UCONN
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Source Code Transformation for GPU-Enhanced Deterministic Global Optimization

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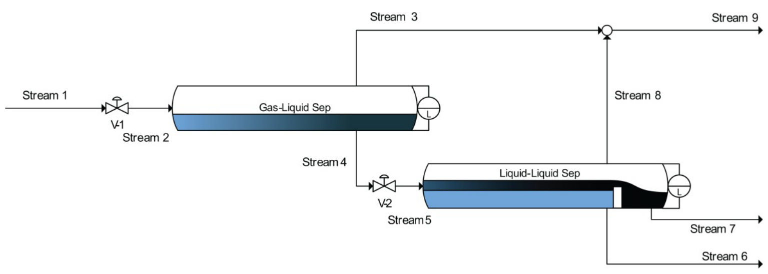
2023 AIChE ANNUAL MEETING

Process Systems and Operations Research Laboratory

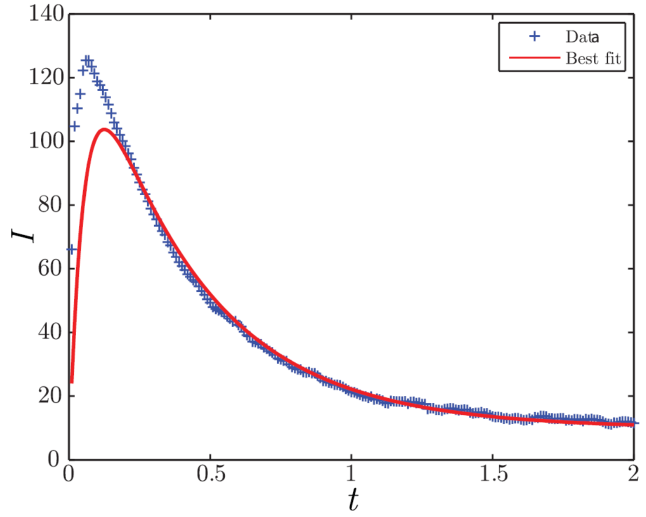
Deterministic Global Optimization

- **Nonconvex problems** naturally arise in many applications
- Guaranteed global solutions require specialized algorithms such as **branch-and-bound (B&B)**
- B&B is **computationally expensive**
  - Solvable problems typically have very few decision variables

***Worst-Case Design and Safety-Critical Systems*[1]**



***Parameter Estimation and Model Validation*[2]**



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Deterministic Global Optimization

Can we **speed up B&B** with **parallelized computing architectures**?

- No…
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- Gu…
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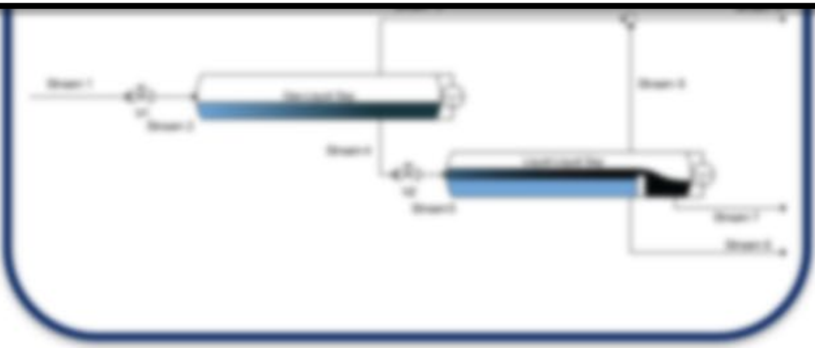
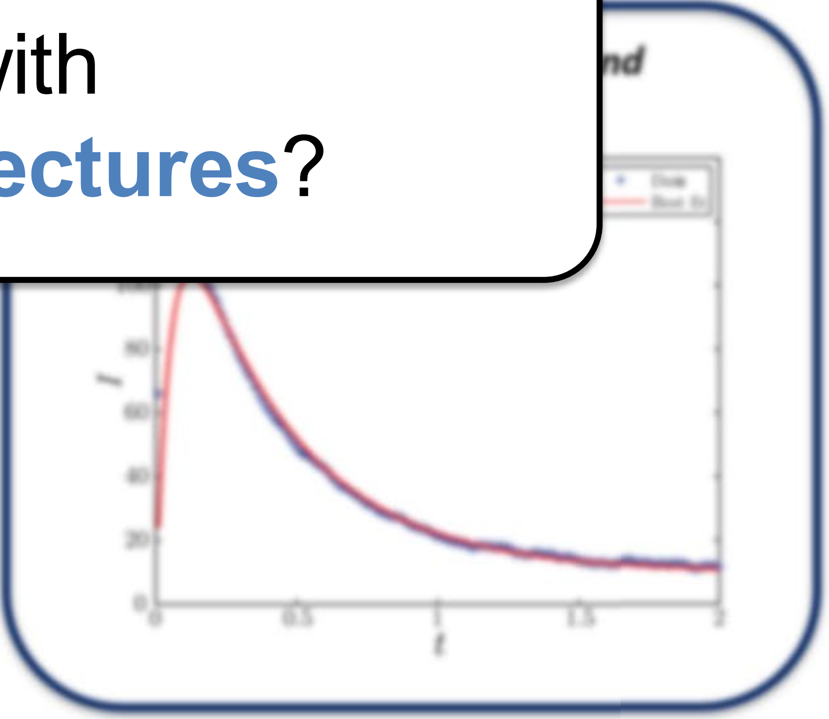
- B&B is **computationally expensive**
  - Solvable problems typically have very few decision variables





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Deterministic Global Optimization

Can we **speed up B&B** with **parallelized computing architectures**?

GPUs have been successfully used for **ML**, **data analysis**, etc.

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Why GPUs?

Strengths

- Faster calculation speed
- More efficient energy utilization
- More cost effective than CPUs for scale-up

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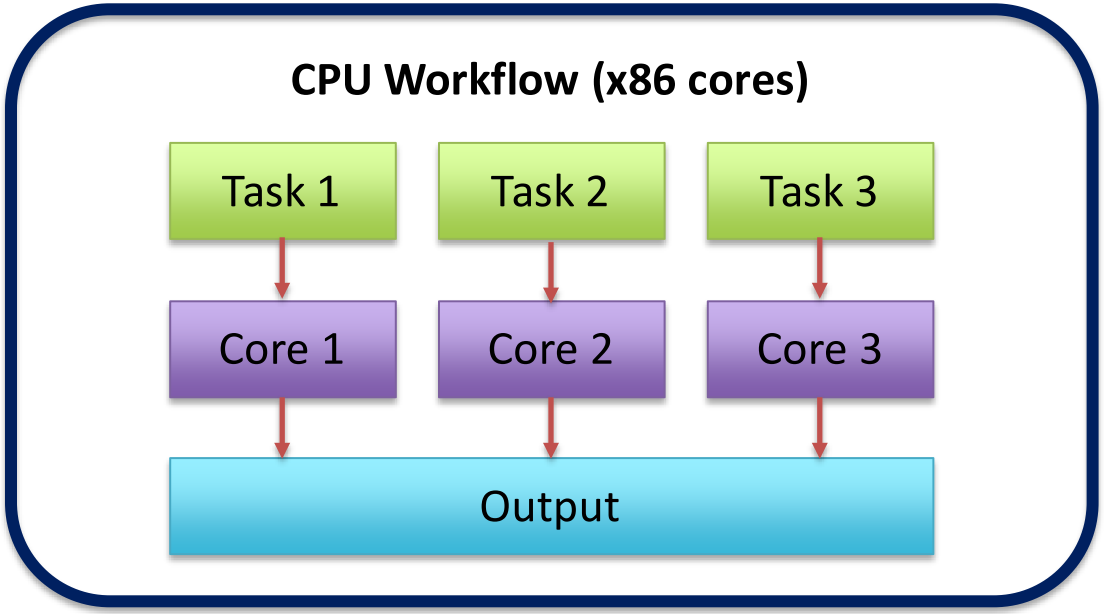
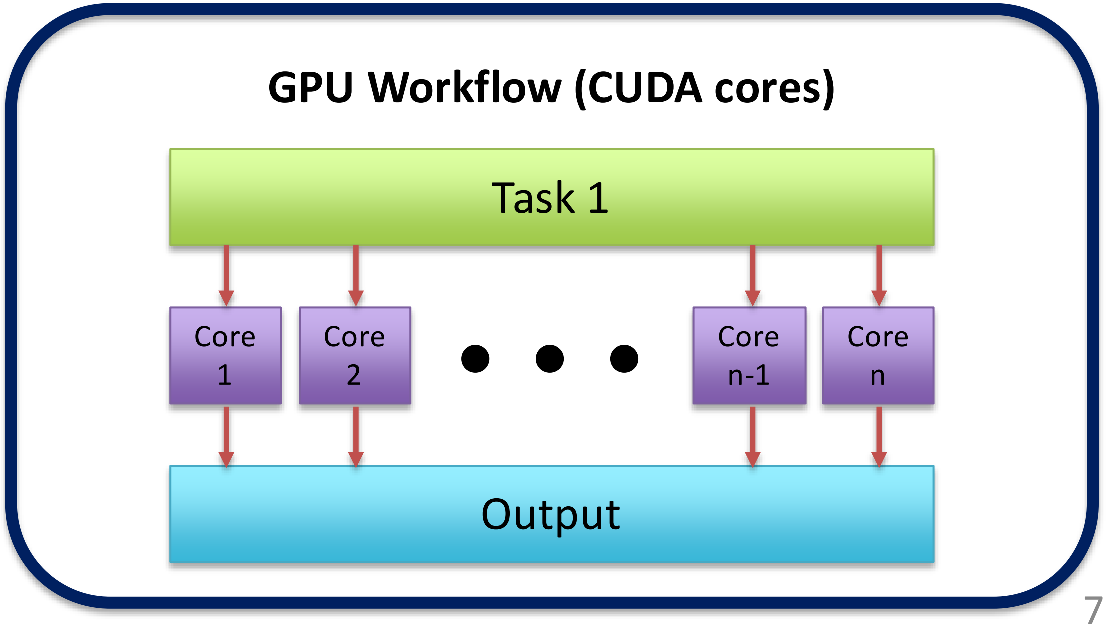
Weaknesses

