Sebastian Sager

PDE constrained mixed-integer optimal control

Magdeburg, January 9, 2020

Otto-von-Guericke University Magdeburg

DFG-Graduiertenkolleg
MATHEMATISCHE
KOMPLEXITÄTSREDUKTION

Application-driven theory & algorithms

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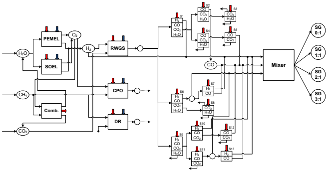

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- A generator is turned on or off
- Switch to different operating mode
- Location of materials / units / devices

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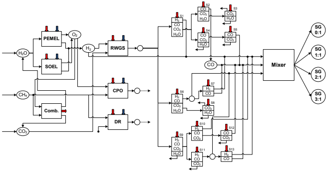

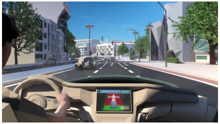

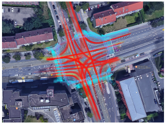

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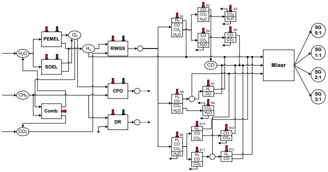

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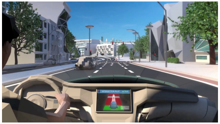

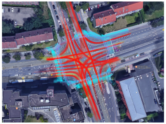

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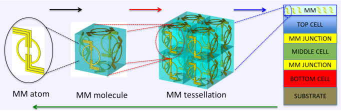

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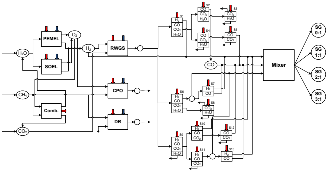

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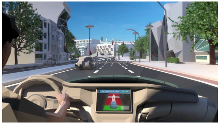
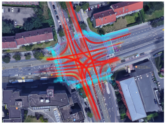

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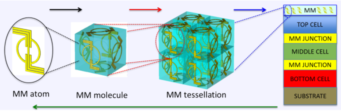

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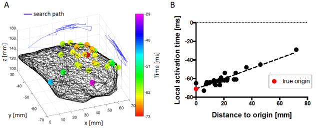

- A certain combination of drugs is given
- Inverse simulation: a signal is blocked
- A certain measurement is done or not
- …

Setting for this talk

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- Combination nonlinearity & integrality $\Rightarrow$ (MINLP) is $\mathcal{NP}$-hard

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The situation is different for mixed-integer optimal control (MIOCP)

$$\min_{y,u,v} F[y] \quad \text{s.t.} \quad G[y,u,v] = 0, \quad (y,u,v) \in \mathcal{X}$$

with independent and dependent variables

- Controls u and v (integer)
- States y uniquely determined for fixed (u,v) via G

  (in practice however we prefer all-at-once / one-shot approaches)

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The situation is

- worse, because fine discretizations $\Rightarrow$ many variables
- better, if one avoids discretization as long as possible

Motivating example: Knapsack

Consider (burglar putting objects in his knapsack)

$$\max_{\omega} \sum_{i=1}^{n_\omega} c_i \omega_i \quad \text{s.t.} \quad \sum_{i=1}^{n_\omega} a_i \omega_i \leq M, \quad \omega_i \in \{0, 1\} \tag{1}$$

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versus (wikileaks guy downloading data on his USB stick)

$$\max_{\omega} \int_0^1 \sum_{i=1}^{n_\omega} c_i \omega_i(\tau) \;\mathrm{d}\tau \;\text{ s.t. }\; \int_0^1 \sum_{i=1}^{n_\omega} a_i \omega_i(\tau) \;\mathrm{d}\tau \leq M, \; \omega_i(t) \in \{0,1\} \; \forall \; t \tag{2}$$

Which one is more difficult?!?

Dynamic knapsack

(Trivial) Lemma.

