} \quad J_2$$

$$\text{s.t.} \quad \boldsymbol{g}_1(\boldsymbol{u}_1^f) + \boldsymbol{g}_2(\boldsymbol{u}_2) \leq 0, \tag{3.15}$$

which satisfies

$$J_2(\boldsymbol{u}_2^{cd}) \leq J_2(\boldsymbol{u}_2^f). \tag{3.16}$$

The same manner then can be followed for computing $\boldsymbol{u}_1^{cd}$ considering $\boldsymbol{u}_2^f$ which yields

$$J_1(\boldsymbol{u}_1^{cd}) \leq J_1(\boldsymbol{u}_1^f). \tag{3.17}$$

Summing up the both sides of Eqs. (3.16) and (3.17) results in

$$J_1(\boldsymbol{u}_1^{cd}) + J_2(\boldsymbol{u}_2^{cd}) \leq J_1(\boldsymbol{u}_1^f) + J_2(\boldsymbol{u}_2^f), \tag{3.18}$$

and consequently relation (3.13) is proven.

If the Lagrange multipliers, found from (1.7), resulting from the coordinate descent procedure, $\boldsymbol{\lambda}_i$, are equal to each other, then we reached the global optimum, otherwise, we proceed with the constraint negotiation steps (`start2`).

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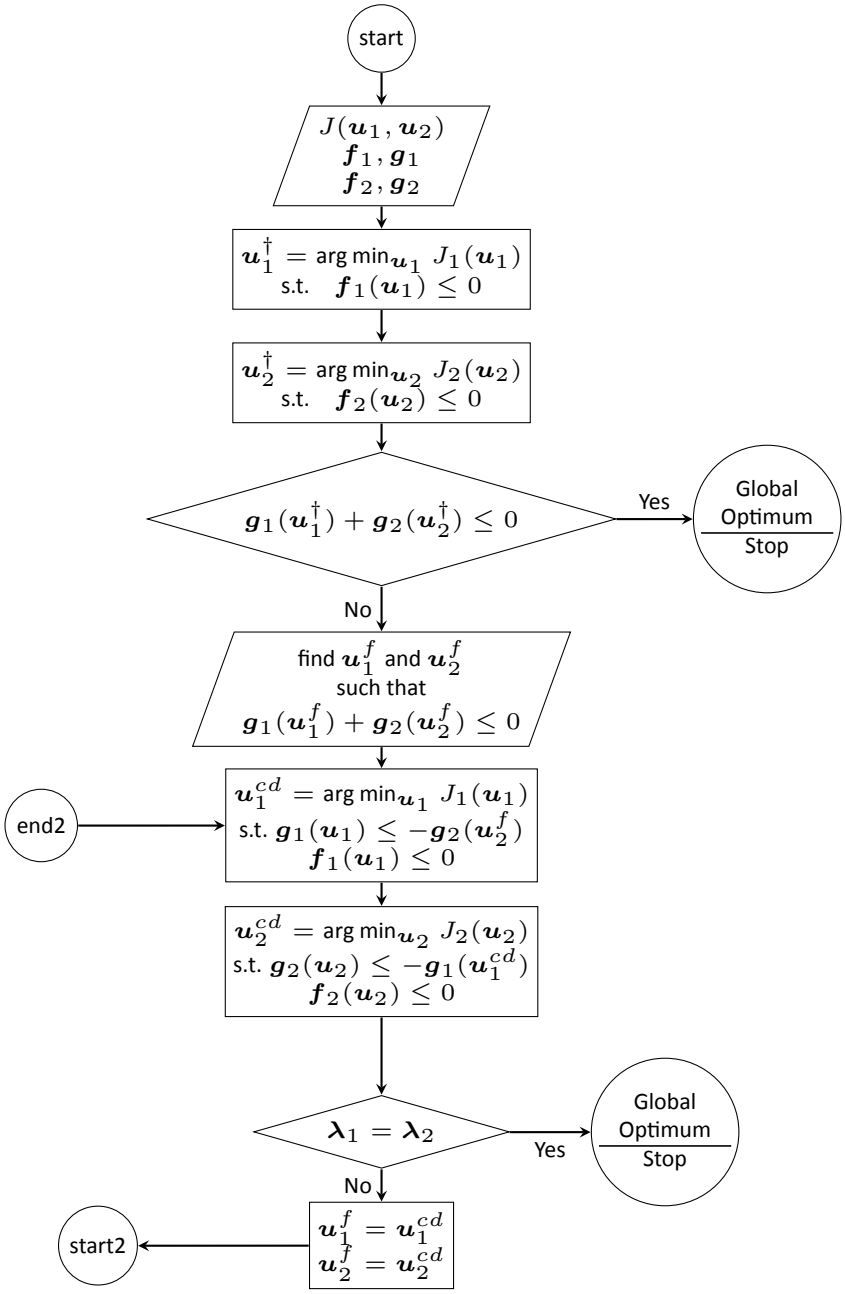

Figure 2: Coordinate Descent Algorithm.

