



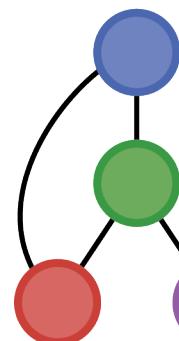
GPU-Accelerated Deterministic Global Optimization

Robert Gottlieb, PhD Student

Matthew Stuber, P&W Associate Professor in
Advanced Systems Engineering

July 23, 2024

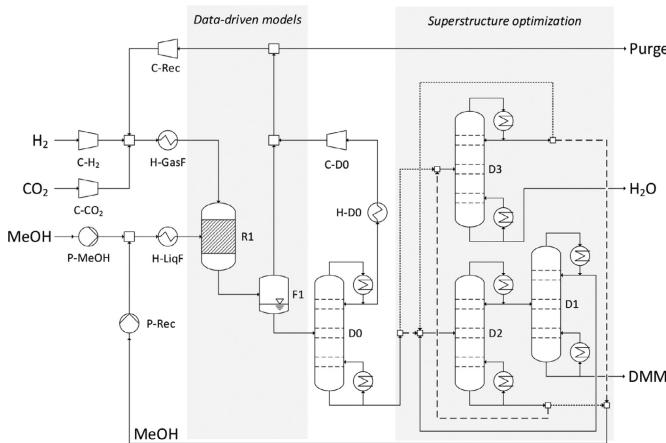
{ ISMP
2024 }



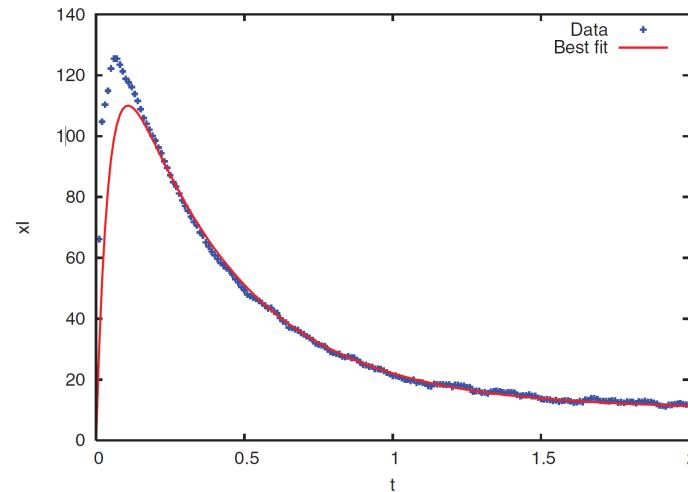
Process Systems and
Operations Research
Laboratory

Deterministic Global Optimization

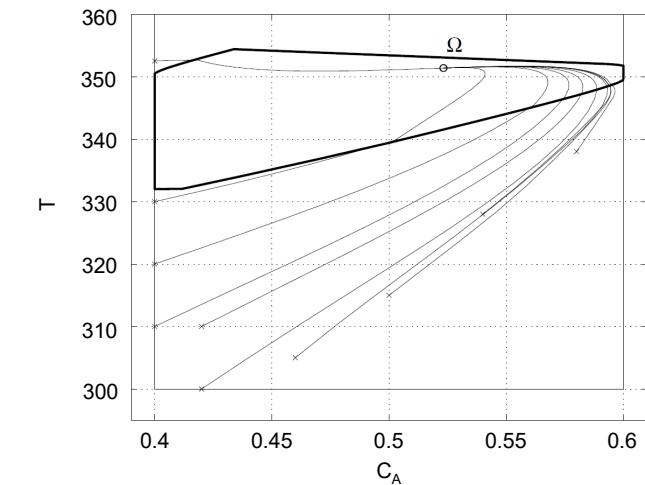
Design Improvements¹



Parameter Estimation and Model Validation²



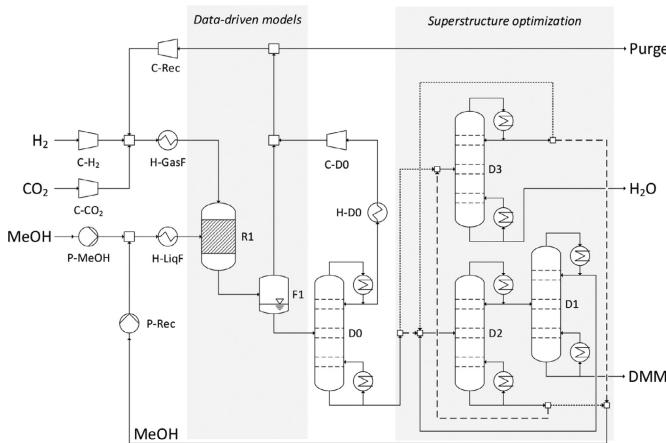
Safety and Robust Control³



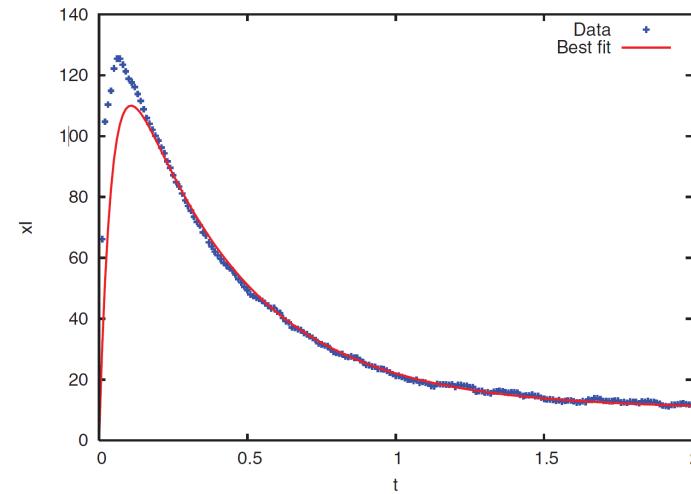
1. Burre, J., et al. **Global flowsheet optimization for reductive dimethoxymethane production using data-driven thermodynamic models**. *Computers & Chemical Engineering*, (2022): 107806.
2. Mitsos, A., et al. **McCormick-based relaxations of algorithms**. *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
3. Limon, D. et al. **Robust MPC of constrained nonlinear systems based on interval arithmetic**. *IEEE Proceedings – Control Theory and Applications* 152(3), 325-332 (2005).

Deterministic Global Optimization

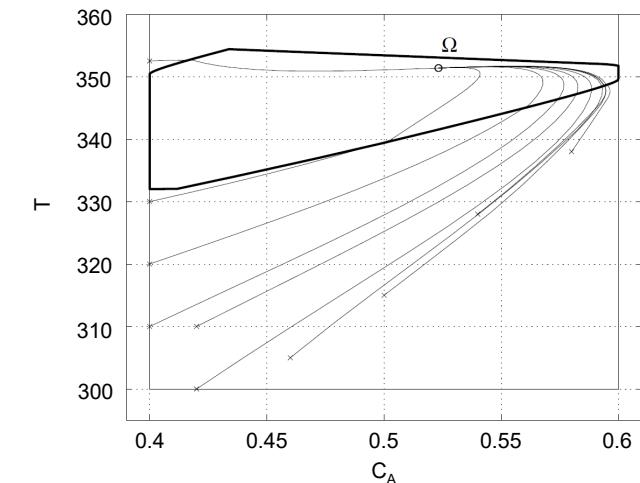
Design Improvements¹



Parameter Estimation and Model Validation²



Safety and Robust Control³



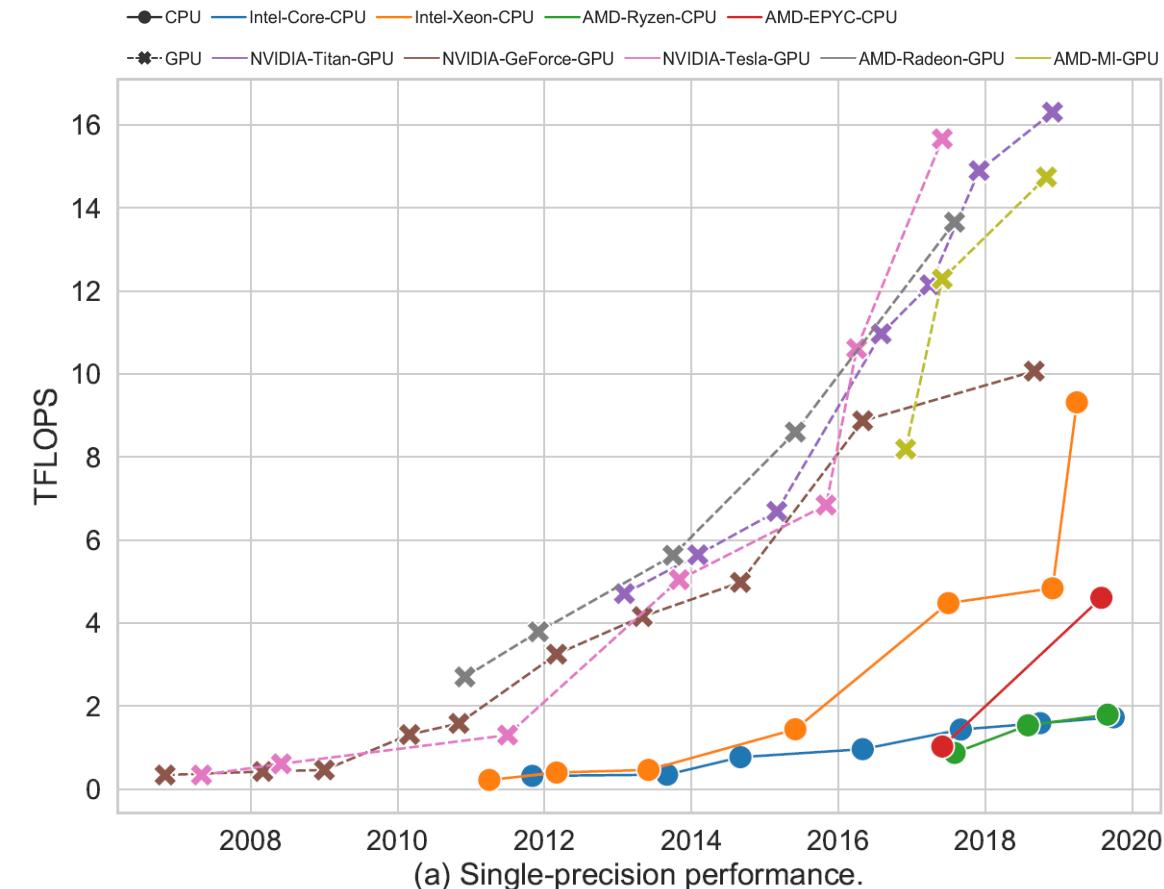
Problems are NP-hard: worst-case exponential runtime

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High-Performance Computing

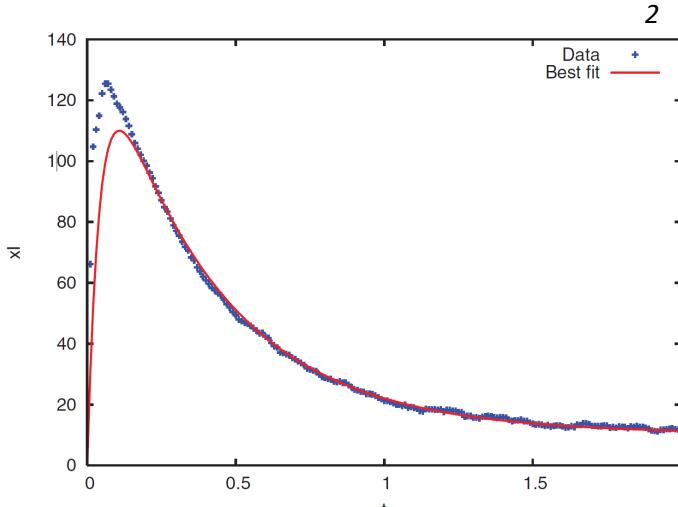
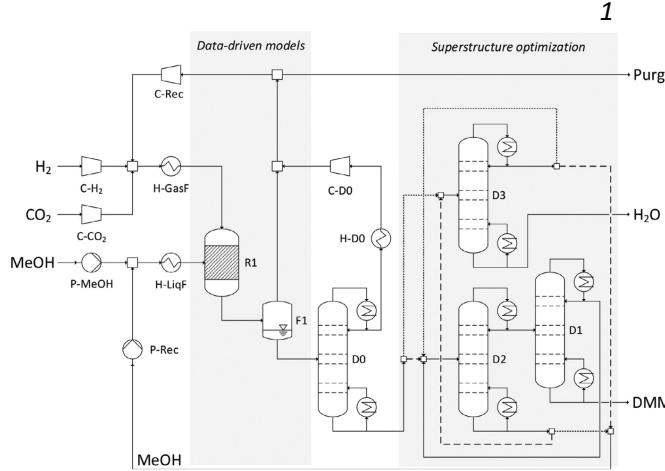
Graphics Processing Units (GPUs)

- Graphics rendering
- Machine learning model training
 - Generative AI
- Data analysis
- Large-scale simulations
 - Molecular dynamics
 - CFD modeling
- Supercomputing
- [...]



4. Sun, Y., et al. Summarizing CPU and GPU design trends with product data. *arXiv*, nov 2019. arXiv: 1911.11313

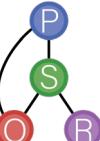
GPUs for Global Optimization?



Accelerate using
GPUs?



