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Lukas Samuel Maxeiner

Dual-based methods for distributed optimization of interconnected systems

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Chemieingenieurwesen

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Declaration of Authorship

I, Lukas Samuel Maxeiner, declare that this thesis titled, “Dual-based methods for distributed optimization of interconnected systems” and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Publications leading to this thesis

Most of the developments, findings and results that are presented in this thesis were published beforehand. In order to show the connection between these publications and the work, in the following the publications are assigned to different chapters. In addition, the author's share of this work will be presented briefly and to the best of his memory.

To classify the share of the work, the following scheme is defined:

- *largely* - an author's share is classified as largely if most of the work or development has been done (for the most part or solely) by the author.
- *partly* - an author's share is classified as partly if the work or development has been jointly by a group of researchers.
- *little* - an author's share is classified as little if the work or development was mostly done by other researchers.

Maxeiner, L. S.; Engell, S. Comparison of dual based optimization methods for distributed trajectory optimization of coupled semi-batch processes. *Optimization and Engineering* **2020.**
Related chapter: 5
Contribution by the author: development of the ideas (*largely*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Maxeiner, L. S.; Engell, S. An accelerated dual method based on analytical extrapolation for distributed quadratic optimization of large-scale production complexes. *Computers & Chemical Engineering* **2020,** *135,* 106728.
Related chapter: 3
Contribution by the author: development of the ideas (*partly*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Maxeiner, L. S. et al., Price-based coordination of interconnected systems with access to external markets In *13th International Symposium on Process Systems Engineering (PSE 2018),* Eden, M. R. et al., Eds.; Elsevier: Amsterdam, Netherlands, 2018, 877–882.
Related chapter: 4

Contribution by the author: development of the ideas (*partly*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Maxeiner, L. S. et al. *Blockchain in the Chemical Industry;* Tech. Rep. Frankfurt, Germany: Frankfurt School Blockchain Center, 2018.
Related chapter: 6
Contribution by the author: development of the ideas (*partly*), Writing of the paper (*largely*).

Wenzel, S. et al. Virtual splitting of shared resource networks for price-based coordination with portfolio tariffs. *Computer Aided Chemical Engineering* **2018,** *43,* 301–306.
Related chapter: 4
Contribution by the author: development of the ideas (*partly*), implementation of the algorithms (*little*), writing of the paper (*little*).

Maxeiner, L. S. et al., Shared resource allocation in the process industries via price-based coordination for systems with discrete decisions In *Computer Aided Chemical Engineering, 40,* Espuña, A. et al., Eds.; Elsevier: Amsterdam, Netherlands, 2017; Vol. 40, 1897–1902.
Related chapters: 5, 6
Contribution by the author: development of the ideas (*largely*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Maxeiner, L. S.; Engell, S. Hierarchical MPC of batch reactors with shared resources. *IFAC-PapersOnLine* **2017,** *50* (1), 12041–12046.
Related chapter: 5
Contribution by the author: development of the ideas (*largely*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Maxeiner, L. S.; Engell, S., Distributed minimum batch time optimization for batch reactors with shared resources In *Computer Aided Chemical Engineering,* Kravanja, Z., Bogotaj, M., Eds.; Elsevier: Amsterdam, Netherlands, 2016; Vol. 38, 1593–1598.
Related chapter: 5
Contribution by the author: development of the ideas (*largely*), implementation of the algorithms (*largely*), writing of the paper (*largely*).

Stojanovski, G. et al. Real-time shared resource allocation by price coordination in an integrated petrochemical site. **2015,** 1498–1503.
Related chapter: 4
Contribution by the author: development of the ideas (*partly*), implementation of the algorithms (*little*), writing of the paper (*little*).

"*Think different.*"

Apple Inc.

Abstract

Many large-scale challenges can be described as optimal allocation of resources between individual systems that are interconnected and coupled via these shared resources. Even though the different systems may be administratively distributed or autonomous, they must interact and agree in order to perform their tasks or satisfy their needs. A chemical site is such a challenge that consists of many interconnected systems that share resources, as energy and material, via networks. In this case, the optimal allocation of resources enables a more efficient production.