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3.3 Constraint Negotiation Procedure

The procedure of *constraint negotiation* is to distribute the relevant information among the subsystems which leads to the optimal satisfaction of the global (coupling) constraints (1.2c). The skeleton of the presented algorithm is taken from [1] and is further extended to be applicable to the type of systems of systems studied in DYMASOS project and its industrial case studies. The procedure can be conceived as a circular information flow, in which subsystem S_i exchanges information to subsystem S_{i+1}. The basic idea of the procedure of constraint negotiation is that we pick a set of active constraints and perturb a member in the set in the direction that leads to the best decrease of the global cost. For instance, let us consider the case when a set $\boldsymbol{U}^{cd} = (\boldsymbol{u}_1^{cd}, \dots, \boldsymbol{u}_n^{cd})$ satisfies (1.2c). Then we pick a subsystem $i \in \{1, \dots, n\}$ and perform a perturbation on $\boldsymbol{u}_i$ such that $\boldsymbol{u}_i = \boldsymbol{u}_i^{cd} + \boldsymbol{p}_i$. Afterwards we examine the influence of this perturbation on other subsystems in the sequential manner as well as on the global problem. We require the resulting set $\boldsymbol{U}$, after this perturbation, to satisfy local and global constraints and to result in a decrease of the global objective function. The set should be passed to the coordinate descent algorithm (given in Section 3.2) to see whether the global optimality conditions, particularly the equality of (local) Lagrange multipliers, are satisfied or not. It follows from economical theory that, since Lagrange multiplier represents the marginal cost of the constraint, the equality of Lagrange multipliers leads to market clearing as in the market-based approaches referenced in Section 2.

In fact the perturbations can be iterated with different $i \in \{1, \dots, n\}$ and the system S_{i^*} whose perturbation (negotiation proposal) results in the biggest decrease of the overall objective function can be selected as the driver of the negotiation. The proposed distribution of shared resources, i.e. the one which results in a biggest decrease of the global objective, is accepted and implemented. If the Lagrange multipliers for the new point do not match, $\boldsymbol{\lambda}_1 \neq \boldsymbol{\lambda}_2 \neq \cdots \neq \boldsymbol{\lambda}_n$, the new point is used for further improvement, i.e. the negotiation procedure is repeated, so the iterative procedure is established and continued until the point such that the resulting solution from constraint negotiation results in equality of Lagrange multipliers.

To perform the constraint negotiation procedure, the following steps are executed;

1. Compute the Lagrange multipliers corresponding to global constraints to each subsystem.

2. Pick a subsystem S_i, $i \in \{1, \dots, n\}$.

3. Solve the following optimization problem

$$\boldsymbol{p}_i = \underset{\boldsymbol{p}_i}{\text{argmin}} \left(\frac{1}{n-1} \sum_{j \neq i} \boldsymbol{\lambda}_j^T \nabla \boldsymbol{g}_i(\boldsymbol{u}_i)\big|_{\boldsymbol{u}_i^{cd}} + \nabla J_i(\boldsymbol{u}_i)\big|_{\boldsymbol{u}_i^{cd}} \right)^T \boldsymbol{p}_i + \frac{1}{2} \boldsymbol{p}_i^T \nabla^2_{\boldsymbol{u}_i} J_i(\boldsymbol{u}_i)\big|_{\boldsymbol{u}_i^{cd}} \boldsymbol{p}_i, \tag{3.19}$$

$$\text{s.t.} \quad \boldsymbol{f}_i(\boldsymbol{u}_i^{cd} + \boldsymbol{p}_i) \leq 0. \tag{3.20}$$

4. Compute $\Delta J_i = J_i(\boldsymbol{u}_i^{cd} + \text{diag}(\boldsymbol{\alpha})\boldsymbol{p}_i) - J_i(\boldsymbol{u}_i^{cd})$ for some $0 < \alpha_i \leq 1$ and also $\boldsymbol{g}_i(\boldsymbol{u}_i^{cd} + \text{diag}(\boldsymbol{\alpha})\boldsymbol{p}_j)$.