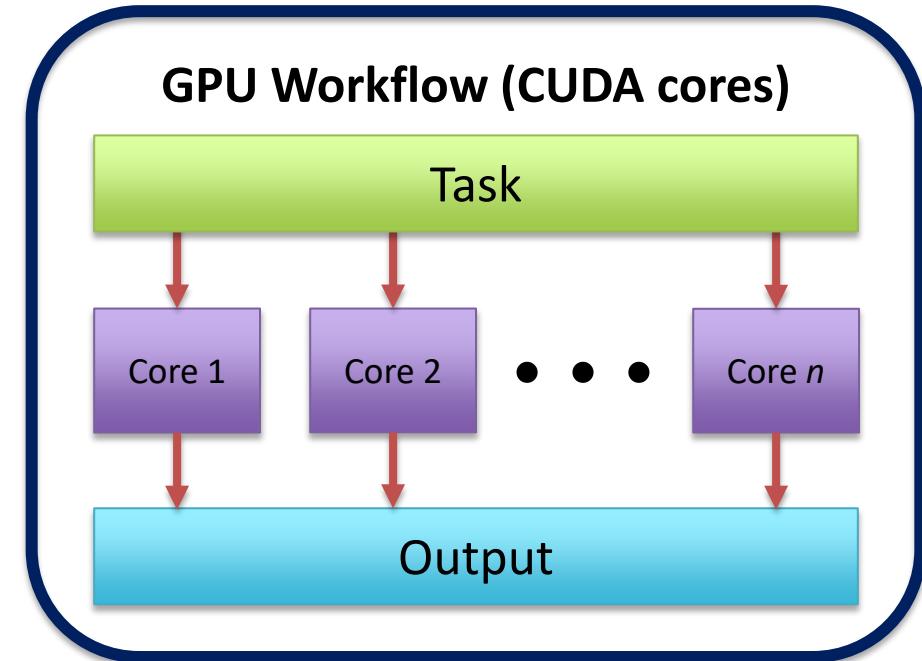
Energy.gov



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GPU Concepts

- GPUs are built for **data parallelism (SIMD)**
 - Thousands of GPU cores (threads) execute tasks simultaneously
 - Large chunks of **identical** data processing (I.e., the **inputs** change, not the math)



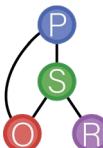
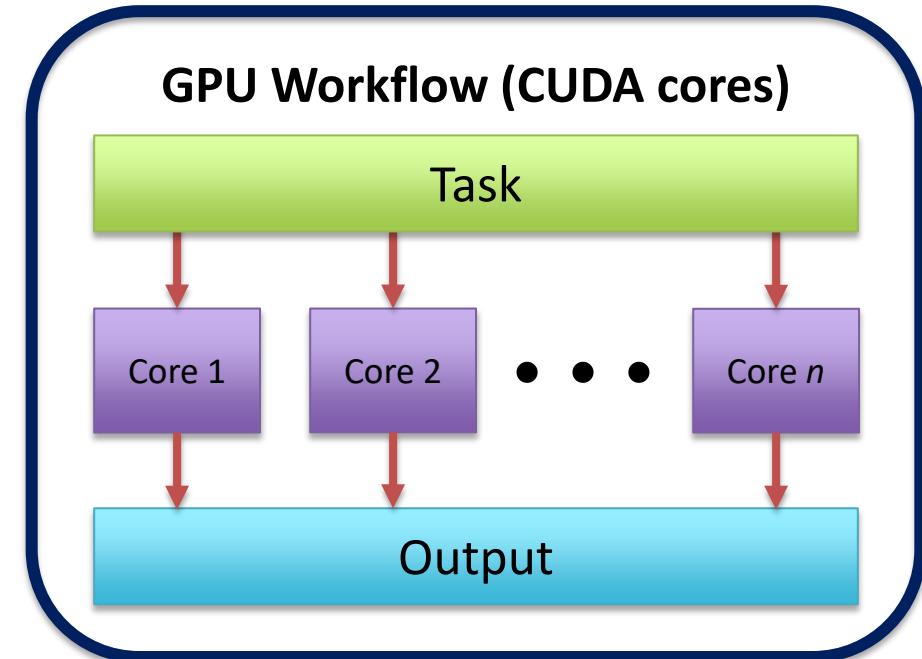
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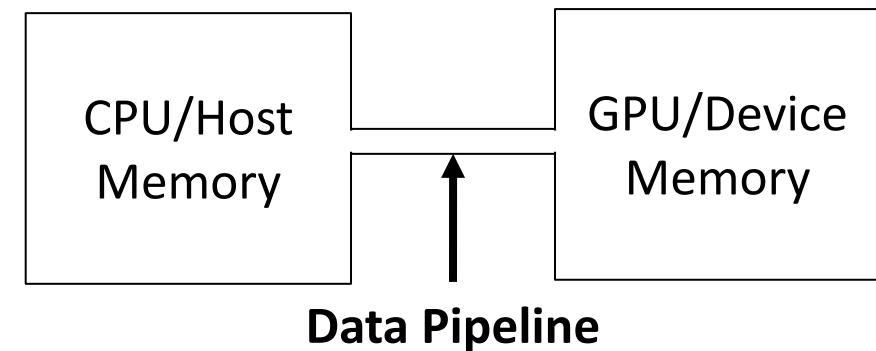
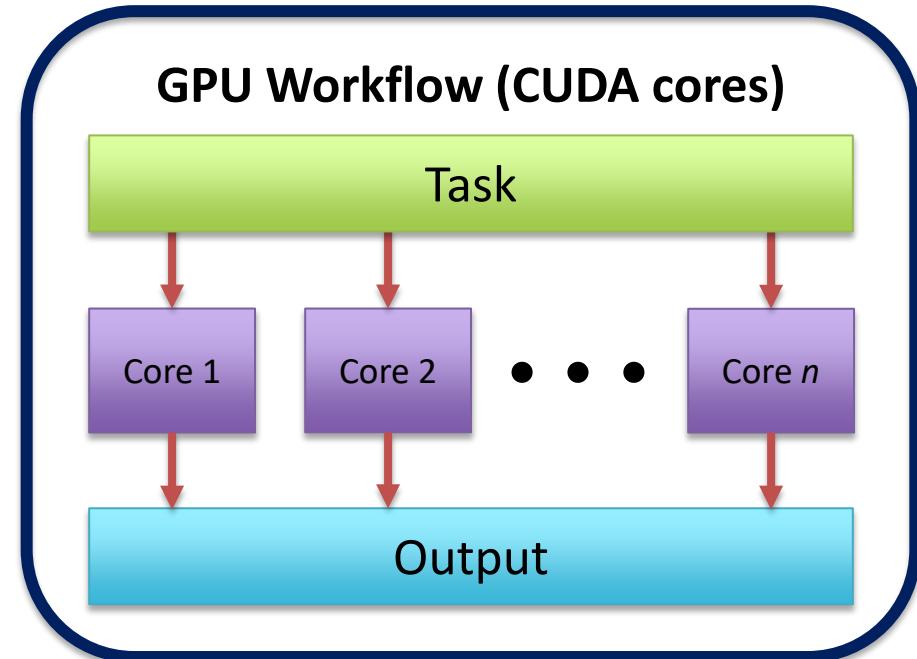
Branch-and-bound (B&B) nodes:

- **Same** optimization problem
- **Same** processing technique
- Different **domains**



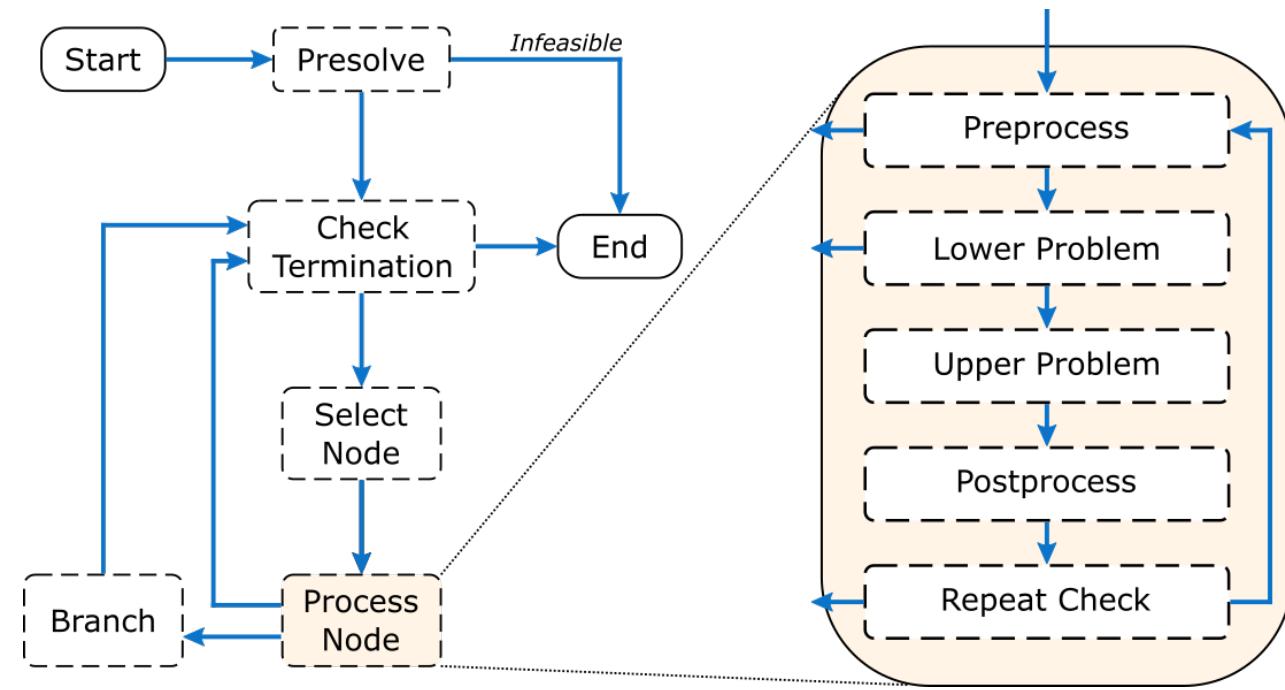
GPU Concepts

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 - Thousands of GPU cores (threads) execute tasks simultaneously
 - Large chunks of **identical** data processing (I.e., the **inputs** change, not the math)
- **Major GPU bottlenecks:**
 - Code branches bad for performance
 - High data transfer overhead cost



Adapting Branch-and-Bound (B&B)

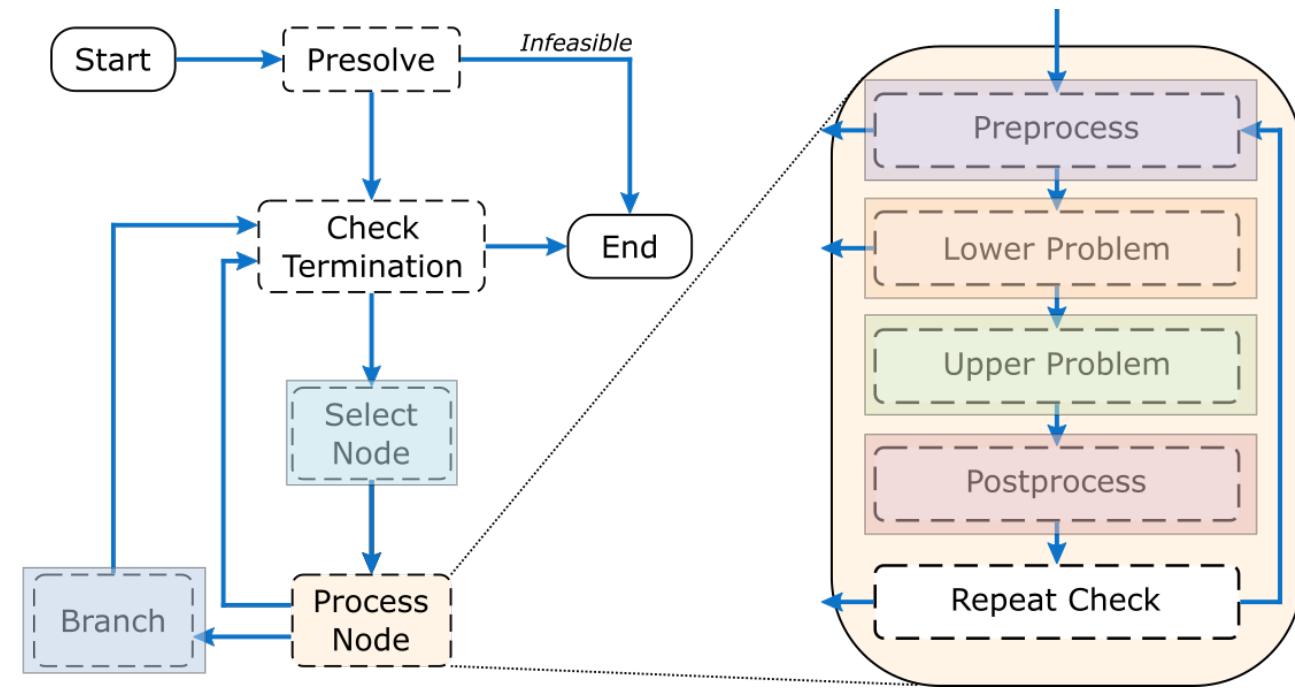
What aspects of B&B should be parallelized?



5. Wilhelm, M.E. and Stuber, M.D. **EAGO.jl**: easy advanced global optimization in Julia. *Optimization Methods and Software*, 37(2):425–450, aug 2022. doi:10.1080/10556788.2020.1786566.

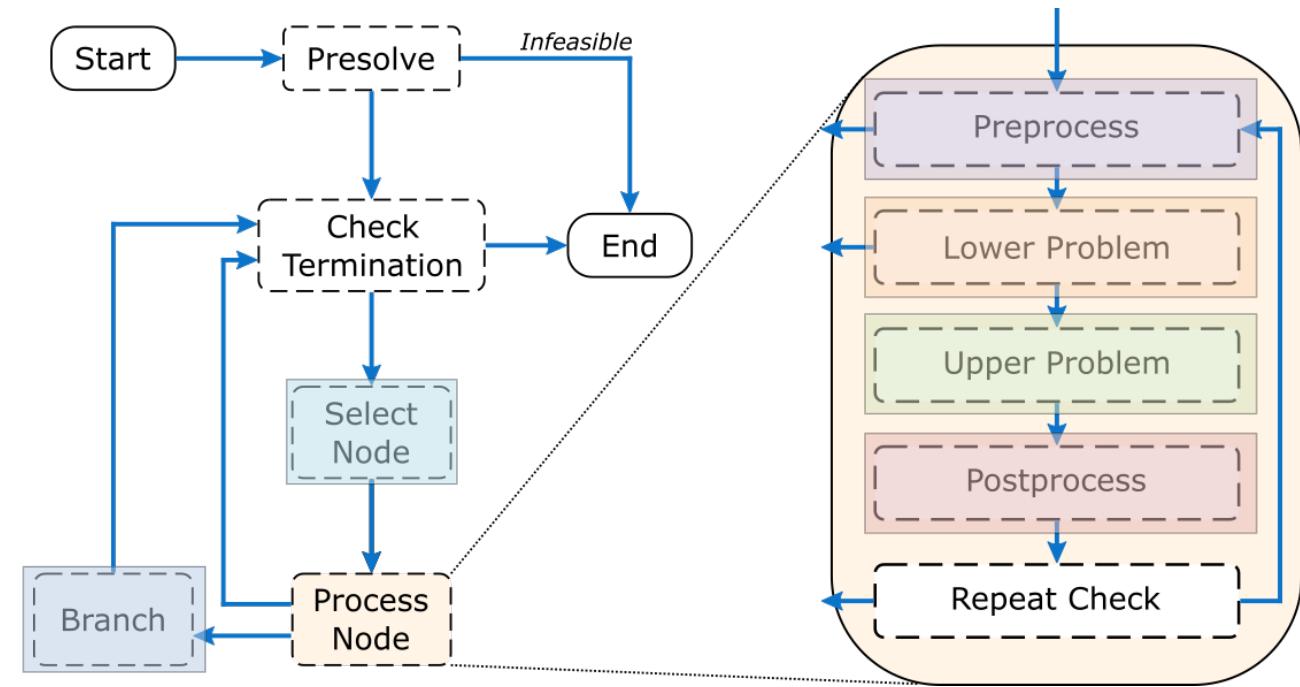
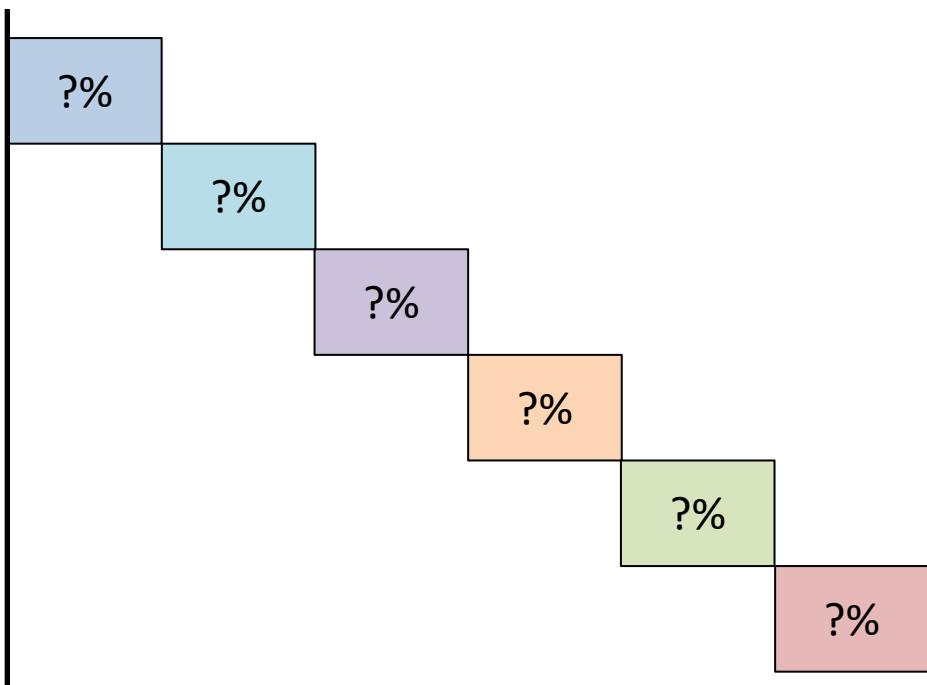
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B&B Step Timing



