Mixed-Integer PDE-Constrained Optimization
US-México Workshop on Optimization and Applications

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Outline

1. Introduction
   - Source Inversion as MIP with PDE Constraints
   - Problem Classification and Challenges

2. Early Theoretical & Numerical Results
   - Eliminating the PDE & State Variables
   - Numerical Experience with Source Inversion
   - Control Regularization: Not All Norms Are Equal
   - Heat Equation: Actuator Design

3. Rounding-Based Heuristic for Cloaking

4. Conclusions
Mixed-Integer PDE-Constrained Optimization (MIPDECO)

PDE-constrained MIP ... \( u = u(t, x, y, z) \Rightarrow \) infinite-dimensional!

- \( t \) is time index; \( x, y, z \) are spatial dimensions

\[
\begin{align*}
\text{minimize} & \quad F(u, w) \\
\text{subject to} & \quad C(u, w) = 0 \\
& \quad u \in \mathcal{U}, \text{ and } w \in \mathbb{Z}^p \text{ (integers)},
\end{align*}
\]

- \( u(t, x, y, z) \): PDE states, controls, & design parameters
- \( w \) discrete or integral variables

MIPDECO Warning

\( w = w(t, x, y, z) \in \mathbb{Z} \) may be infinite-dimensional integers!
Mixed-Integer PDE-Constrained Optimization (MIPDECO)

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It’s a MIP, Jim, but not as we know it!
Grand-Challenge Applications of MIPDECO

- **Topology optimization** [Sigmund and Maute, 2013]
- Nuclear plant design: select core types & control flow rates [Committee, 2010]
- Well-selection for remediation of contaminated sites [Ozdogan, 2004]
- Design of next-generation solar cells [Reinke et al., 2011]
- Design of wind-farms [Zhang et al., 2013]
- Design & control of gas networks, [De Wolf and Smeers, 2000, Martin et al., 2006, Zavala, 2014]
- Design of accelerators ... many more
Source Inversion as MIP with PDE Constraints

Simple Example: Locate number of sources to match observation \( \bar{u} \)

\[
\begin{align*}
\text{minimize} & \quad J = \frac{1}{2} \int_{\Omega} (u - \bar{u})^2 d\Omega \\
\text{subject to} & \quad -\Delta u = \sum_{k,l} w_{kl} f_{kl} \quad \text{in } \Omega \\
& \quad \sum_{k,l} w_{kl} \leq S \quad \text{and } w_{kl} \in \{0, 1\} 
\end{align*}
\]

least-squares fit
Poisson equation
source budget

with Dirichlet boundary conditions \( u = 0 \) on \( \partial \Omega \).

E.g. Gaussian source term, \( \sigma > 0 \), centered at \( (x_k, y_l) \)

\[
f_{kl}(x, y) := \exp\left(\frac{-\| (x_k, y_l) - (x, y) \|^2}{\sigma^2}\right),
\]

Motivated by porous-media flow application to determine number of boreholes, [Ozdogan, 2004, Fipki and Celi, 2008]
Consider 2D example with $\Omega = [0, 1]^2$ and discretize PDE:

- 5-point finite-difference stencil; uniform mesh $h = 1/N$
- Denote $u_{i,j} \approx u(ih, jh)$ approximation at grid points

\[
\begin{align*}
\text{minimize} & \quad J_h = \frac{h^2}{2} \sum_{i,j=0}^{N} (u_{i,j} - \bar{u}_{i,j})^2 \\
\text{subject to} & \quad \frac{4u_{i,j} - u_{i,j-1} - u_{i,j+1} - u_{i-1,j} - u_{i+1,j}}{h^2} = \sum_{k,l=1}^{N} w_{kl} f_{kl}(ih, jh) \\
& \quad u_{0,j} = u_{N,j} = u_{i,0} = u_{i,N} = 0 \\
& \quad \sum_{k,l=1}^{N} w_{kl} \leq S \quad \text{and} \quad w_{kl} \in \{0, 1\}
\end{align*}
\]

$\Rightarrow$ finite-dimensional (convex) MIQP
Potential source locations (blue dots) on $16 \times 16$ mesh
Create target $\bar{u}$ using red square sources
Source Inversion as MIP with PDE Constraints