Let $\alpha \in [0,1]^{n_\omega}$ be the solution of the relaxed problem (1).
Then an optimal solution of (2) is given by

$$\omega_i(t) = \begin{cases} 1 & \text{if } t \in [0, \alpha_i] \\ 0 & \text{else} \end{cases}$$

with

$$\int_0^1 \sum_{i=1}^{n_\omega} c_i \omega_i(\tau)\,\mathrm{d}\tau = \sum_{i=1}^{n_\omega} c_i \alpha_i \quad \text{and} \quad \int_0^1 \sum_{i=1}^{n_\omega} a_i \omega_i(\tau)\,\mathrm{d}\tau = \sum_{i=1}^{n_\omega} a_i \alpha_i = M.$$

MIOCPs with distributed integer variables

$$
\begin{aligned}
\inf_{y,u,v} \quad & F(y) \\
\text{s.t.} \quad & G(y) = f(y,u,v) \\
& \Gamma[y] = 0 \\
& 0 \le c(y,u) && \text{a.e.} \\
& v(t,x) \in \{v^1, \dots, v^{n_\omega}\} && \text{a.e.}
\end{aligned} \tag{MIOCP}
$$

with F, f, c sufficiently smooth (Lipschitz continuous).

Possible settings

- $G(y) = \dot{y} - Ay$, where A generates a C_0-semigroup, $\Gamma(y) = y(0) - y_0$, and $v : [0,T] \to \{v^1, \dots, v^{n_\omega}\}$, e.g., heat eq., reaction-diffusion eq., semilinear hyperbolic
- $G(y) = -\Delta y$, Robin boundary conditions, and $f(y,u,v) = f(v)$, $v : \Omega \to \{v^1, \dots, v^{n_\omega}\}$, e.g., Poisson eq.

MIOCPs with distributed integer variables

$$\begin{aligned} \inf_{y,u,v} \quad & F(y) \\ \text{s.t.} \quad G(y) &= f(y,u,v) \\ \Gamma[y] &= 0 \\ 0 &\leq c(y,u) && \text{a.e.} \\ v(t,x) &\in \{v^1,\ldots,v^{n_\omega}\} && \text{a.e.} \end{aligned} \tag{MIOCP}$$

Partial Outer Convexification: the switches $\omega(t,x)$ are the extremal points of a n_ω-simplex forming a *one-hot encoding* of the discrete choices:

$$\begin{aligned} \inf_{y,u,\omega} \quad & F(y) \\ \text{s.t.} \quad G(y) &= \sum_{i=1}^{n_\omega} \omega_i f(y,u,v^i) \\ \Gamma[y] &= 0 \\ 0 &\leq c(y,u) && \text{a.e.} \\ \omega(t,x) &\in \{0,1\}^{n_\omega} && \text{a.e.} \\ 1 &= \sum_{i=1}^{n_\omega} \omega_i(t,x) && \text{a.e.} \end{aligned} \tag{MIPOC}$$

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\end{aligned}
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Relaxation: consider relaxed controls $\alpha(t,x) \in L^\infty([0,t_\mathrm{f}] \times \Omega, [0,1]^{n_\omega})$ of the binary controls $\omega(t,x)$:

$$
\begin{aligned}
\min_{y,u,\alpha} \quad & F(y) \\
\text{s.t.} \quad & G(y) = \textstyle\sum_{i=1}^{n_\omega} \alpha_i f(y,u,v^i) \\
& \Gamma[y] = 0 \\
& 0 \le c(y,u) && \text{a.e.} \\
& \alpha(t,x) \in [0,1]^{n_\omega} && \text{a.e.} \\
& 1 = \textstyle\sum_{i=1}^{n_\omega} \alpha_i(t,x) && \text{a.e.}
\end{aligned}
\tag{POC}
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Short survey of (MIOCP) $\approx$ (POC) + (MILP)