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B&B Step Timing

Example 1

Typical “Short” Problem
(<60s runtime)

Branching/Fathoming: 0.3%

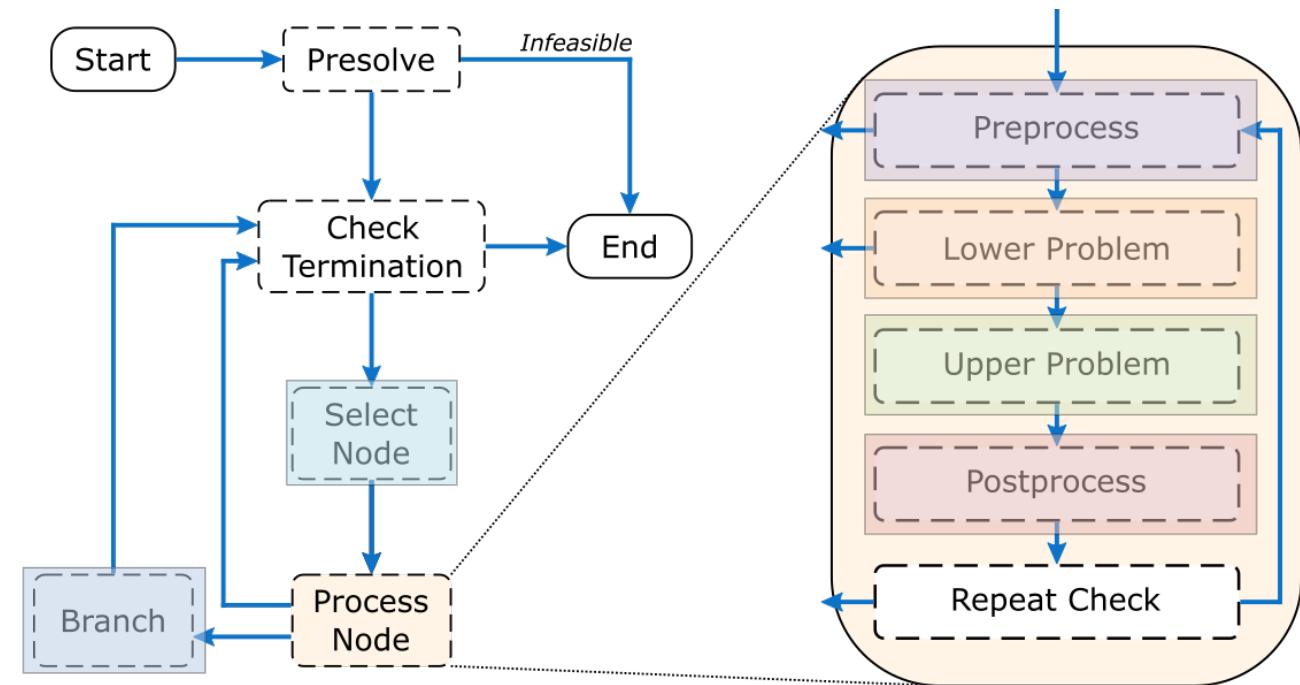
Node Selection: 0.5%

Preprocessing: 1.1%

Lower Problem: 56.9%

Upper Problem: 41.4%

Postprocessing: 0.0%



5. Wilhelm, M.E. and Stuber, M.D. **EAGO.jl**: easy advanced global optimization in Julia. *Optimization Methods and Software*, 37(2):425–450, aug 2022. doi:10.1080/10556788.2020.1786566.

B&B Step Timing

Example 2 Typical “Long” Problem (>2h runtime)

Branching/Fathoming: 0.2%

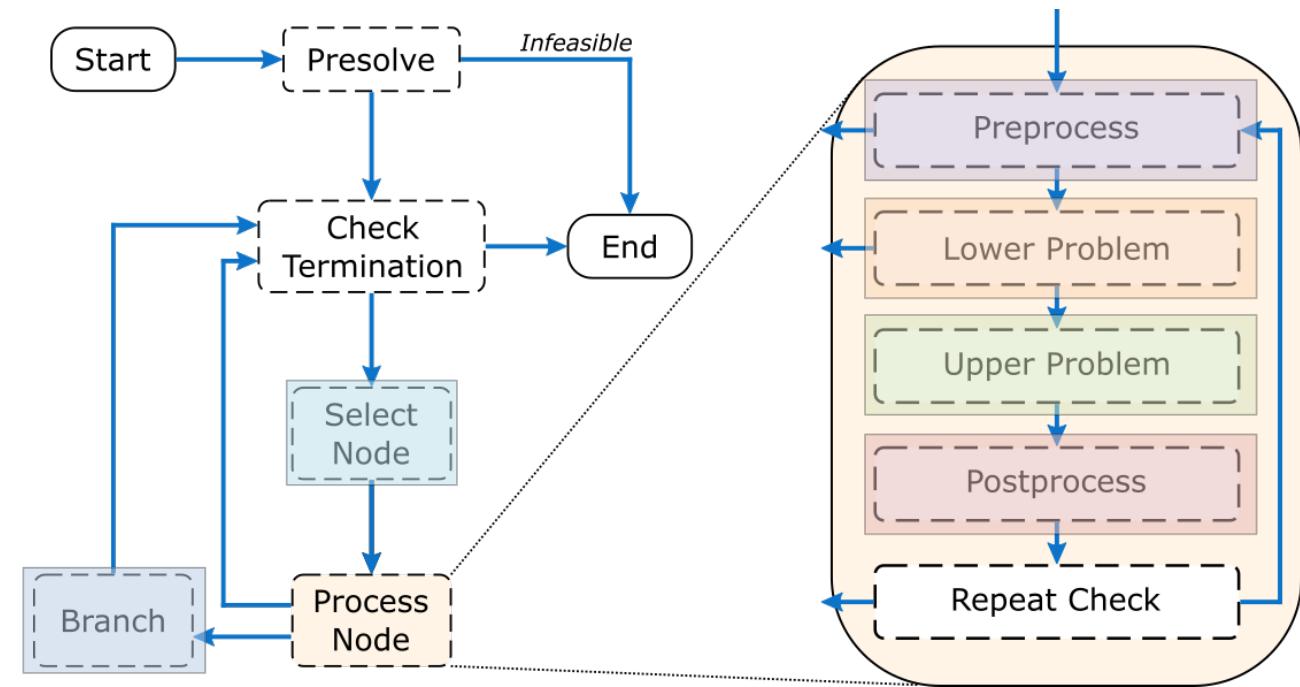
Node Selection: 0.3%

Preprocessing: 0.3%

Lower Problem: 98.9%

Upper Problem: 0.3%

Postprocessing: 0.0%



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B&B Step Timing

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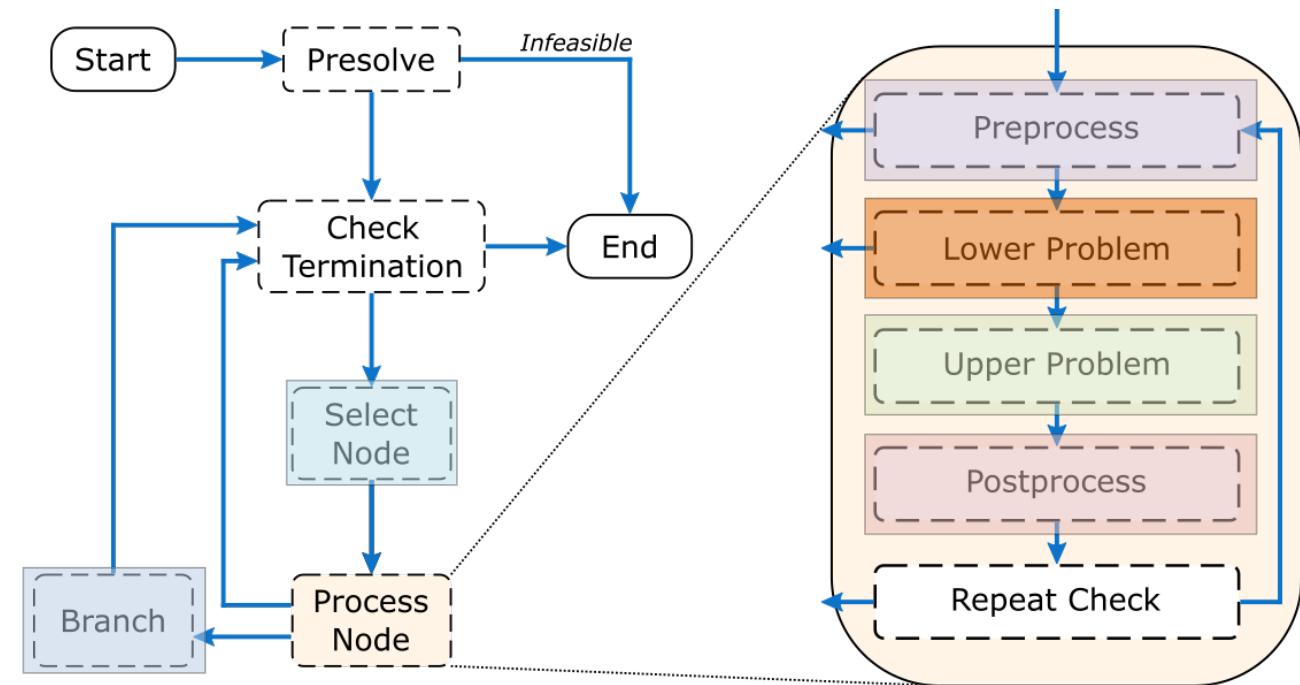
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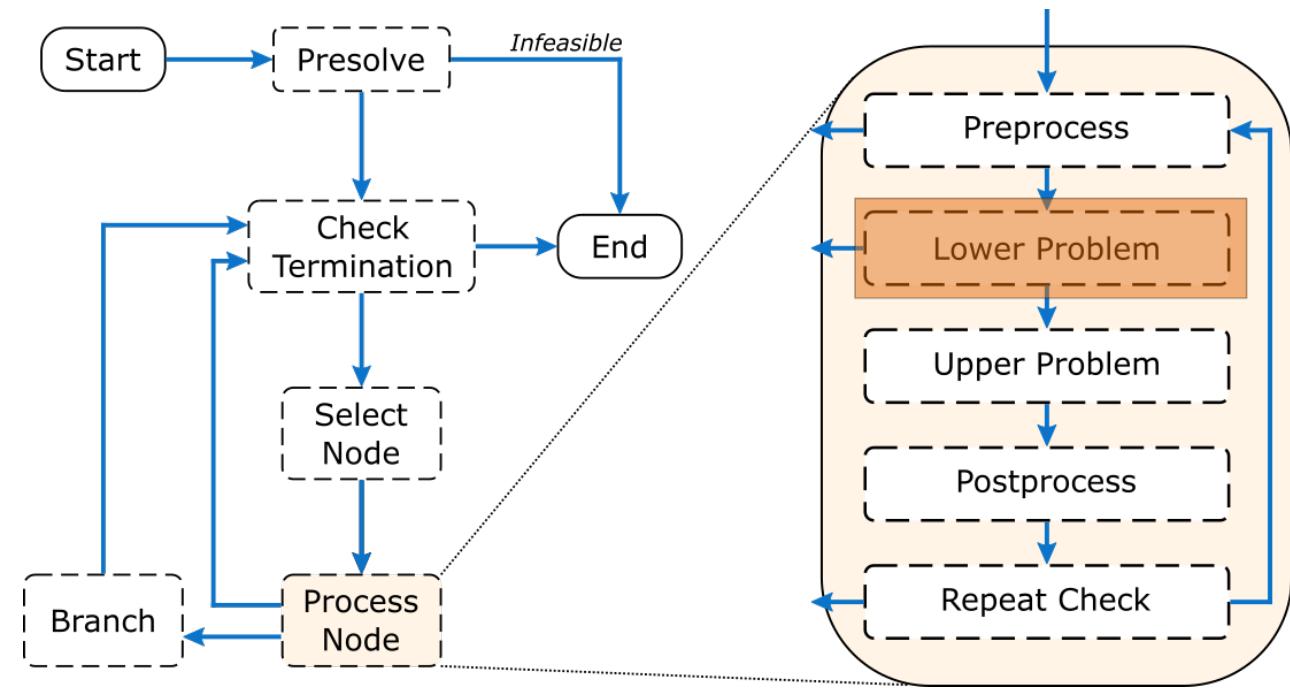
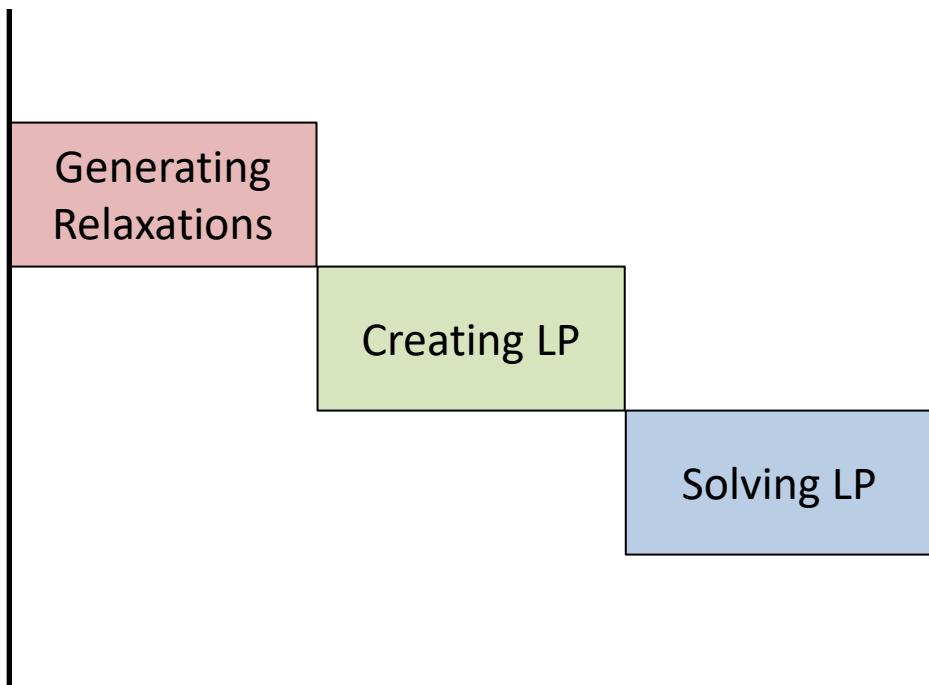
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B&B Step Timing