- Standard B&B software not automatically compatible with GPUs
  - Requires re-architecting algorithms to be data-parallel
- "Branches" in code massively degrade performance

CPU vs. GPU Parallelism

- Multicore CPUs use **task parallelism (MIMD)**
  - Different cores perform **different tasks** independently
- GPUs use **data parallelism (SIMD)**
  - Different cores perform the **same task** on **different portions of data**
  - **Efficient** with a pipeline: minimal decision-making, minimal branches based on data

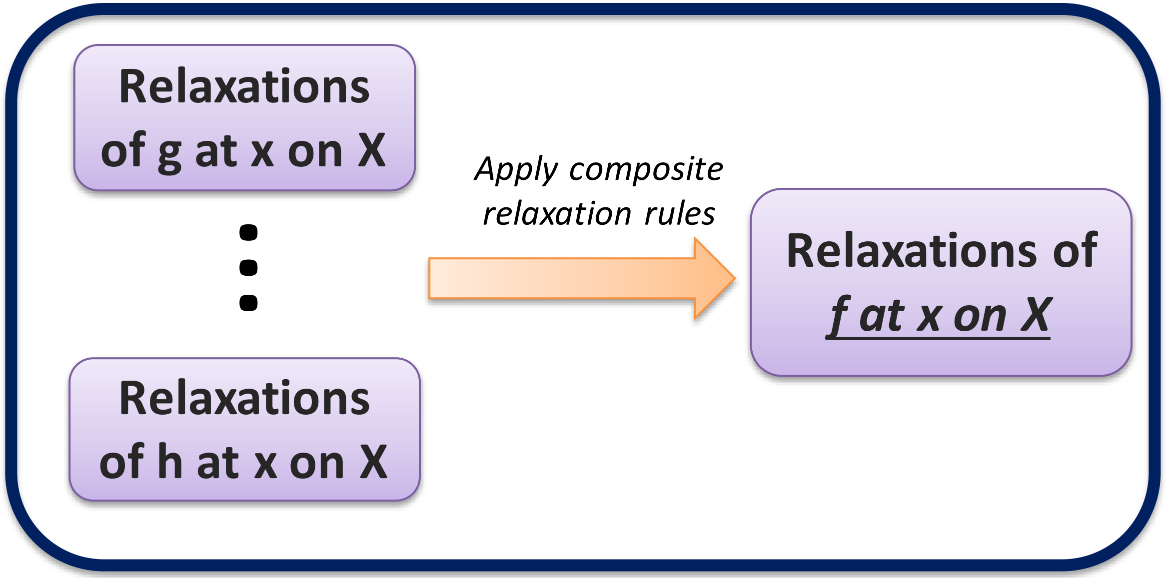




McCormick Relaxations of Factorable Functions

$$\mathbf{y} = \mathbf{f}(\mathbf{g}(\mathbf{x}), \ldots, \mathbf{h}(\mathbf{x}))$$

McCormick-Based Relaxations[5,6]



https://www.github.com/PSORLab/EAGO.jl

5. Mitsos, A., et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
6. Scott, J.K., et al. **Generalized McCormick relaxations.** *Journal of Global Optimization* 51.4 (2011): 569-606.

McCormick.jl

1) Create a library of math operators, overloaded* to apply McCormick rules

$$\exp\left(x / y\right) - xy^2 / \left(y+1\right)$$

*Multiple dispatch, in Julia

McCormick.jl

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3) Evaluate the math expression using McCormick objects

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$$\exp\left(x / y\right) - xy^2 / \left(y + 1\right)$$

Relaxations at specified values/bounds of *x*, *y*

1) Create a library of math operators, overloaded* to apply McCormick rules

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*Multiple dispatch, in Julia

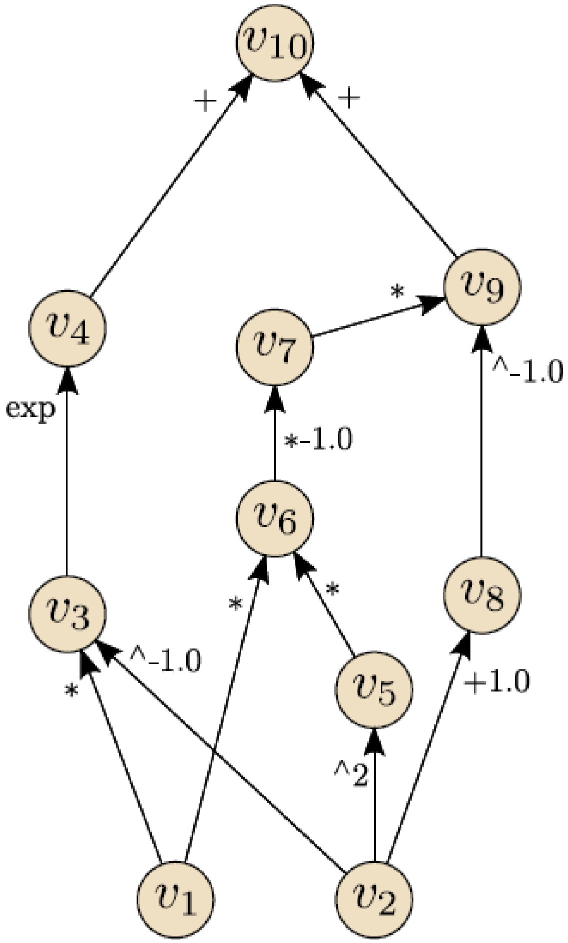
SourceCodeMcCormick.jl

$$\exp\left(x / y\right) - xy^2 / \left(y + 1\right)$$

SourceCodeMcCormick.jl

$$\exp\left(x \,/\, y\right) - xy^2 \,/\, \left(y + 1\right) \longrightarrow$$

$$\begin{aligned}
v_1 &= x \\
v_2 &= y \\
v_3 &= v_1 / v_2 \\
v_4 &= \exp(v_3) \\
v_5 &= v_2^2 \\
v_6 &= v_1 v_5 \\
v_7 &= -v_6 \\
v_8 &= v_2 + 1.0 \\
v_9 &= v_7 / v_8 \\
v_{10} &= v_4 + v_9
\end{aligned}$$



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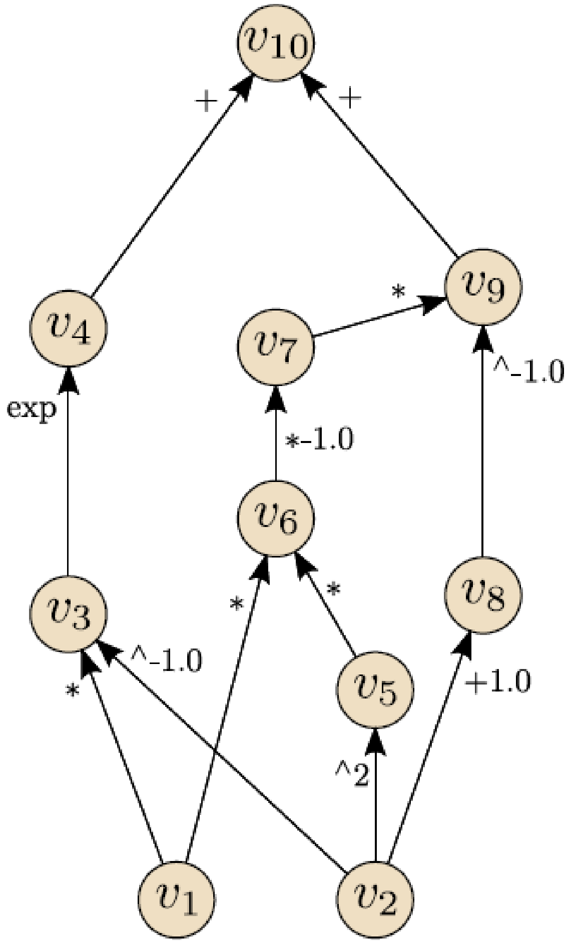

