UCONN
UNIVERSITY OF CONNECTICUT

Improvements to EAGO.jl: Consolidation and Performance

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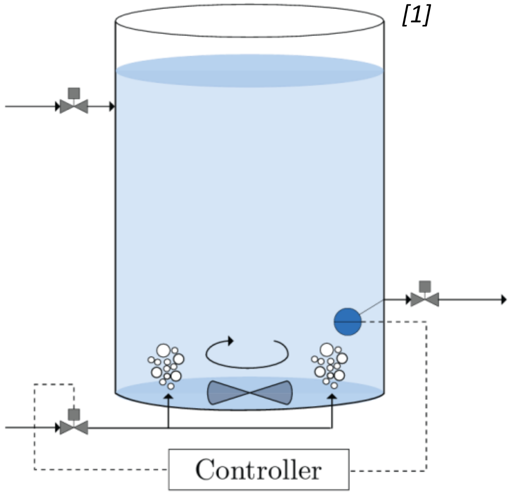
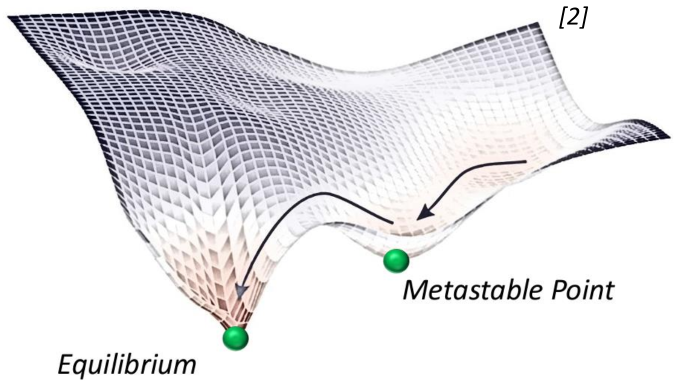
2024 AIChE ANNUAL MEETING

Process Systems and Operations Research Laboratory

Global Optimization

- Complex problems arise in many applications
  - Advanced control systems
  - Thermodynamic stability
  - Kinetic parameter estimation
  - Design under uncertainty
  - Etc.





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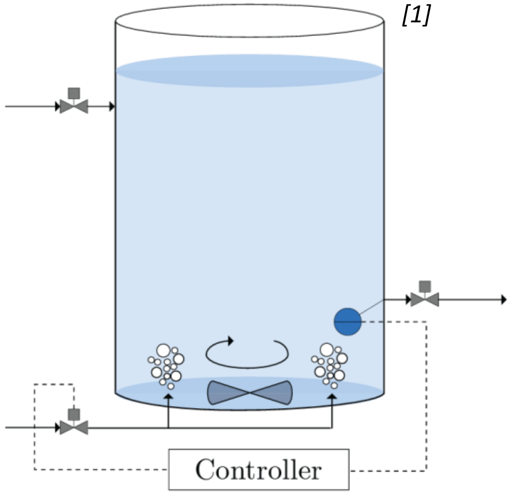
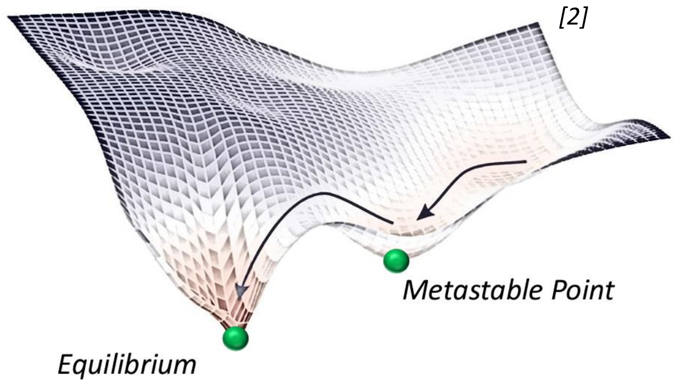
- Certificate of optimality





