TRR 154 | Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks

Simulation based mixed integer programming

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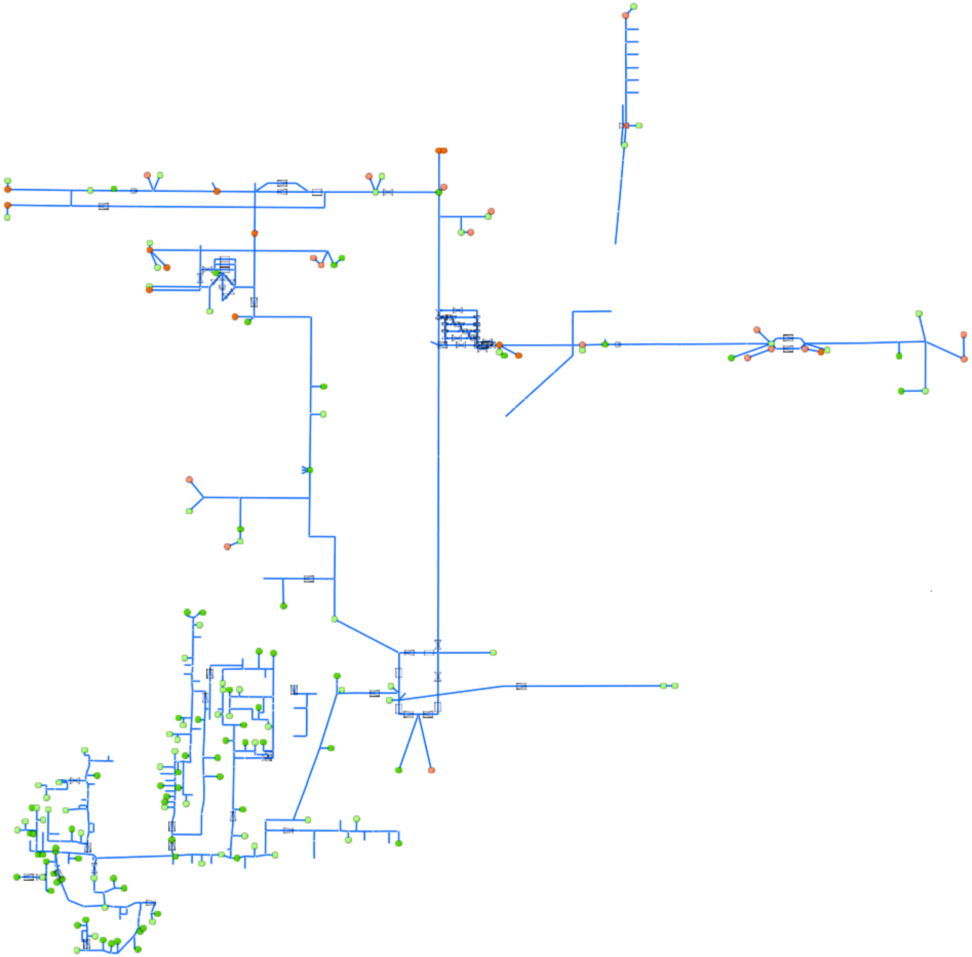
A typical network flow problem

- 661 vertices
- 689 arcs
- 32 sources
- 142 sinks



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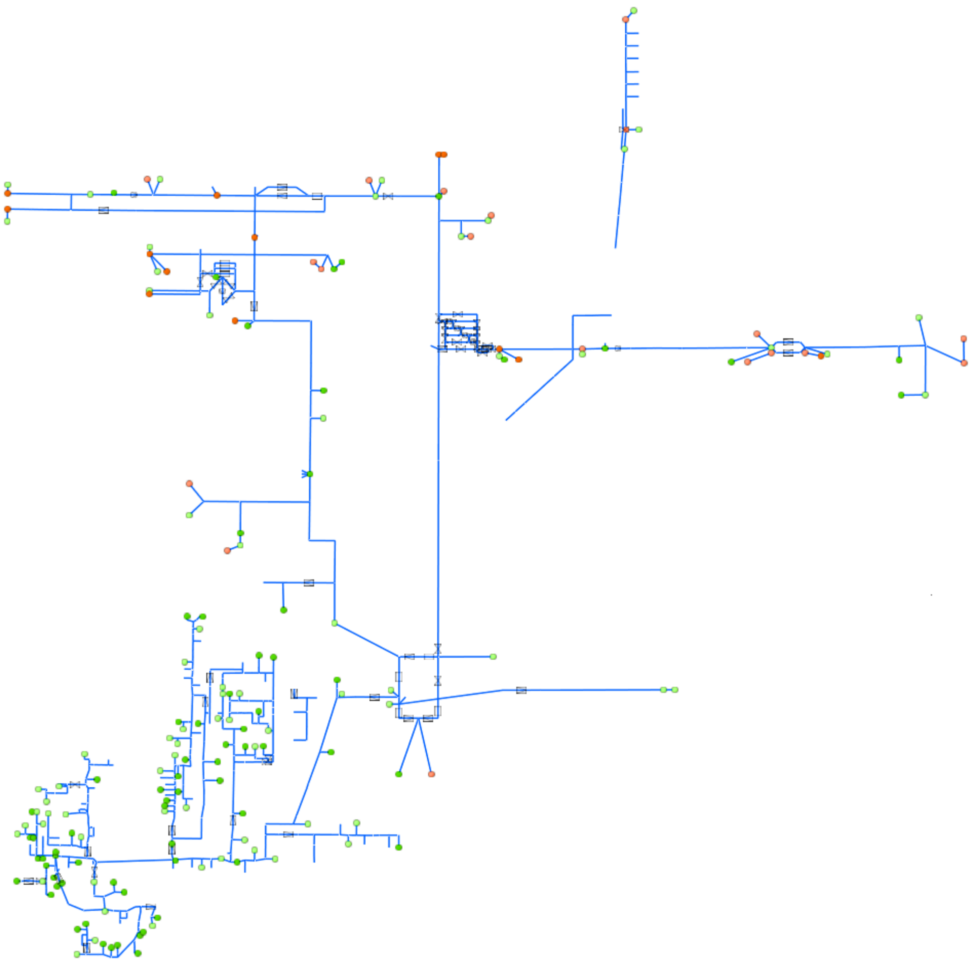
- except that the "flow" is gas



Gas networks

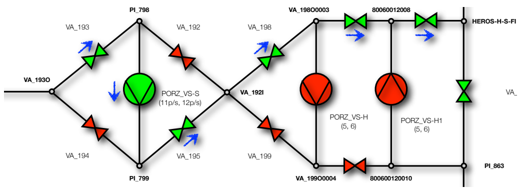
- Physics are inherently continuous

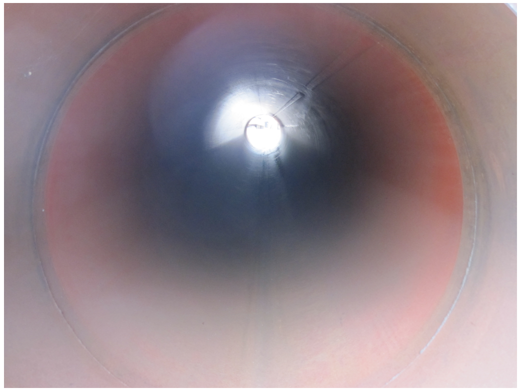
$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} &= 0 \\
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho v^2 + p)}{\partial x} + \hat{g}\rho\frac{\partial h}{\partial x} + \frac{\hat{\lambda}}{2\hat{D}}\rho|v|v &= 0 \\
\frac{\partial E}{\partial t} + \frac{\partial (Ev + pv)}{\partial x} + \hat{A}\rho v\hat{g}\frac{\partial h}{\partial x} + \pi\,\hat{D}\,\hat{k}\,(T - T_{\mathrm{soil}}) &= 0.
\end{aligned}
$$

- Networks are inherently discrete with edges that can be switched on or off

Valve a with switching variable $s_a \in \{0, 1\}$

$$
\begin{aligned}
s_a = 0 &\Rightarrow q_a = 0 \\
s_a = 1 &\Rightarrow p_i = p_j
\end{aligned}
$$





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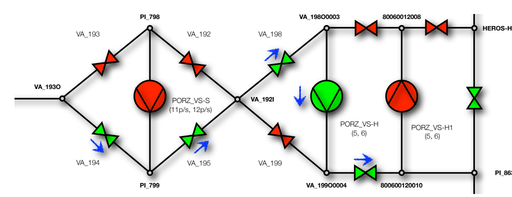

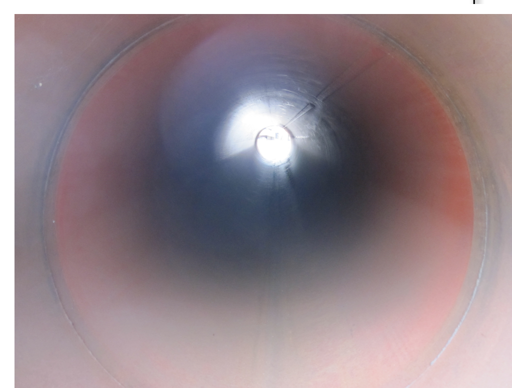

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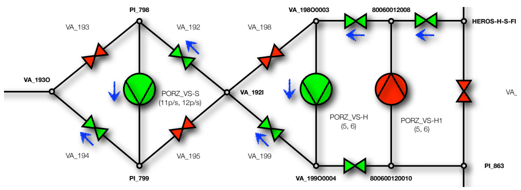
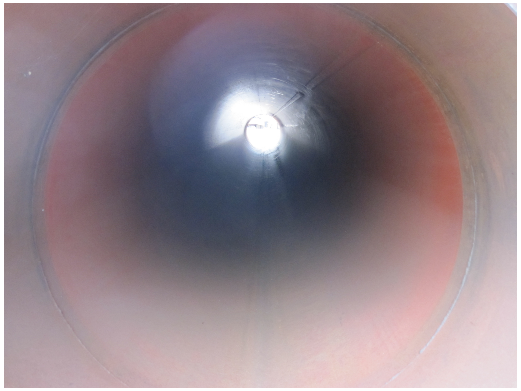
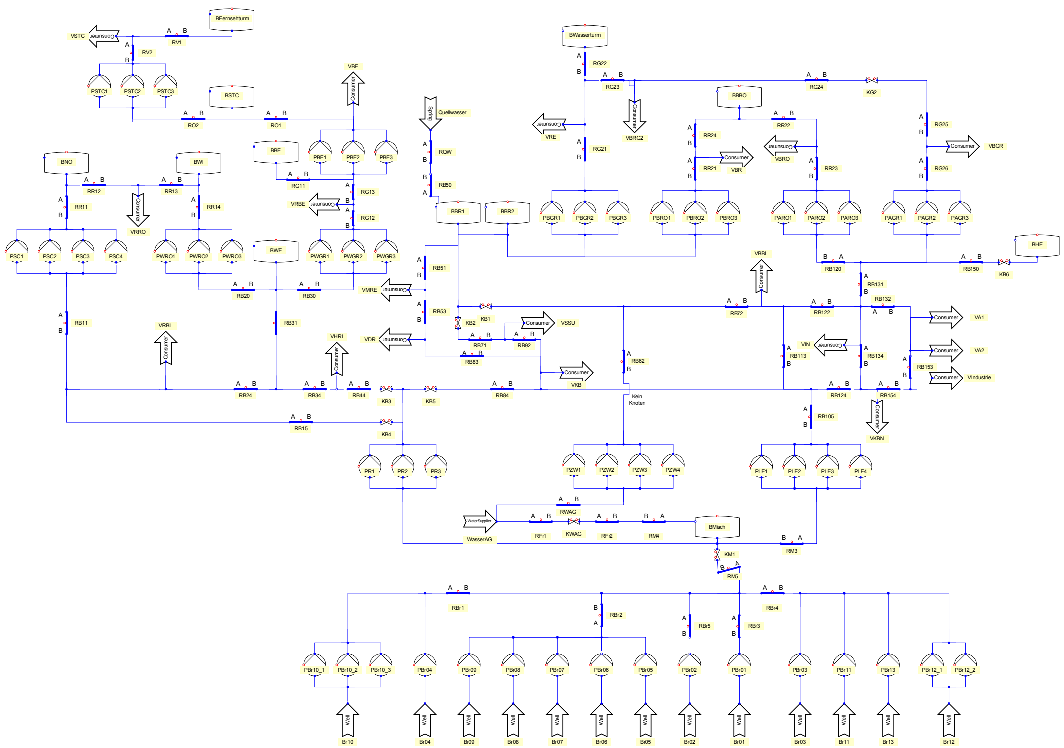




A typical network flow problem (2)

- 188 vertices
- 225 arcs
- 15 suppliers
- 21 consumers



A typical network flow problem (2)

- 188 vertices
- 225 arcs
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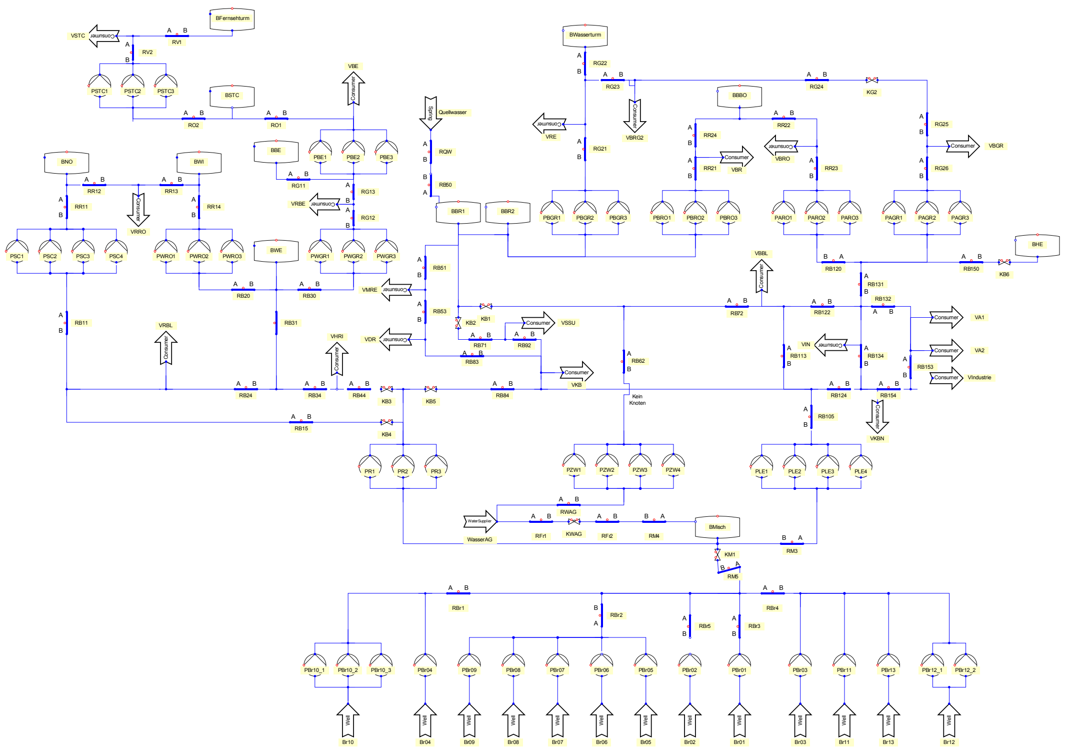
- except that the "flow" is water