1) Factor original math expression

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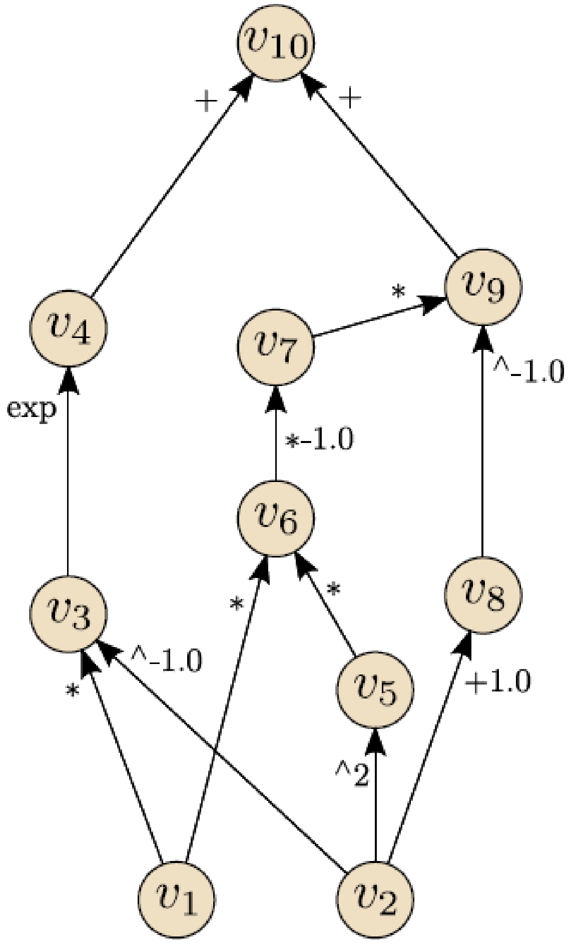

1) Factor original math expression

2) Replace each factor with code capturing all variations of that McCormick rule

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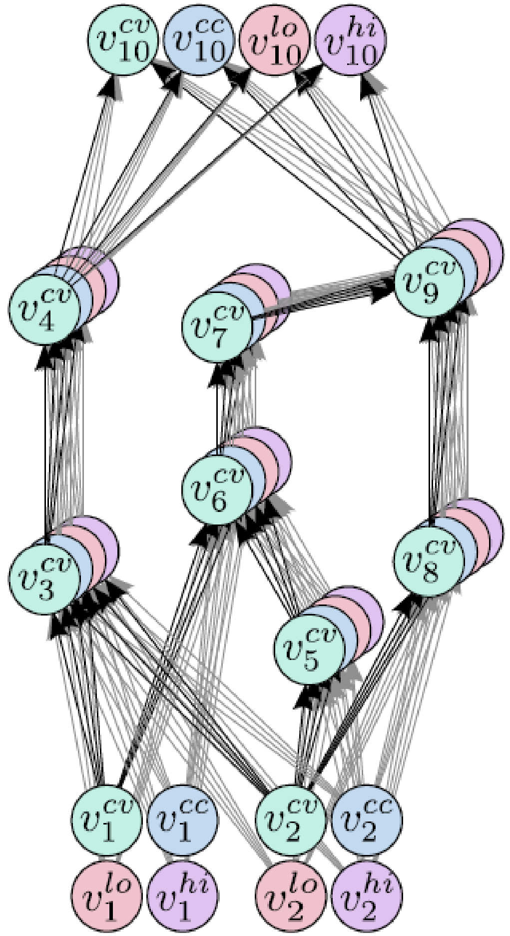

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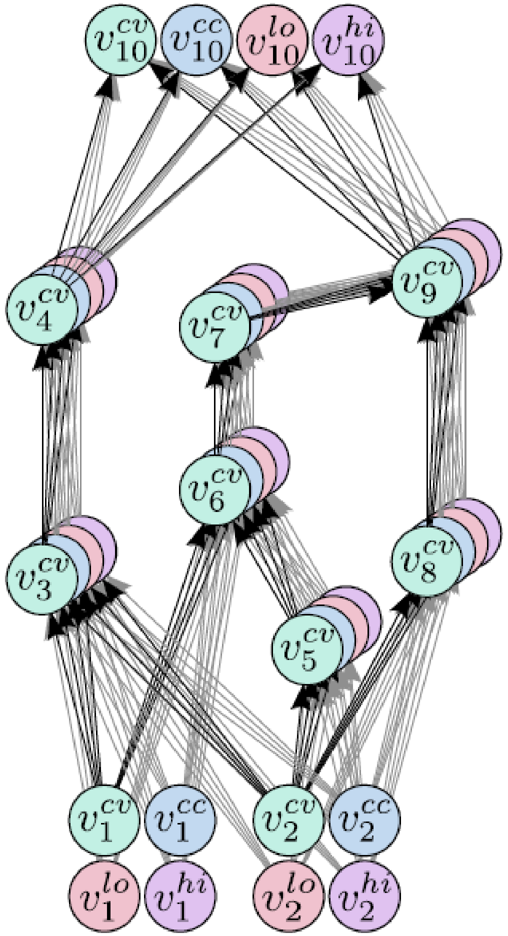

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2) Replace each factor with code capturing all variations of that McCormick rule
3) Compile code into an “evaluator function”

SourceCodeMcCormick.jl

$$\exp\left(x / y\right) - xy^2 / \left(y + 1\right)$$

↓

new_func(x^{cv}, x^{cc}, x^L, x^U, y^{cv}, y^{cc}, y^L, y^U)

↓

Plug in values/bounds of *x*, *y* to obtain relaxations

1) Factor original math expression

2) Replace each factor with code capturing all variations of that McCormick rule

3) Compile code into an "evaluator function"

SourceCodeMcCormick.jl

$$\exp(x/y) - xy^2/(y+1)$$

1) Factor original math expression
2) Replace each factor with code

to obtain relaxations

Fully compatible with GPUs

Pointwise evaluations **~3 OOM faster** than McCormick.jl

Past Hurdles

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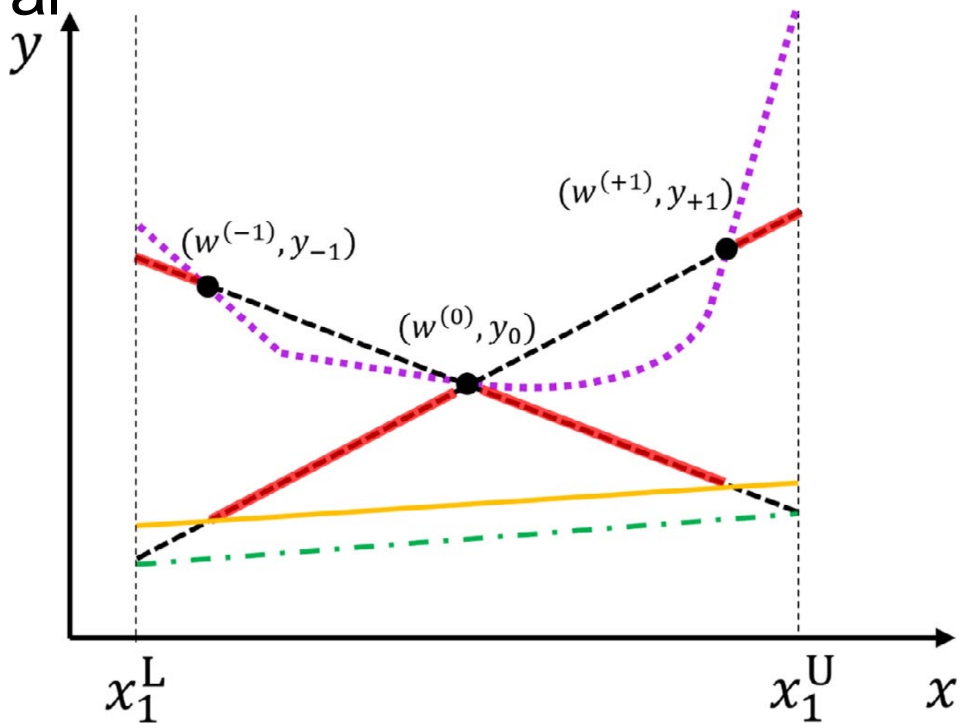
1) Only returned **relaxations** and natural interval extensions (**no subgradients**)
   - ➢ Reliant on subgradient-free lower-bounding methods
   - ➢ Cannot handle non-trivial constraints



4. Song, Y., et al. **Bounding convex relaxations of process models from below by tractable black-box sampling.** *Computers & Chemical Engineering* 153 (2021), 107413.