However, optimization across system boundaries, in the example of the chemical site across the business unit or company boundaries, can be one of the main contributions towards a more economical and ecological operation, as such problems are in general not tackled efficiently. The conventional approach, monolithic optimization, is mostly not possible, since the different systems act autonomously and require a certain degree of confidentiality, especially when different systems compete with each other.

To overcome this, dual-based distributed optimization methods can be applied. Instead of solving the problem directly, the optimal solution is iteratively determined via optimization on the system level as well as communication of marginal information between the systems and a neutral coordinator.

In this thesis, an extensive overview of such methods as well as of their domains of application are given. A newly proposed method, analytical extrapolation, reduces the effort to solve quadratic problems with relatively few overarching constraints. Distributed optimization methods are applied and compared for static and dynamic optimization problems. In the static case, the optimal allocation of resources in a chemical park is investigated. In the dynamic case, the optimal distribution of resources between inherently discontinuous processes using the example of chemical semi-batch reactors is analyzed. The resulting economic benefits are analyzed, and practical considerations for the implementation of dual-based distributed optimization are outlined.

Kurzfassung

Viele große Herausforderungen lassen sich als optimale Verteilung von Ressourcen zwischen einzelnen Systemen, die über diese gemeinsamen Ressourcen miteinander verbunden und gekoppelt sind, beschreiben. Auch wenn die verschiedenen Systeme administrativ verteilt oder autonom sind, müssen sie interagieren und sich abstimmen, um ihre Aufgaben zu erfüllen oder ihre Bedürfnisse zu befriedigen. Ein Chemiestandort ist ein Beispiel dafür, da dieser aus vielen miteinander verbundenen Systemen besteht, welche Energie sowie Rohstoffe und Utilities über Netzwerke gemeinsam nutzen.

In diesem Fall ermöglicht die optimale Allokation der Ressourcen eine effizientere Produktion. Die Optimierung über Systemgrenzen hinweg, im Beispiel des Chemiestandortes über Geschäftsbereichs- oder Unternehmensgrenzen hinweg, ist jedoch eine der größten Herausforderungen auf dem Weg zu einem wirtschaftlicheren und ökologischeren Betrieb, da solche Probleme in der Regel nicht effizient angegangen werden. Der konventionelle mathematische Ansatz, die monolithische Optimierung, kann nicht angewendet werden, da die verschiedenen Systeme autonom agieren und ein gewisses Maß an Vertraulichkeit erfordern, insbesondere wenn verschiedene Systeme miteinander konkurrieren.

Um trotzdem eine optimale Lösung zu finden, können Methoden der verteilten Optimierung angewendet werden, welche auf der dualen Dekomposition basieren. Anstatt das Problem direkt zu lösen, wird die optimale Lösung iterativ durch Optimierung auf Systemebene sowie durch Kommunikation zwischen den Systemen und einem neutralen Koordinator ermittelt.

In dieser Arbeit wird eine umfangreiche Übersicht über derartige Methoden und ihre Anwendungsgebiete gegeben. Eine neu entwickelte Methode, die analytische Extrapolation, reduziert den Aufwand zur Lösung von Problemen mit relativ wenigen übergreifenden Randbedingungen. Verteilte Optimierungsmethoden werden für statische und dynamische Optimierungsprobleme angewendet und verglichen. Im statischen Fall wird die optimale Allokation von Ressourcen in einem Chemiepark untersucht. Im dynamischen Fall wird die optimale Verteilung von Ressourcen auf inhärent diskontinuierliche Prozesse am Beispiel von chemischen Semi-Batch-Reaktoren untersucht. Die sich daraus ergebenden wirtschaftlichen Vorteile werden analysiert und praktische Aspekte zur Implementierung einer Optimierung basierend auf der dualen Dekomposition erleutert.

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