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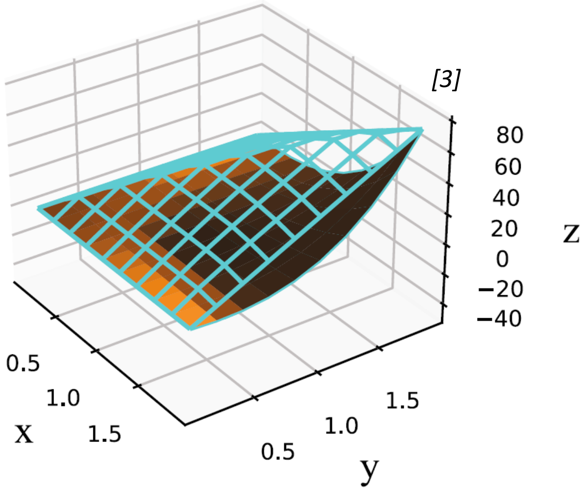
Easy Advanced Global Optimization

- Open-source deterministic global solver for nonconvex MINLPs
  - Semi-infinite programs (SIPs)
  - Dynamic optimization
  - User-defined functions
- Applies McCormick-based relaxations for convex lower-bounding problems
- Designed in Julia for performance and extensibility
  - Improved user experience through JuMP.jl



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Parameter Estimation Example

- Oxidation of cyclohexadienyl
- Dynamic optimization problem

$$\min_{\mathbf{p}} \phi(\mathbf{p},t) = \sum_{i=0}^{N} (I_i^{calc} - I_i^{exp})^2 \quad [3]$$

$$\text{s.t.} \;\; \mathbf{p} \in [\mathbf{p}^L, \mathbf{p}^U]$$

$$I_i^{calc} = x_{A,i} + \frac{2}{21} x_{B,i} + \frac{2}{21} x_{D,i}$$

$$\frac{dx_A}{dt} = k_1 x_Z x_Y - c_{O_2}(k_{2f} + k_{3f}) x_A + \frac{k_{2f}}{K_2} x_D + \frac{k_{3f}}{K_3} x_B - k_5 x_A^2$$

$$\frac{dx_B}{dt} = c_{O_2} k_{3f} x_A - \left(\frac{k_{3f}}{K_3} + k_4 \right) x_B$$

$$\frac{dx_D}{dt} = c_{O_2} k_{2f} x_A - \frac{k_{2f}}{K_2} x_D$$

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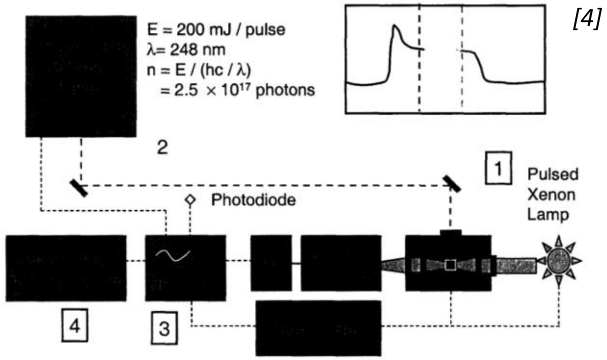

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- Dynamic optimization problem
  - Simplify using explicit Euler

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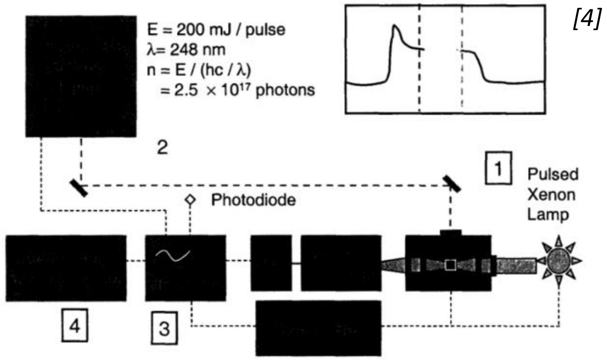