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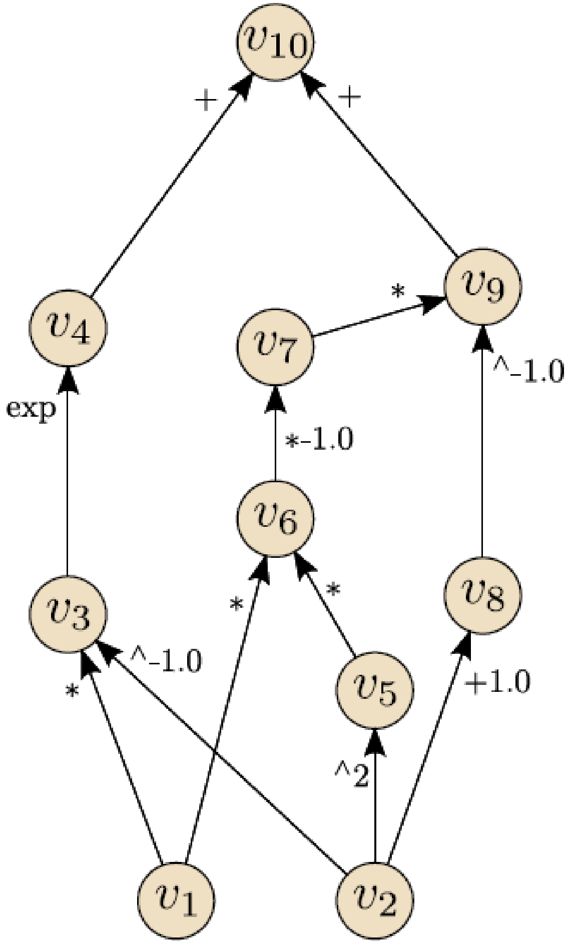
   - Greater chance of branching in rules



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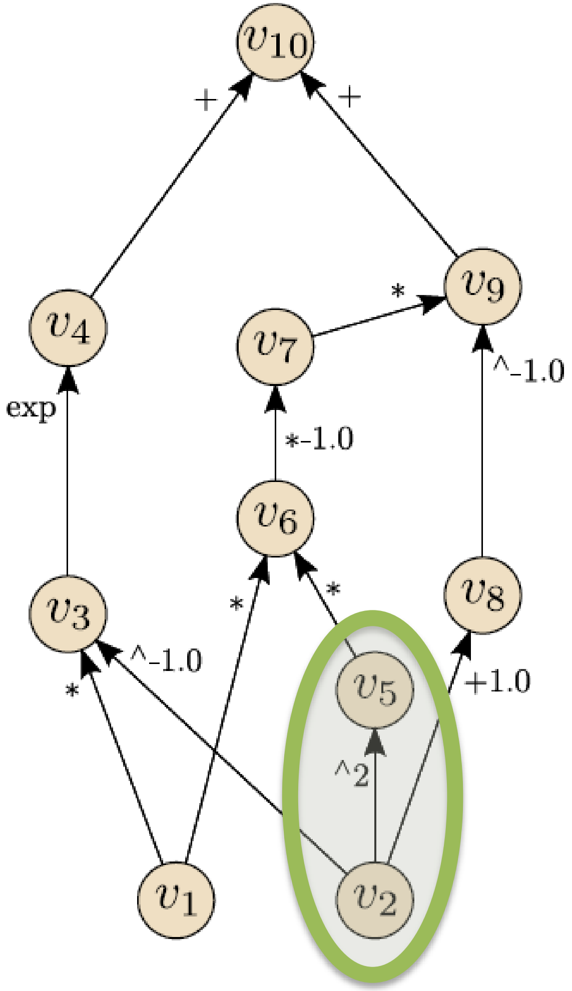

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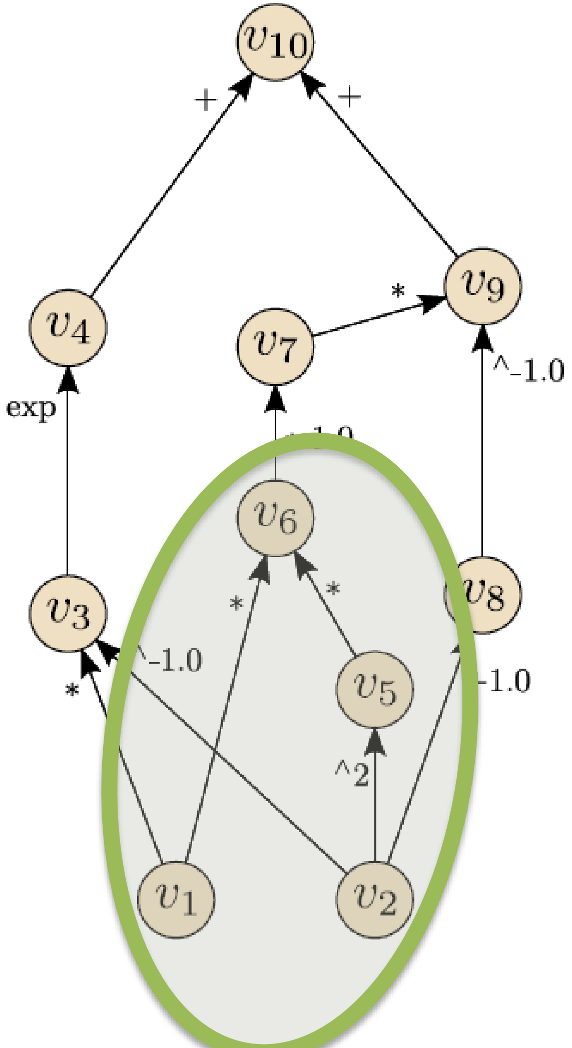

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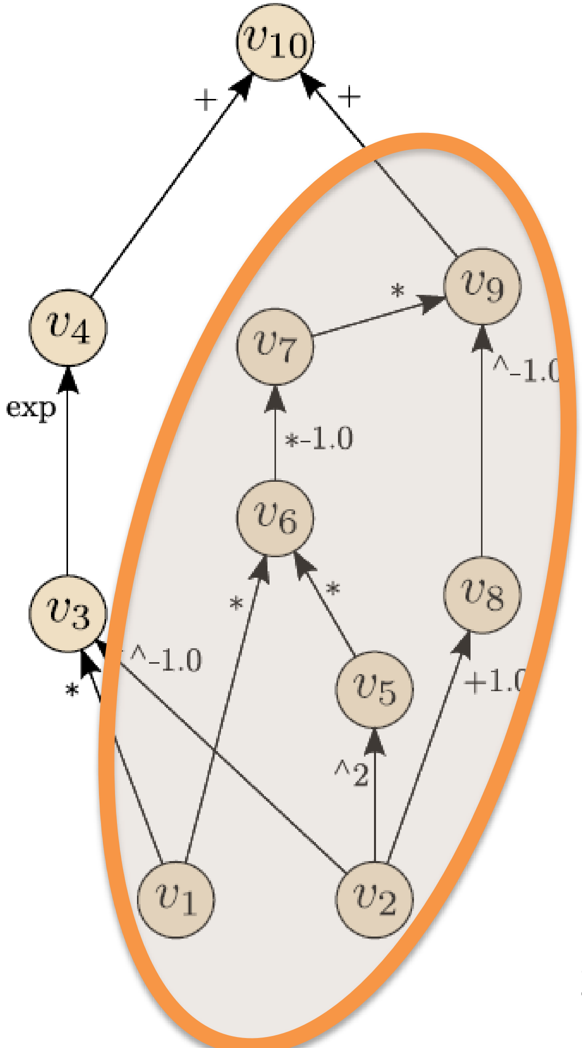

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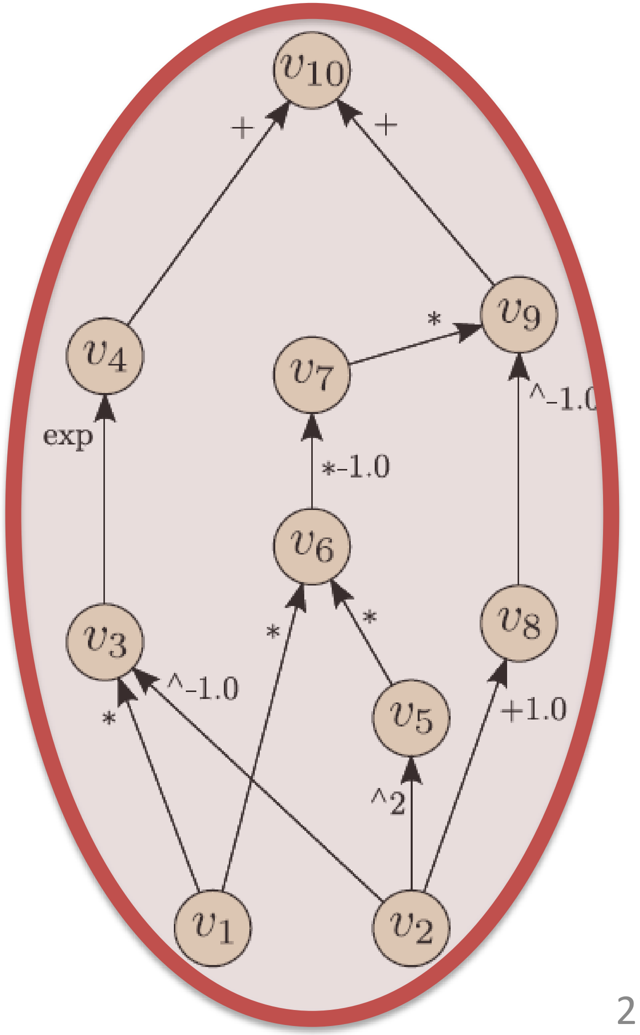