Water networks

- Networks are inherently discrete/switching

  Valve a with switching variable $s_a \in \{0, 1\}$

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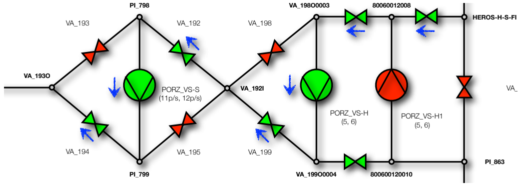
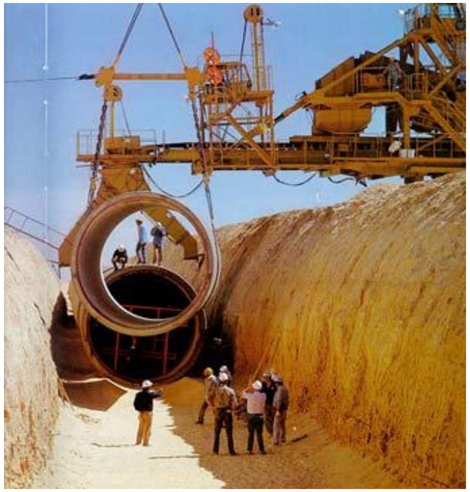
\begin{aligned}
s_a = 0 \;&\Rightarrow\; q_a = 0 \\
s_a = 1 \;&\Rightarrow\; p_i = p_j
\end{aligned}
$$

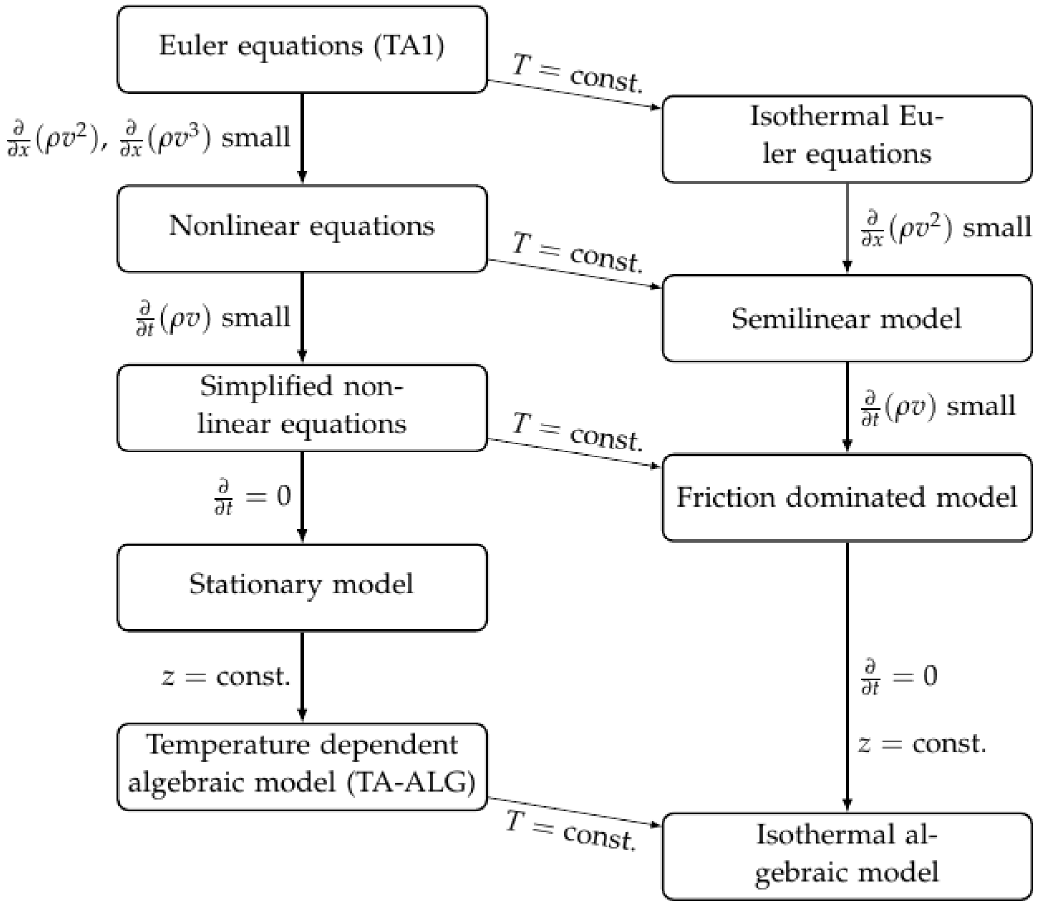
- Physics are inherently continuous/switching

$$
\begin{aligned}
\frac{\partial h}{\partial t} + \frac{a^2}{gA}\frac{\partial q}{\partial x} &= 0 \\
\frac{\partial q}{\partial t} + gA\frac{\partial h}{\partial x} &= -\lambda \frac{q|q|}{2DA}
\end{aligned}
$$





Model hierarchy for pipes



MINLP model

- Variables:
  - Pressure p_i for nodes $i \in \mathbb{V}$
  - Standard volumetric flow q_a for arcs $a \in \mathbb{A}$
  - Compressor power P_a for compressors $a \in \mathbb{A}$
- Nonlinear constraints:
  - Pressure loss over a pipe $a = (i, j)$: $p_j^2 = \left(p_i^2 - \Lambda_a |q_a| q_a \frac{e^{S_a} - 1}{S_a}\right) e^{-S_a}$
  - Pressure loss over a resistor $a = (i, j)$:

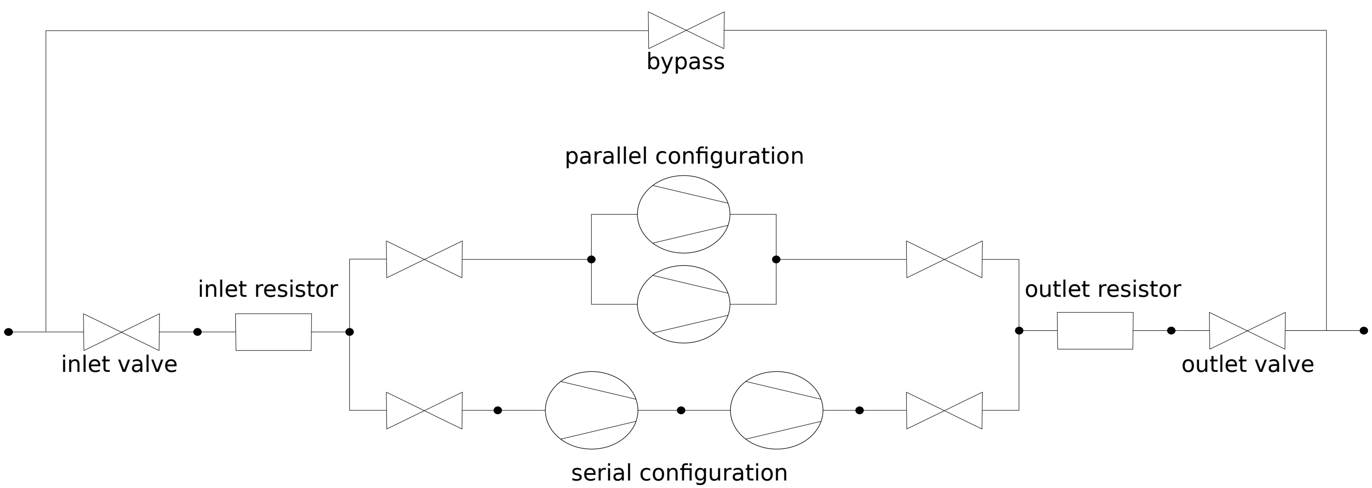
$$p_i^2 - p_j^2 + |\Delta_{ij}|\Delta_{ij} = \frac{16 \rho_0 p_0 z_m}{\pi^2 z_0 T_0} \frac{\xi_a T}{D_a^4} |q_a| q_a, \quad \Delta_{ij} = p_i - p_j$$

  - Power consumption of a compressor unit $a = (i, j)$:

$$P_a = \frac{\kappa}{\kappa - 1} \frac{\rho_0 R T_i z_i}{\eta_{ad,a} m} \left(\left(\frac{p_j}{p_i} \right)^{\frac{\kappa - 1}{\kappa}} - 1 \right) q_a$$

MINLP model

- Switching variables $s_a \in \{0, 1\}$ for active elements $a \in \mathcal{A}$
- Combinatorial constraints:
  - Valve: $s_a = 0 \to q_a = 0$, $s_a = 1 \to p_i = p_j$
  - Control valves: $s_a = 0 \to q_a = 0$, $s_a = 1 \to p_i - p_j \in [\Delta_a^-, \Delta_a^+]$
  - Compressors: $s_a = 0 \to q_a = 0$, $s_a = 1 \to p_j = f(P_a, q_a, p_i)$
  - Configurations: $\sum_{c \in C} s_c + s_{bypass} \leq 1$

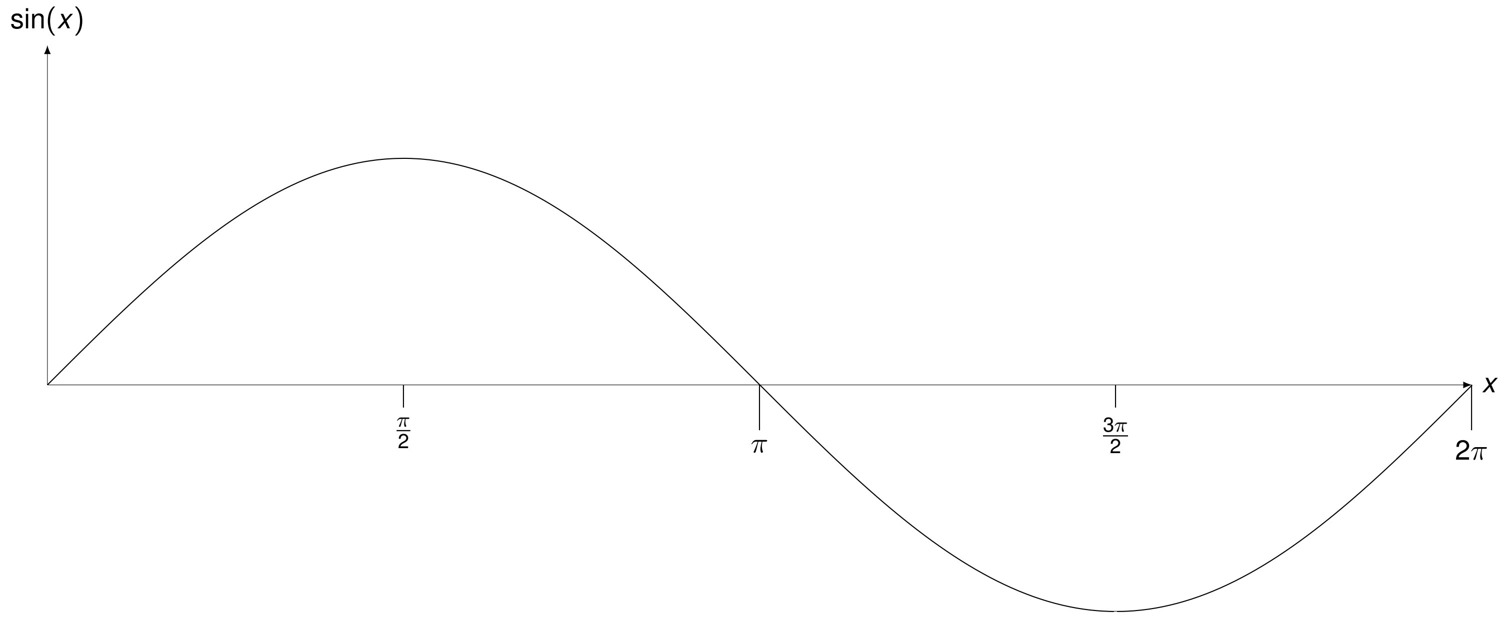


Solution methods for MINLPs

1. Approaches using outer approximation and spatial branching
    - Baron (Tawarmalani, Sahinidis 2005)
    - Couenne (Belotti, Lee, Liberti, Margot, Wächter 2009)
    - SCIP (Vigerske 2013)
    - alphaECP (Westerlund, Lindquist 2003)
    - Bonmin (Bonami, Biegler, Conn, Cornuejols, Grossmann, Laird, Lee, Lodi, Margot, Sawaya, Wächter 2005)
    - ...
2. Approaches using piecewise linear approximation and relaxtion
    - Lots of branching experiences for (M)IPs
    - Polyhedral combinatorics help to avoid parts of branching

Approach: MIP relaxations of MINLPs

e. g. $\sin(x) = 0.5$ instead of $p_j^2 = \left(p_i^2 - \Lambda_a |q_a| q_a \frac{e^{S_a}-1}{S_a}\right) e^{-S_a}$



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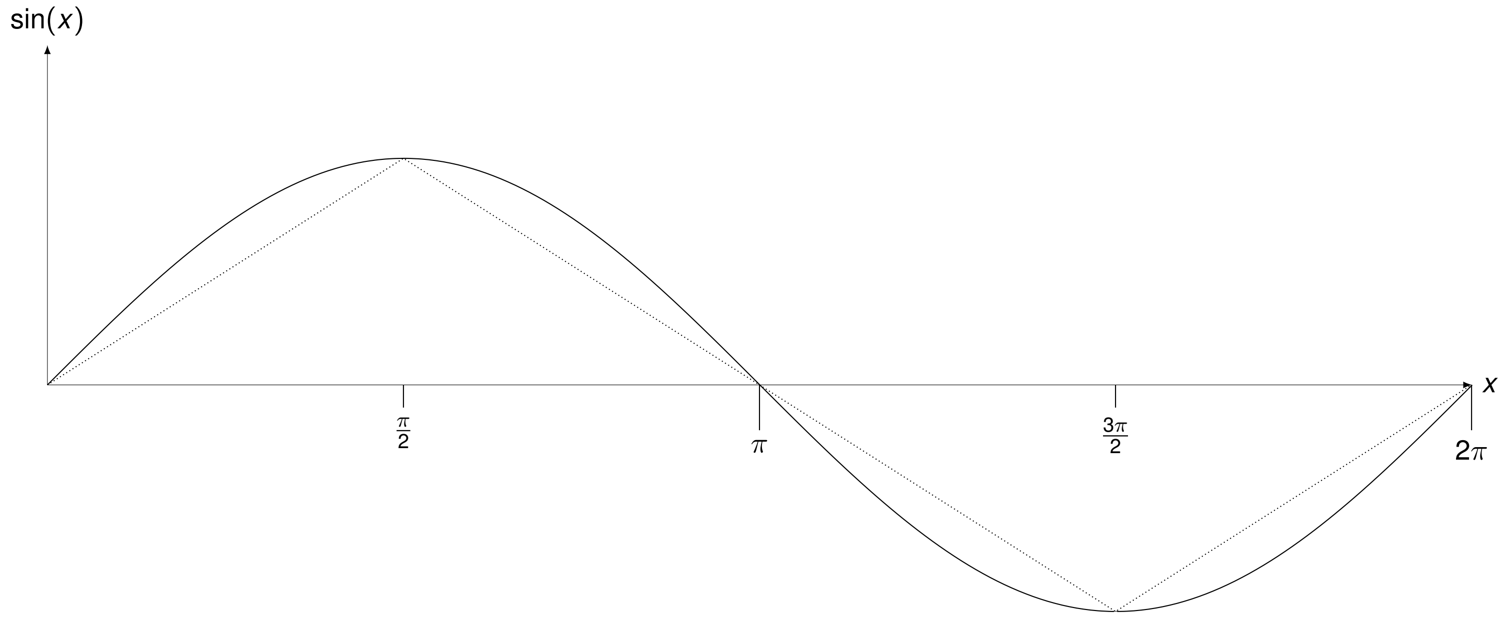