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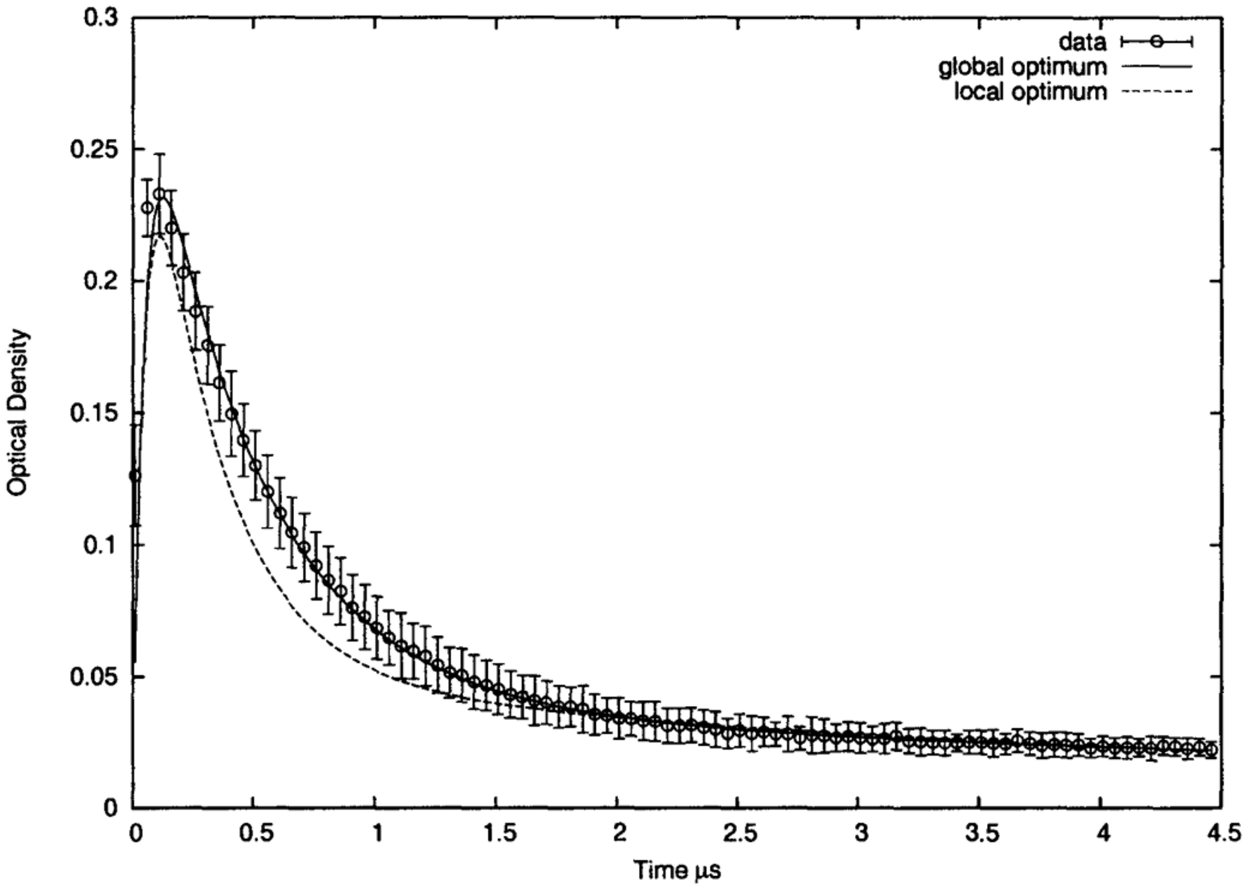

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EAGO v0.8.x

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@NLconstraint(model, e1, -x[1]*(1.12 + 0.13167*x[8] - 0.00667*(x[8])^2) + x[4] == 0.0)
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→