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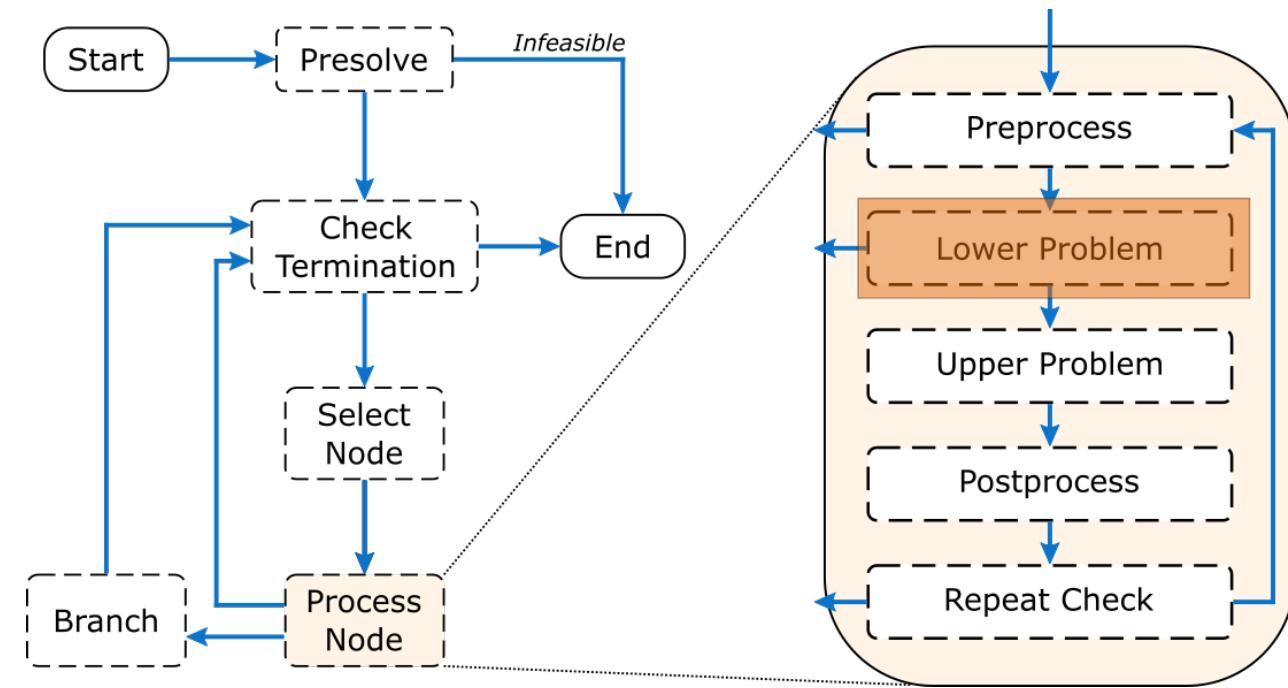
Simple Expressions

Higher Dimensionality

Generating Relaxations: 34.4%

Creating LP: 12.0%

Solving LP: 53.6%



5. Wilhelm, M.E. and Stuber, M.D. **EAGO.jl**: easy advanced global optimization in Julia. *Optimization Methods and Software*, 37(2):425–450, aug 2022. doi:10.1080/10556788.2020.1786566.

B&B Step Timing

Example 2

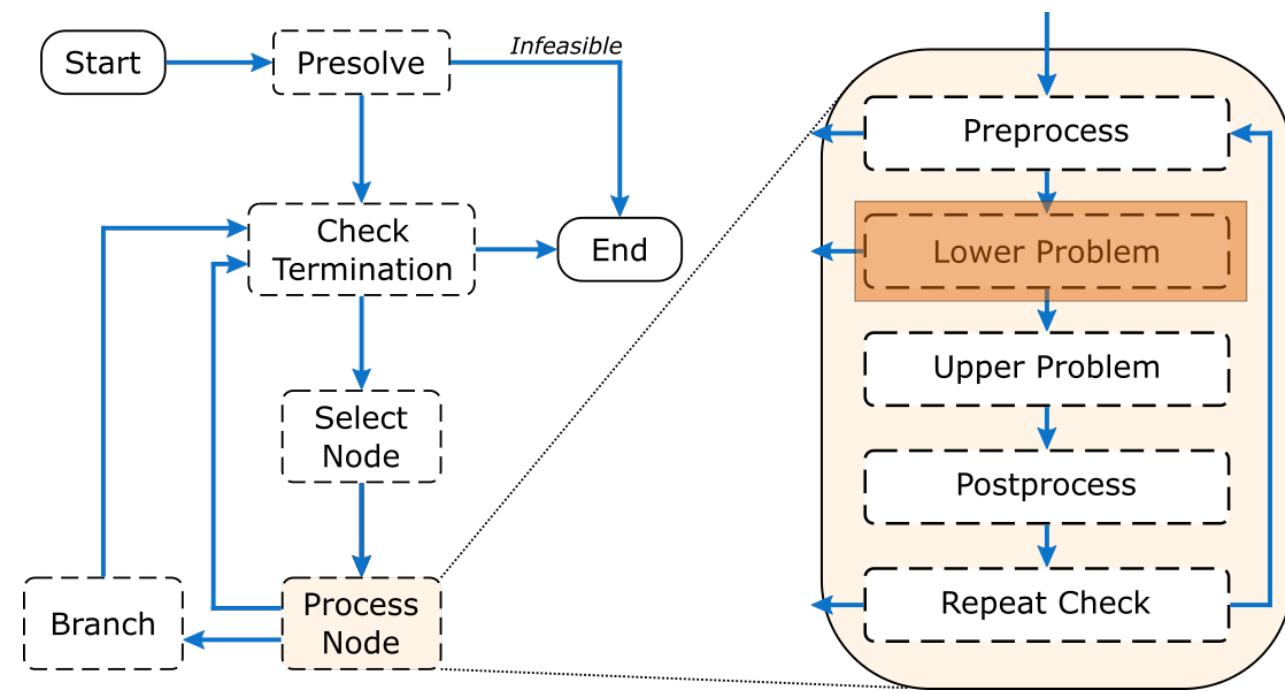
Complex Expressions

Lower Dimensionality

Generating Relaxations:
64.0%

Creating LP: 12.7%

Solving LP: 23.3%

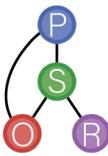
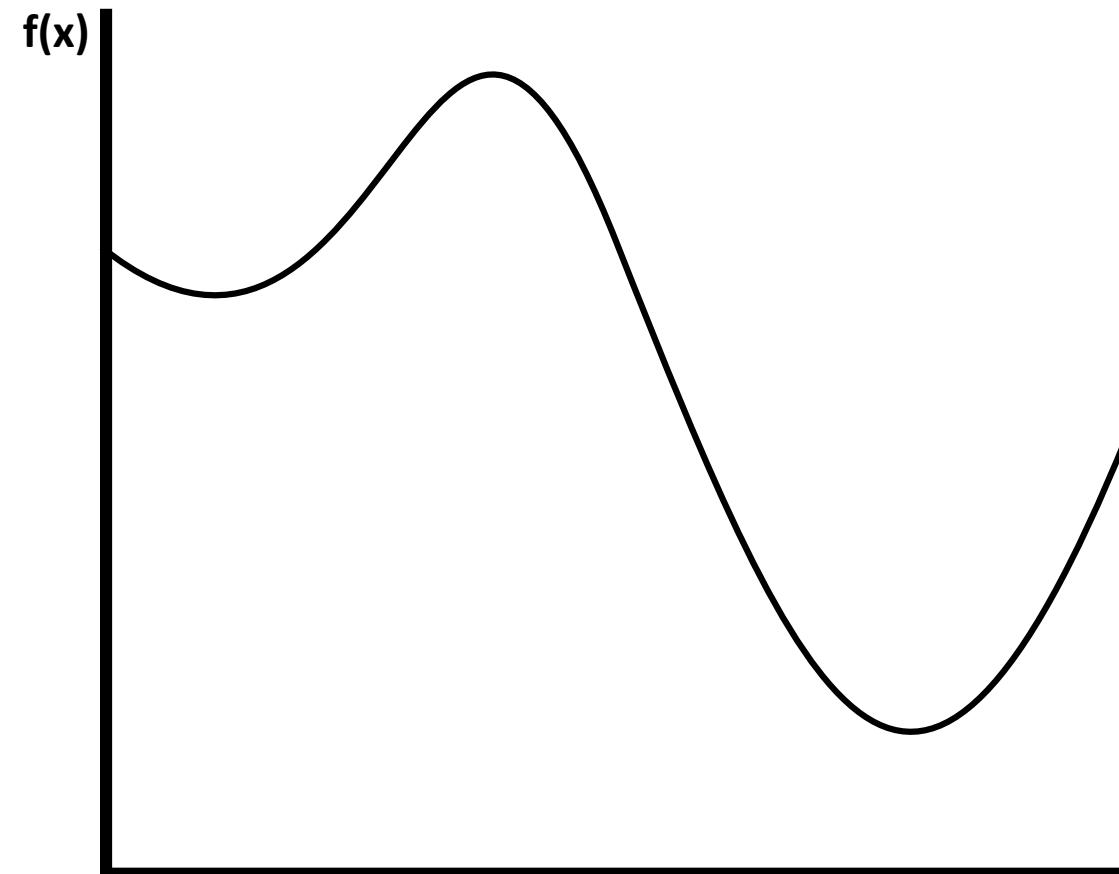


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GPU Parallelization Targets

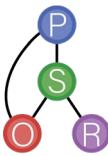
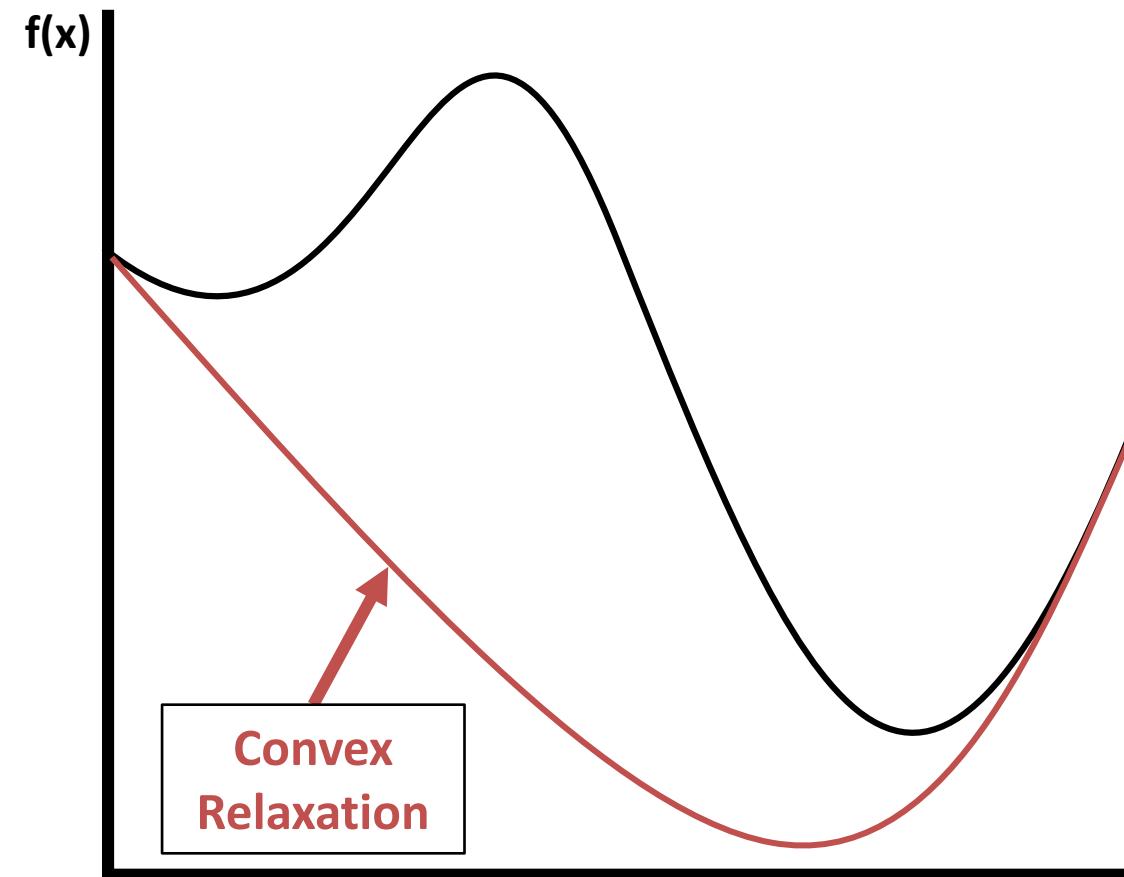
3 Main Parallelization Targets:



GPU Parallelization Targets

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1. Relaxation Generation

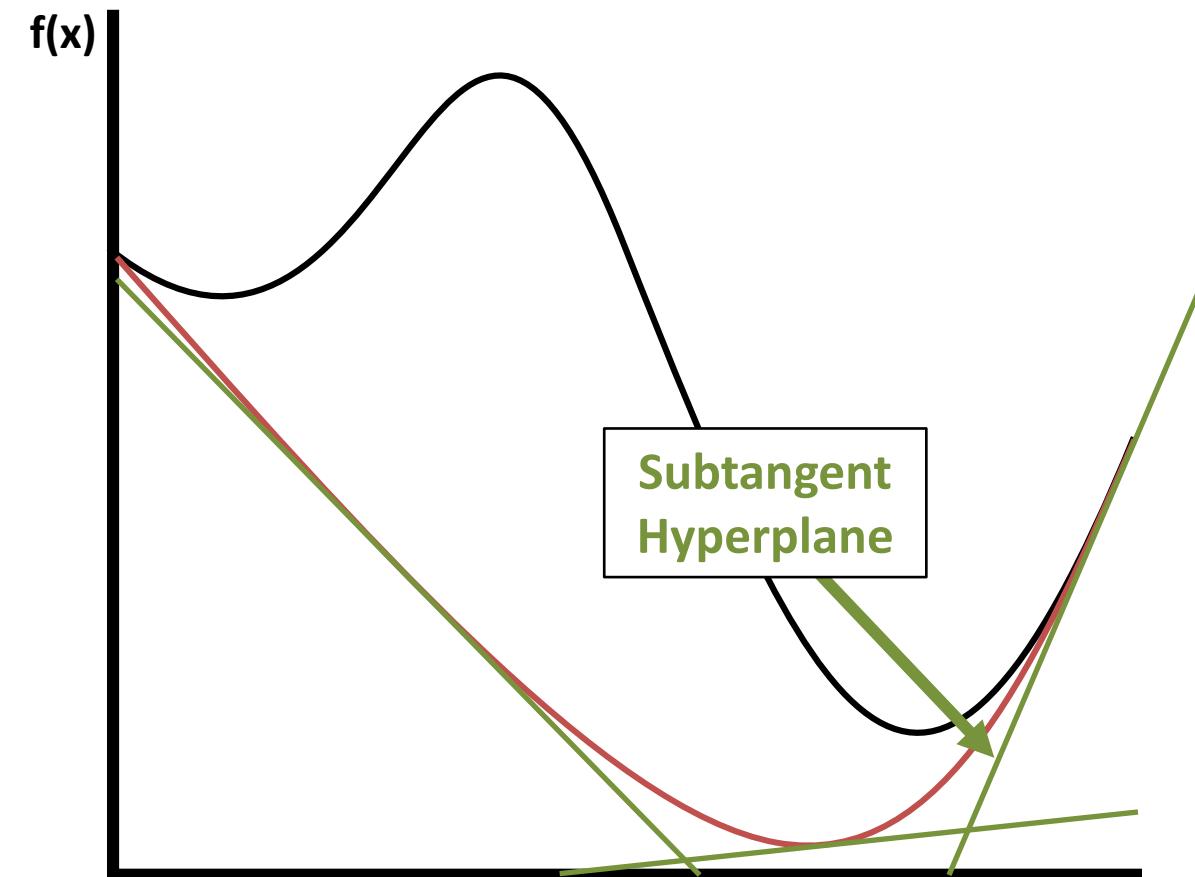


GPU Parallelization Targets

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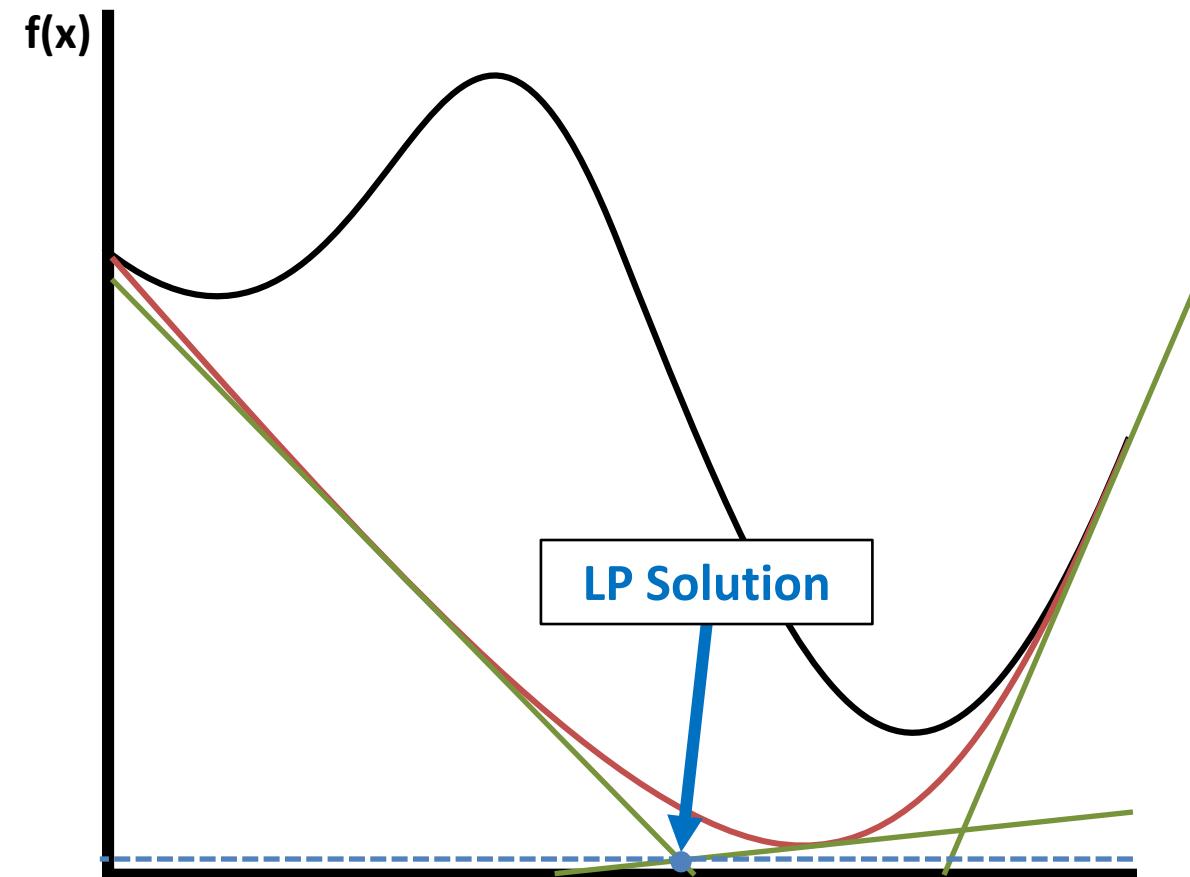
2. Linear Program (LP) Creation



GPU Parallelization Targets

3 Main Parallelization Targets:

1. Relaxation Generation
2. Linear Program (LP) Creation
3. LP Solution

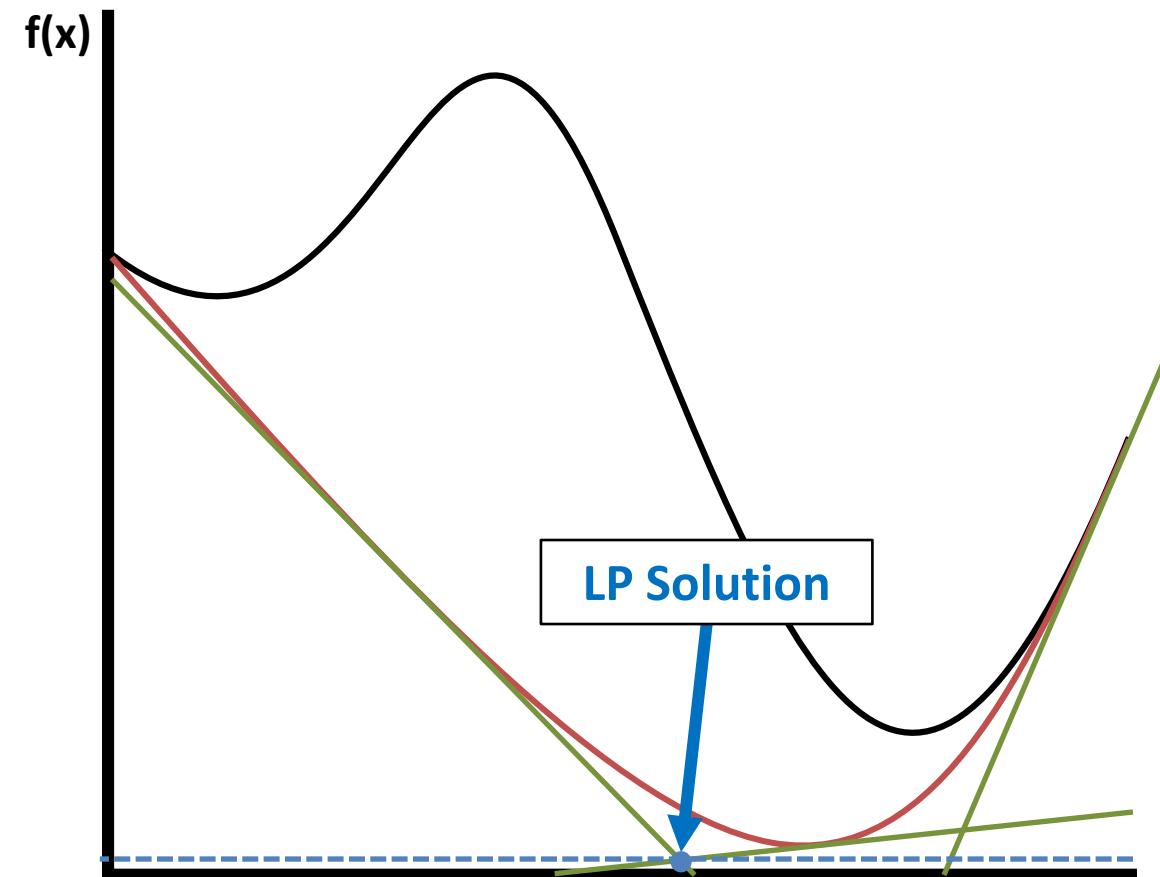


GPU Parallelization Targets

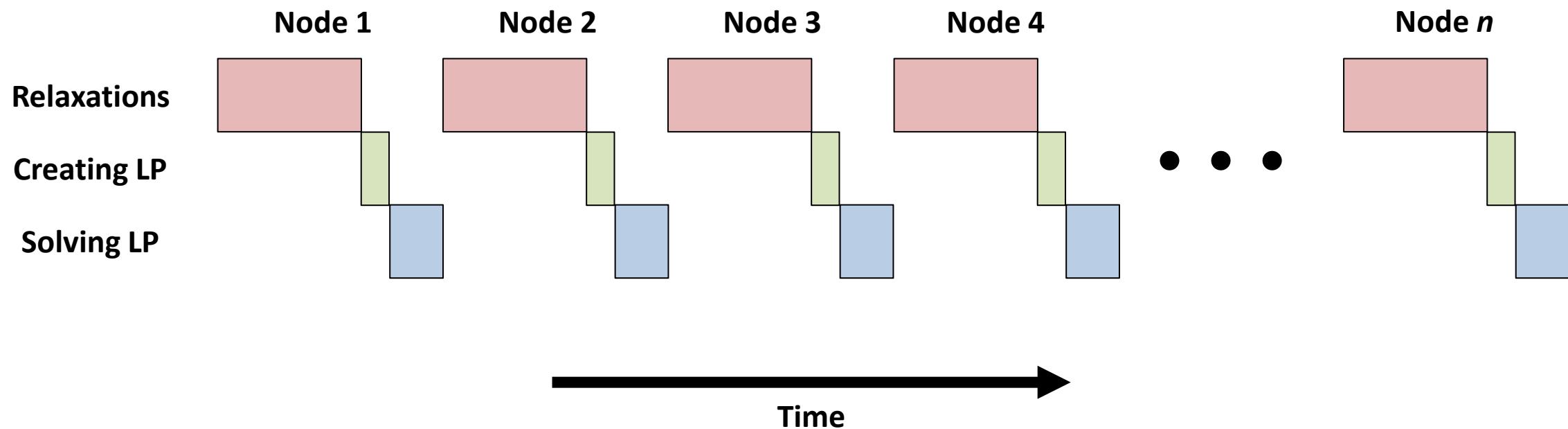
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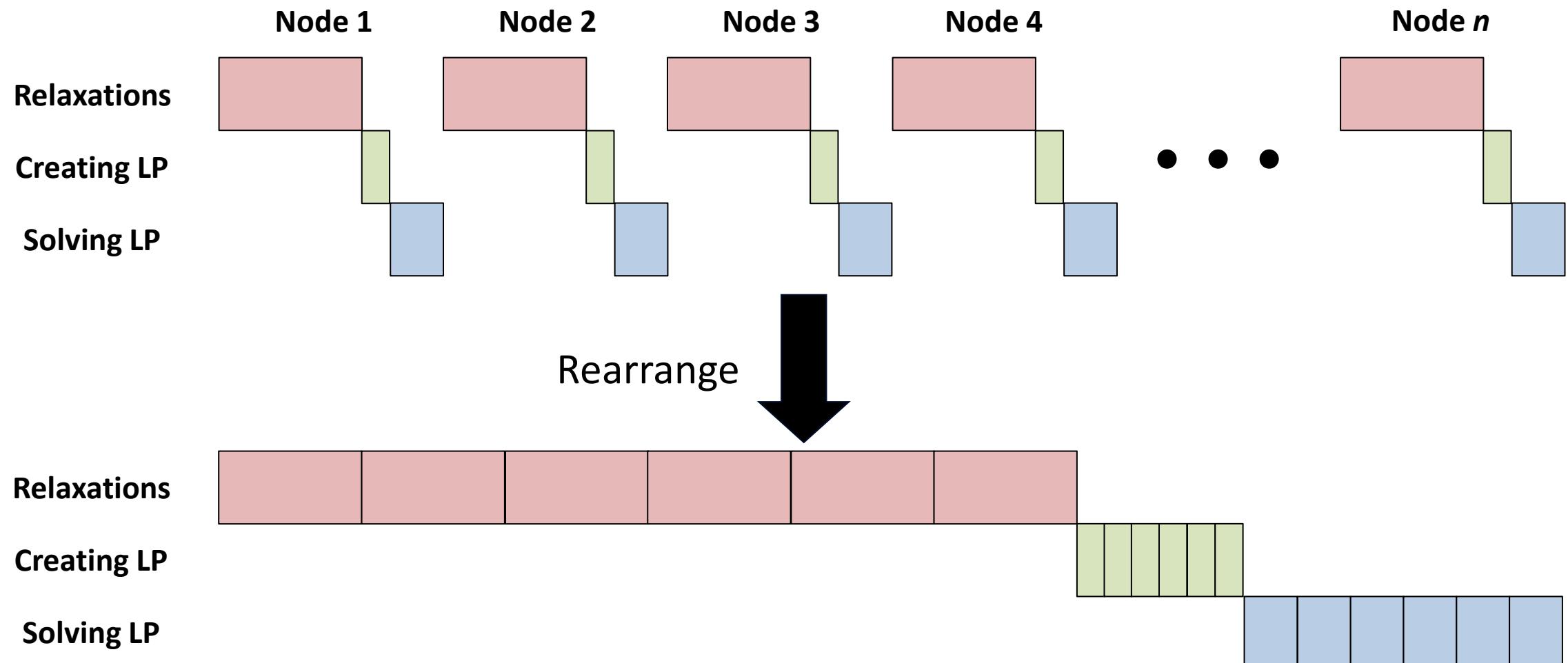
If these tasks can be efficiently parallelized, we can run B&B on powerful GPU hardware