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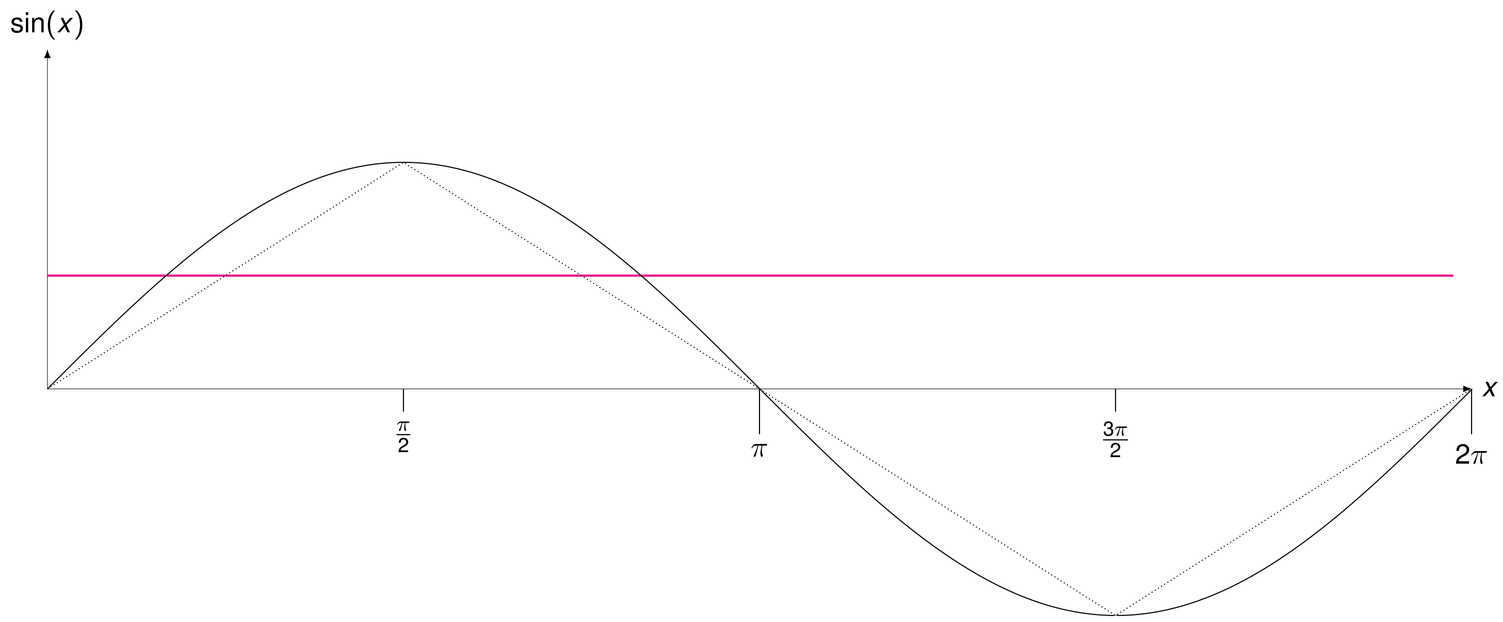

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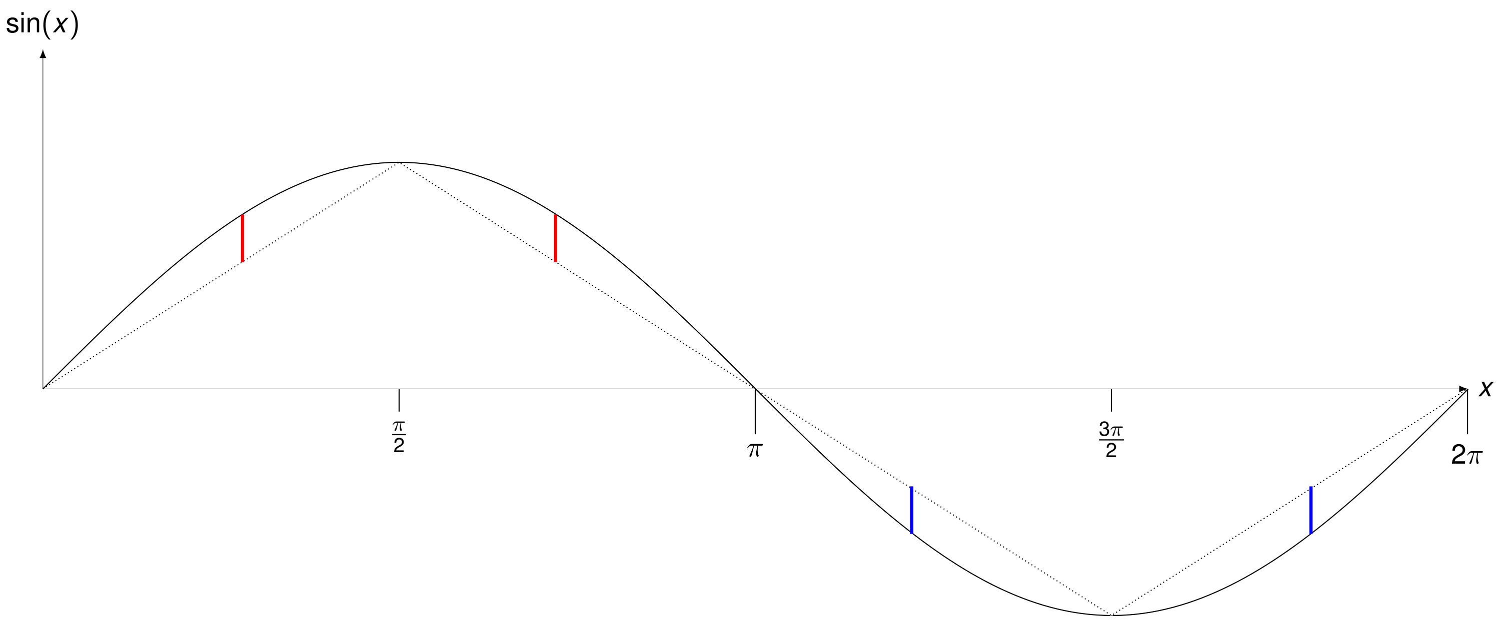

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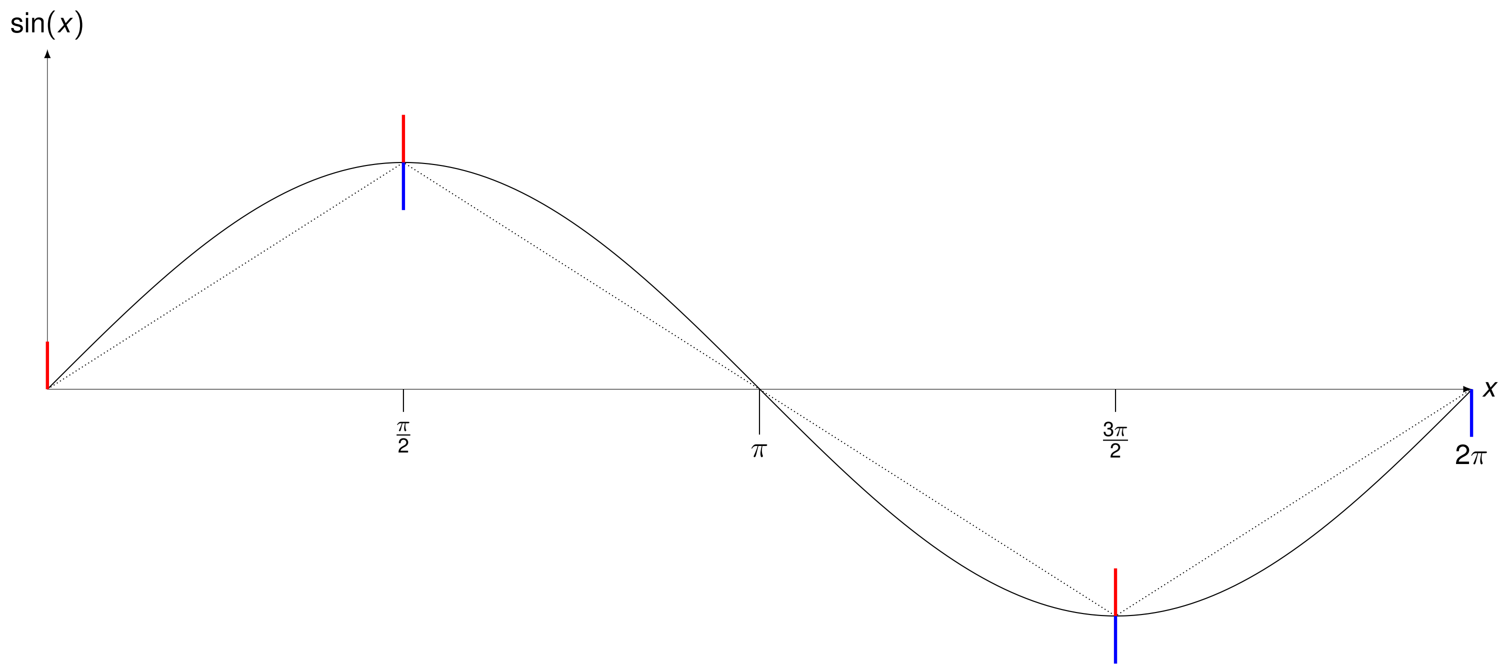

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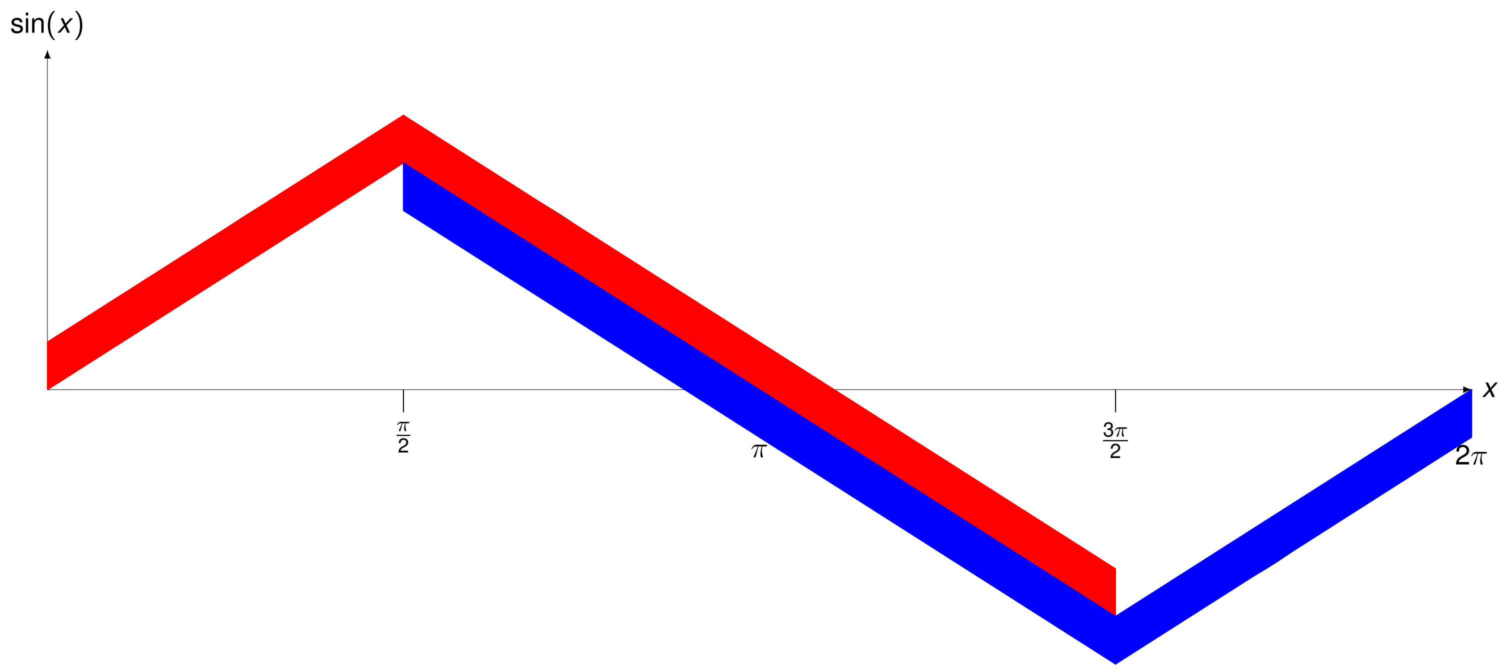

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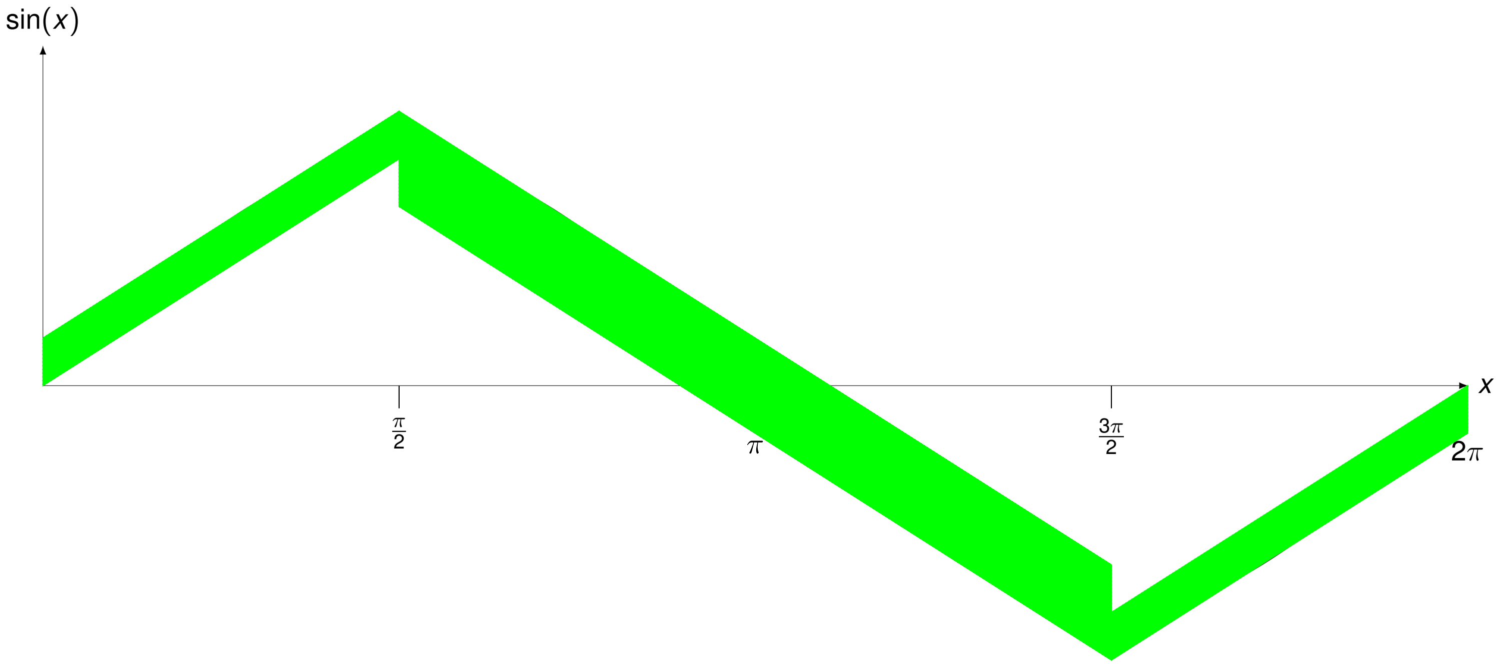