- Basic ideas introduced for ODE case [S. Phd 2005]
  - Partial Outer Convexification (POC) problem in $[0, 1]$ variables
  - No integer gap between (MIOCP) and (POC)
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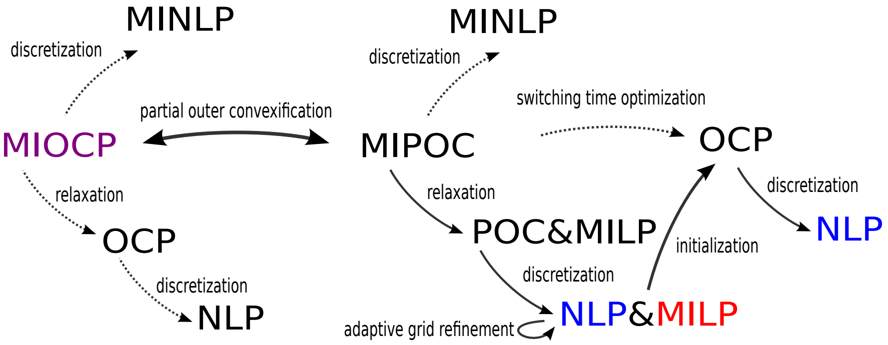
  - Concept of space filling curves
- Generalizations of CIA decomposition [Zeile, S., 3 papers submitted]
  - Exploit objective; consider combinatorial constraints

Convexification, relaxation, discretization



- Discretization: e.g., direct simultaneous (“all-at-once”) method
- Relaxation: $\alpha_j(\cdot) \in [0, 1]$ instead of $\omega_j(\cdot) \in \{0, 1\}$
- (Partial Outer) Convexification: $\omega_j(\cdot) = 1 \iff v(\cdot) = v^j \in \mathcal{V}$

Main result of decomposition approach

Example: ordinary differential equation (switched system)

Consider for $\mathcal{T} := [0, t_\mathrm{f}]$ given L^∞ control functions
$\omega_i : \mathcal{T} \mapsto \{0, 1\}$ and $\alpha_i : \mathcal{T} \mapsto [0, 1]$ with $\sum_{i=1}^{n_\omega} \omega_i(t) = \sum_{i=1}^{n_\omega} \alpha_i(t) = 1$.

Let $y(\cdot)$ be the solution of $\dot{y}(t) = f_0(y(t)) + \sum_{i=1}^{n_\omega} \omega_i(t) f_i(y(t)), y(0) = y_0$,
let $z(\cdot)$ be the solution of $\dot{z}(t) = f_0(z(t)) + \sum_{i=1}^{n_\omega} \alpha_i(t) f_i(z(t)), z(0) = y_0$.

Let all f_i be sufficiently smooth.

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Let all f_i be sufficiently smooth. Then $\|y(t) - z(t)\|$ is small for all t, if

$$\left\| \int_0^t \alpha(\tau) - \omega(\tau) \, \mathrm{d}\tau \right\|$$

is small for all times $t \in \mathcal{T}$.

Combinatorial Integral Approximation

Definition

We define the *Combinatorial Integral Approximation Problem* as

$$\min_{\omega} \max_{t} \left\| \int_0^t \alpha(\tau) - \omega(\tau) \, \mathrm{d}\tau \right\| \text{ s.t. } \ldots \qquad (\mathrm{CIA}_\alpha)$$

- Combinatorial: using $\{0, 1\}$ variables / functions
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- Combinatorial: using $\{0, 1\}$ variables / functions
- Integral Approximation: trying to get close to integrated function
- (CIA_α) on finite grid with constant controls equivalent to MILP

$$\begin{array}{llll} \min\limits_{\eta,p} & \eta & \text{subject to} & \\ & \eta & \geq \left| \sum_{j=1}^{i} (q_{k,j} - p_{k,j}) \Delta_j \right|, & k = 1..n_\omega, \; i = 1..n_t, \\ & \sum_{k=1}^{n_\omega} p_{k,i} & = 1, & i = 1..n_t, \\ & p_{k,i} & \in \{0, 1\}, & k = 1..n_\omega, \; i = 1..n_t. \end{array}$$

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Combinatorial Integral Approximation Decomposition

1. Solve relaxed problem (POC) to get continuous $\alpha(\cdot)$
2. Calculate binary controls $\omega(\cdot)$ via (CIA$_\alpha$)
3. Simulate / reoptimize (MIOCP) with fixed $v(\cdot)$ (derived from $\omega(\cdot)$)
4. Optionally refine control grid, go to 2.