Modern

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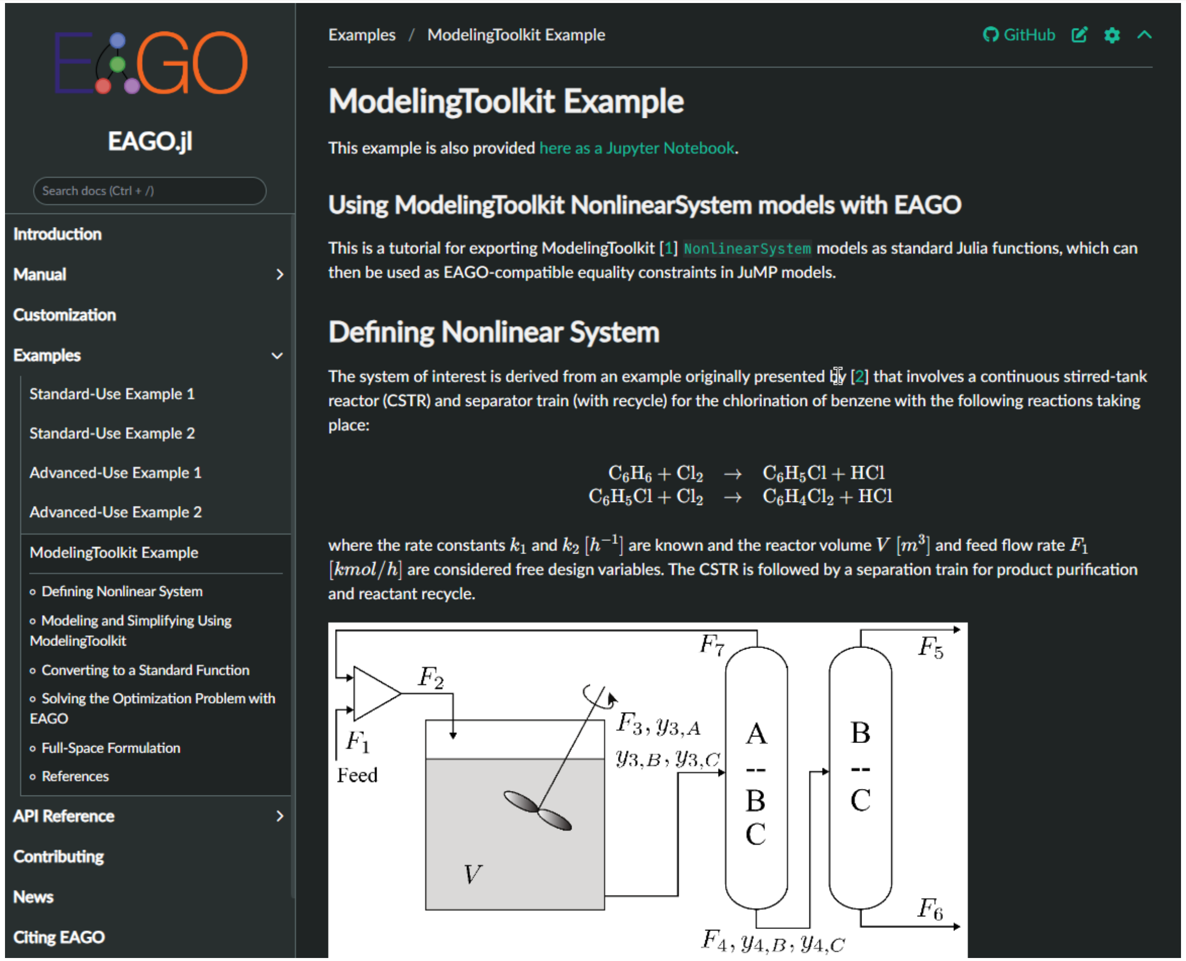
Automatic Generation of Reduced-Space Optimization Formulations of Process Systems for Faster Deterministic Global Optimization in Julia

Joseph Choi



Active Projects

- Integrate GPU-based methods

[5]

OPTIMIZATION METHODS & SOFTWARE
https://doi.org/10.1080/10556788.2024.2396297

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Automatic source code generation for deterministic global optimization with parallel architectures