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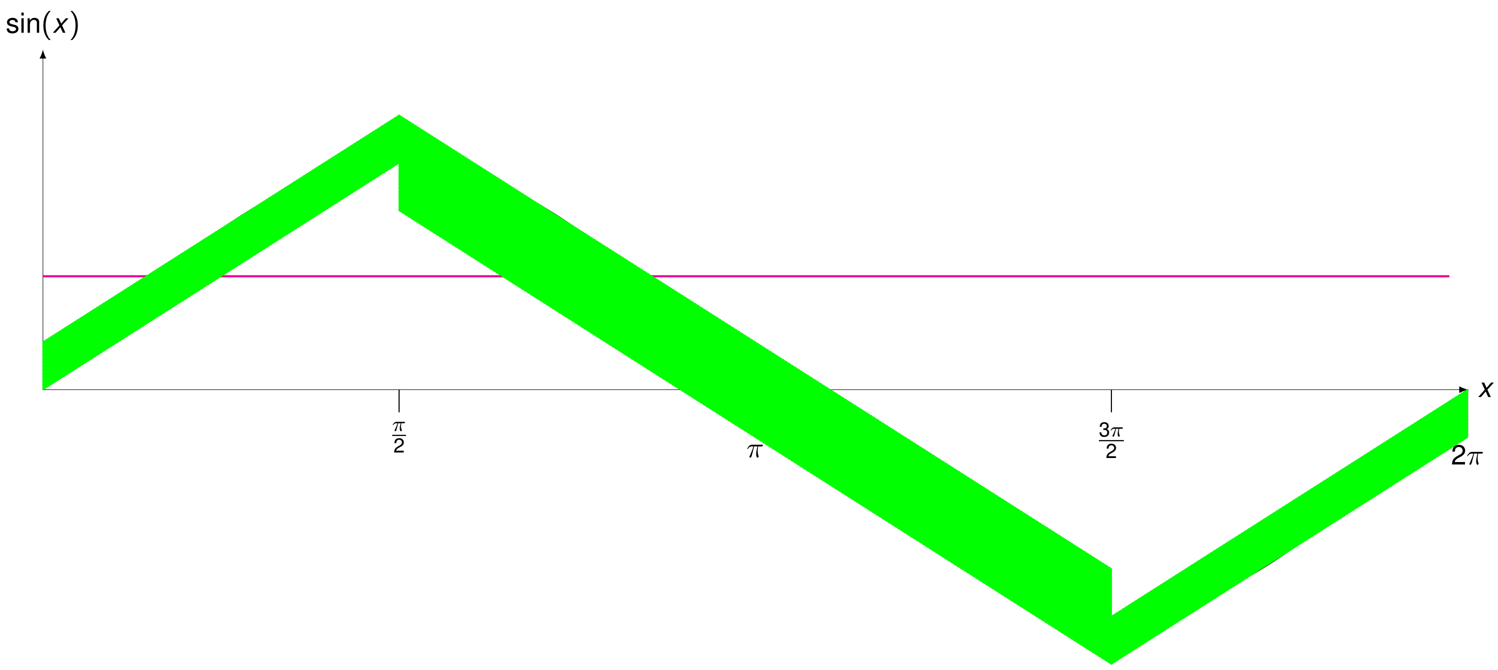

Consistent hierarchical modeling approach

(1) Determine relaxation error ϵ

(2) Set up the MIP relaxation with accuracy ϵ

(3) Solve the MIP relaxation

(4) If MIP is infeasible $\rightarrow$ STOP (MINLP is infeasible)

(5) Fix the discrete decision variables in the MINLP model according to the MIP solution

(6) Solve the remaining NLP model

(7) If NLP is feasible $\rightarrow$ STOP
(feasible MINLP solution found; solution quality within ϵ)

(8) Reduce ϵ, goto (2)

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Burlacu and Schewe (2018)

An adaptive version of this algorithm together with a so-called ϵ-precise refinement procedure is correct and terminates after a finite number of steps.

MIP models for piecewise linear functions

- (linear) convex combination models
  - Linear number of cont. variables
  - Linear number of binaries
  - Linear number of constraints
- (logarithmic) convex combination models (Nemhauser, Vielma 2008)
  - Linear number of cont. variables
  - Logarithmic number of binaries
  - Logarithmic number of constraints
  - Locally ideal formulation
- incremental model (Markowitz, Manne 1957)
  - Linear number of cont. variables
  - Linear number of binaries
  - Linear number of constraints
  - Locally ideal formulation
- Also possible: SOS branching (Beale, Tomlin 1970)

Incremental model for piecewise linear functions

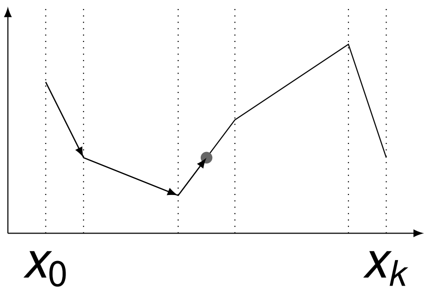
$$x = x_0 + \sum_{i=1}^{k} (x_i - x_{i-1})\delta_i$$

$$y = y_0 + \sum_{i=1}^{k} (y_i - y_{i-1})\delta_i$$

$$\delta_{i+1} \leq z_i \leq \delta_i \qquad i = 1, \ldots, k-1$$

$$0 \leq \delta_i \leq 1 \qquad i = 1, \ldots, k$$

$$z_i \in \{0, 1\} \qquad i = 1, \ldots, k-1$$



Incremental model for piecewise linear relaxations

$$x = x_0 + \sum_{i=1}^{k} (x_i - x_{i-1})\delta_i$$

$$y = y_0 + \sum_{i=1}^{k} (y_i - y_{i-1})\delta_i + e$$

$$\delta_{i+1} \leq z_i \leq \delta_i \qquad i = 1, \ldots, k-1$$

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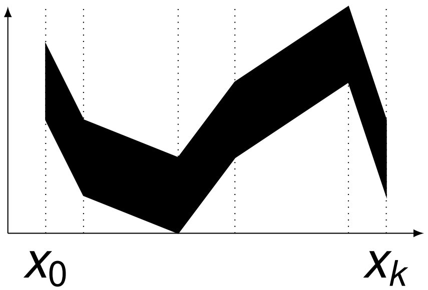
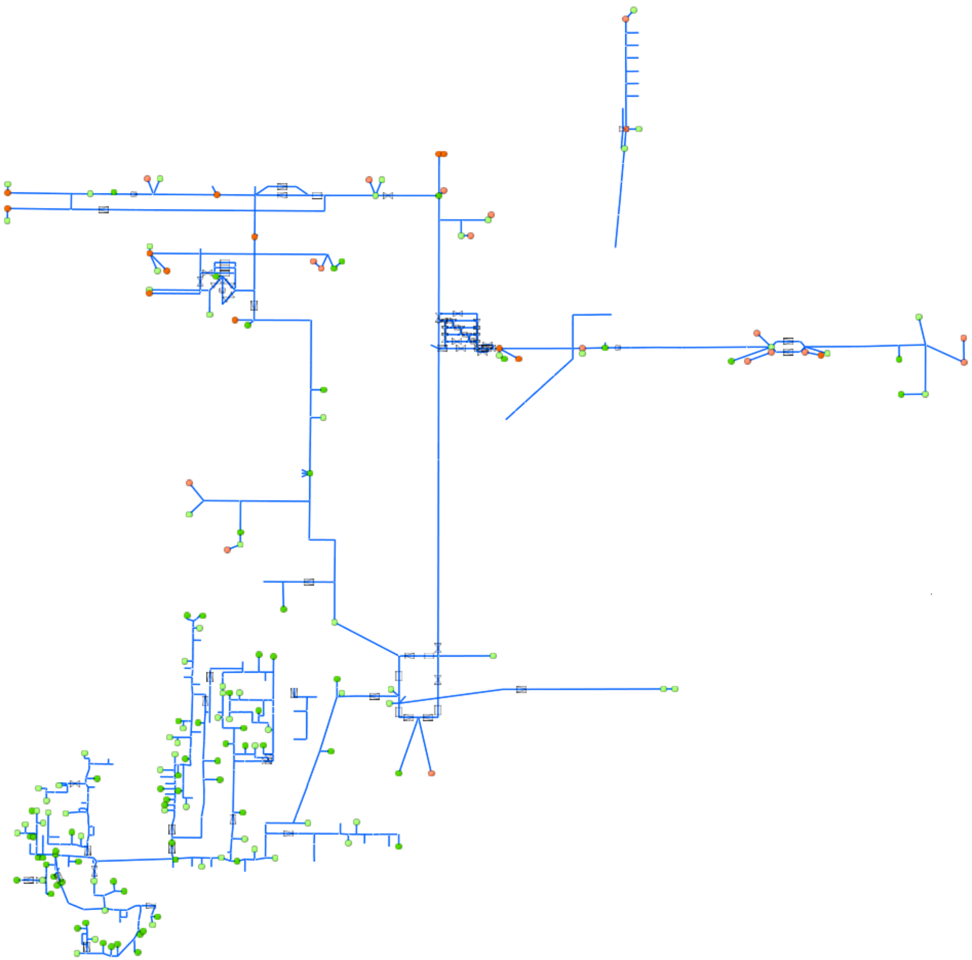
$$z_i \in \{0, 1\} \qquad i = 1, \ldots, k-1$$

$$-\epsilon \leq e \leq \epsilon$$

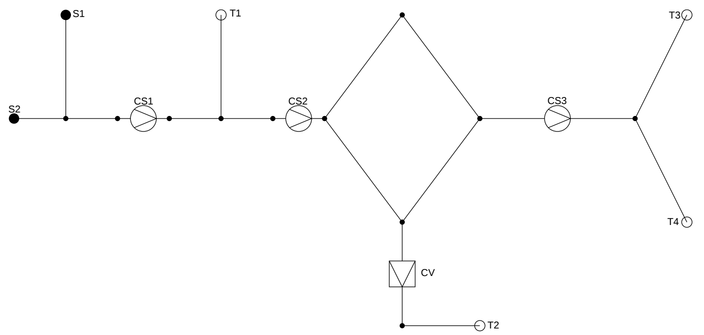


Numerical results: Gas networks

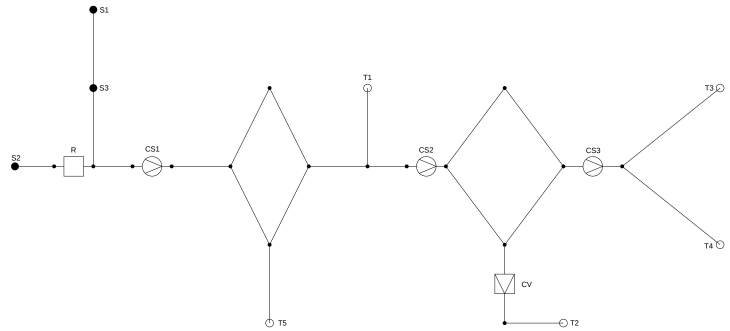


Intances I - small test networks

- Net 1:

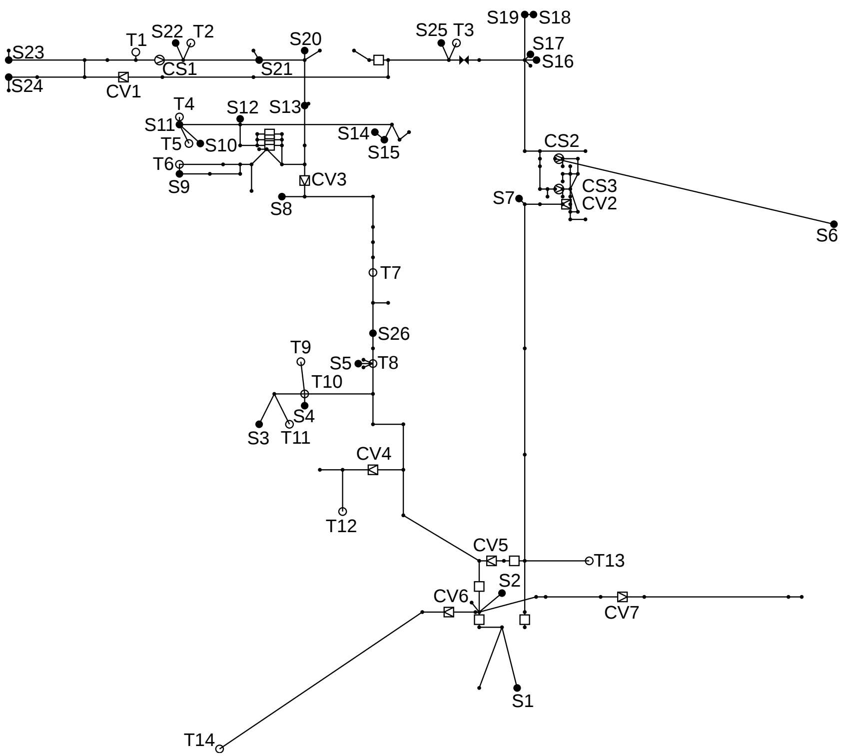


- Net 2:

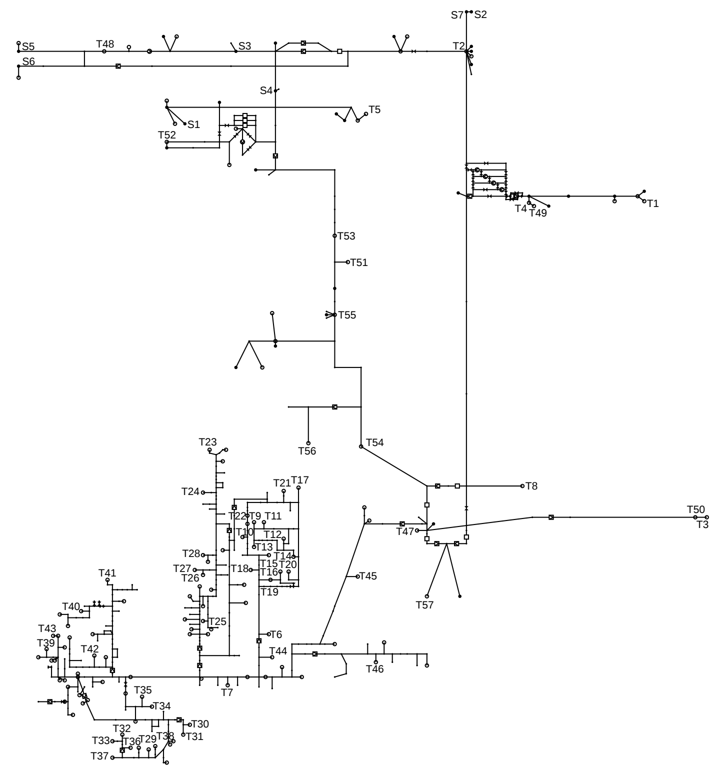


Instances II - real gas networks

- Net 3:



- Net 4:



Results on small (real) instances

net	ϵ	cont	bin	cons	t_{MIP}	feas	t_{NLP}
1	10.0	377	42	685	0.01s	y	0.11s
1	5.0	380	45	694	0.01s	y	0.15s
1	2.5	387	52	714	0.01s	y	0.06s
1	1.0	423	88	823	0.02s	y	0.20s
2	10.0	450	67	859	0.05s	y	0.26s
2	5.0	479	96	946	0.09s	y	0.20s
2	2.5	543	160	1138	0.11s	y	0.09s
2	1.0	816	433	1957	0.13s	y	0.26s
3	10.0	2099	418	3868	1.24s	n	12.94s
3	5.0	2412	713	4807	1.51s	y	1.48s
3	2.5	3058	1377	6745	6.03s	y	1.32s
3	1.0	5185	3504	13126	22.04s	y	1.59s
4	10.0	4825	1663	10994	21.65s	n	41.33s
4	5.0	6012	2850	14555	51.26s	y	30.83s
4	2.5	8433	5217	21818	132.96s	y	36.65s
4	1.0	16343	13181	45548	600.00s	-	-