5. Pick a subsystem S_j, $j = i + 1$. Initialize the index sets $\mathcal{I}_p := i + 1$ and $\mathcal{I}_e := \{1, \dots, n\} \setminus \{i, i+1\}$.

6. Solve the following optimization problem

$$\begin{aligned} \min_{\boldsymbol{p}_j} \quad & J_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j) \\ \text{s.t} \quad & 0 \geq \boldsymbol{f}_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j), \\ & 0 \geq \boldsymbol{g}_i(\boldsymbol{u}_i^{cd} + \text{diag}(\boldsymbol{\alpha})\boldsymbol{p}_i) + \sum_{k \in \mathcal{I}_p} \boldsymbol{g}_k(\boldsymbol{u}_k^{cd} + \boldsymbol{p}_k) + \sum_{k \in \mathcal{I}_e} \boldsymbol{g}_k(\boldsymbol{u}_k^{cd}). \end{aligned} \tag{3.21}$$

7. Repeat step 6 with j taken as a first element of $\mathcal{I}_e$ (when j is picked perform $\mathcal{I}_e := \mathcal{I}_e \ominus j$ and $\mathcal{I}_p := \mathcal{I}_p \oplus j$) until $\mathcal{I}_e = \emptyset$.

8. Pick i^* such that $\sum_{i=1}^{n} \Delta J_i$ is the smallest.

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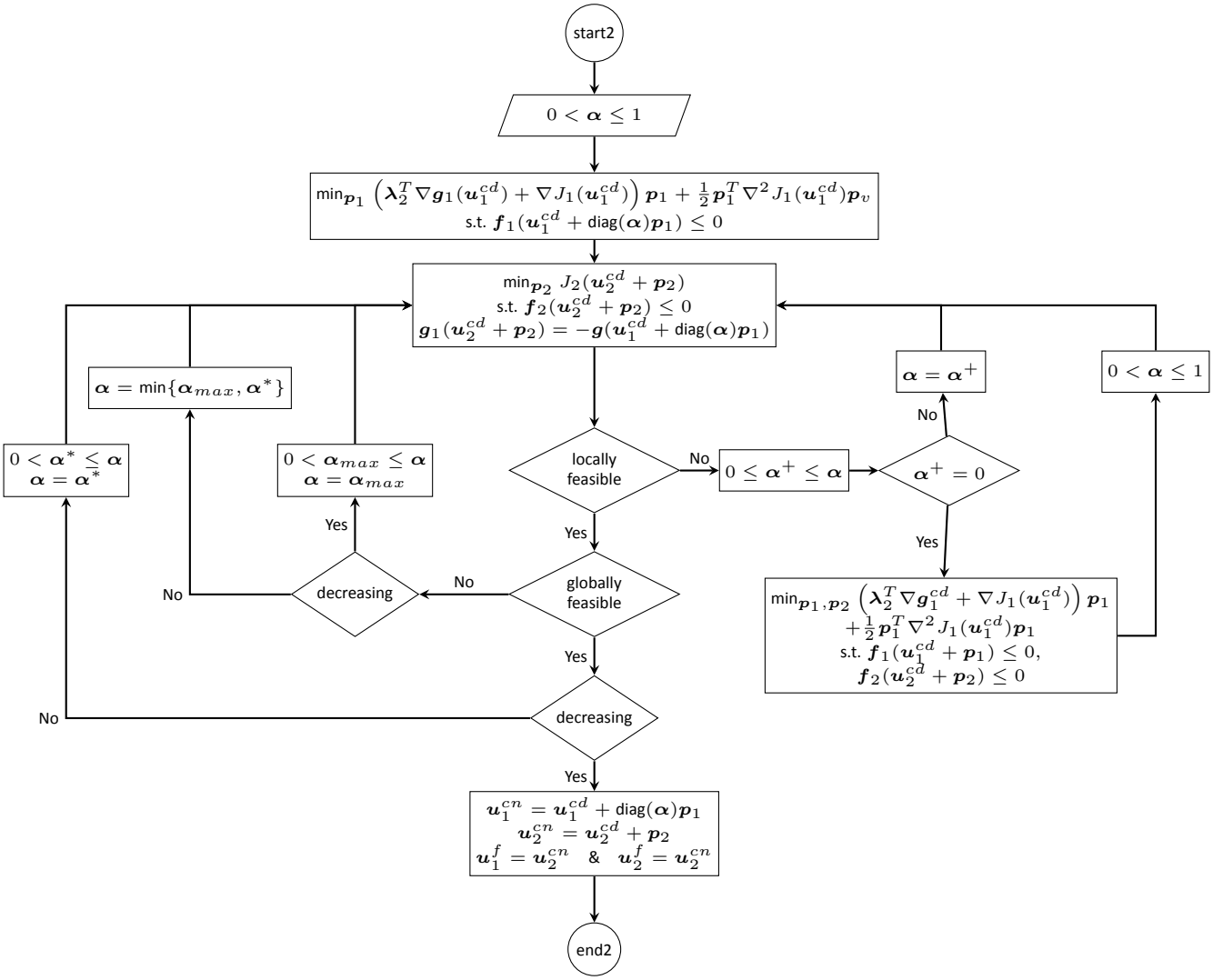