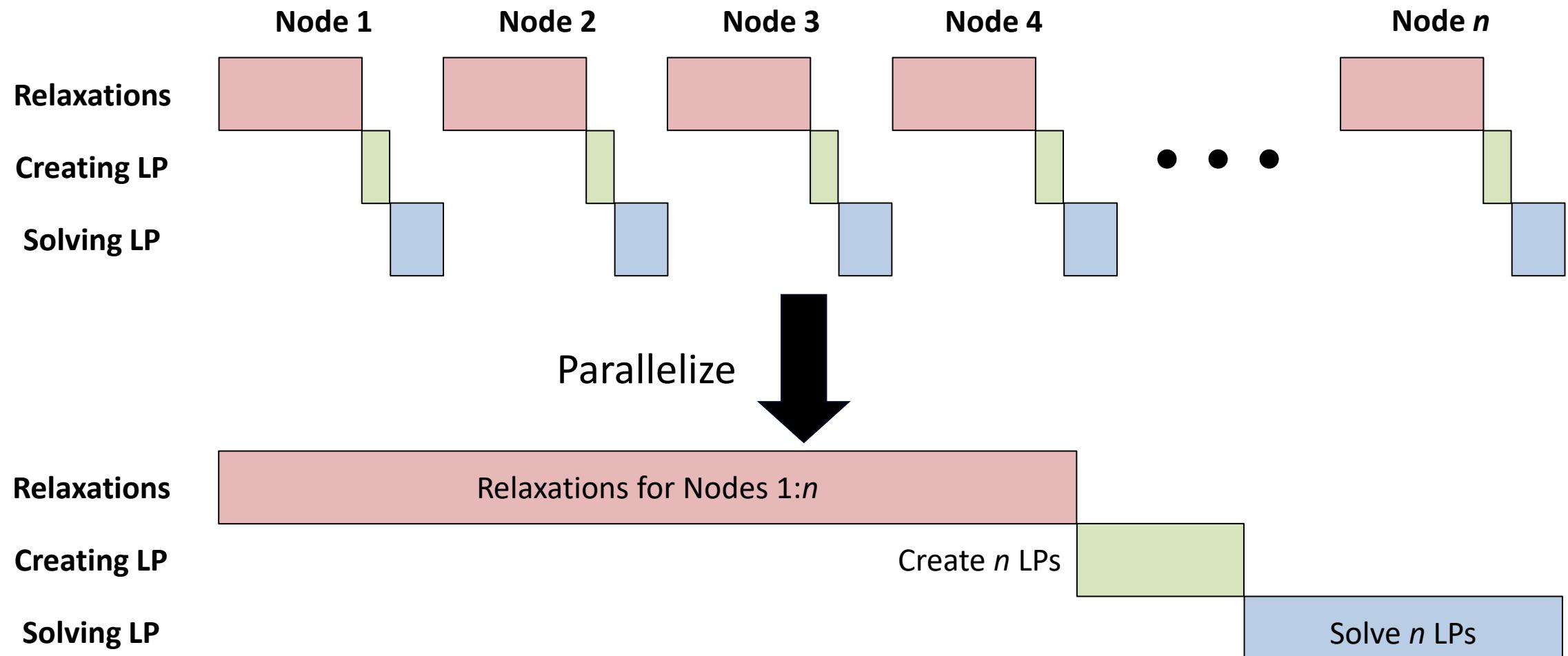
Parallelization Strategy



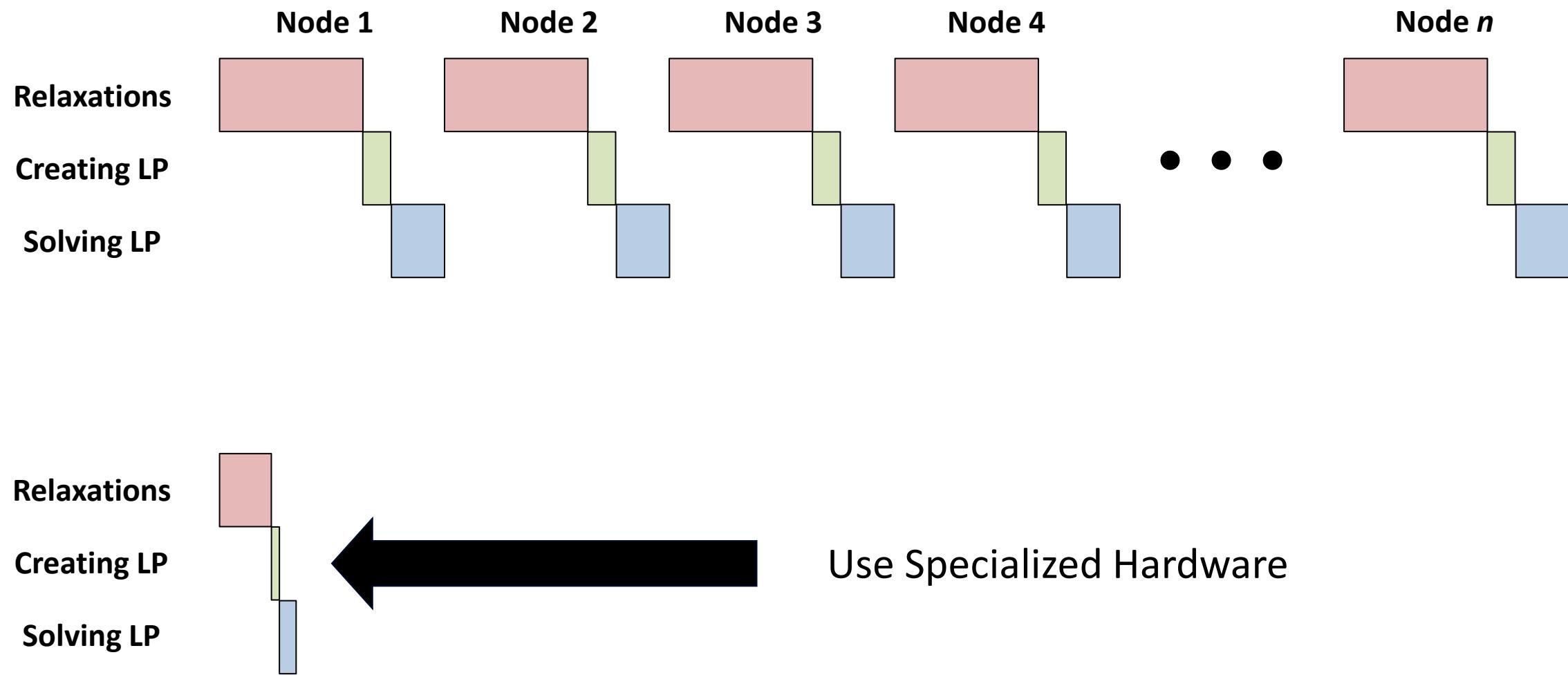
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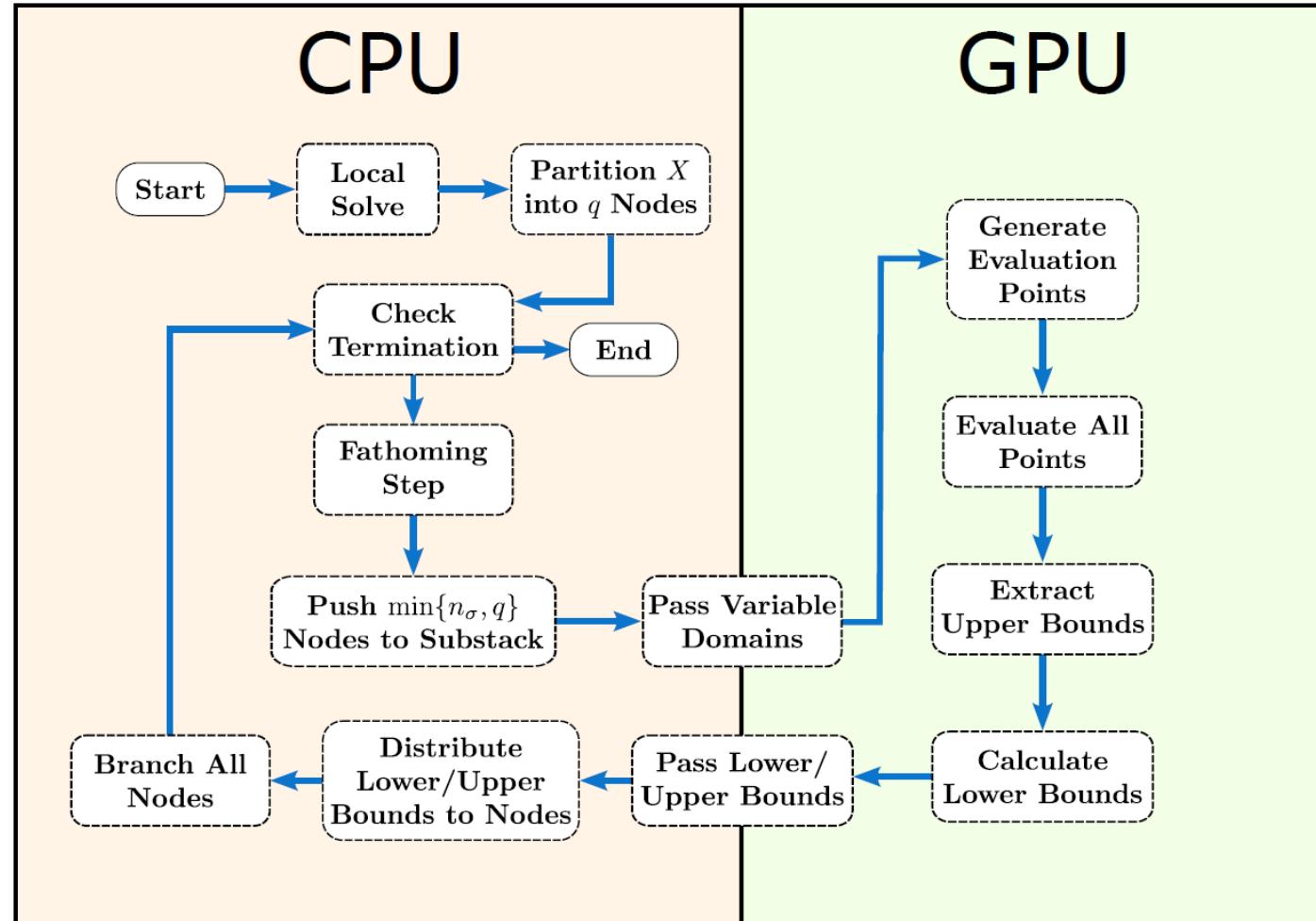
Parallelization Strategy



Parallelization Strategy



ParBB Algorithm



6. Gottlieb, R.X., et al., *Automatic source code generation for deterministic global optimization with parallel architectures*, *Under Review*.



3 Key Parallelization Targets

Relaxations

LP Generation

LP Solves



GPU-Accelerated Relaxations

SourceCodeMcCormick.jl

Enables **GPU-compatible** McCormick relaxations through:

- Primal trace generation
- Creation of subfunctions for:
 - Interval extensions
 - Relaxations
 - Subgradients of relaxations
- Connecting subfunctions using generalized McCormick theory
- Constructing **evaluator functions** for original expressions

```
using SourceCodeMcCormick, Symbolics
Symbolics.@variables x, y
expr = (4 + (-2.1+x^2/4)*x^2)*x^2 + x*y + (-4+4*y^2)*y^2
func = fgen(expr, [:cv, :lo, :cvgrad])
```



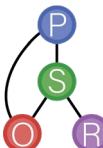
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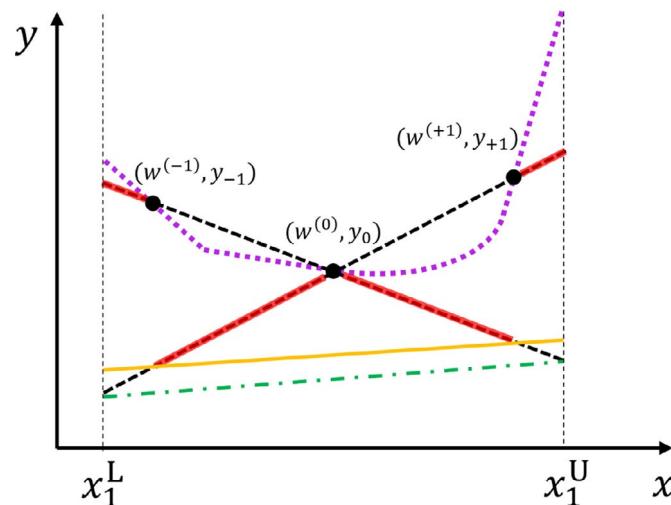
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Subgradient Utility

Before Adding Subgradients

- Black-box sampling technique⁷ for lower bounds
- No nontrivial constraints



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

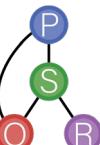
After Adding Subgradients

- Tighter, subgradient-based lower-bounding method
- Nontrivial constraints via LP generation

E·GO



Same method,
but on **GPU**



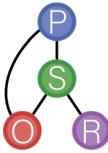
3 Key Parallelization Targets



Relaxations

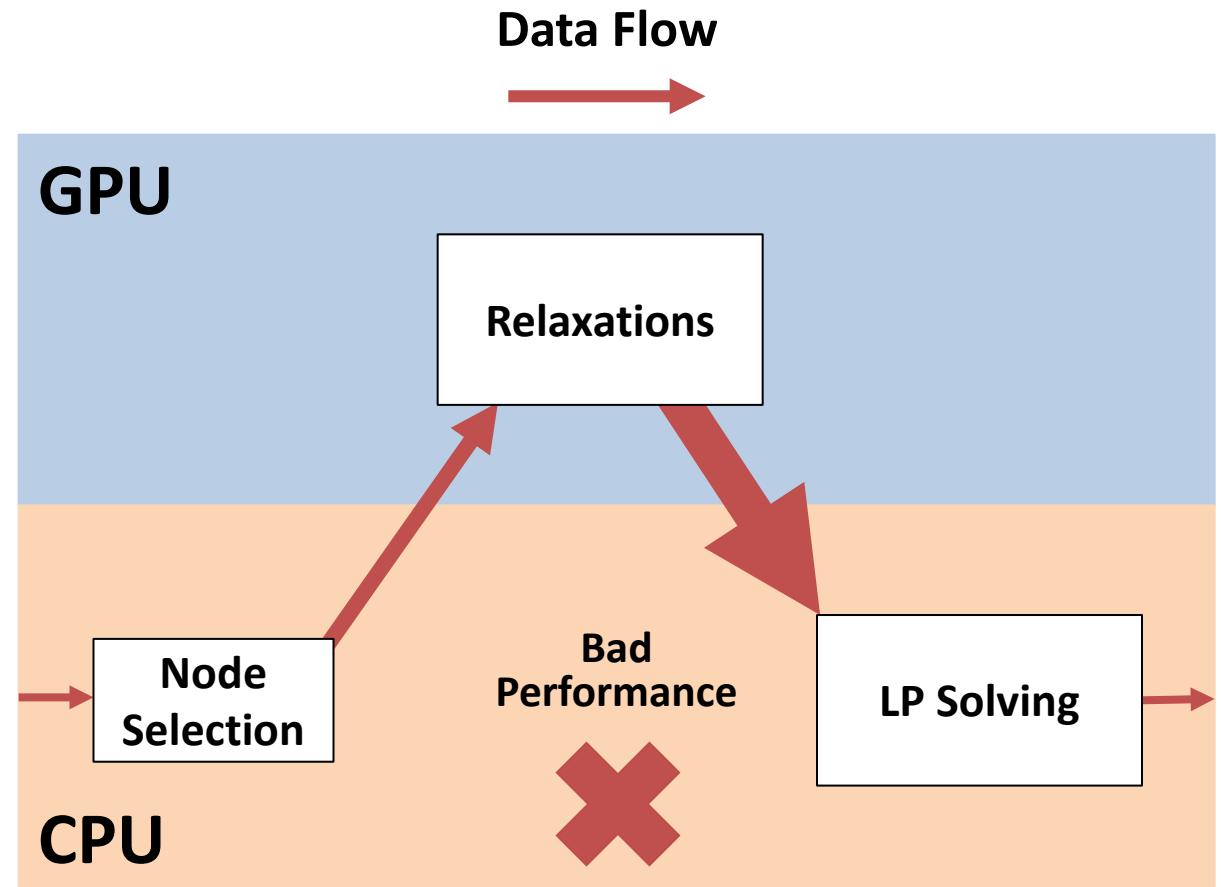
LP Generation

LP Solves



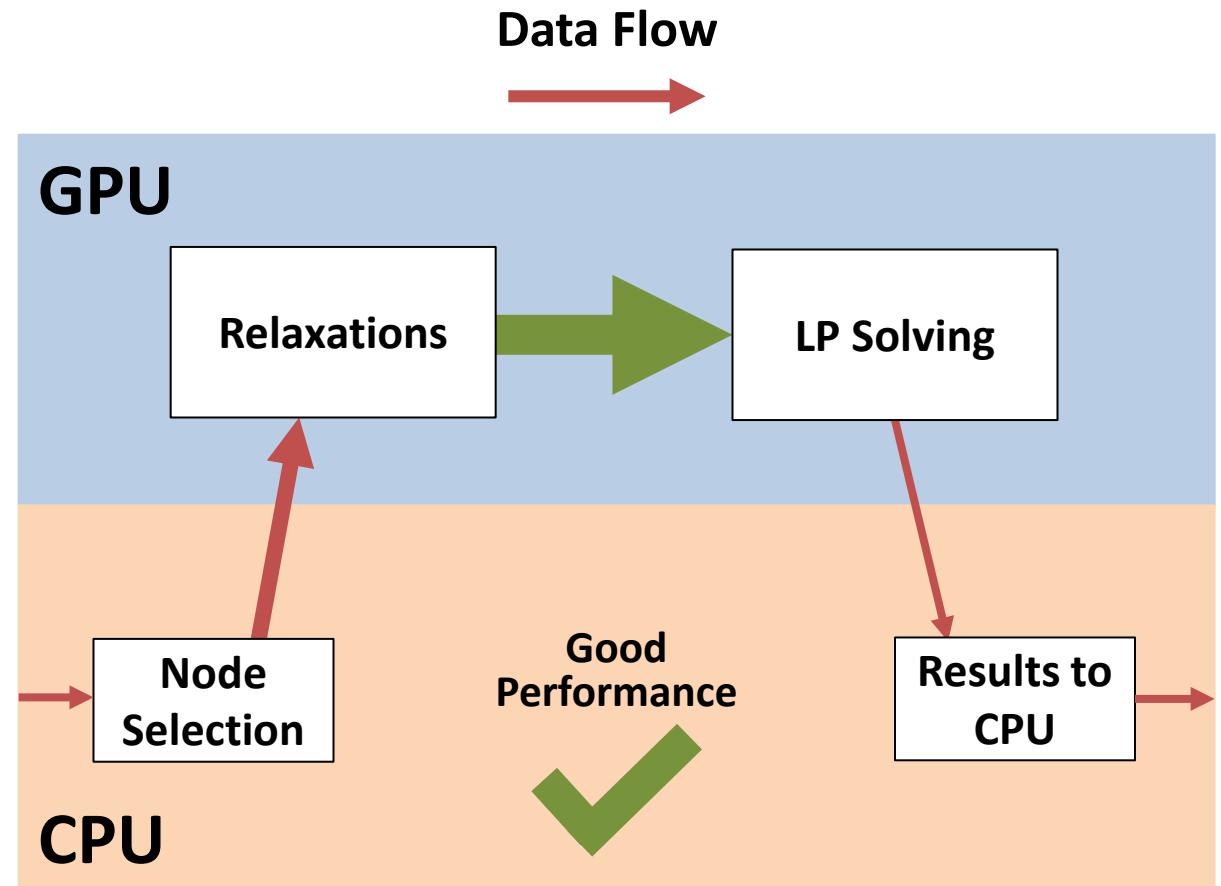
We Need GPU LPs!