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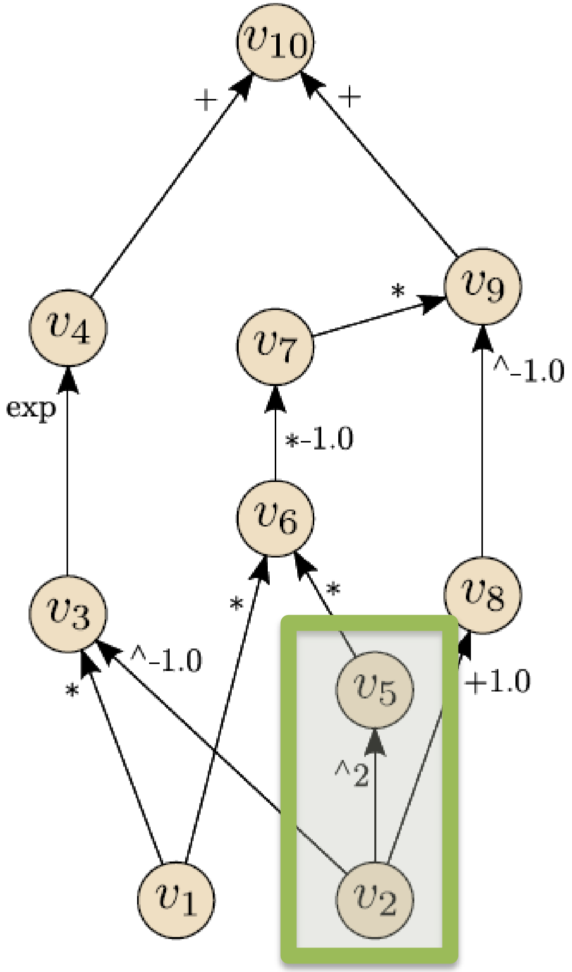

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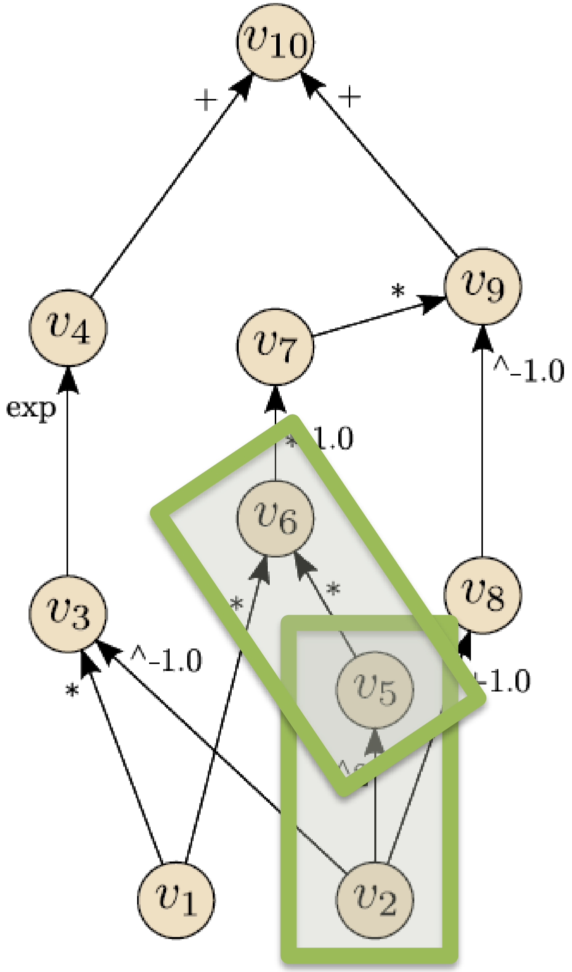

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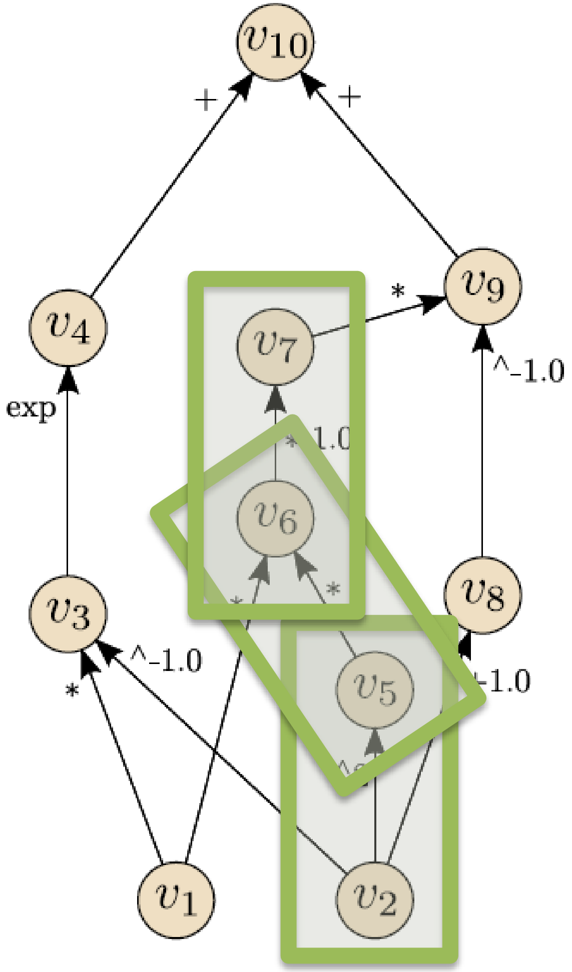

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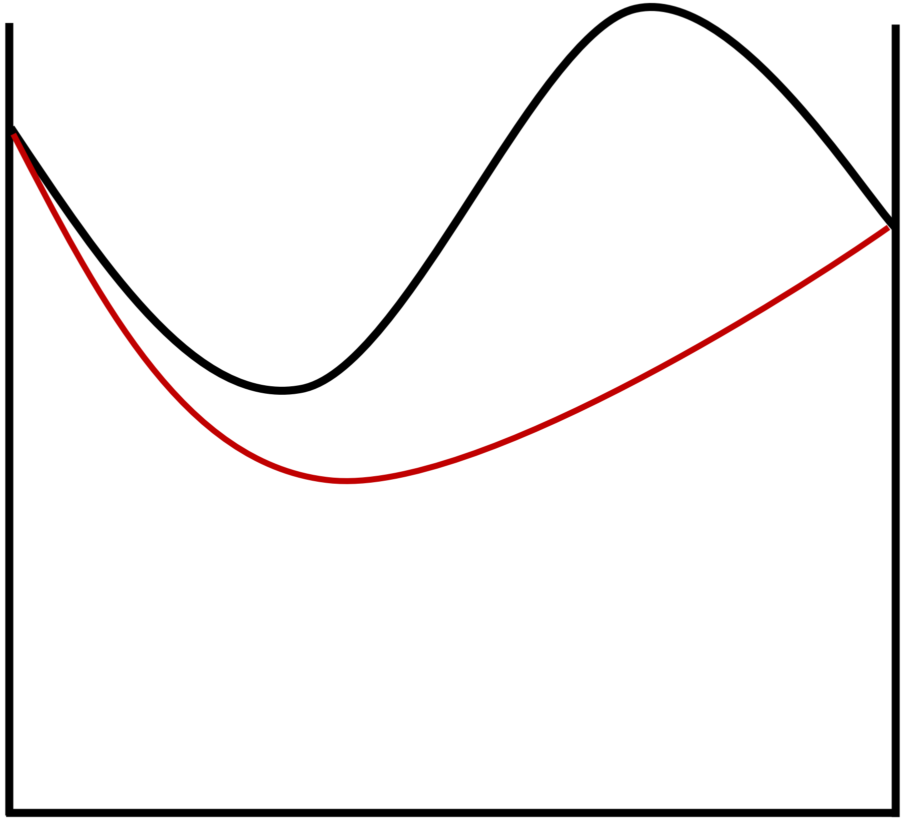
Newest Improvements

1) Can now handle subgradients!