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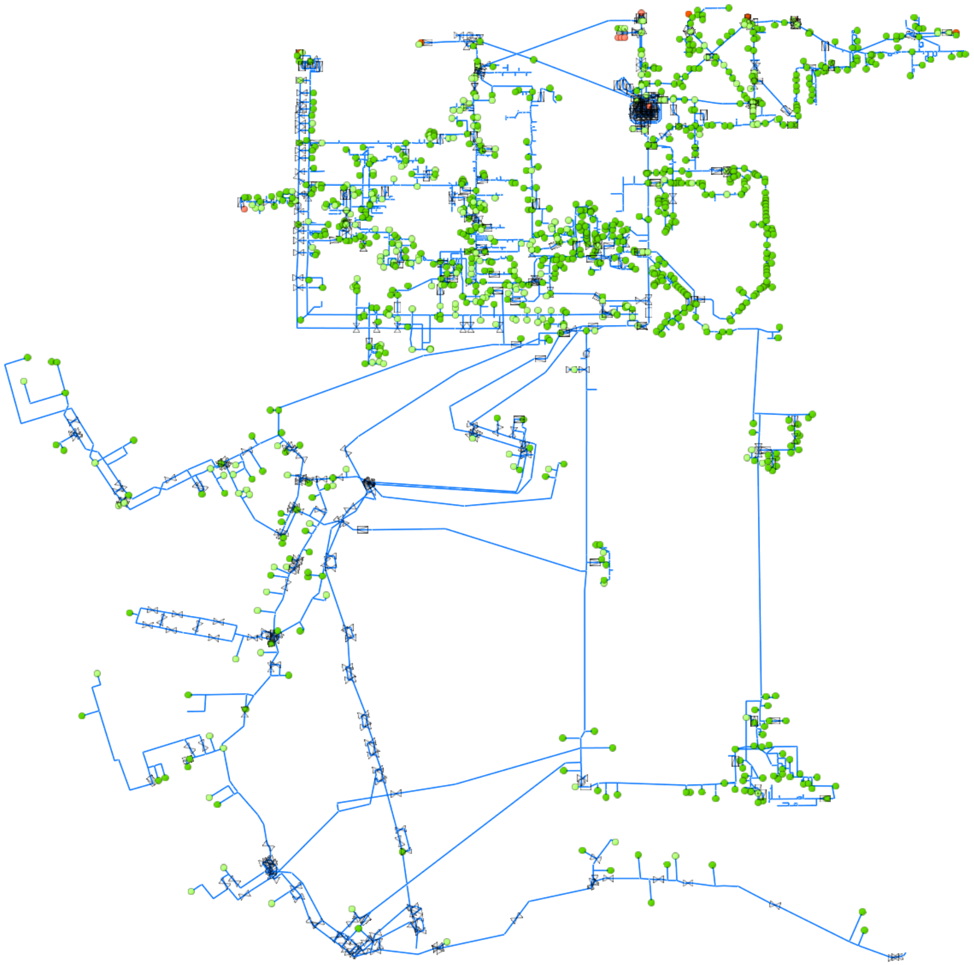
Results on small (real) instances: a comparison

net	Baron (MINLP)	SCIP (MINLP)	MIP	NLP	MIP+NLP
1	$<$1s	$<$1s	$<$1s	$<$1s	$<$1s
2	$<$1s	$<$1s	$<$1s	$<$1s	$<$1s
3	456s	2s	2s	1s	3s
4	$>$1h	$>$1h	51.26s	30.83s	82.09s

L-Gas network of Open Grid Europe, Germany

- 13 entries
- 1,062 exits
- 3,632 pipes
- 26 resistors
- 305 valves
- 120 control valve stations
- 12 compressor stations
- 25,000 variables
  (5,000 binary)



Computing time for 51 *expert scenarios*:

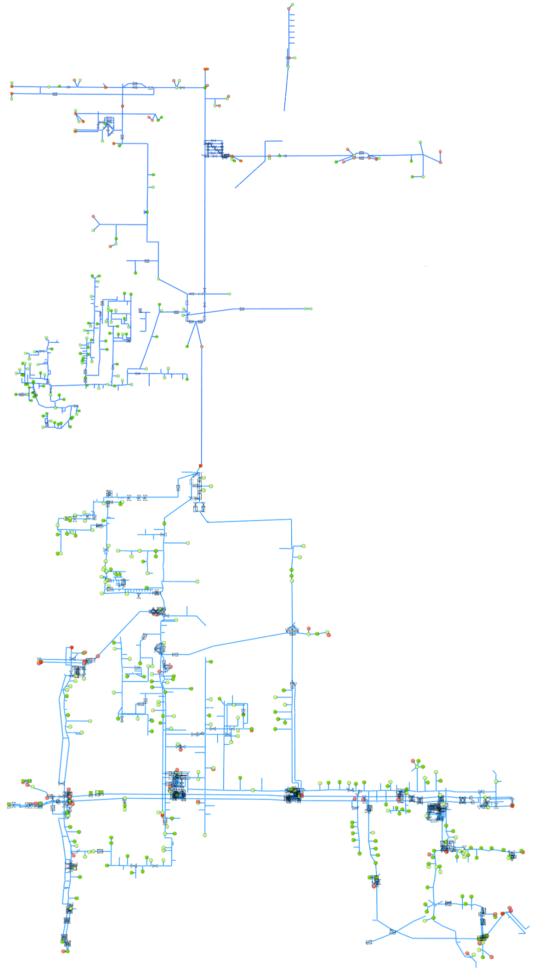
- 5 min to 70 min
- average: 34 min

H-Gas network of Open Grid Europe, Germany

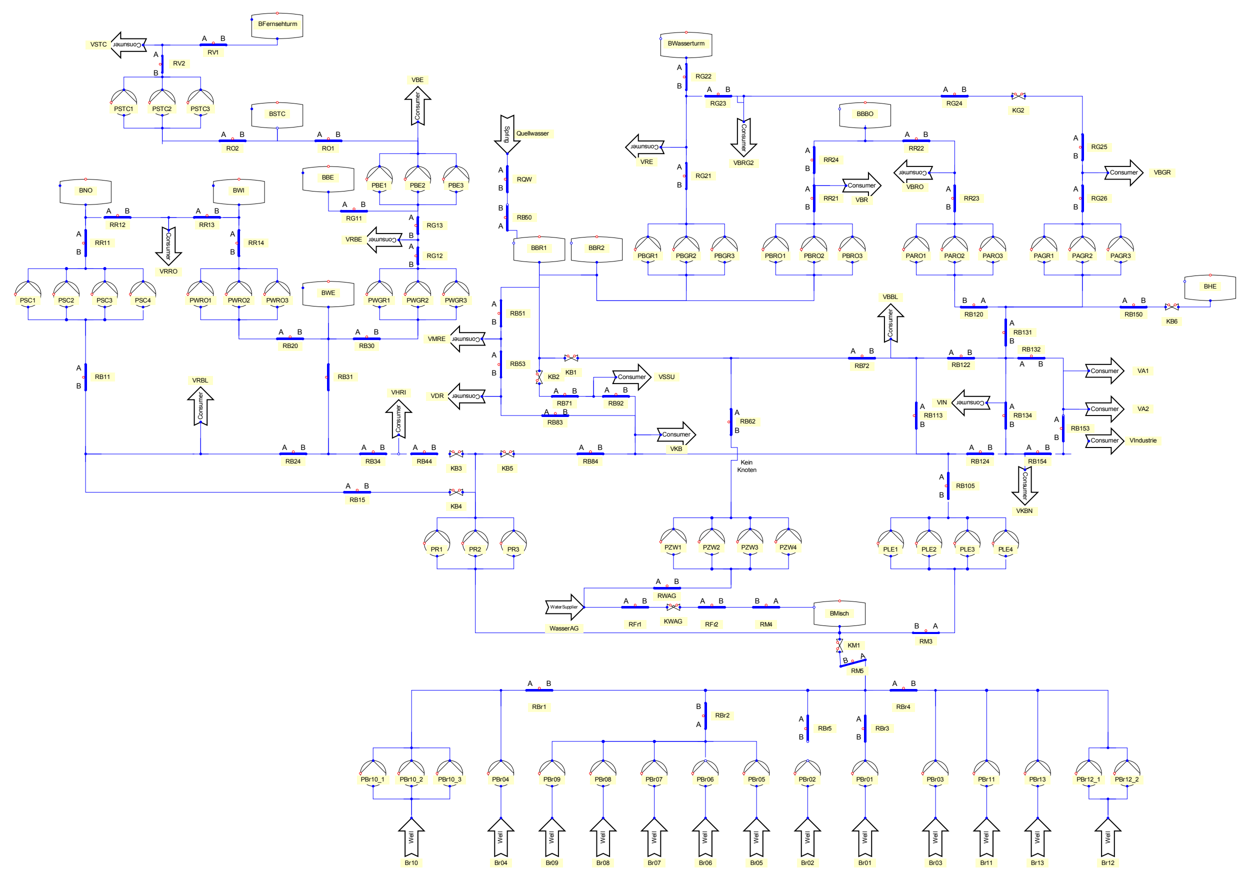
- 78 entries
- 395 exits
- 1,588 pipes
- 56 resistors
- 264 valves
- 101 control valve stations
- 35 compressor stations
- 35,000 variables
  (14,000 binary)

Computing time for 29 *expert scenarios*:

- 18 min to 10 hours
- average: 168 min

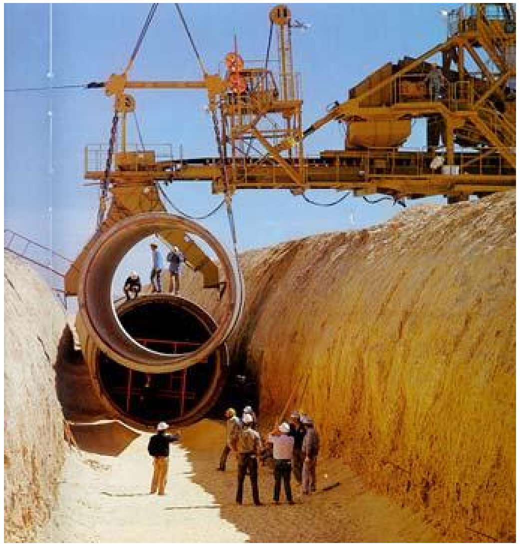


Numerical results: Water networks



Pipe details – 'Water Hammer Equations'

- Fundamental description by a system of hyperbolic partial differential equations (PDE)



continuity equation

$$\frac{\partial h}{\partial t} + \frac{a^2}{gA}\frac{\partial q}{\partial x} = 0$$

momentum equation

$$\frac{\partial q}{\partial t} + gA\frac{\partial h}{\partial x} = -\lambda \frac{q|q|}{2DA}$$

$$\frac{1}{\sqrt{\lambda}} = -2\log_{10}\left(\frac{k}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{\lambda}}\right)$$

$$\mathrm{Re} = \frac{D}{\nu A}|q|$$

$h = h(x,t)$	(pressure) head
$q = q(x,t)$	flow
$\lambda = \lambda(q)$	friction factor
A	cross-sectional area
D	diameter
L	length

Pipe details – 'Water Hammer Equations'

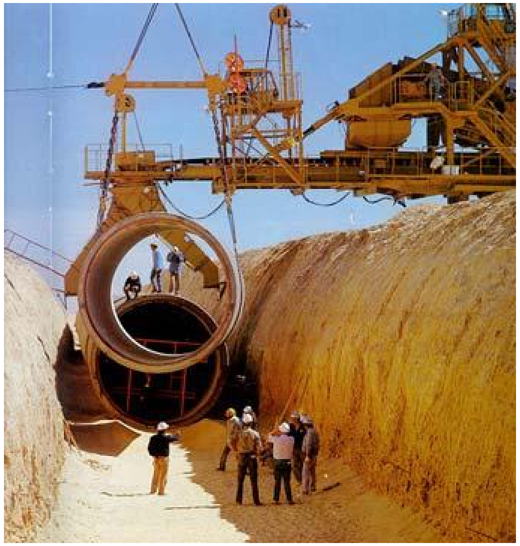
- After applying an implicit box scheme [Wendroff, 1960; Kolb, Lang, Bales, 2010]

discretized continuity equation

$$\frac{h_w^{t+1} + h_v^{t+1}}{2\Delta t} - \frac{h_w^t + h_v^t}{2\Delta t} + \frac{a^2}{gA}\frac{q_w^{t+1} - q_v^{t+1}}{L} = 0$$

discretized momentum equation

$$\frac{q_w^{t+1} + q_v^{t+1}}{2\Delta t} - \frac{q_w^t + q_v^t}{2\Delta t} + gA\frac{h_w^{t+1} - h_v^{t+1}}{L}$$
$$= -\frac{1}{2DA}\left(\lambda_v^{t+1}\frac{q_v^{t+1}|q_v^{t+1}|}{2} + \lambda_w^{t+1}\frac{q_w^{t+1}|q_w^{t+1}|}{2}\right)$$



$h = h(x,t)$	(pressure) head
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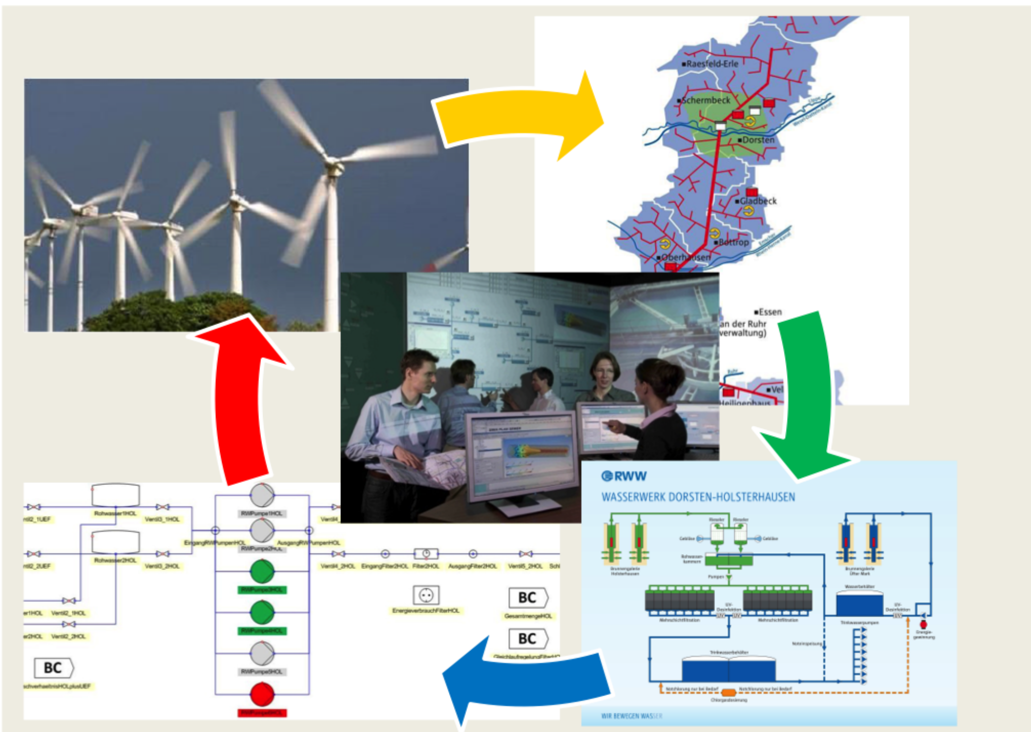
Energy Efficient Water Supply