Figure 3: Constraint negotiation algorithm as proposed in [1].

9. Compute $\boldsymbol{u}_i^{cn}$, $\forall i \in \{0, \ldots, N\}$ (as described in the flowchart in Fig. 3) and go to the coordinate descent algorithm.

The described procedure is illustrated in Fig. 3 for 2 subsystems. Hence Step 9 of the procedure adjusts the value(s) of $\boldsymbol{\alpha}$ such that the result of the constraint negotiation is:

- *locally feasible* i.e. Eq. (1.2b) is satisfied,
- *global feasibility* i.e. Eq. (1.2c) is satisfied,
- *decreasing* i.e. means that $\sum_{i=1}^{n} \Delta J_i < 0$.

According to the flowchart in Fig. 3, if the local or global feasibility is violated or if the perturbation results in non-decreasing value of the objective function (i.e. $\sum_{i=1}^{n} \Delta J_i \geq 0$), the values of $\boldsymbol{\alpha}$ should be modified to meet the constraints. The different possibilities illustrated in Fig. 3 are described in detail in [1]. In this study we propose a novel approach for calculation of the vector $\boldsymbol{\alpha}$ that serves as a *proposal execution rate* or *negotiation parameter*.

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3.3.1 Proposed Calculation of α

The original constraint negotiation algorithm, presented in [1], involves a multi-step process of evaluation and adaptation of the parameter $\boldsymbol{\alpha}$ to arrive at the acceptable performance in terms of feasibility and decrease of objective value. The choice of parameter $\boldsymbol{\alpha}$ might not be straightforward, although for simple small-scale case studies presented in next section, the choice of $\alpha = 1/2$ is optimal regarding the rate of convergence of the constraint negotiation procedure. The authors of the original constraint negotiation procedure [1] propose a use of scalar *negotiation parameter*. However, for multivariate decision vector $\boldsymbol{u}_i$, it might turn out that, in order to achieve a faster convergence of the coordination procedure, taking the *negotiation parameter* as a vector would be necessary. This will apply in the cases when the initial point from which the negotiation starts is very far from a global optimum or when a substantial diversity appears in the magnitudes of the constraints, decisions and local objective functions that is not properly regularized. The practice gives often rise to these situations.

We suggest to formulate the choice of $\boldsymbol{\alpha}$ as an optimization problem. We propose two different procedures which involve different optimization objectives and different degrees of freedom and also require different amount of local information to be present to these methods.

As it was mentioned above, the coordination procedure must enforce the optimality conditions (1.7). The objective function for identifying the best value of negotiation parameter $\boldsymbol{\alpha}$, with respect to the rate of negotiation convergence, can thus follow two goals (the index i^* can be selected using the procedure described in Section 3.3 with some a priori chosen value of $\alpha \in (0, 1)$):