Target (3 sources), reconstructed sources, & error on 32 × 32 mesh
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Mixed-Integer PDE-Constrained Optimization (MIPDECO)

\[
\begin{aligned}
\text{minimize} & \quad \mathcal{F}(u, w) \\
\text{subject to} & \quad \mathcal{C}(u, w) = 0 \\
& \quad u \in \mathcal{U}, \quad \text{and} \quad w \in \mathbb{Z}^p \quad (\text{integers}),
\end{aligned}
\]

- \(u(t, x, y, z)\): PDE states, controls, & design parameters
- \(w\) discrete or integral variables

Towards a problem characterization

- **Type of PDE**: different classes of PDEs
e.g. elliptic, parabolic, hyperbolic, nonlinear, ...
- **Class of Integers**: binary, general integers, etc
- **Type of Objective**: functional form of objective
- **Type of Constraints**: characterize c/s other than PDE
- **Discretization**: discretization method & CUTEr classification
Mesh-Independent & Mesh-Dependent Integers

Definition (Mesh-Independent & Mesh-Dependent Integers)

1. The integer variables are mesh-independent, iff number of integer variables is independent of the mesh.
2. The integer variables are mesh-dependent, iff the number of integer variables depends on the mesh.

Mesh-Independent

- Manageable tree size
- Theory possible

Mesh-Dependent

- Exploding tree size
- Theory???

... also mixed: mesh-dependent in time, $t$, but not space
Theoretical Challenges of MIPDECO

**Functional Analysis** *(mesh-dependent integers)*

Denis Ridzal: What function space is $w(x, y) \in \{0, 1\}$?

- Consistently approximate $w(x, y) \in \{0, 1\}$ as $h \to 0$?
- Conjecture: $\{w(x, y) \in \{0, 1\}\} \neq L_2(\Omega)$
  - e.g. binary support of Cantor set not integrable
- Likely need additional regularity assumptions

**Coupling between Discretization & Integers**

Discretization scheme (e.g. upwinding for wave equation) depends on direction of flow (integers).

- Application: gas network models with flow reversals
  
  ... open postdoc position at Argonne!
Computational Challenges of MIPDECO

- Approaches for **humongous branch-and-bound trees**
  ... e.g. 3D topology optimization with $10^9$ binary variables

- **Warm-starts** for PDE-constrained optimization (nodes)
- Guarantees for nonconvex (nonlinear) PDE constraints
  ... factorable programming approach hopeless for $10^9$ vars!

$$\ldots \ f(x_1, x_2) = x_1 \log(x_2) + x_2^3$$
MIPDECO: Two Cultures Collide

Observation

PDE-optimization & MIP developed separately ⇒ different assumptions, methodologies, and computational kernels!

<table>
<thead>
<tr>
<th><strong>PDE-Optimization</strong></th>
<th><strong>Mixed-Integer Programming</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Obtain good solutions efficiently</td>
<td>Deliver certificate of optimality</td>
</tr>
<tr>
<td>Nonlinear optimization:</td>
<td>Combinatorial optimization:</td>
</tr>
<tr>
<td>Newton’s method</td>
<td>branch-and-cut</td>
</tr>
<tr>
<td>Iterative Krylov solvers</td>
<td>Factors &amp; rank-one updates</td>
</tr>
<tr>
<td>Run on bleeding-edge HPC</td>
<td>Limited HPC developments</td>
</tr>
</tbody>
</table>

Potential for Disaster, or Opportunity for Innovation!
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Source Inversion as MIP with PDE Constraints

Find number and location of sources to match observation $\bar{u}$

$$\begin{aligned}
\text{minimize} \quad & J = \frac{1}{2} \int_{\Omega} (u(w) - \bar{u})^2 \, d\Omega \\
\text{subject to} \quad & -\Delta u = \sum_{k, l} w_{kl} f_{kl} \quad \text{in} \quad \Omega \quad \text{Poisson equation} \\
& \sum_{k, l} w_{kl} \leq S \quad \text{and} \quad w_{kl} \in \{0, 1\} \quad \text{source budget}
\end{aligned}$$

- MIP with convex quadratic objective on $\Omega = [0, 1]^2$
- 5-point finite-difference stencil; uniform mesh $h = 1/N$
- Denote $u_{i,j} \approx u(ih, jh)$ approximation at grid points
Cool MIPDECO Trick: Eliminating the PDE

Discretized PDE constraint (Poisson equation)

\[
\frac{4u_{i,j} - u_{i,j-1} - u_{i,j+1} - u_{i-1,j} - u_{i+1,j}}{h^2} = \sum_{k,l} w_{kl} f_{kl}(ih,jh), \; \forall \; i,j
\]

\[\Leftrightarrow \quad A u = \sum w_{kl} f_{kl}, \text{ where } w_{kl} \in \{0, 1\} \text{ only appear on RHS!}\]