- Calculating relaxations on GPUs is fast, but creates **lots of data**
 - Relaxations; intervals; subgradients
- **Memory transfer overhead** could negate benefits of GPU relaxations



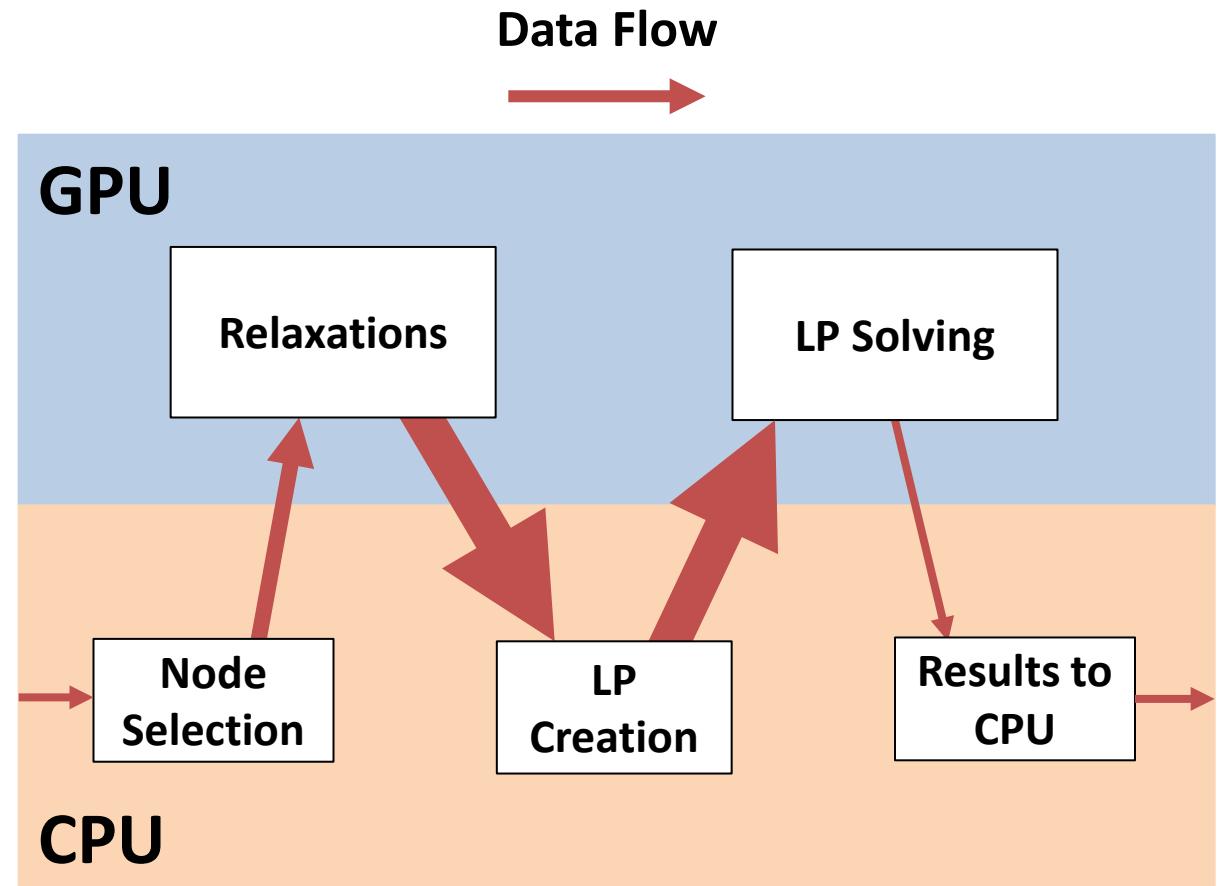
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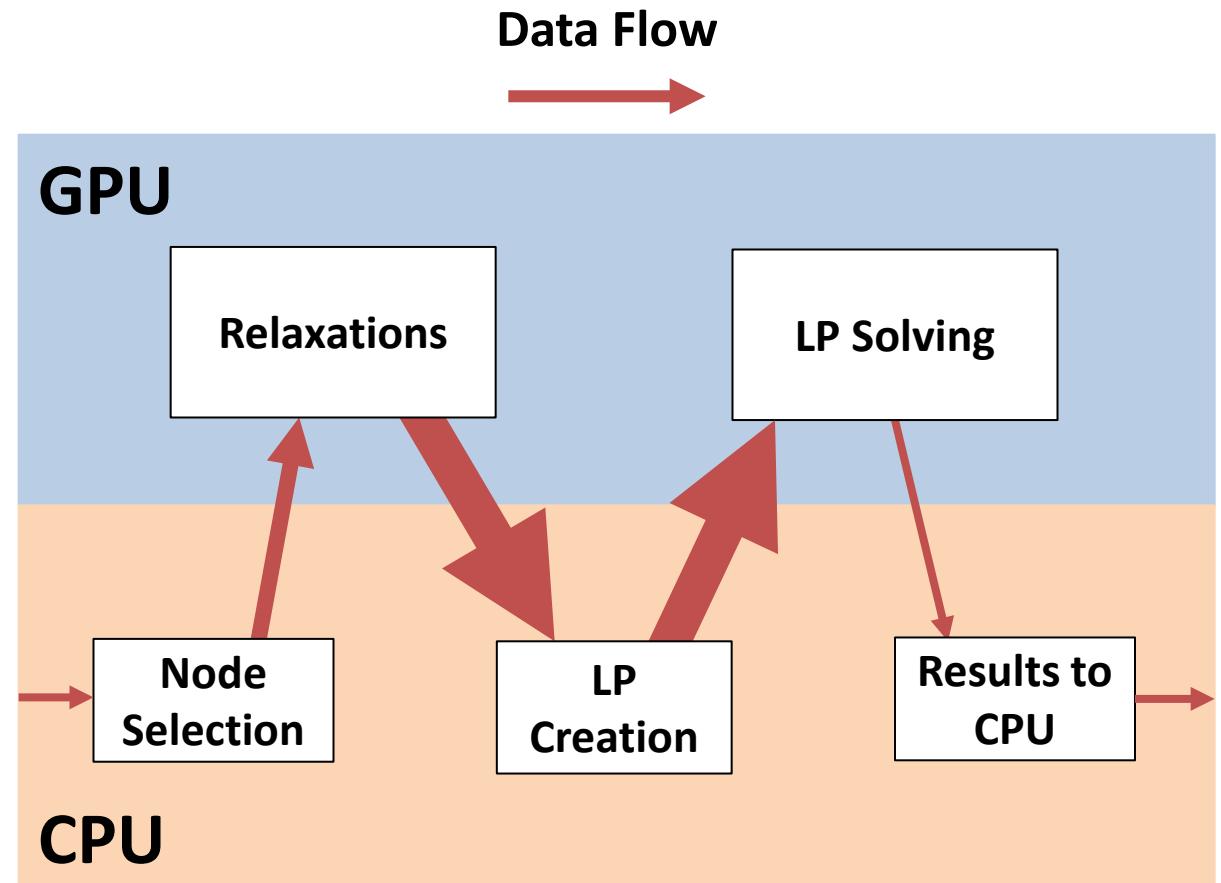
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- **Memory transfer overhead** could negate benefits of GPU relaxations
- **GPU-based LP solver is needed**
 - LP creation must also be on GPU
 - Need a **custom LP solver**



LPs on GPUs?

Does Gurobi support GPUs?



Greg Glockner

10 months ago · Updated

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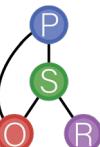
The Gurobi development team is watching GPUs (Graphics Processing Units) closely, but up to this point, all of the evidence indicates that they aren't well suited to the needs of an LP/MIP/QP solver. Specifically:

- GPUs don't work well for sparse linear algebra, which dominates much of linear programming. GPUs rely on keeping hundreds or even thousands of independent processors busy at a time. The extremely sparse matrices that are typical in linear programming don't admit nearly that level of parallelism.
- GPUs are built around SIMD computations, where all processors perform the same instruction in each cycle (but on different data). Parallel MIP explores different sections of the search tree on different processors. The computations required at different nodes in the search tree are quite different, so SIMD computation is not well suited to the needs of parallel MIP.

Note that CPUs and GPUs are both improving parallelism as a means to increase performance. The Gurobi Optimizer is designed to effectively exploit multiple cores in a CPU, so you'll definitely see a benefit from more parallelism in the future.



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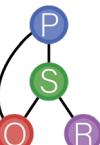
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all of the evidence indicates that they aren't well suited to the needs of an LP/MIP/QP solver.

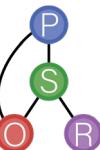
- * GPUs don't work well for sparse linear algebra, which dominates much of linear programming. GPUs are built around SIMD computations, where all processors compute the same operation each cycle (but on different data). Parallel MIP explores different subproblems on different processors. The computations required at different nodes in the tree are very different, so SIMD computation is not well suited to the needs of parallel optimization.
- * GPUs are built around SIMD computations, where all processors compute the same operation each cycle (but on different data). Parallel MIP explores different subproblems on different processors. The computations required at different nodes in the tree are very different, so SIMD computation is not well suited to the needs of parallel optimization.

Note that CPUs and GPUs are both improving parallelism as a means to increase performance. Gurobi Optimizer is designed to effectively exploit multiple cores in a CPU, so we expect to benefit from more parallelism in the future.



Gurobi.com

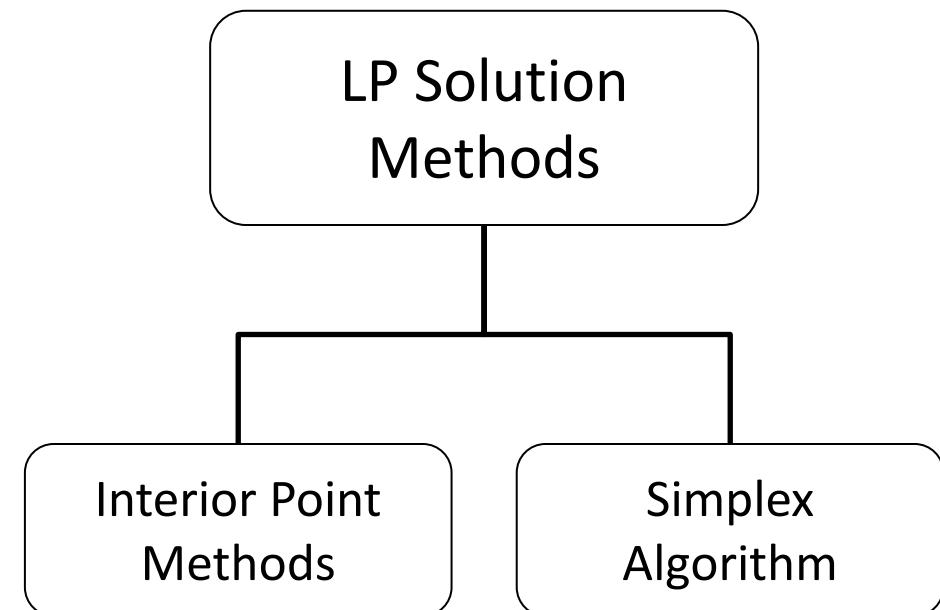
Linear subproblems in deterministic global optimization are small and dense



Custom LP Solver

Goal is to parallelize LPs that are all:

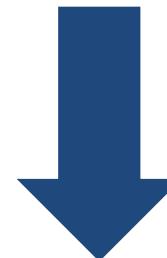
- Small
- Dense
- The same size
- Of similar complexity



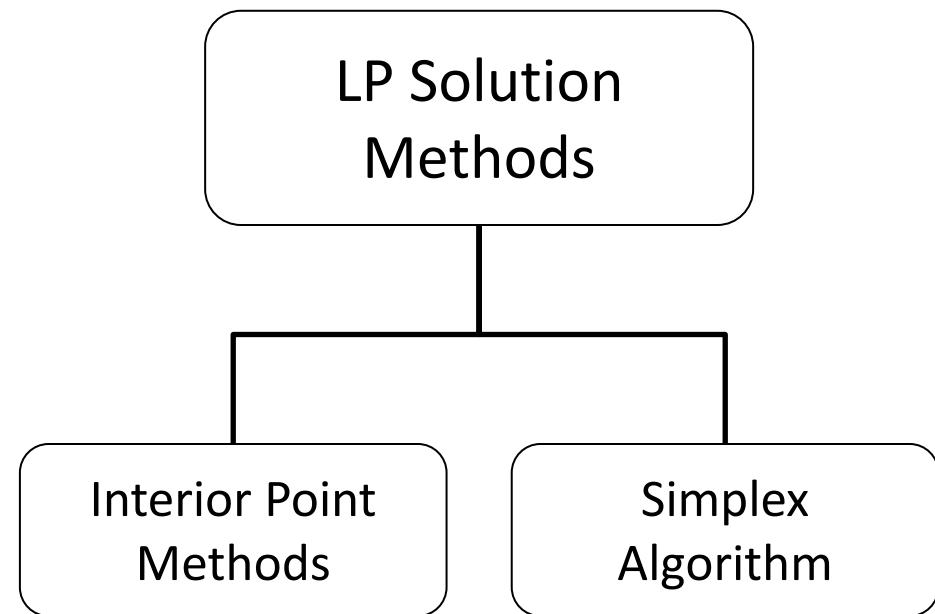
Custom LP Solver

Goal is to parallelize LPs that are all:

- Small
- Dense
- The same size
- Of similar complexity



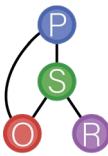
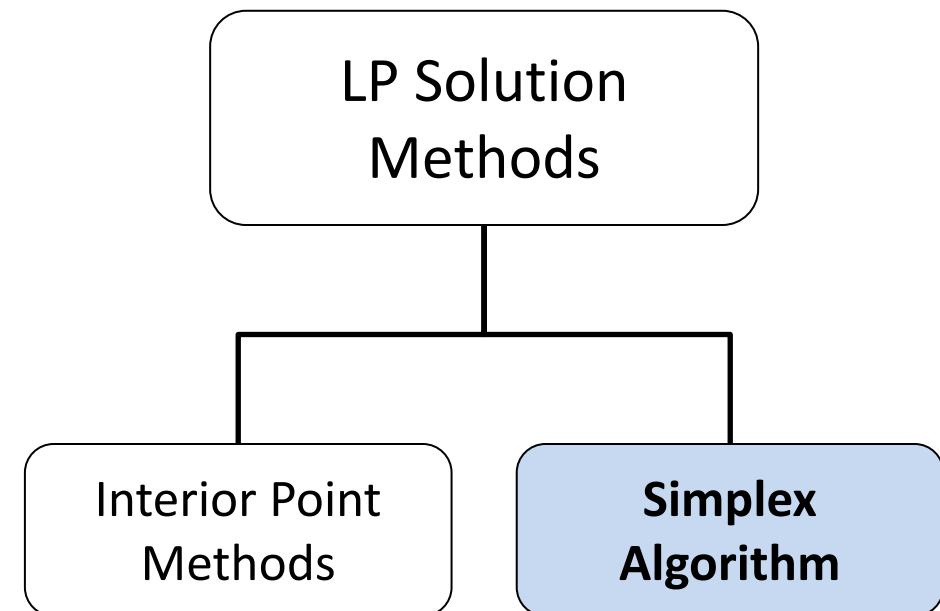
**Typical heuristics for GPU-based LP methods
may not apply**



Custom LP Solver

Implementing **two-phase Simplex method**

- Intuitive
- Simple to set up tableau(s)
- Straightforward to find BFS(s)
- No matrix inversion needed



Custom LP Solver

Implementing **two-phase Simplex method**

- Intuitive
- Simple to set up tableau(s)
- Straightforward to find BFS(s)
- No matrix inversion needed

- Not the only solution! Other methods may work as well (or better!)