- Global (primal) optimality

  To this end we consider the following optimization problem:

$$\min_{\boldsymbol{\alpha}, \boldsymbol{p}_j,\ 1\le j\le n,\ j\neq i^*} J_{i^*}(\boldsymbol{u}_{i^*}^{cd} + \mathrm{diag}(\boldsymbol{\alpha})\boldsymbol{p}_{i^*}) + \sum_{j\neq i^*} J_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j), \tag{3.22a}$$

$$\text{s.t. } 0 \ge \boldsymbol{f}_{i^*}(\boldsymbol{u}_{i^*}^{cd} + \mathrm{diag}(\boldsymbol{\alpha})\boldsymbol{p}_{i^*}), \tag{3.22b}$$

$$0 \ge \boldsymbol{f}_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j), \qquad 1 \le j \le n,\ j \neq i, \tag{3.22c}$$

$$0 \ge \boldsymbol{g}_{i^*}(\boldsymbol{u}_{i^*}^{cd} + \mathrm{diag}(\boldsymbol{\alpha})\boldsymbol{p}_{i^*}) + \sum_{j\neq i^*} \boldsymbol{g}_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j). \tag{3.22d}$$

  We remark that if functions $\boldsymbol{J}(\cdot)$, $\boldsymbol{f}(\cdot)$, or $\boldsymbol{g}(\cdot)$ are nonlinear, a linearization of a constraint or of the objective function can take place in order to simplify the problem (3.23) and express it in the form of sequential linear programming. Hence in this approach the subsystems communicate the sensitivities of the constraints and objectives w.r.t. shared resources. Note that similar schemes based on sharing the derivative information have been applied in price-based coordination in order to enhance the convergence [30].

- Optimal resource allocation (market clearing)

  The aim here is enforce the equality of the local Lagrange multipliers of the subsystems. Practically, we can formulate an optimization problem that minimizes the difference of Lagrange multipliers w.r.t. to the mean value of the local Lagrange multipliers among individual constraints. The problem can be formulated as

$$\min_{\boldsymbol{\lambda}, \boldsymbol{\alpha}, \boldsymbol{p}_j,\ 1\le j\le n,\ j\neq i^*} \left\| \boldsymbol{\lambda} - \frac{\mathbf{1}^T\boldsymbol{\lambda}}{n} \right\|_1, \tag{3.23a}$$

$$\text{s.t. } 0 \ge \boldsymbol{f}_{i^*}(\boldsymbol{u}_{i^*}^{cd} + \mathrm{diag}(\boldsymbol{\alpha})\boldsymbol{p}_{i^*}), \tag{3.23b}$$

$$0 \ge \boldsymbol{f}_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j), \qquad 1 \le j \le n,\ j \neq i, \tag{3.23c}$$

$$0 \ge \boldsymbol{g}_{i^*}(\boldsymbol{u}_{i^*}^{cd} + \mathrm{diag}(\boldsymbol{\alpha})\boldsymbol{p}_{i^*}) + \sum_{j\neq i^*} \boldsymbol{g}_j(\boldsymbol{u}_j^{cd} + \boldsymbol{p}_j), \tag{3.23d}$$

$$\text{Eq. (1.7).} \tag{3.23e}$$

  It is clear that this second proposal involves a bigger number of degrees of freedom and constraints. On the other hand, if the values of the underlying objectives are not available to coordinator or the problem is

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highly nonlinear and, a linearization is required (as discussed in the above one paragraph), the proposed approach will provide a reasonable trade-off between computational complexity and convergence of constraint negotiation.

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4. Examples

4.1 Example 1: Two Coupled Systems with One Shared Resource

Consider the following optimization problem

$$\begin{aligned} \min_{u_1,u_2} \quad & u_1^2 + u_2^2 \\ \text{s.t.} \quad & 1 - u_1 - u_2 \leq 0. \end{aligned} \tag{4.1}$$

This problem has a clear geometrical interpretation as a minimization of the radius of a sphere centered at point $(0,0)^T$ which intersects the line $u_2 = 1 - u_1$. This rather simple problem with a solution $(1/2, 1/2)^T$ can also be regarded as joint optimization over two subsystems with quadratic cost functions and one shared resource, hence a coupling via a linear inequality is present.

The decomposition into local optimization problems can be performed as follows

$$S_1 : \min_{u_1} \quad u_1^2, \tag{4.2}$$

$$S_2 : \min_{u_2} \quad u_2^2, \tag{4.3}$$

where we clearly observe that both systems are identical. The solutions of the subsystems' problems are $\{u_1^\dagger = 0,\ u_2^\dagger = 0\}$ which do not fulfill the global constraint condition.

Table 1: Summary of a coordinate descent procedure for Example 1.