Elimination of PDE and states \(u(x,y,z)\)

- \(Au = \sum w_{kl} f_{kl} \Leftrightarrow u = A^{-1} \left( \sum w_{kl} f_{kl} \right) = \sum w_{kl} A^{-1} f_{kl}\)
- Solve \(n^2 \ll 2^n\) PDEs: \(u^{(kl)} := A^{-1} f_{kl}\)
- Eliminate \(u = \sum w_{kl} u^{(kl)}\) from Source Inversion
Cool MIPDECO Trick: Eliminating the PDE

Eliminating \( u = \sum_{k,l} w_{kl} u^{(kl)} \) in MINLP gives:

\[
\begin{align*}
\min_w J_h &= \frac{h^2}{2} \sum_{i,j=0}^{N} \left( \sum_{k,l} w_{kl} u^{(kl)}_{ij} - \bar{u}_{i,j} \right)^2 \\
\text{subject to} \quad \sum_{k,l=1}^{N} w_{kl} &\leq S \quad \text{and} \quad w_{kl} \in \{0, 1\}
\end{align*}
\]

- Eliminates the states \( u \) (\( N^2 \) variables)
- Eliminates the PDE constraint (\( N^2 \) constraints)

... generalizes to other PDEs (with integer controls on RHS)

Simplified model is quadratic knapsack problem
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Numerical Experience with Source Inversion

Find number and location of sources to match observation $\bar{u}$

$$\min_{u,w} J = \frac{1}{2} \int_{\Omega} (u(w) - \bar{u})^2 d\Omega \quad \text{least-squares fit}$$

subject to

$$-\Delta u = \sum_{k,l} w_{kl} f_{kl} \quad \text{in } \Omega \quad \text{Poisson equation}$$

$$\sum_{k,l} w_{kl} \leq S \text{ and } w_{kl} \in \{0, 1\} \quad \text{source budget}$$

MIP with convex quadratic objective

Computational Experiments:

1. Test NLP-plus-rounding heuristic versus MINLP
2. Effect of mesh-dependent vs. mesh-independent integers
   - Mesh-independent: pick sources from 36 potential locations
   - Mesh-dependent: all nodes are potential locations
3. Effect of state-elimination trick
Potential source locations (blue dots) on 16 × 16 mesh
Create target $\bar{u}$ using red square sources
**Approach 1: NLP-Solve, Knapsack Rounding, and MIP**

### Knapsack Rounding

1. Solve continuous relaxation using NLP solver
2. Round largest $S$ locations, $w_i$, to one & set all others to zero
Approach 1: NLP-Solve, Knapsack Rounding, and MIP

**Knapsack Rounding**

1. Solve continuous relaxation using NLP solver
2. Round largest $S$ locations, $w_i$, to one & set all others to zero

Knapsack-rounded NLP (left) and MINLP (right)

MINLP solution better: $\text{NLP-err} = 0.0388 > 0.0307 = \text{MIP-err}$
Mesh-Independent Source Inversion: MINLP Solvers

Number of Nodes and CPU time for Increasing Mesh Sizes

- **Number of Nodes independent of mesh size!**
- **MINLP & Minotaur**: filterSQP runs out of memory for $N \geq 32$
- **BonminOA** takes roughly 100 iterations ... quadratic objective
Mesh-Dependent (all) Source Inversion: MINLP Solvers

Number of Nodes and CPU time for Increasing Mesh Sizes

- **Number of nodes explodes with mesh size!**
- **OA <BREAK> after 130,000 seconds**
Elimination of States & PDEs: Source Inversion

CPU Time for Increasing Mesh Sizes: Simplified vs. Original Model

Eliminating PDEs is two orders of magnitude faster!
Elimination of States & PDEs: Source Inversion

CPU Time for Increasing Mesh Sizes: Simplified vs. Original Model

<table>
<thead>
<tr>
<th></th>
<th>8 × 8</th>
<th>16 × 16</th>
<th>32 × 32</th>
</tr>
</thead>
<tbody>
<tr>
<td>Presolve Time</td>
<td>0.05</td>
<td>1.30</td>
<td>62.51</td>
</tr>
<tr>
<td>Simplified Model</td>
<td>0.18</td>
<td>0.50</td>
<td>2.38</td>
</tr>
<tr>
<td>Total Simplified</td>
<td>0.23</td>
<td>1.80</td>
<td>64.89</td>
</tr>
<tr>
<td>Full PDE Model</td>
<td>2.10</td>
<td>29.43</td>
<td>1013.21</td>
</tr>
</tbody>
</table>