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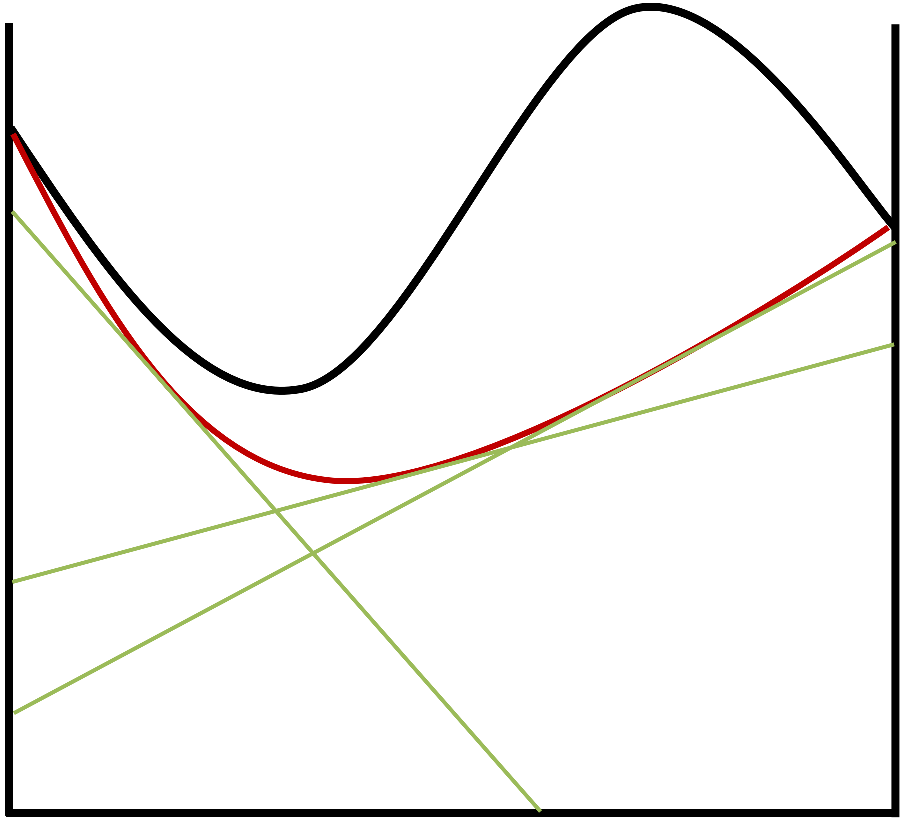

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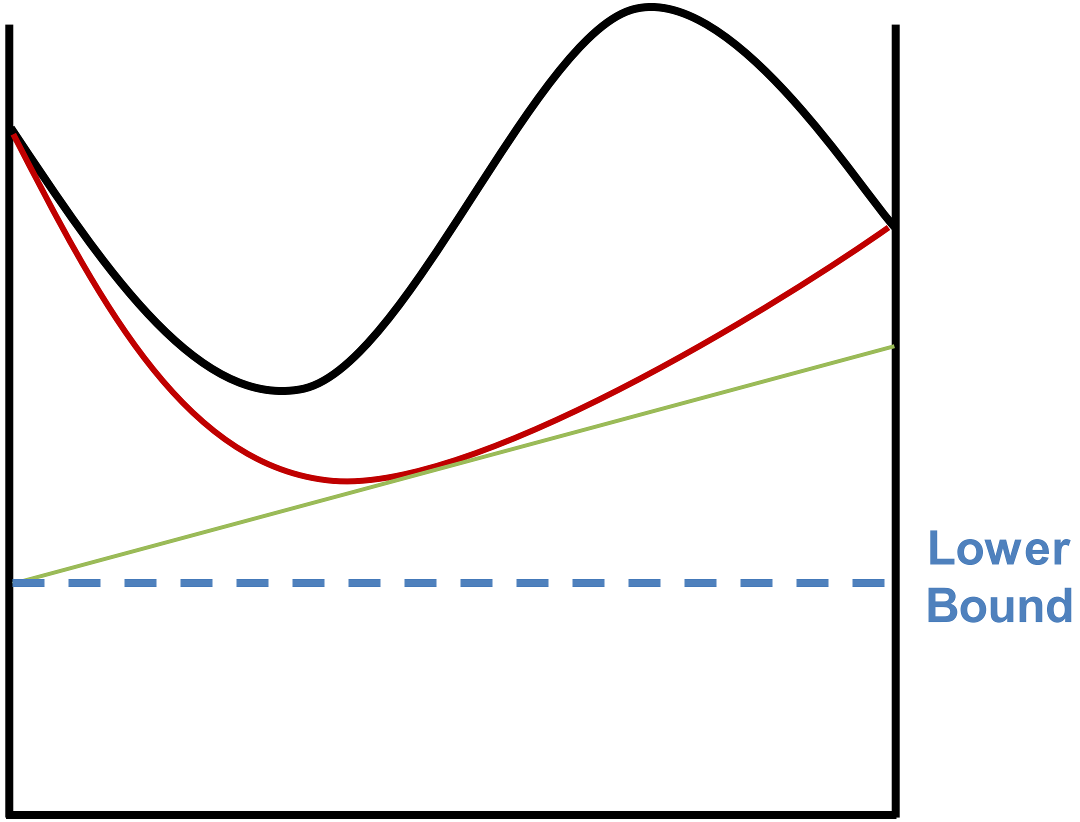

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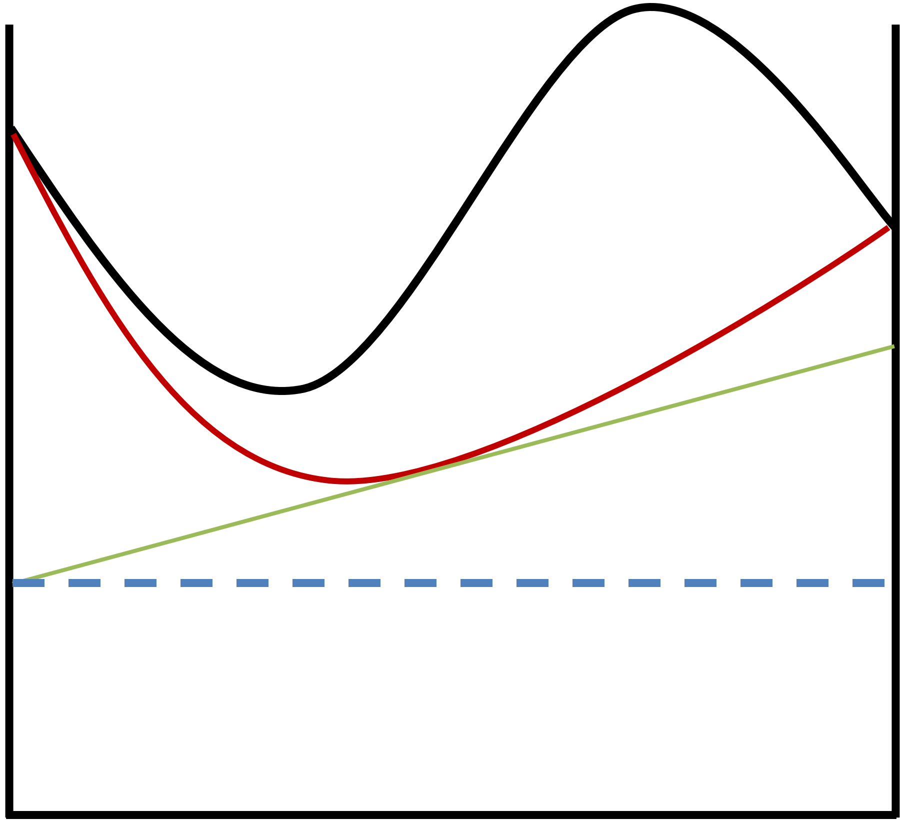
   - Does not address nontrivial constraints



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   - ➢ Evaluator functions stitched into larger function
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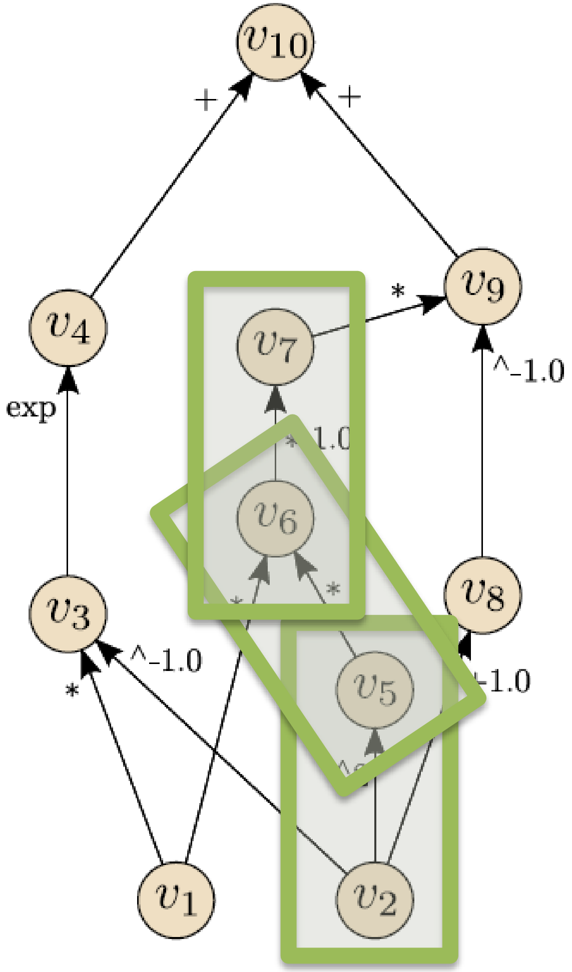