S_1	$\Rightarrow$	S_2
$\min_{u_1} \quad u_1^2$ s.t. $\quad 1 - u_1 - u_2^f \leq 0$		$\min_{u_2} \quad u_2^2$ s.t. $\quad 1 - u_1^{cd} - u_2 \leq 0$
$\Downarrow$		$\Downarrow$
$\min_{u_1} \quad u_1^2$ s.t. $\quad -u_1 \leq 0$ $\Rightarrow u_1^{cd} = 0$		$\min_{u_2} \quad u_2^2$ s.t. $\quad 1 - u_2 \leq 0$ $\Rightarrow u_2^{cd} = 1$

We consider $\{u_1^f = 0, u_2^f = 1\}$ as an initial point which is located on the (active) global constraint. We proceed as suggested above by coordinate descent procedure. This is summarized in Tab. 1. We first solve the subsystem S_1 while passing it the value u_2^f, i.e. the amount of shared resource taken by S_2. We remark here that having more than two subsystem results in this step again in communication of a quantity that corresponds to aggregated usage of the shared resource. Once the optimum of S_1 for a given u_2^f is determined, the optimal solution u_1^{cd} is passed to S_2 which determines now a new local solution u_2^{cd}.

For our particular choice of $\boldsymbol{U}^f$, the coordinate descent procedure results in exchange of the initial local solutions between the subsystems. The same phenomenon takes place when the order of communication (S_2 proposes to change the allocation of the shared resource) is reverted. We proceed now with the constraint negotiation procedure as described in Section 3.3. The information required as input to the algorithm is given in Tab. 2. The reported Lagrange multipliers correspond to local solutions from the coordinate descent step.

According to Eq. (3.19) and by picking the first subsystem, we solve the following optimization problem

$$\min_{p_1} \quad p_1^2 - 2p_1,$$

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Table 2: Instance of constraint negotiation procedure for Example 1.

	S_1	S_2
u_i^{cd}	0	1
λ_i	0	2
g_i	$-u_1$	$-u_2$
$\nabla g_i\big\|_{u_i^{cd}}$	-1	-1
$\nabla J_i\big\|_{u_i^{cd}}$	0	2
$\nabla^2 J_{u_i}\big\|_{u_i^{cd}}$	2	2

which has the solution $p_1 = 1$. Considering $\alpha = \frac{1}{2}$ we have $\Delta J_1 = J_1(u_1^{cd} + \alpha p_1) - J_1(u_1^{cd}) = \frac{1}{4}$. Continuing with the procedure of constraint negotiation, we solve the following problem (from Eq. (3.21))

$$\begin{aligned} \min_{p_2} \quad & \left(u_2^{cd} + p_2\right)^2 \\ \text{s.t.} \quad & 1 - u_2^{cd} + p_2 = u_1^{cd} + \alpha p_1, \end{aligned} \tag{4.4}$$

which yields the solution $p_2 = -\frac{1}{2}$ and decrease of

$$\Delta J_2 = J_2(u_2^{cd} + p_2) - J_2(u_2^{cd}) = -\frac{3}{4}.$$

Therefore the total decrease is

$$\sum_{i=1}^{2} \Delta J_i = -\frac{1}{2}, \tag{4.5}$$

which shows an improvement in the objective function value. The resulting solution after the constraint negotiation steps is

$$\begin{aligned} u_1^{cn} &= u_1^{cd} + \alpha p_1 = \frac{1}{2}, \\ u_2^{cn} &= u_2^{cd} + p_2 = \frac{1}{2}, \end{aligned} \tag{4.6}$$

which is a globally optimal point. It is easy to investigate that continuing with this point through the coordinate descent procedure, i.e. first part of flow chart (Fig. 2), we end up with a justification of this point to be a global optimum since it holds that

$$\lambda_1 = \lambda_2 = 1.$$

Starting the negotiation with solving the subsystem S_2 and picking $\alpha = 0.5$, the procedure terminates after the first application of the constraint negotiation procedure with the same solution.

4.2 Example 2: Three Coupled Systems with Two Shared Resources

We consider the following optimization problem

$$\begin{aligned} \min_{u_1, \boldsymbol{u}_2, u_3} \quad & u_1^2 + \boldsymbol{u}_2^T I \boldsymbol{u}_2 + u_3^2 \\ \text{s.t.} \quad & 1 - u_1 - u_{21} \leq 0, \\ & 1 - u_{22} - u_3 \leq 0, \\ & -2u_{21} + u_{22} \leq 0. \end{aligned} \tag{4.7}$$

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The problem can be interpreted as a plant-wide optimization of the site that comprises of three production units which share two resources and there are local constraints present in subsystem 2. This problem is structurally similar to the motivating example presented in Fig. 1 but the number of shared resources is reduced for lucidity.