Approximation theorem yields bound on gap to (MIOCP) solution

Main decomposition result (slide courtesy of Paul Manns)

Claim: If grid size $\overline{\Delta} \to 0$ then $F^*(MIOCP) \to F^*(POC)$.

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Approximation argument chain:

$\overline{\Delta} \to 0$

Let y, u, α solve (POC).

1. $\omega^{\overline{\Delta}} = \arg\min_\omega$ (CIA$_\alpha$) for rounding grid $\mathcal{S}_j$ with coarseness $\overline{\Delta}$.

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Approximation argument chain:

$$\overline{\Delta} \to 0 \quad \Rightarrow \quad d(\omega^{\overline{\Delta}}, \alpha) \to 0 \quad \Rightarrow \quad \omega^{\overline{\Delta}} \rightharpoonup^* \alpha$$

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1. $\omega^{\overline{\Delta}} = \arg\min_\omega$ (CIA$_\alpha$) for rounding grid $\mathcal{S}_j$ with coarseness $\overline{\Delta}$.
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   (note that we can't drive $\alpha - \omega^{\overline{\Delta}}$ to zero in the norm topology!)

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3. Approximation of (POC) optimal state with (MIOCP) feasible state
4. Continuity of objective $F(\cdot)$ (and of constraint functions)

Multi-dimensional CIA decomposition

Main question: how to refine the control mesh?

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Definition: order conserving domain dissection [Manns, Kirches SPP1962-080]

$\left(\left\{S_1^{(n)}, \dots, S_{N^{(n)}}^{(n)}\right\}\right)_n \subset 2^{\mathcal{B}(\Omega)}$ is an **order conserving domain dissection** if

- $N^{(0)} = 1,\ S_1^{(0)} = \Omega$
- $\bigcup_i S_i^{(n)} \subset \Omega,\ S_i^{(n)} \cap S_j^{(n)} = \emptyset$ for all $i \neq j$ and $\lambda\left(\bigcup_i S_i^{(n)}\right) = \lambda(\Omega)$
- $\lambda(S_i^{(n)}) > 0 \quad \forall n, i \in [N^{(n)}]$
- $\exists j < k$ s.t. $\bigcup_{l=j}^k S_l^{(n)} \subset S_i^{(n-1)}$ and $\lambda\left(\bigcup_{l=j}^k S_l^{(n)}\right) = \lambda(S_i^{(n-1)})\ \forall n, i \in [N^{(n-1)}]$
- $\max_{i \in \{1,\dots,N^{(n)}\}} \lambda(S_i^{(n)}) \to 0$
- $\sigma\left(\bigcup_{n=1}^{\infty}\left\{S_1^{(n)}, \dots, S_{N^{(n)}}^{(n)}\right\}\right) = \mathcal{B}(\Omega).$

Multi-dimensional CIA decomposition

Theorem [Manns, Kirches SPP1962-080]

Let

$$\omega^{(n)} := \arg\min_{\omega} \max_{i} \left\| \int_{\bigcup_{j=1}^{i} S_j^{(n)}} \alpha - \omega \right\|_{\infty}$$

for a given order conserving domain dissection $\left(\left\{S_1^{(n)}, \ldots, S_{N^{(n)}}^{(n)}\right\}\right)_n$.

Then,

$$\omega^{(n)} \rightharpoonup^* \alpha \text{ in } L^{\infty}.$$

Consequently,

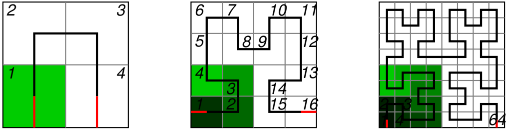
$$y(\omega^{(n)}) \to y(\alpha)$$

under suitable regularity assumptions for elliptic PDEs.