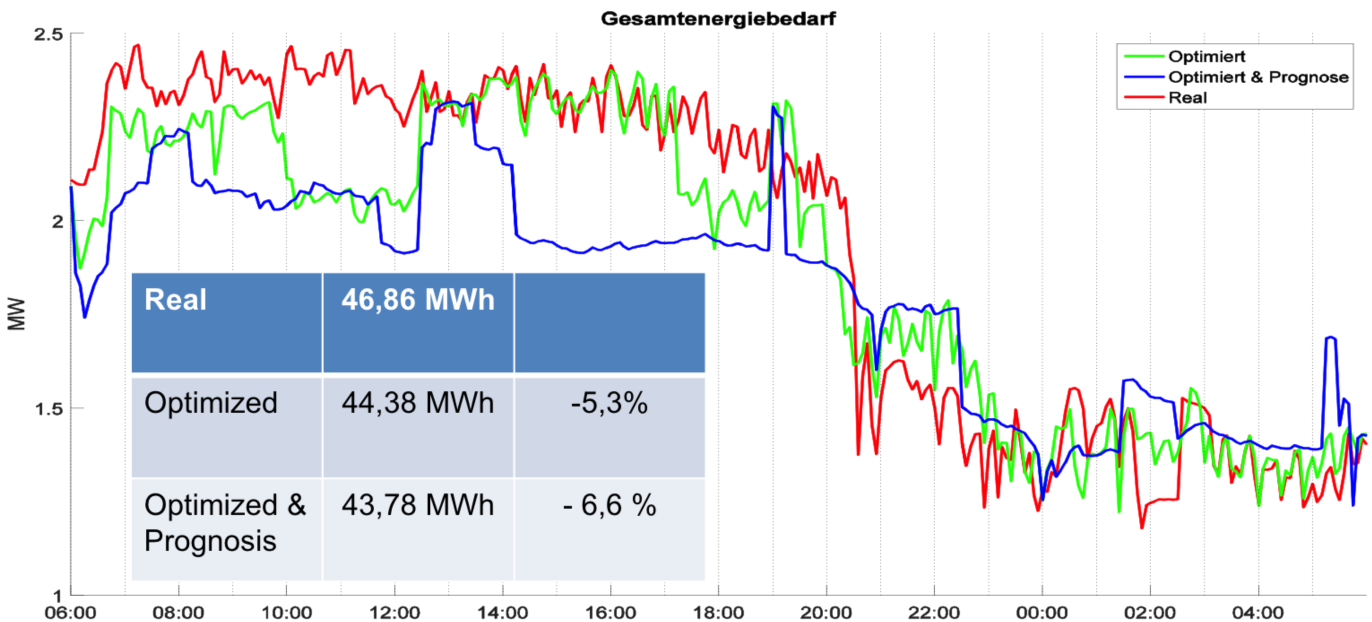
Develop local energy management systems to improve energy optimal operating plans using the example of water supply



Federal Ministry of Education and Research

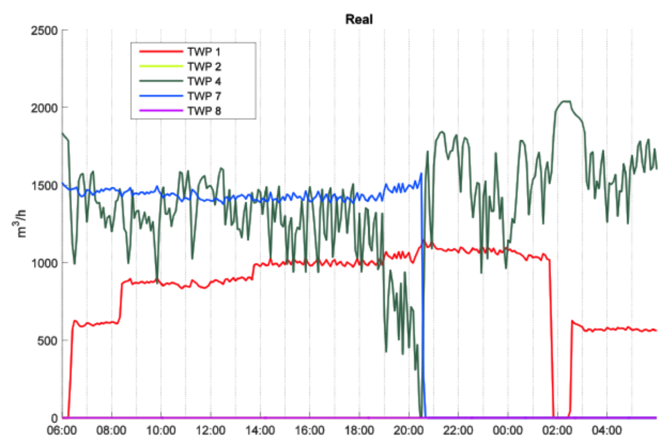
Results

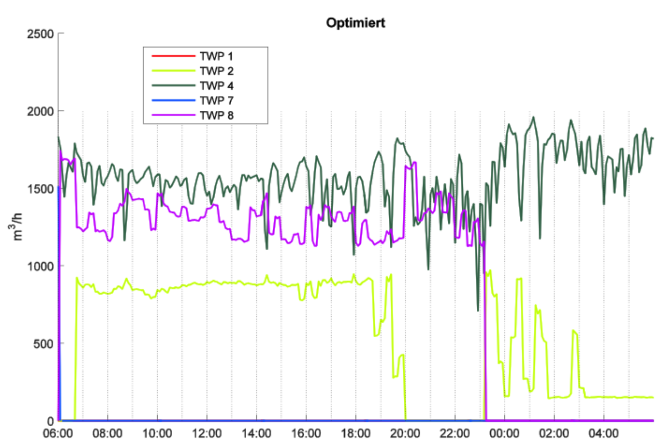
Total energy consumption

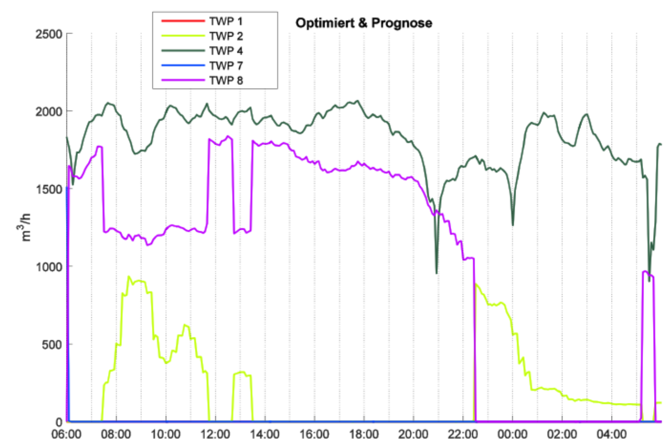


Real	46,86 MWh	
Optimized	44,38 MWh	-5,3%
Optimized & Prognosis	43,78 MWh	- 6,6 %

Optimized Pumping Schedule







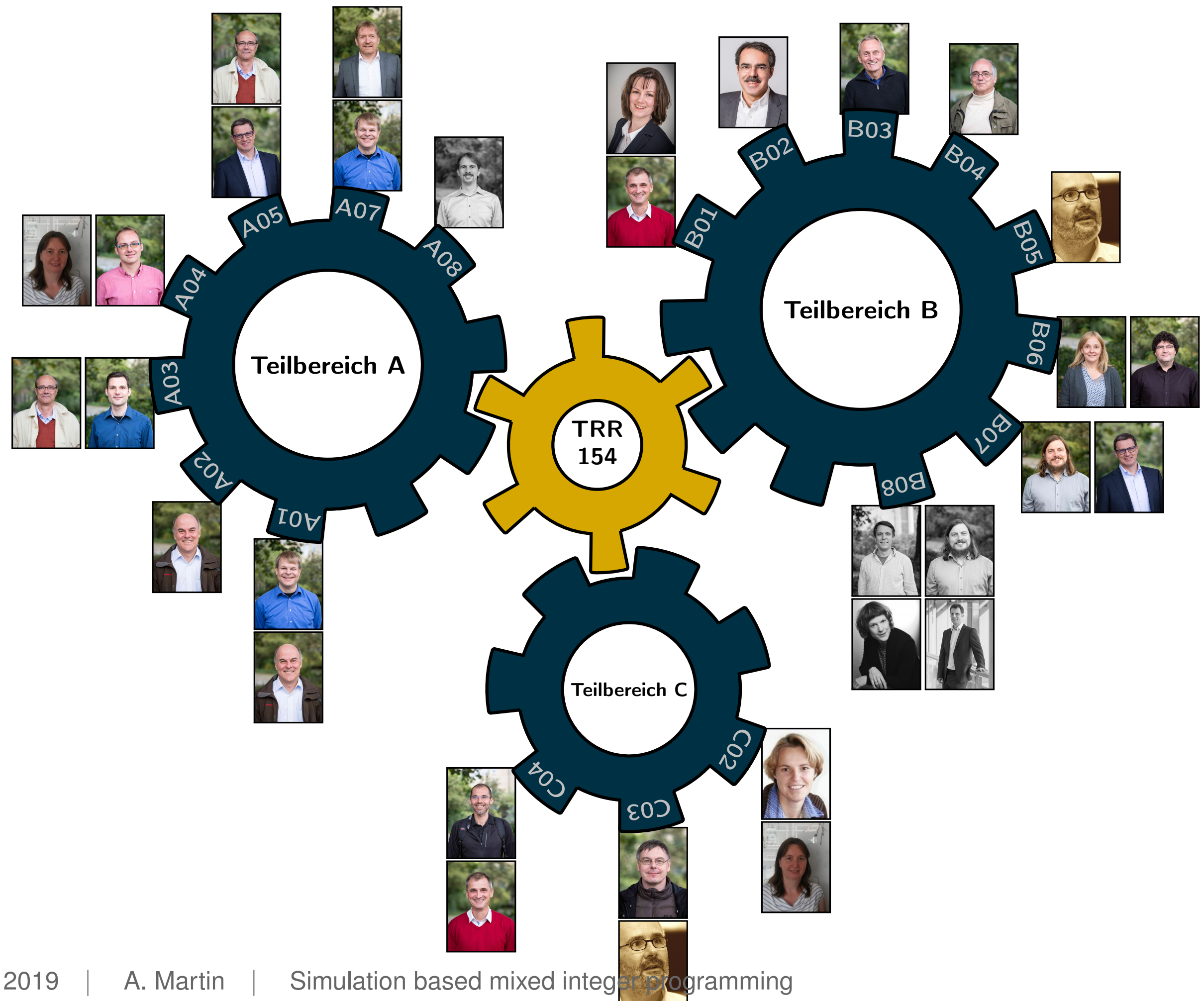
Where we are

- The stationary case is "solvable",
  i. e., the underlying nonlinearities are in closed form
- Purely polyhedral view on (mixed-integer) nonlinear problems
- Convincing computational results, including large-scale real-life instances
- Consistent hierarchy of models from MIP to MINLPs,
  if the number of variables of each nonlinear function is small

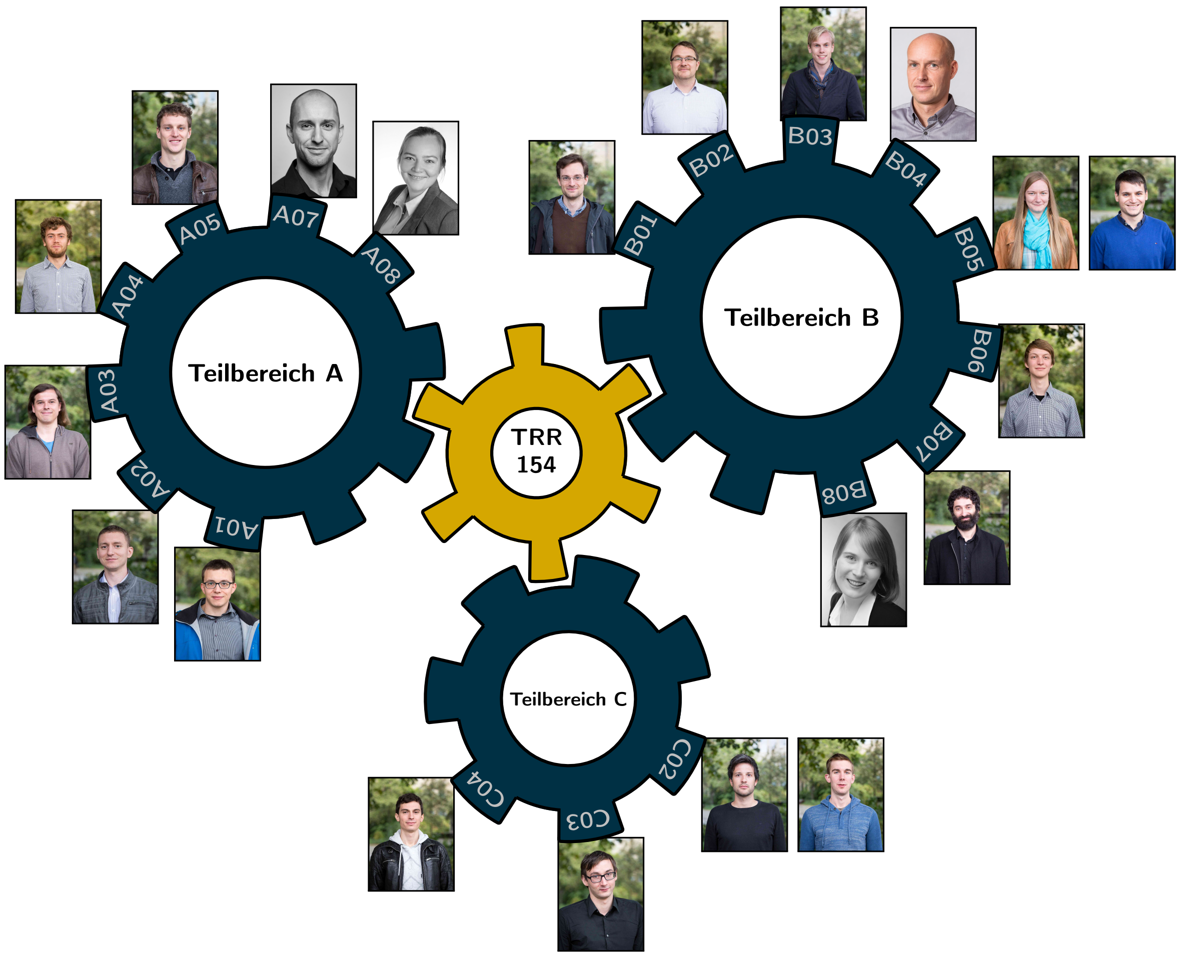
Where to go

- The non-steady case
- Dynamically coupling of time and space is necessary
- Coupling of methods from various disciplines PDE, NLP, MIP necessary
- Remodeling may not be the way to go
- Research Grant: Cooperate Research Center CRC 154
  supported by the German Science Foundation (DFG)

CRC 154: All PIs



CRC 154: All PhDs/PostDocs



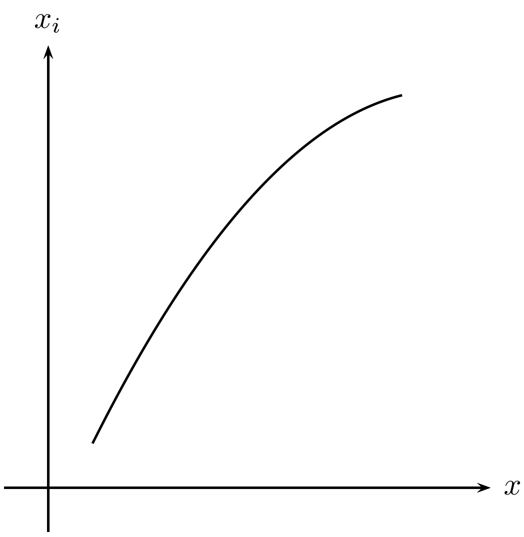
One possible way (without remodeling)

Definition (Masterproblem = MIP)

$$\begin{aligned} \min\ & c^T x + d^T y \\ \text{s.t. } & Ax + Bz \leq b \\ & \text{linearize}(\mathcal{X}) \qquad\qquad \text{MIP}(\mathcal{X}) \\ & x \in [\underline{x}, \overline{x}],\ z \in [\underline{z}, \overline{z}] \\ & (x, z) \in \mathbb{R}^n \times \mathbb{Z}^m \end{aligned}$$

Definition (Subproblem $\in \{AE, PDE, \ldots\}$)

$$\begin{aligned} & F(x, x_i, Dx_i, \ldots, D^{n-1}x_i) = 0 \\ & \forall i \in 1, \ldots, n \end{aligned} \qquad (\mathcal{X})$$



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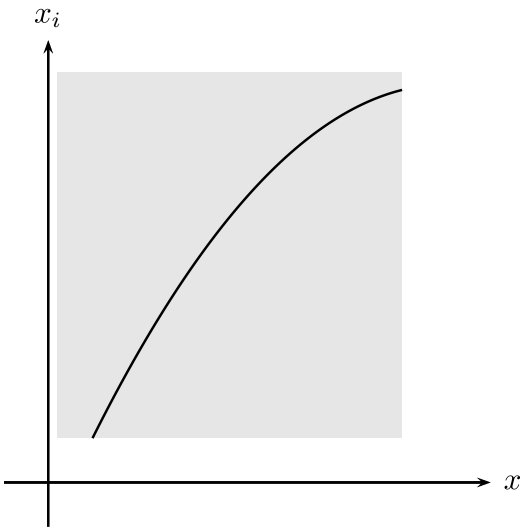

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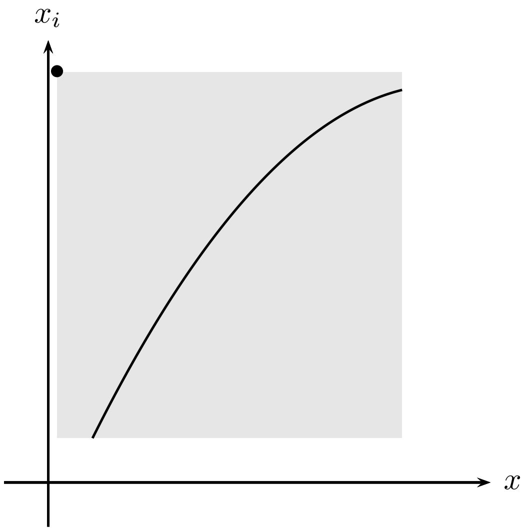