... using NLP solve for PDE (inefficient)

Presolve is cheap ... simplified model solves much faster!
First Conclusions: Source Inversion

Numerical Results

- **Solve mesh-independent** problems with coarse discretization
- **Mesh-dependent** instances cannot be solved
- Outer Approximation (Bon-OA) inefficient for these instances
- Trick # 1: elimination of states and PDE constraint
- Nonlinear solvers run into storage issues
First Conclusions: Source Inversion

Numerical Results

- **Solve mesh-independent** problems with coarse discretization
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- Outer Approximation (Bon-OA) inefficient for these instances
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... not surprising: **MIPDECO trees grow like tribbles!**
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Control Regularization: Not All Norms Are Equal


\[
\begin{align*}
\text{minimize} & \quad \| u - u_d \|^2_{L^2(\Omega)} + \alpha \| w \|^2_{L^x} \\
\text{subject to} & \quad u_t - \Delta u = 0 \quad \text{in} \quad [0, T] \times \Omega \\
& \quad u(0, x) = 0 \quad \text{in} \quad \Omega \quad \text{and} \quad \frac{\partial u}{\partial x}(t, 0) = 0 \quad \text{in} \quad (0, T) \\
& \quad \frac{\partial u}{\partial x}(t, 1) = b(w(t) - u(t, 1)) \quad \text{in} \quad (0, T) \\
& \quad w(t) \in \{-1, 0, 1\}
\end{align*}
\]

$L^1$ or $L^2$ regularization term for control $w(t) \in \{-1, 0, 1\}$?

**Good Norms for MIPs**

MIP’ers prefer polyhedral norms ... promote integrality

- Old MIP trick: $w^2(t) = |w(t)|$ for $w(t) \in \{-1, 0, 1\}$
  \[ \Rightarrow L^1\text{-norm same as } L^2\text{-norm on binary variables!} \]
Not All Norms Are Equal

Consider **Robin Boundary Control** for increasing \((x, t)\)-mesh

<table>
<thead>
<tr>
<th>Mesh</th>
<th>CPU for (L^2) Regularization</th>
<th>(L^1) Regularization</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Minotaur</td>
<td>B-BB</td>
</tr>
<tr>
<td>8x8</td>
<td>0.04</td>
<td>0.80</td>
</tr>
<tr>
<td>16x16</td>
<td>6.61</td>
<td>72.21</td>
</tr>
<tr>
<td>32x32</td>
<td>Time</td>
<td>Time</td>
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Consider **Robin Boundary Control** for increasing \((x, t)\)-meshes.

### CPU for \(L^2\) Regularization

<table>
<thead>
<tr>
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<th>Minotaur</th>
<th>B-BB</th>
<th>B-Hyb</th>
<th>B-OA</th>
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<tbody>
<tr>
<td>8x8</td>
<td>0.04</td>
<td>0.80</td>
<td>2.54</td>
<td>126.81</td>
</tr>
<tr>
<td>16x16</td>
<td>6.61</td>
<td>72.21</td>
<td>1305.00</td>
<td>Time</td>
</tr>
<tr>
<td>32x32</td>
<td>Time</td>
<td>Time</td>
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### CPU for \(L^1\) Regularization

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<tbody>
<tr>
<td>8x8</td>
<td>0.03</td>
<td>0.48</td>
<td>0.21</td>
<td>0.04</td>
</tr>
<tr>
<td>16x16</td>
<td>0.11</td>
<td>3.62</td>
<td>0.66</td>
<td>0.20</td>
</tr>
<tr>
<td>32x32</td>
<td>0.18</td>
<td>62.66</td>
<td>3.53</td>
<td>0.74</td>
</tr>
</tbody>
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- \(L^1\) regularization is equivalent to \(L^2\), but faster
- Many fewer nodes in tree-searches \(\Rightarrow\) solve up to \(128 \times 128\)
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Problem 2: Actuator Placement and Operation [Falk Hante]

Goal: Control temperature with actuators

- Select sequence of control inputs (actuators)
- Choose continuous control (heat/cool) at locations
- Match prescribed temperature profile

... “de-mist bathroom mirror with hair-drier”