Space filling curves as order conserving domain dissections

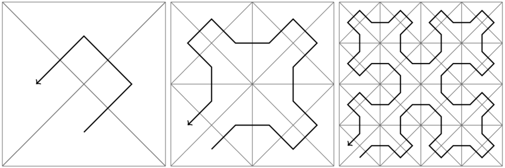
Hilbert curve:

[Image by Paul Manns]



Sierpinski curve:

[Image by Mirko Hahn]



[Manns, Kirches SPP1962-080]: Iterates of space-filling curves induce an ordered discretization that satisfies the required properties allowing to establish

$$d(\omega^{(n)}, \alpha) \to 0 \quad \Rightarrow \quad \omega^{(n)} \rightharpoonup^{*} \alpha$$

in the multi-dimensional setting.

Numerical illustration [Hahn, Kirches, Manns, S., Zeile 2019]

Poisson equation on $\Omega = [0,1]^2$ with Robin boundary conditions

Relaxed problem from [Clason, Kunisch, 2014]:

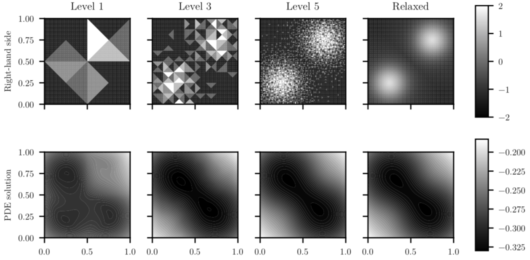
$$\begin{aligned} \min \ & \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} \\ -\Delta y &= u \\ \frac{\partial y}{\partial \nu} - y &= 0 \quad \text{a.e. on } \partial\Omega \\ -2 \leq u &\leq 2 \text{ a.e.} \end{aligned} \tag{RC}$$

and integer control problem with substituted u

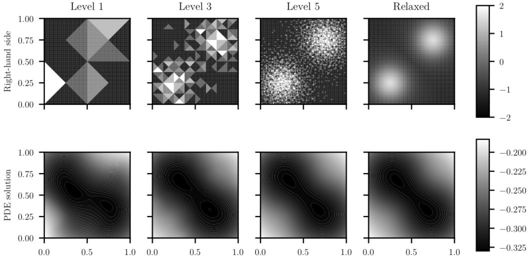
$$u = \sum_{i=1}^{5} \omega_i v^i \in \{-2, -1, 0, 1, 2\} \tag{MIPOC}$$

Numerical illustration [Hahn, Kirches, Manns, S., Zeile 2019]

- Finite element method with continuous first-order Lagrange elements on a structured triangular mesh iterated over according to the Sierpinski curve



Sum Up Rounding



(CIA_{α})

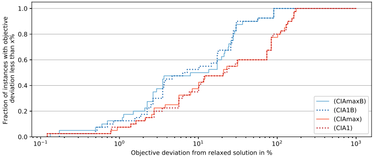
Recent CIA results

Consider solution of CIA problem (CIA$_\alpha$)

$$\eta^* := \min_{\omega} \max_{t} \left\| \int_0^t \alpha(\tau) - \omega(\tau) \, \mathrm{d}\tau \right\|_\infty \quad \text{s.t. constraints}$$

Extensions [Zeile, S., 3 papers submitted]

- (CIA$_\alpha$) in backwards direction $\int_t^{t_\mathrm{f}}$ for problems with specific BCs



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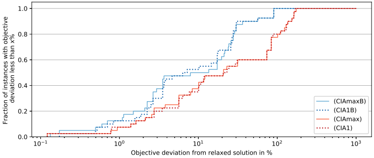

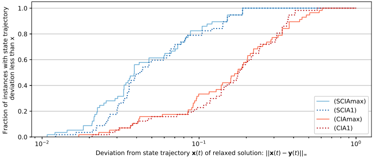

Scaled CIA $\Leftarrow$ Dual Weighted Residuals [Becker, Rannacher]

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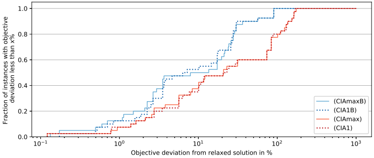