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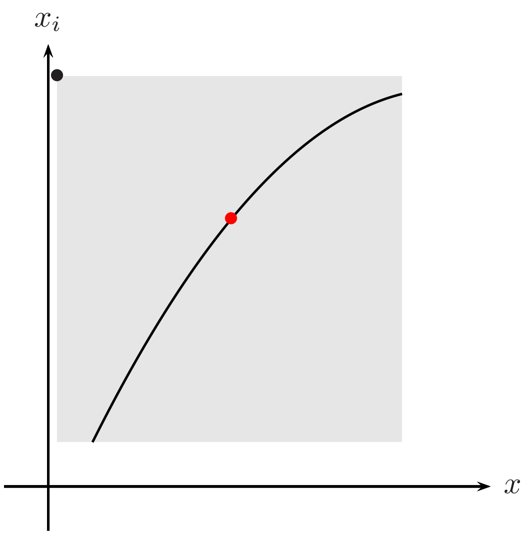

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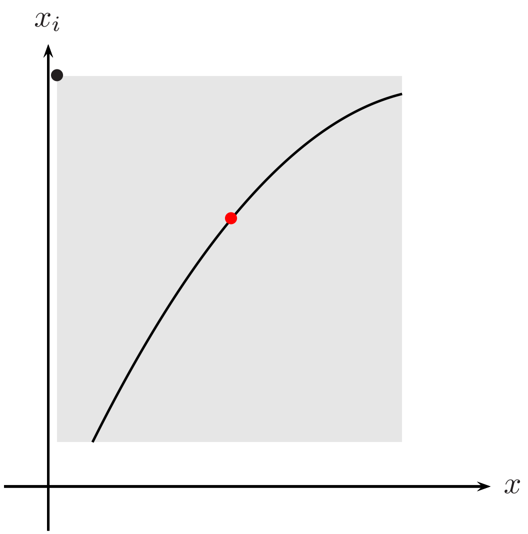

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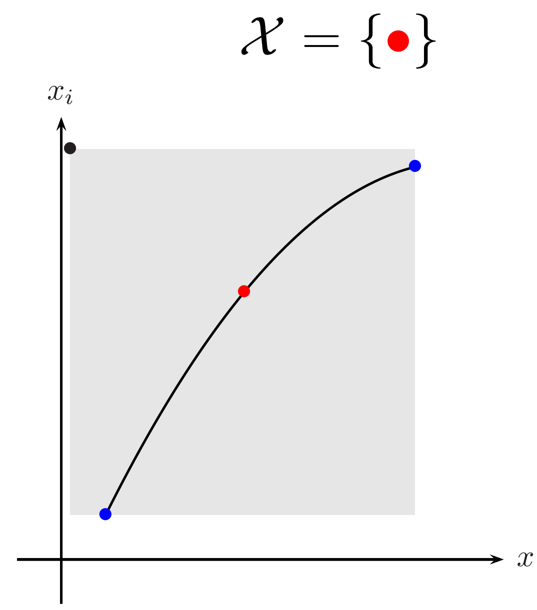

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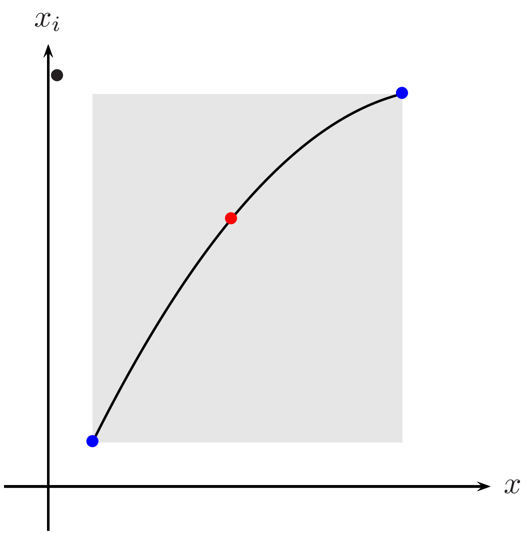

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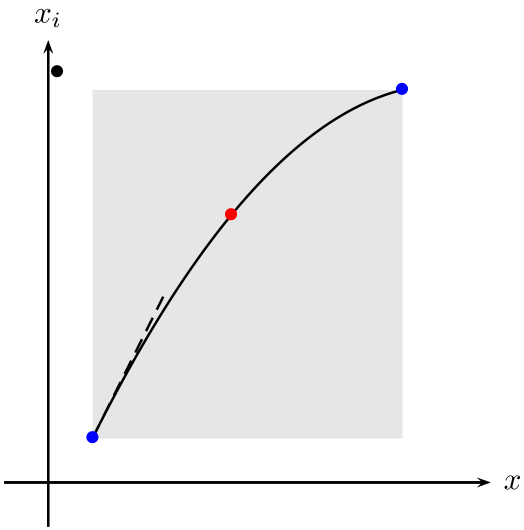

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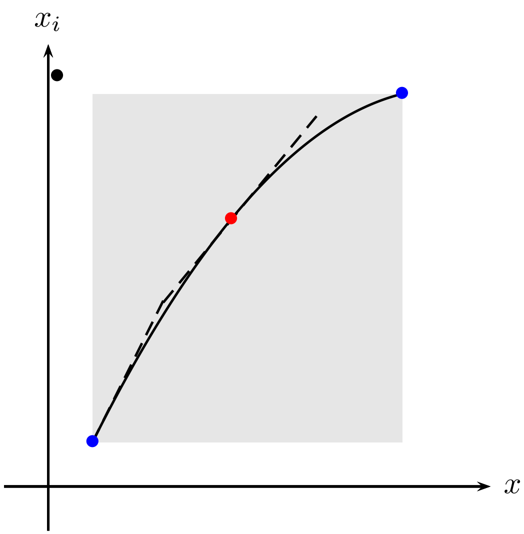

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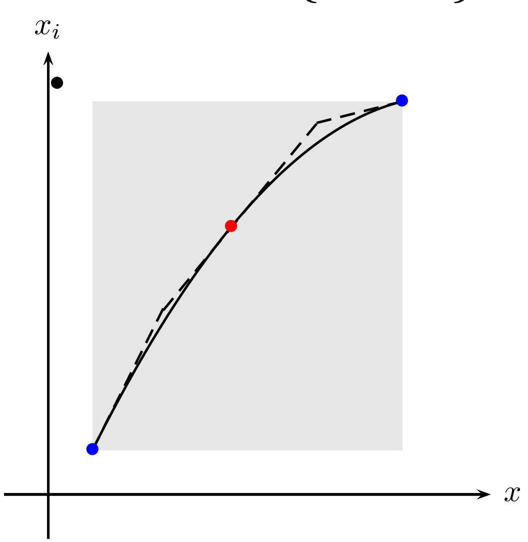

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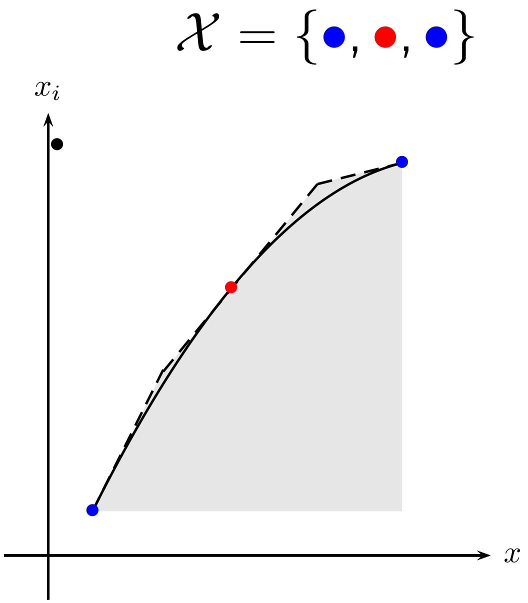

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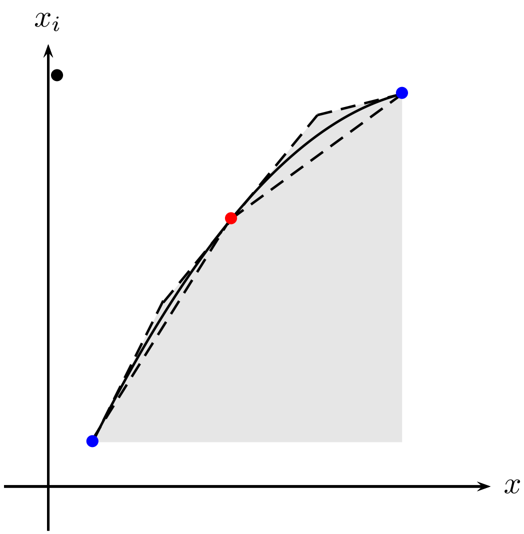

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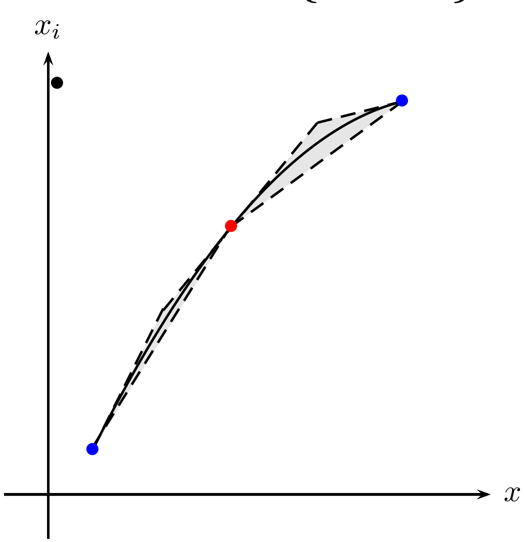

A first step: The 1-dimensional case

$$
\begin{aligned}
\min_{x} \quad & c^\top x \\
\text{s.t.} \quad & Ax \geq b \\
& x_{i_2} = f_i(x_{i_1}) \qquad \text{for all } i \in [\sigma] \\
& \hat{x} \leq x \leq \bar{x} \\
& x_{\mathcal{C}} \in \mathbb{R}^{|\mathcal{C}|},\ x_{\mathcal{I}} \in \mathbb{Z}^{|\mathcal{I}|}
\end{aligned}
$$

Assumption

The functions f_i are

- not known explicitly
- strictly monotonic
- strictly concave or convex
- differentiable with bounded first derivative

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Example

- Ordinary differential equation

$$y' = g(x, y(x)), \quad y(0) = y_0, \quad x \in [0, L]$$

- Solution $y = y(x; y_0)$
- f maps y_0 onto solutions of initial value problem, i.e., $f(y_0) = y(L; y_0)$

Algorithm

Set $L_i := \{l_{i_1}, u_{i_1}\}$, $C_i := \{l_{i_2}, u_{i_2}\}$, and $G_i := \{f'(l_{i_1}), f'(u_{i_1})\}$ for all $i \in [\sigma]$.

for $k = 0, 1, 2, \ldots$ **do**

Solve master problem for $P_d(L_i, C_i)$, and G_i.

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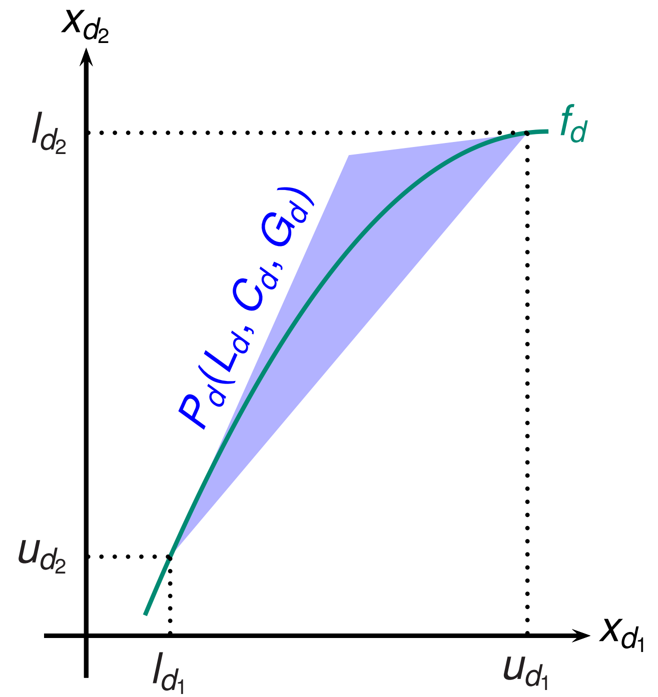

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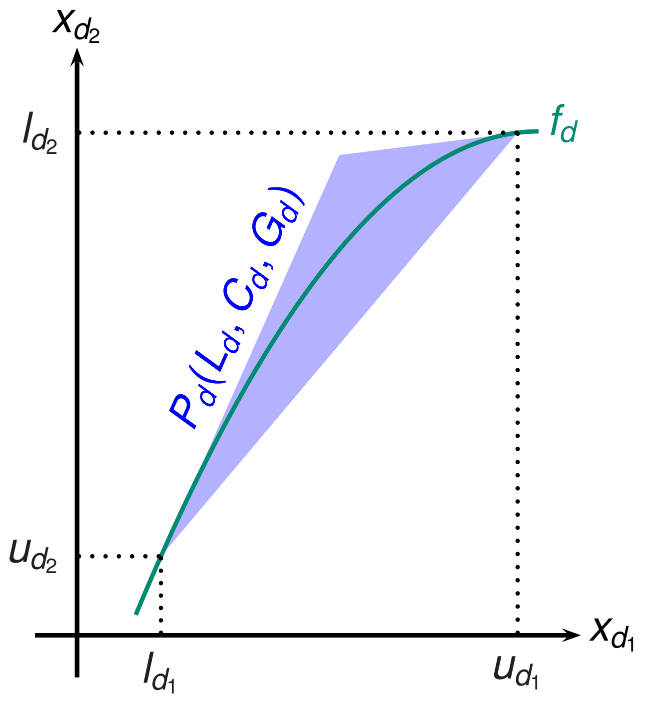

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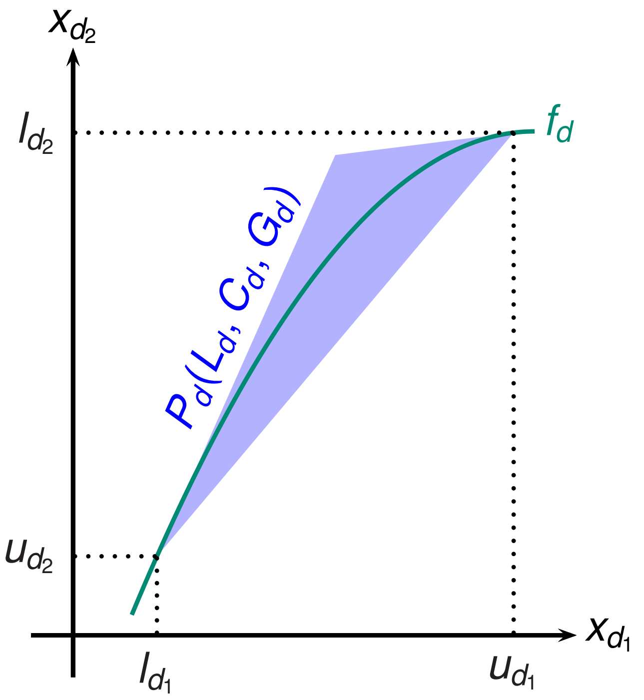
if master infeasible **return** "infeasible".