More concretely, the problem (4.7) can be separated into three subproblems as

$$S_1 : \min_{u_1} \quad u_1^2, \tag{4.8}$$

$$S_2 : \min_{\boldsymbol{u}_2} \quad u_1^2 + u_2^2, \text{ s.t. } -2u_{21} + u_{22} \leq 0, \tag{4.9}$$

$$S_3 : \min_{u_3} \quad u_3^2. \tag{4.10}$$

As in the previous case, the individual optima of the three systems will not result in a feasible point for the global optimization as $u_1^\dagger = 0, u_{21}^\dagger = 0, u_{22}^\dagger = 0, u_3^\dagger = 0)$. The optimal solution of the problem is, similarly to previous example, $(1/2, 1/2, 1/2, 1/2)^T$ which shows a symmetry in the problem. We proceed with the coordinate descent step where we select the initial feasible point $\boldsymbol{U}^f = (1/2, 1/2, 1, 0)$ where the diversity of the local solutions is motivated by the observed symmetry of the problem; simply speaking, starting with $\boldsymbol{U}^f = (0, 1, 1, 0)$ would lead to follow the same procedures for S_1 negotiating with S_2 and for S_3 communicating with S_2. Instead we would like to study the behavior of the aforementioned algorithms when initialized at the partial optimum (hence variables u_1 and u_{21} are initialized at the optimal points). The required input information is given in Tab. 4.

Table 3: Summary of a coordinate descent procedure for Example 2.

S_1	$\Rightarrow$	S_2	$\Rightarrow$	S_3
$\min_{u_1} \; u_1^2$ s.t. $1 - u_1 - u_{21}^f \leq 0$		$\min_{\boldsymbol{u}_2} \; u_{21}^2 + u_{22}^2$ s.t. $1 - u_1^{cd} - u_{21} \leq 0$ $1 - u_{22} - u_3^f \leq 0$ $-2u_{21} + u_{22} \leq 0$		$\min_{u_2} \; u_2^2$ s.t. $1 - u_{22}^{cd} - u_3 \leq 0$
$\Downarrow$		$\Downarrow$		$\Downarrow$
$\min_{u_1} \; u_1^2$ s.t. $1/2 - u_1 \leq 0$		$\min_{\boldsymbol{u}_2} \; u_{21}^2 + u_{22}^2$ s.t. $1/2 - u_{21} \leq 0$ $1 - u_{22} \leq 0$ $-2u_{21} + u_{22} \leq 0$		$\min_{u_3} \; u_3^2$ s.t. $-u_3 \leq 0$
$\Rightarrow u_1^{cd} = 1/2$		$\Rightarrow \boldsymbol{u}_2^{cd} = (1/2, 1)^T$		$\Rightarrow u_3^{cd} = 0$

The proceeding of the coordinate descent algorithm is presented in Tab. 3. We first solve the subsystem S_1 while passing it the value u_{21}^f, i.e. the amount of the first shared resource taken by S_2. The optimum for S_1 for the given u_2^f is determined to be the same as u_1^f and the similar situation occurs when subsystem S_2 solves its local optimization, i.e. $u_{21}^{cd} = u_{21}^f$ when it is passed the solution from S_1. As S_2 does not propose to change its solution (resource allocation) w.r.t. $\boldsymbol{U}^f$, and S_3 gives $u_3^{cd} = u_3^f$ consequently. For our particular choice of $\boldsymbol{U}^f$, the coordinate descent procedure results in the starting point.

We proceed now with the constraint negotiation procedure as described in Section 3.3. The information required as input to the algorithm is given in Tab. 4. The reported Lagrange multipliers correspond to the local solutions from the coordinate descent step.

Instead of starting the negotiation with subsystem S_1, as in the coordinate descent step, we start with the subsystem S_2. This choice is motivated by the fact that S_2 plays an active role in both global constraints. Such situation might very frequently appear in the practice, for instance, the cracker unit is the initiator of the negotiation in practice in the case study provided by project partner INEOS as most of its products serve as intermediates for other plants.

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Table 4: Instance of constraint negotiation procedure for Example 2.