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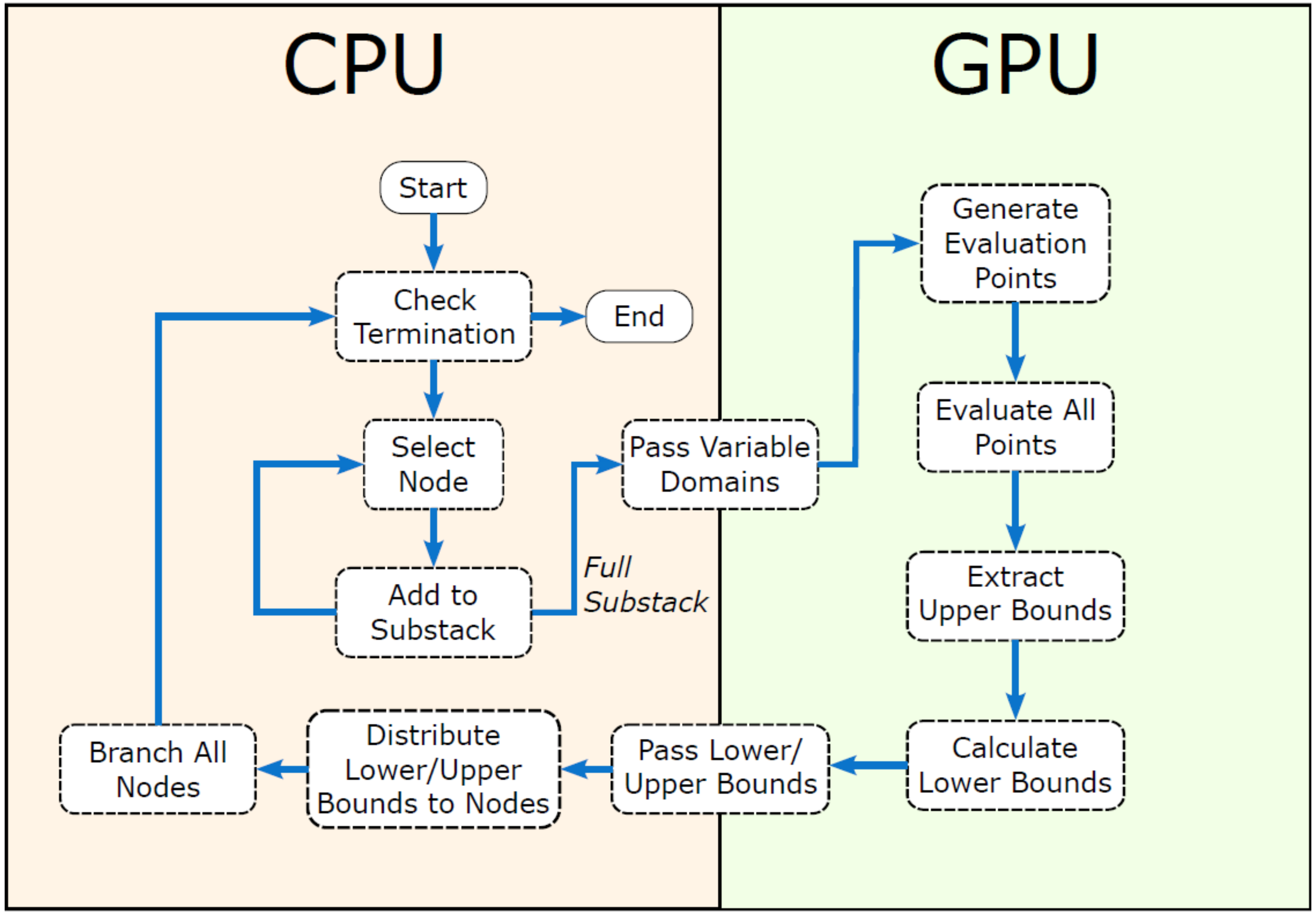
$$\log(\pi^{\text{calc}}) = \sum_{i=0}^{2} a_i w^i + \frac{\sum_{i=0}^{2} b_i w^i}{T}$$

```
@variables a0, a1, a2, b0, b1, b2, data, W, T
expr = exp(a0 + a1*W + a2*W^2 + (1/T)*(b0 + b1*W + b2*W^2))

new_func = fgen(((expr-data)/data)^2, constants=[data, W, T])
```

ParBB



6. Gottlieb, R.X., Xu, P., Stuber, M.D. **Automatic source code generation for deterministic global optimization with parallel architectures.** *Under Review.*

Kinetic Parameter Estimation

Concentrations after an initial laser flash pyrolysis are modeled using the system of ODEs:[8]

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

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

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

$$\frac{dx_Y}{dt} = -k_{1s}x_Z x_Y,$$

$$\frac{dx_Z}{dt} = -k_1 x_z x_Y, \quad x_A(0) = x_B(0) = x_D(0) = 0, \quad x_Y(0) = 0.4, \quad x_Z(0) = 140.$$

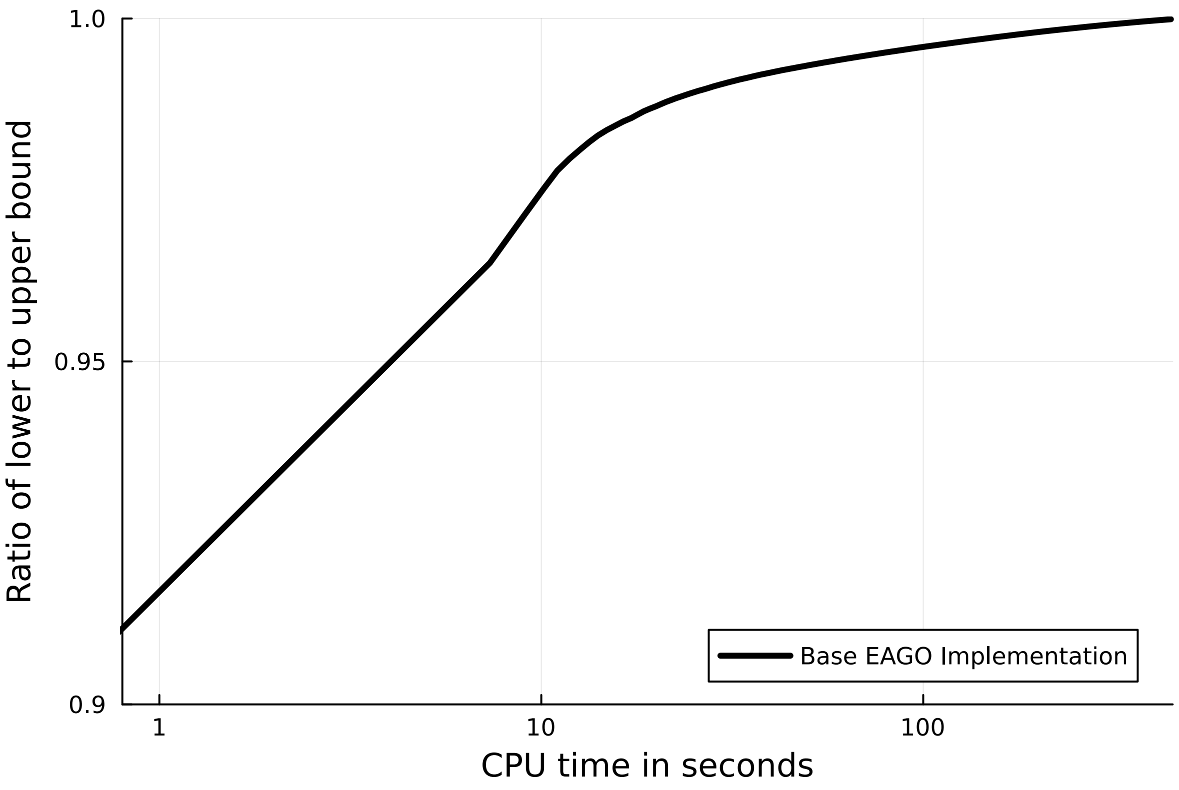
$$I = x_A + \frac{2}{21}x_B + \frac{2}{21}x_D$$

$$f(\mathbf{p}) = \sum_{i=0}^{N}\left(I^{\mathrm{calc}}(\mathbf{x}_i, \mathbf{p}) - I_i^{\exp}\right)^2$$

7. Taylor, J. W. **Direct Measurement and Analysis of Cyclohexadienyl Oxidation.** Ph.D. thesis, Massachusetts Institute of Technology.