Potential Actuator Locations \( l = 1, \ldots, L \)
Problem 2: Actuator Placement and Operation

Find optimal sequence of actuators, $w_l(t)$, and controls, $v_l(t)$:

\[
\begin{align*}
\text{minimize} & \quad \| u(t_f, \cdot) \|_\Omega^2 + 2\| u \|_{T \times \Omega}^2 + \frac{1}{500} \| v \|_T^2 \\
\text{subject to} & \quad \frac{\partial u}{\partial t} - \kappa \Delta u = \sum_{l=1}^{L} v_l(t) f_l \quad \text{in} \quad T \times \Omega \\
& \quad w_l(t) \in \{0, 1\}, \quad \sum_{l=1}^{L} w_l(t) \leq W, \quad \forall t \in T \\
& \quad L w_l(t) \leq v_l(t) \leq U w_l(t), \quad \forall l = 1, \ldots, L, \quad \forall t \in T
\end{align*}
\]

where

\[
f_l(x, y) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{\| (x, y) - (x_l, y_l) \|^2}{2\sigma} \right)
\]

point-source for actuators at $(x_l, y_l)$ ... movies!
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Design of cloaking device on domain $\Omega$

- Cloak subdomain $\Omega_0$ (red dashes) by preventing (complex) wave from entering domain
- Design scatterer in subdomain $\hat{\Omega}$
  ...$w(x, y) \in \{0, 1\}$
- PDE: 2D Helmholtz (over $\mathbb{C}$) with Robin boundary conditions
- Incident wave is $\exp(ik_0y)$ for wavelength $k_0 = 6\pi$

where $i = \sqrt{-1}$
Control: $w = w(x, y)$ in $\hat{\Omega}$
States: $u = u(x, y)$ in $\Omega$
Target: $u_0 = u_0(x, y)$ in $\Omega_0$

minimize $J(u) = \frac{1}{2} \|u + u_0\|_{2, \Omega_0}^2$
subject to $-\Delta u - k_0^2 (1 + qw) u = k_0^2 q w u_0$ in $\Omega$
$\frac{\partial u}{\partial n} - ik_0 u = 0$ on $\partial \Omega$
$w \in \{0, 1\}$ in $\hat{\Omega}$.

Discretization: finite-differences with $l = 3$ nodes per scatter element, $w(x, y)$. 

Strip Rounding Heuristic

Cannot solve on reasonable mesh/domain with any MINLP solver.

Algorithm: Strip Rounding Heuristic
Solve continuous relaxation & initialize $i = 1$

for $i=1,...,N$ do
    Round a strip $w(x_i, y_j)$ for all $j$
    Resolve relaxation with $w(x_k, y)$ fixed for all $k \leq i$
end

Round fractional $w(x, y)$ following direction of wave
Strip Rounding Heuristic

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end

Round fractional $w(x, y)$ following direction of wave
Results for Strip Rounding

Scatterer, $w(x, y)$

States $u(x, y)$

... resolve PDE on finer mesh for fixed controls
... Solution Not Physical!

Coarse States  
... not clear we’re getting the correct physics!

Resolved States
Conclusions

Mixed-Integer PDE-Constrained Optimization (MIPDECO)
- Class of challenging problems with important applications
  - Subsurface flow: oil recovery or environmental remediation
  - Design and operation of gas-/power-networks
- On-going work: Building library of test problems
- Classification: mesh-dependent vs. mesh-independent
- Elimination of PDE and state variables $u(t, x, y, z)$
- Discretized PDEs $\Rightarrow$ huge MINLPs ... push solvers to limit
- Need new ideas, solvers, software for real applications

Outlook and Extensions
- Consider multi-level in space (network) and time
- Move toward truly multi-level approach similar to PDEs
  ... our five-year mission ...
To boldly go where no optimizer has gone before …

… to explore strange new PDEs & MIPs!
Advanced fuel pellet materials and fuel rod design for water cooled reactors.

The gas transmission problem solved by an extension of the simplex algorithm.

An integer programming model to optimize resource allocation for wildfire containment.
*Forest Science*, 61(2).

The use of multilateral well designs for improved recovery in heavy oil reservoirs.
In *IADV/SPE Conference and Exhibition*, Orlanda, Florida. SPE.

Mixed integer models for the stationary case of gas network optimization.

OPTPDE (2014).
OPTPDE — a collection of problems in PDE-constrained optimization.
http://www.optpde.net.

Optimization of well placement under time-dependent uncertainty.