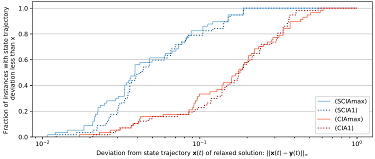

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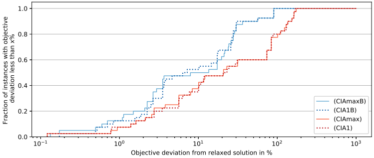

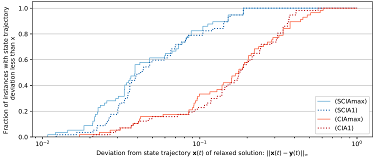

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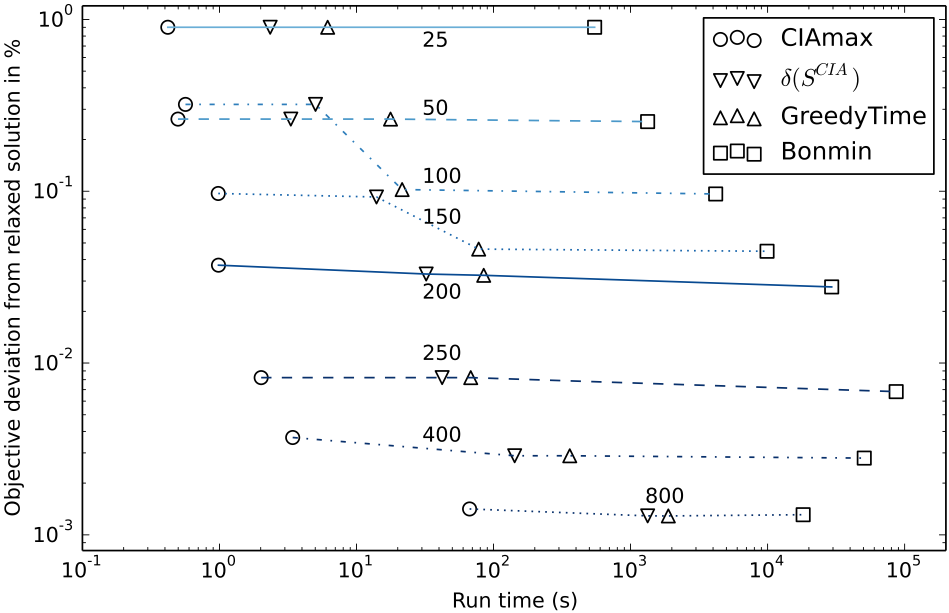
- Total Variation constraints $\quad \eta^* \leq \frac{t_\mathrm{f}}{\sigma_{\max} + 2} + \bar{\Delta}$ for all α



CIAmax
$\delta(S^{CIA})$
GreedyTime
Bonmin
25
50
100
150
200
250
400
800
Objective deviation from relaxed solution in %
Run time (s)
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-1}
10^0
10^1
10^2
10^3
10^4
10^5

MIOC via CIA decomposition

Advantages

- More powerful modeling compared to sparse control with $\|\cdot\|_1$
  - Allows combinatorial constraints
- Interesting connections to topology optimization, switched systems, hybrid systems, machine learning, ...

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- Independent of how (POC) is solved
  - One-shot, low-rank tensor, model order reduction, semi-smooth Newton, parareal / multiple shooting, regularization, multigrid, ...
  - Uncertainty treatment: MC, scenario trees, robust, PC, CVaR, ...

Software

Using and combining different software packages, e.g.,

- FEniCS, Gascoigne
- ipopt, qpOASES
- cplex, gurobi
- CasADi
- pyMOR

MathOpt software packages

- pycombina
- blockSQP (standard NLP solver in CasDAi)
- ampl_mintoc
- GloOptCon
- plus problem–specific codes

BMBF Mathematics for Innovation

- Project *Power2Chemicals*
- with Peter Benner, Martin Stoll, Kai Sundmacher
- new algorithms based on CIA decomposition, B&B, MOR, low rank

Summary: MIOC – a growing field

- MIOC projects important part of funding initiatives, e.g.,
  - DFG Gas Transregio 154
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Thank you for your attention!