	S_1	S_2	S_3
$\boldsymbol{u}_i^{cd}$	$1/2$	$(1/2,1)^T$	0
$\boldsymbol{\lambda}_i$	$(1,0)^T$	$(1,2)^T$	$(0,0)^T$
$\boldsymbol{g}_i$	$(-u_1,0)^T$	$(-u_{21},-u_{22})^T$	$(0,-u_3)^T$
$\nabla \boldsymbol{g}_i\big\vert_{\boldsymbol{u}_i^{cd}}$	$(-1,0)^T$	$((-1,0)^T,(0,-1)^T)$	$(0,-1)^T$
$\boldsymbol{f}_i$	–	$(-2,1)^T$	–
$\nabla J_i\big\vert_{\boldsymbol{u}_i^{cd}}$	1	$(1,2)^T$	0
$\nabla^2 J_i\big\vert_{\boldsymbol{u}_i^{cd}}$	2	2	2

According to Eq. (3.19) we solve

$$\begin{aligned} &\min_{\boldsymbol{p}_2} (0,2)^T \boldsymbol{p}_2 + \boldsymbol{p}_2^T I \boldsymbol{p}_2, \\ &\text{s.t.} -2u_{21} + u_{22} \leq 0. \end{aligned} \tag{4.11}$$

which gives the solution $\boldsymbol{p}_2 = (0,-1)^T$. Considering $\alpha = \frac{1}{2}$ we have $\Delta J_2 = J_2(\boldsymbol{u}_2^{cd} + \alpha \boldsymbol{p}_2) - J_2(\boldsymbol{u}_2^{cd}) = -\frac{3}{4}$.

Continuing with the procedure of constraint negotiation, the subsystem S_1 responds with $p_1 = 0$, as $\alpha p_{21} = 0$, and the subsystem S_3 responds with $p_3 = 1/2$. This negotiation leads to the biggest decrease in the global objective.

Evaluation of the proposal by subsystem S_1 is trivial as there is no proposed change (reallocation) of the global constraint corresponding to S_1 and S_2. Evaluation of the proposal by subsystem S_3 follows a solution to optimization problem

$$\begin{aligned} \min_{p_3} \quad & \left(u_3^{cd} + p_3\right)^2 \\ \text{s.t.} \quad & 1 - \left(u_{22}^{cd} + \alpha p_{22}\right) - \left(u_3^{cd} + p_3\right) \leq 0, \end{aligned} \tag{4.12}$$

which results in $p_3 = 1/2$ and $\Delta J_{u_2} = 1/4$. The total decrease is

$$\sum_{i=1}^{3} \Delta J_i = -\frac{1}{2}.$$

The resulting point after this round of negotiation is

$$\begin{aligned} u_1^{cn} &= u_1^{cd} + \alpha p_1 = 1/2, \\ \boldsymbol{u}_2^{cn} &= \boldsymbol{u}_2^{cd} + 1/2 p_2 = (1/2, 1/2)^T \\ u_3^{cn} &= u_3^{cd} + p_3 = 1/2. \end{aligned} \tag{4.13}$$

which is a global optimum. It is easy to verify that this point results in equality of local Lagrange multipliers that confirms the optimality and makes constraint negotiation to terminate.

We finally note that by picking the subsystem S_1 to be the system that proposes the reallocation of shared resources, the proposal would be zero and no decrease in the value of global objective would be achieved. If the constraint negotiation starts at S_3, the global optimum would be achieved.

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5. Conclusions and Future Work

In this report we presented an algorithm adapted from open literature for the management of physically coupled systems of systems that uses a principle of multi-agent negotiation over the set of active coupling constraints that is a specific type of problems investigated in the framework of the DYMASOS project. We also presented the recently developed extensions of the constraint negotiation algorithm that enhance its convergence.

The presented algorithm is particularly suitable for the management of small-scale systems of systems, i.e. networks with tens of constituting subsystems, that exhibit nonlinear behavior. This type of systems of systems is naturally present in chemical production complexes such as the case studies of DYMASOS provided by the partners BASF and INEOS. Moreover, the presented management method is a feasible-path iterative procedure, in contrast to infeasible-path price-based algorithms studied in WP 2 of DYMASOS, and thus well suited for the robust implementation in chemical industry that might be relatively conservative with respect to the application of new management methodologies.

The algorithmic developments presented in this report will be further applied to the case studies from the area of chemical industry provided by partners BASF and INEOS for demonstration of their applicability as one of the final results of DYMASOS.

This project has received funding from the European Union's Seventh Programme for research, technological development and demonstration under grant agreement No 611281.

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