Robert X. Gottlieb, Pengfei Xu and Matthew D. Stuber

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ABSTRACT
Trends over the past two decades indicate that much of the performance gains of commercial optimization solvers is due to improvements in x86 hardware. To continue making progress, it is critical to consider alternative/specialized massively parallel computing architectures. In this work, we detail the development of an open-source source code transformation approach built using `Symbolics.jl` to construct McCormick-based relaxations of functions that enables their effective parallelized evaluation. We then apply this approach in a novel parallelized branch-and-bound routine that offloads lower- and upper-bounding problems to a GPU. The effectiveness of this new approach is demonstrated on three nonconvex problems of interest, where it yields convergence time improvements of 22–118x compared to an equivalent serial CPU implementation and in two cases outperforms vanilla branch-and-bound versions of existing state-of-the-art solvers that use tighter bounding techniques. This work exemplifies how deterministic global optimizers using alternative hardware architectures can compete with—or eventually outclass—even the most powerful serial CPU implementations, and to the best of the authors' knowledge, represents the first successful demonstration of deterministic global optimization using a GPU.

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KEYWORDS
Dynamical systems; parameter estimation; factorable programing; open-source software; McCormick relaxations

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90C26; 90-04; 65G30; 26B25; 65Y05

[5] Gottlieb, R.X., Xu, P., and Stuber, M.D. Automatic Source Code Generation for Deterministic Global Optimization With Parallel Architectures. *Optimization Methods & Software*. (2024).

Active Projects

- Integrate GPU-based methods
- Update advanced functionality
  - SIP algorithms
  - Dynamic optimizer
  - Implicit routines

[5]

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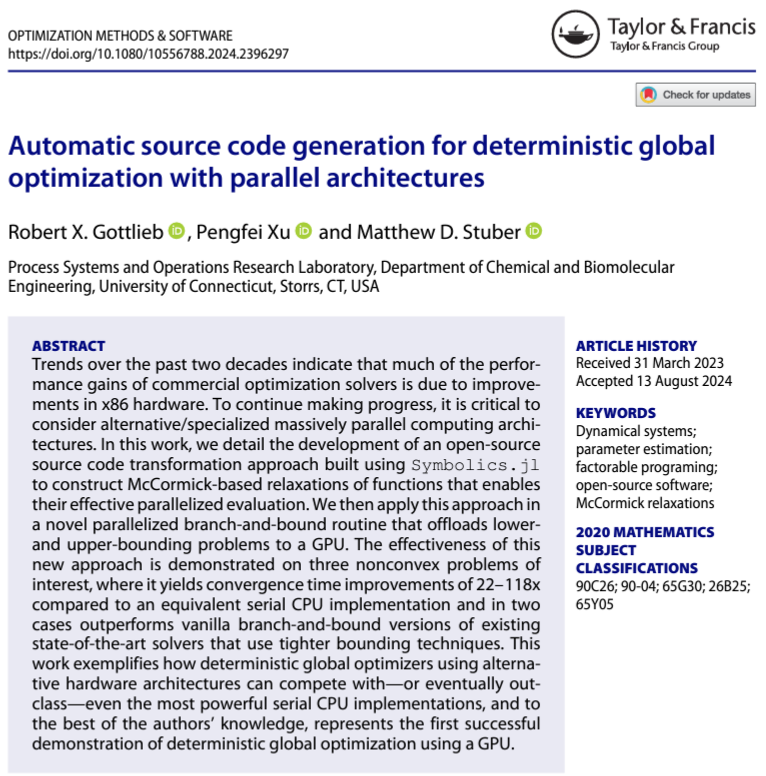
P S O R

Active Projects

- Integrate GPU-based methods
- Update advanced functionality
  - SIP algorithms
  - Dynamic optimizer
  - Implicit routines
- Continue to update documentation and examples



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Questions?

EAGO

https://psorlab.github.io/EAGO.jl/dev/

EAGO-notebooks

https://github.com/PSORLab/EAGO-notebooks