Results

Solution Method	Convergence Time (s)	Nodes Accessed
Base EAGO	445.1	8.4E5



CPU: Intel W-2195
GPU: NVIDIA Quadro GV100

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Solution Method	Convergence Time (s)	Nodes Accessed
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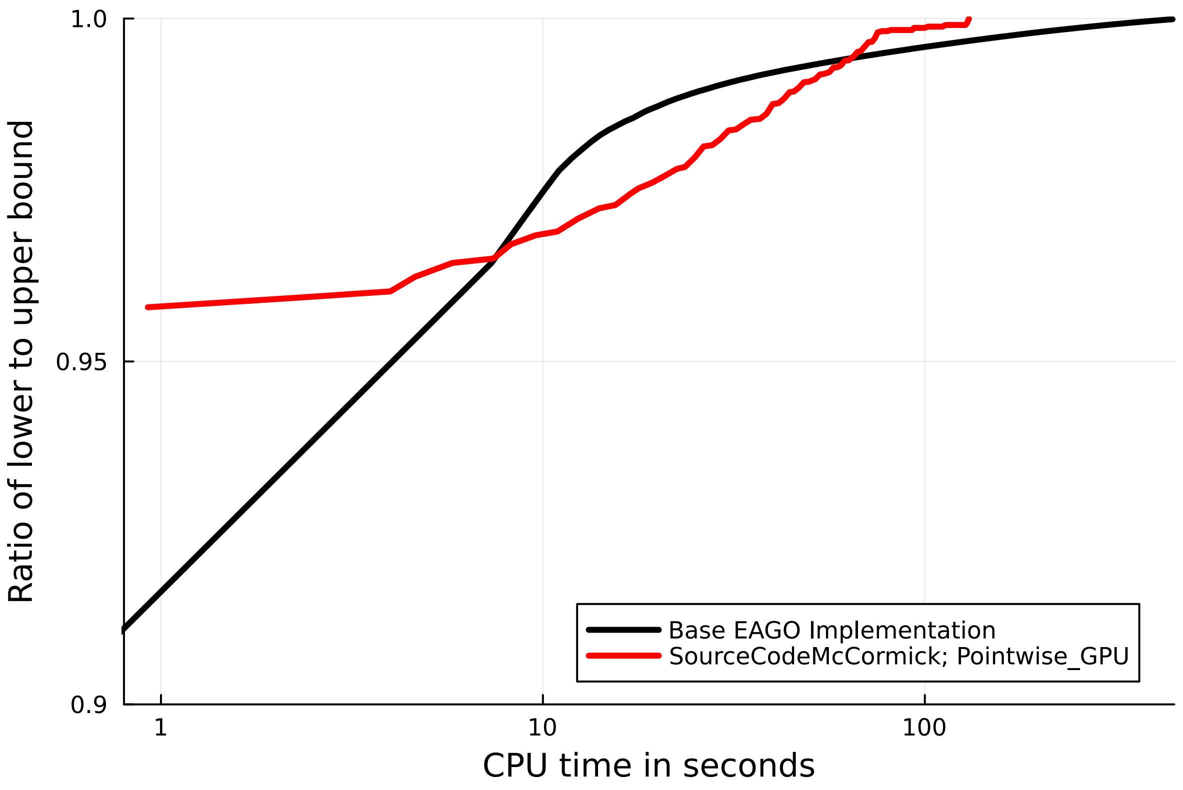

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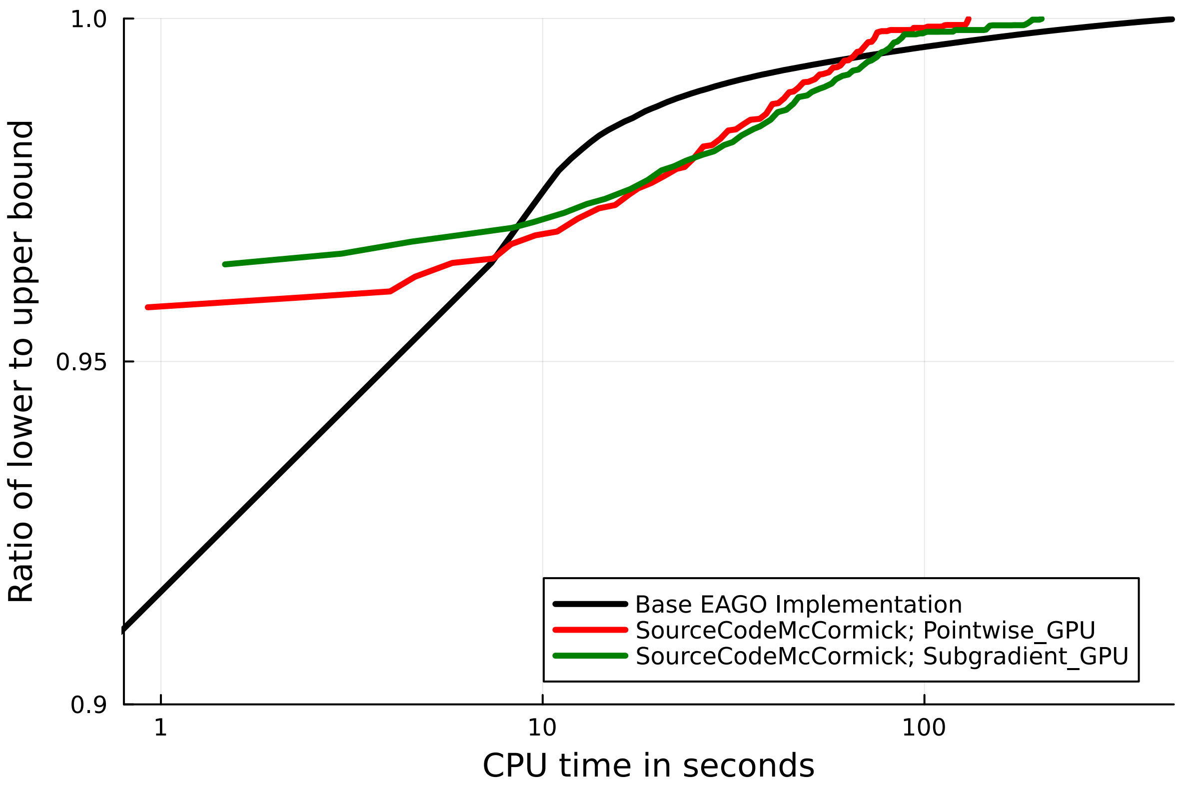
Subgradient GPU	202.7	5.2E6



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Conclusions

- Evaluations of relaxations and subgradients **performant on GPU**
- GPU-based B&B algorithm **implemented** in SourceCodeMcCormick.jl
- Current method **cannot handle non-trivial constraints**
  - Would require batch parallelized GPU LP solver

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Acknowledgements

Members of the Process Systems and Operations Research Laboratory at the University of Connecticut (https://psor.uconn.edu/)

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Process Systems and Operations Research Laboratory

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Questions?

Process Systems and Operations Research Laboratory

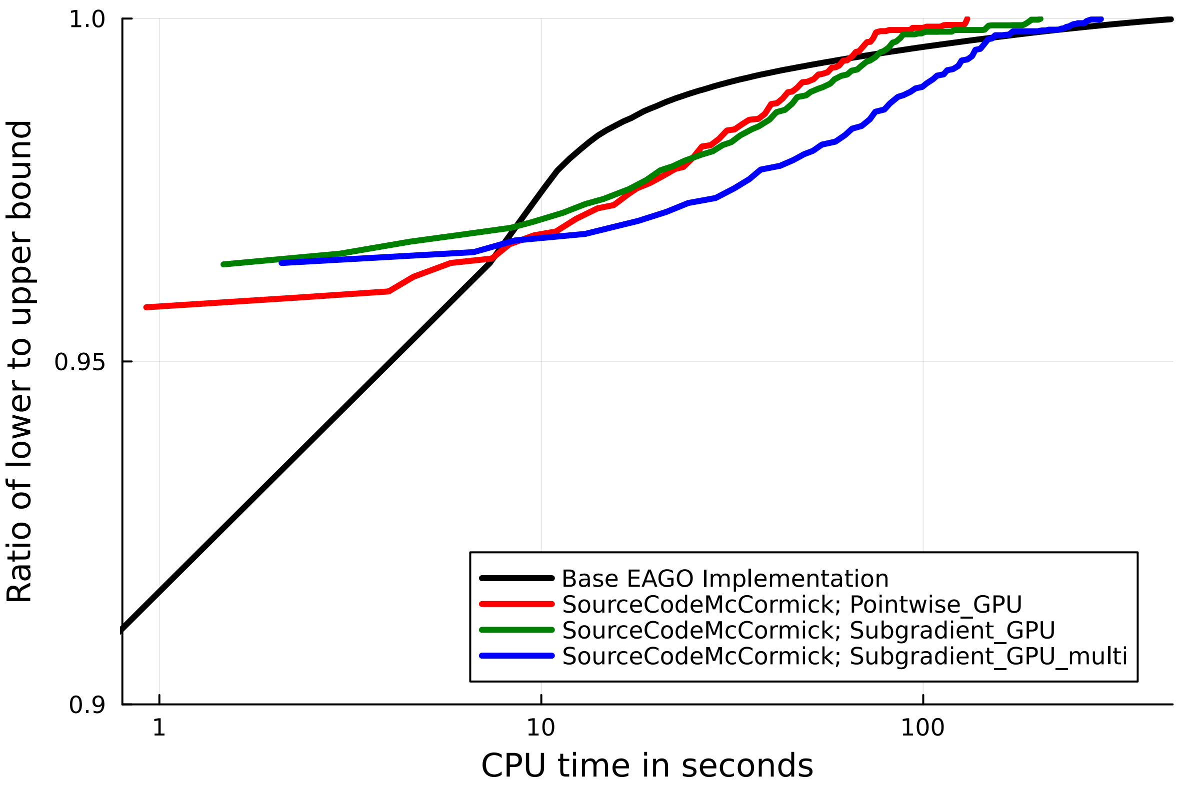
https://www.psor.uconn.edu

EAGO

https://www.github.com/PSORLab/EAGO.jl

Results

Solution Method	Convergence Time (s)	Nodes Accessed
Base EAGO	445.1	8.4E5
Pointwise GPU	130.4	4.5E6
Subgradient GPU	202.7	5.2E6
Subgradient GPU (multi)	291.9	4.3E6



CPU: Intel W-2195
GPU: NVIDIA Quadro GV100