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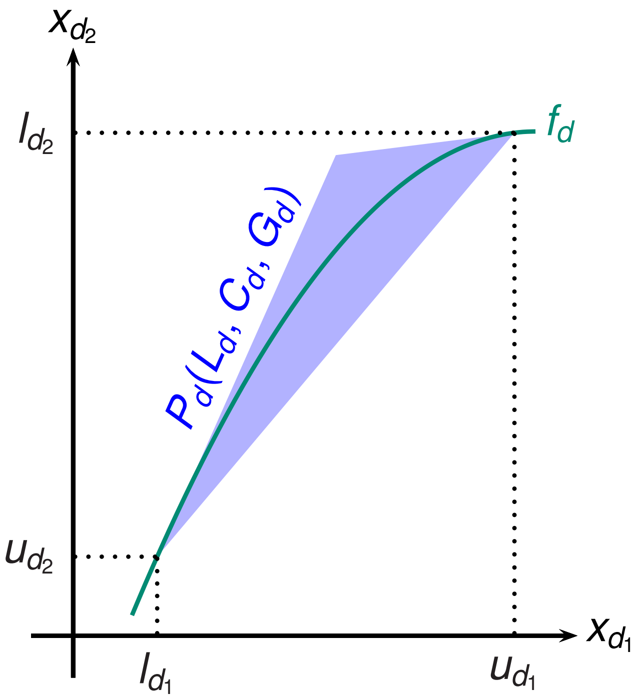
Denote solution of master problem by $\widetilde{x}^k$.



Algorithm

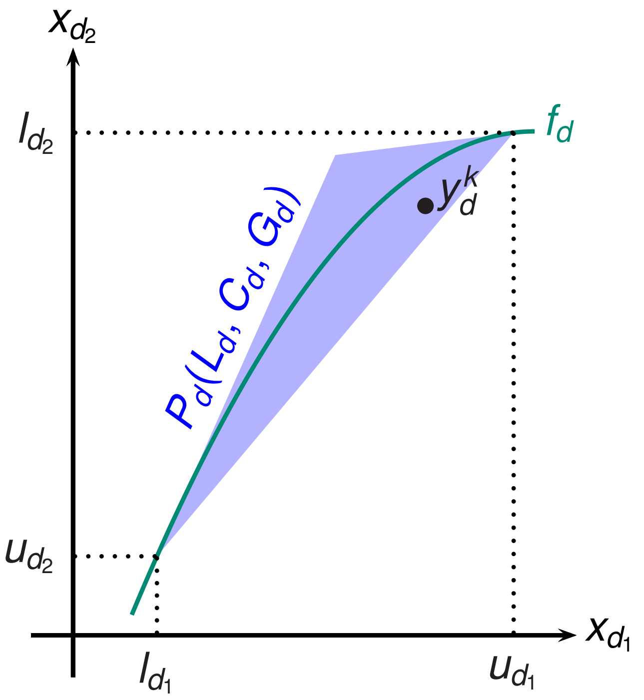
Set $L_i := \{l_{i_1}, u_{i_1}\}$, $C_i := \{l_{i_2}, u_{i_2}\}$, and $G_i := \{f'(l_{i_1}), f'(u_{i_1})\}$ for all $i \in [\sigma]$.

for $k = 0, 1, 2, \ldots$ **do**

Solve master problem for $P_d(L_i, C_i)$, and G_i.

if master infeasible **return** "infeasible".

Denote solution of master problem by $\widetilde{x}^k$.



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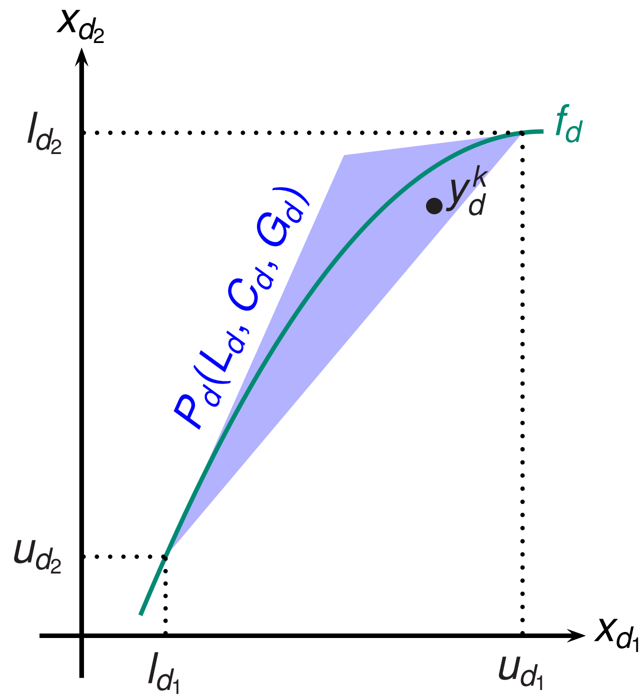
yielding solutions $\mathring{x}_i^k$ and objective values $\psi(\widetilde{x}^k)$.



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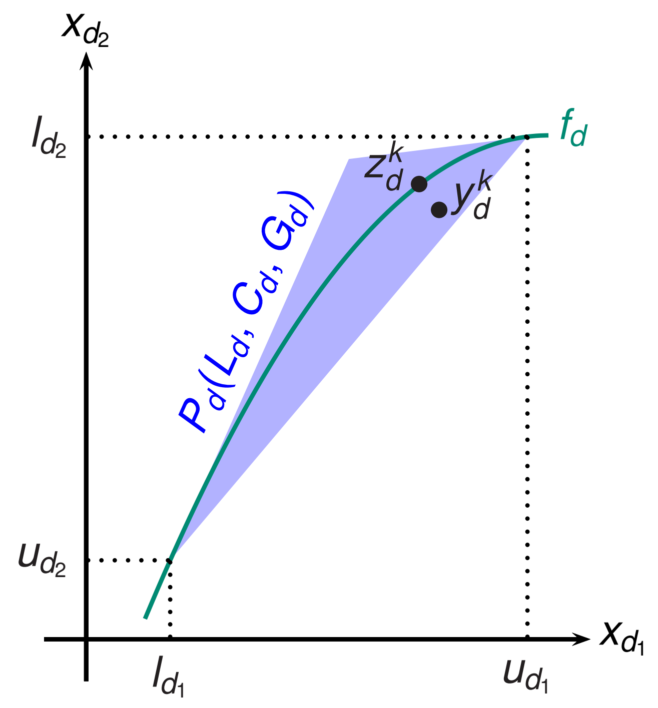

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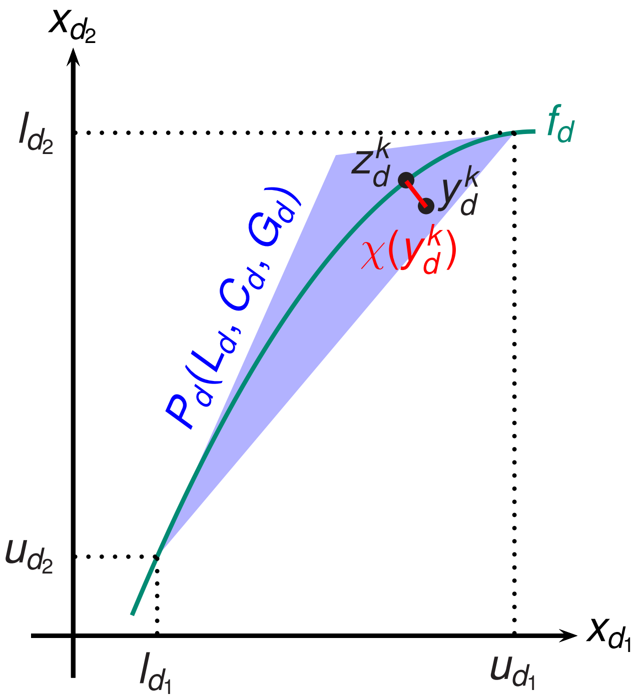

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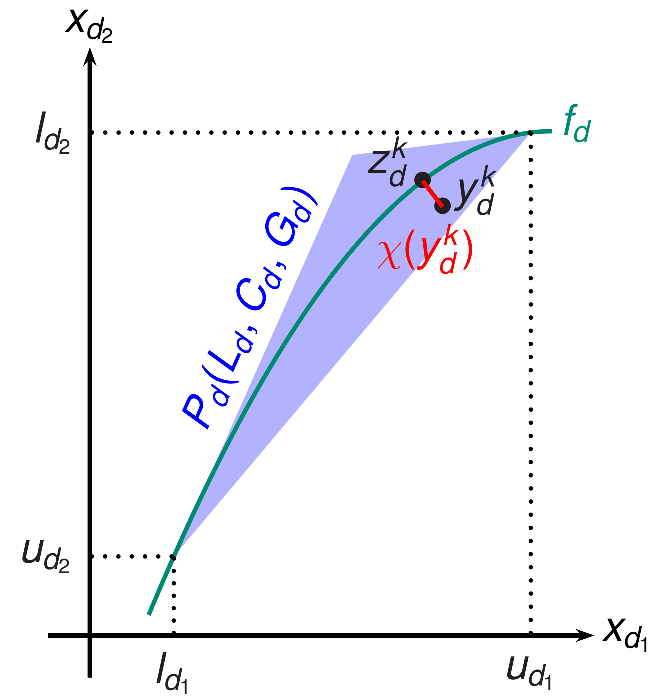

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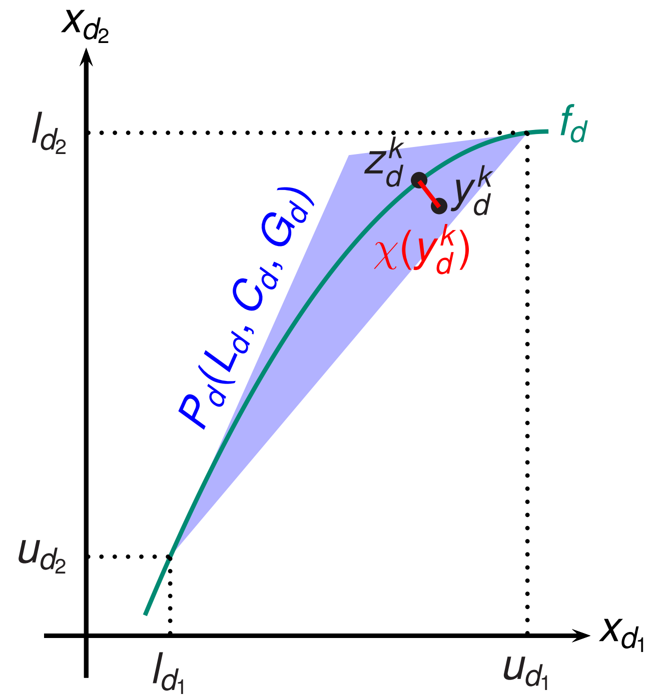

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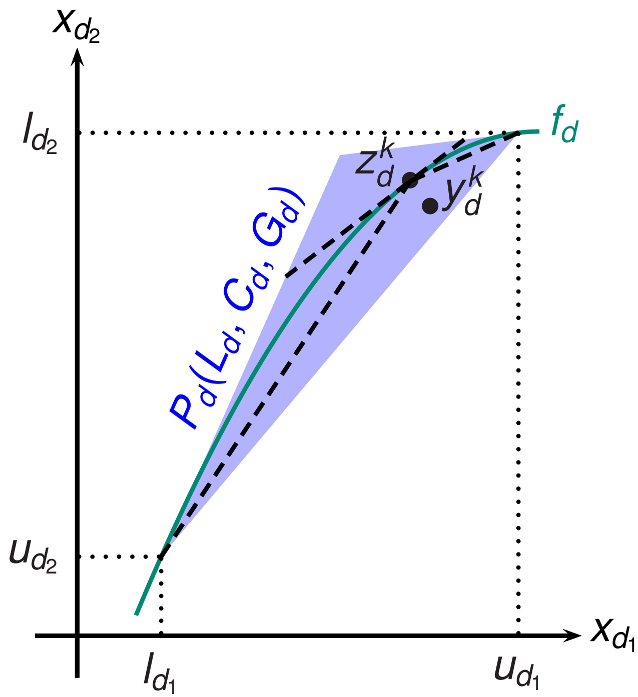

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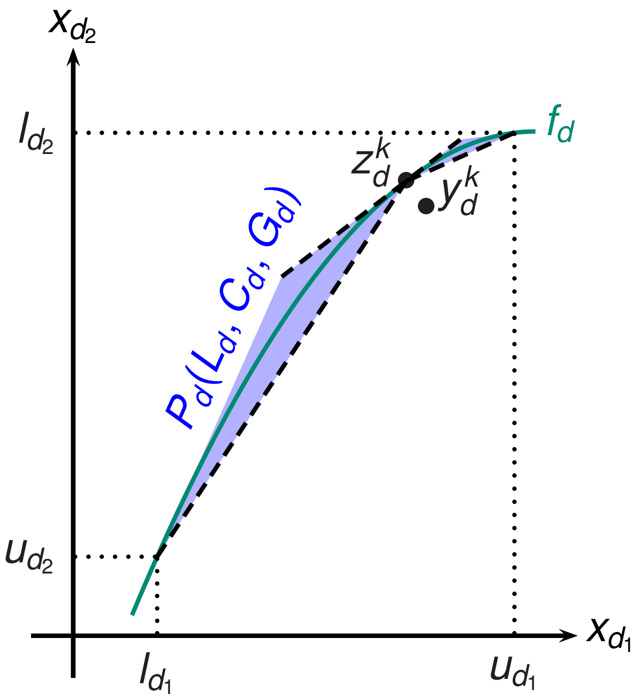

Convergence Results

Theorem

Let

- $\widetilde{x}_i \in P_i(L_i, C_i, G_i)$ be solution of the master problem
- $\mathring{x}_i$ be solution of subproblem with $\psi > \varepsilon > 0$

Then

$$\widetilde{x}_i \notin P_i(L'_i, C'_i, G'_i)$$

with $L'_i = L_i \cup \{\mathring{x}_{i_1}\}$, $C'_i = C_i \cup \{\mathring{x}_{i_2}\}$, $G'_i = G_i \cup \{f'(\mathring{x}_{i_1})\}$

Theorem

The algorithm terminates after a finite number of iterations with

- an ε-feasible solution *or*
- an indication of infeasiblility

Application: Stationary gas transport optimization

Greek Natural Gas Transport Network

Type	Quantity
Entries	3
Exits	45
Inner nodes	86
Pipes	86
Short pipes	45
Control valves	1
Compressors	1

Application: Stationary gas transport optimization

Instance	Status	Obj.	k	Total	Master	Sub
12/23/2011	opt.	262.91	6	29.15	0.13	29.03
04/19/2012	opt.	0	5	23.50	0.14	23.36
10/08/2012	opt.	248.96	6	27.30	0.22	27.09
03/16/2013	inf.	—	2	7.75	0.01	7.74
01/25/2014	opt.	311.4	5	23.73	0.09	23.64
07/04/2014	opt.	335.23	5	23.01	0.06	22.95
09/07/2014	opt.	0	6	26.55	0.38	26.17
11/14/2014	opt.	0	6	33.52	0.30	33.22
08/27/2015	opt.	0	5	22.90	0.14	22.76
11/06/2015	inf.	—	2	8.43	0.01	8.42

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M. Gugat, G. Leugering, A. Martin, M. Schmidt, M. Sirvent, D. Wintergerst: *Towards Simulation Based Mixed-Integer Optimization with Differential Equations*, Networks, 2018, `https://doi.org/10.1002/net.21812`

Summary

- Mixed integer programs with physical side constraints open great challenges.
- If nonlinearities from physics are given in closed form, piecewise linear relaxations are a promising approach.
  - Consistent hierarchy of models from MIP to MINLPs
  - Convincing computational results, including large-scale real-life instances, if the number of variables of each nonlinear function is small
- In the non-steady case, this approach may have its limits
  - Even a stronger need for a consistent hierarchy of models
  - Simulation based solutions of MIPs (including methods from based PDE, NLP) might be one way to go, see `trr154.fau.de`
  - Is there some connection to learning based algorithms or something we can learn from?

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Thanks