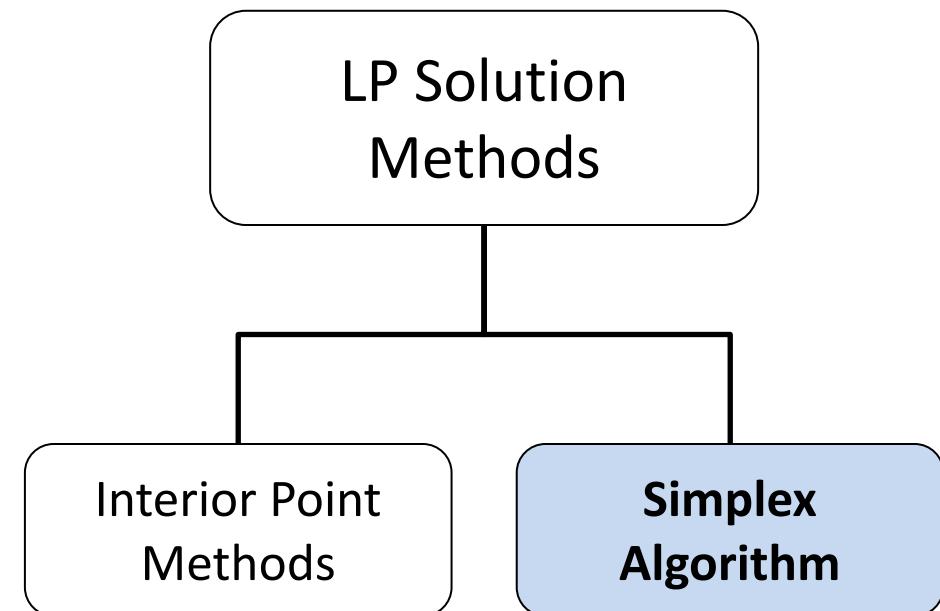


Tableau Generation

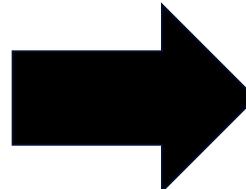
$$\min f_{cv}(x)$$

$$\text{s.t. } 0.8x + 12 \leq f_{cv}(x)$$

$$1.6x + 4 \leq f_{cv}(x)$$

$$-2.8x + 24 \leq f_{cv}(x)$$

$$x_L \leq x \leq x_U$$



- Shifting/scaling domain
- Epigraph reformulation
- Restructuring

$$\min \xi^+ - \xi^-$$

$$\text{s.t. } -\xi^+ + \xi^- \geq f_L$$

$$-\xi^+ + \xi^- + 0.2x \leq -1$$

$$-\xi^+ + \xi^- + 0.4x \leq 1$$

$$-\xi^+ + \xi^- - 0.7x \leq -4$$

$$0 \leq x \leq 1$$

$$0 \leq \xi^+ \leq \text{Inf}$$

$$0 \leq \xi^- \leq \text{Inf}$$

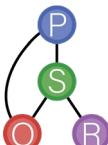
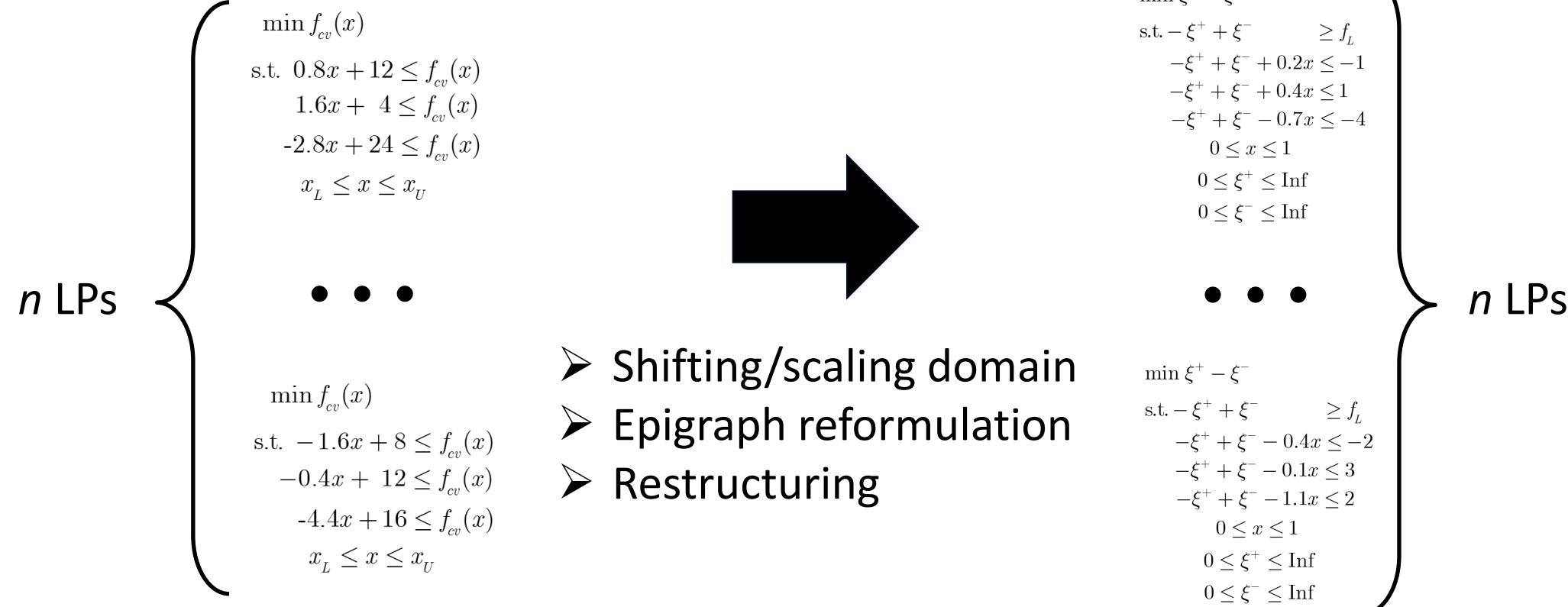


Tableau Generation



- Shifting/scaling domain
- Epigraph reformulation
- Restructuring

Tableau Generation

$$\begin{aligned}
 & \min \xi^+ - \xi^- \\
 \text{s.t.} \quad & -\xi^+ + \xi^- \geq f_L \\
 & -\xi^+ + \xi^- + 0.2x \leq -1 \\
 & -\xi^+ + \xi^- + 0.4x \leq 1 \\
 & -\xi^+ + \xi^- - 0.7x \leq -4 \\
 & 0 \leq x \leq 1 \\
 & 0 \leq \xi^+ \leq \text{Inf} \\
 & 0 \leq \xi^- \leq \text{Inf}
 \end{aligned}$$

• • •

$$\begin{aligned}
 & \min \xi^+ - \xi^- \\
 \text{s.t.} \quad & -\xi^+ + \xi^- \geq f_L \\
 & -\xi^+ + \xi^- - 0.4x \leq -2 \\
 & -\xi^+ + \xi^- - 0.1x \leq 3 \\
 & -\xi^+ + \xi^- - 1.1x \leq 2 \\
 & 0 \leq x \leq 1 \\
 & 0 \leq \xi^+ \leq \text{Inf} \\
 & 0 \leq \xi^- \leq \text{Inf}
 \end{aligned}$$

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
...
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2

LP #1

LP #n

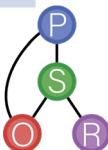


Tableau Generation

$$\begin{aligned}
 & \min \xi^+ - \xi^- \\
 \text{s.t.} \quad & -\xi^+ + \xi^- \geq f_L \\
 & -\xi^+ + \xi^- + 0.2x \leq -1 \\
 & -\xi^+ + \xi^- + 0.4x \leq 1 \quad \leftarrow \\
 & -\xi^+ + \xi^- - 0.7x \leq -4 \\
 & 0 \leq x \leq 1 \\
 & 0 \leq \xi^+ \leq \text{Inf} \\
 & 0 \leq \xi^- \leq \text{Inf}
 \end{aligned}$$

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
...
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2

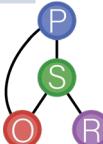


Tableau Generation

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
...
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	$-f_L$
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2

$n * [\text{height of one LP}]$



3 Key Parallelization Targets



Relaxations



LP Generation

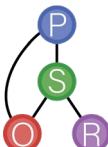
LP Solves



GPU Simplex

Parallelization approach depends on step:

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2

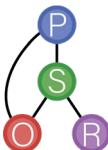


GPU Simplex

Parallelization approach depends on step:

- A) “Vectorized” steps (apply to each row)
- Access column information
 - Find pivot column

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	0	0	0	0	0	0	0	0	-2



GPU Simplex

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- A) “Vectorized” steps (apply to each row)
- Access column information
 - Find pivot column

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	0.5	0	1	0	1	0	1	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	0	0	1	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	0.5	0	1	0	1	0	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	0	0	1	0	0	0	0	0	0	0	0	-2

Thread #1

Thread #2

Thread #3

Thread #n

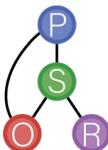


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ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
-1	1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	0	0	0	0	0	0	1	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.1	0	0	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
-1	1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	0	0	0	0	0	0	1	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
1	-1	-1.1	0	0	0	0	0	1	0	0	0	0	2
-1	1	0	0	0	0	0	0	0	0	0	0	0	0
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.1	0	0	0	0	0	0	0	0	0	0	-2



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 - Find pivot column

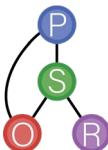
ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	0	1	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	0	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	0	0	0	0	0	0	0	0	-2

Thread #1

Thread #2

Thread #3

Thread #n

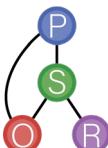


GPU Simplex

Parallelization approach depends on step:

- A) “Vectorized” steps (apply to each row)
- Access column information
 - Find pivot column

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	-0.5	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	0	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1	0	0	0	0	1	0	0	0	0	0	2
1	-1	-0.4	0	0	0	0	0	0	0	0	0	0	0
-1	1	0	0	1	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	-0.5	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	0	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1	0	0	0	0	1	0	0	0	0	0	2
1	-1	-0.4	0	0	0	0	0	0	0	0	0	0	0
-1	1	0	0	1	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1	0	0	0	0	1	0	0	0	0	0	2
1	-1	-0.4	0	0	0	0	0	0	0	0	0	0	0
-1	1	0	0	1	0	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

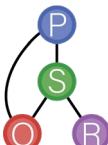
A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

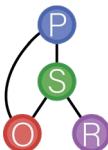
A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	0.1	0	0	0	1	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

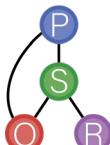
A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	0	0	0	0	0	0	-5
0	0	1	0	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	0.7	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	0.4	0	0	-1	0	0	0	0	1	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

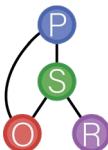
A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0		1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	0	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	0.7	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	0.4	0	0	-1	0	0	0	0	1	0	0	2
1	-1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1		0	0	0	0	0	0	0	0	0	1
-1	1	0		1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	1	0	0	0	0	1	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	1	0	0	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

C) “Batch” steps (apply to each LP)

- Pivoting

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2



GPU Simplex

Parallelization approach depends on step:

A) “Vectorized” steps (apply to each row)

- Access column information
- Find pivot column

B) Parallel reduction steps

- Find minimum ratio (pivot row)

C) “Batch” steps (apply to each LP)

- Pivoting

ξ^+	ξ^-	x	s_1	s_2	s_3	s_4	s_5	a_1	a_2	a_3	a_4	a_5	b
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	1	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
-1	1	0.4	0	0	0	0	0	0	0	1	0	0	2
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	3
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	-0.4	0	0	1	0	0	0	0	0	0	0	0	-2
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	0	0	1	0	0	0	0	0	0	0	0	0	f_L
1	-1	-0.2	0	0	-1	0	0	0	0	1	0	0	1
-1	1	0.4	0	0	0	0	0	0	0	0	0	0	1
1	-1	0.7	0	0	0	0	-1	0	0	0	0	0	4
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-2	2	-0.5	0	0	1	0	1	0	0	0	0	0	-5
0	0	1	1	0	0	0	0	0	0	0	0	0	1
-1	1	0	0	1	0	0	0	0	0	0	0	0	f_L
1	-1	0.4	0	0	-1	0	0	0	0	1	0	0	2
-1	1	-0.1	0	0	0	1	0	0	0	0	0	0	3
-1	1	-1.1	0	0	0	0	1	0	0	0	0	0	2
1	-1	0	0	0	0	0	0	0	0	0	0	0	0
-1	1	-0.4	0	0	1	0	0	0	0	0	0	0	-2

Block #3, Thread #2

Block #3



3 Key Parallelization Targets



Relaxations



LP Generation



LP Solves



Vapor Pressure Parameter Estimation

$$\mathbf{p}^* \in \arg \min_{\mathbf{p} \in P \subset \mathbb{R}^{n_p}} f(\mathbf{p}) = \sum_{i=1}^N \left[\frac{\pi^{calc}(\mathbf{x}_i, \mathbf{p}) - \pi_i^{\exp}}{\pi_i^{\exp}} \right]^2$$

$$\mathbf{p} = (a_0, a_1, a_2, b_0, b_1, b_2)$$

$$\mathbf{x}_i = (w_i, T_i)$$

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

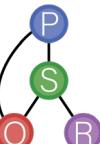
Davidson and
Erickson's working pair²

LiNO₃ + KNO₃ + NaNO₃
(53:28:19)

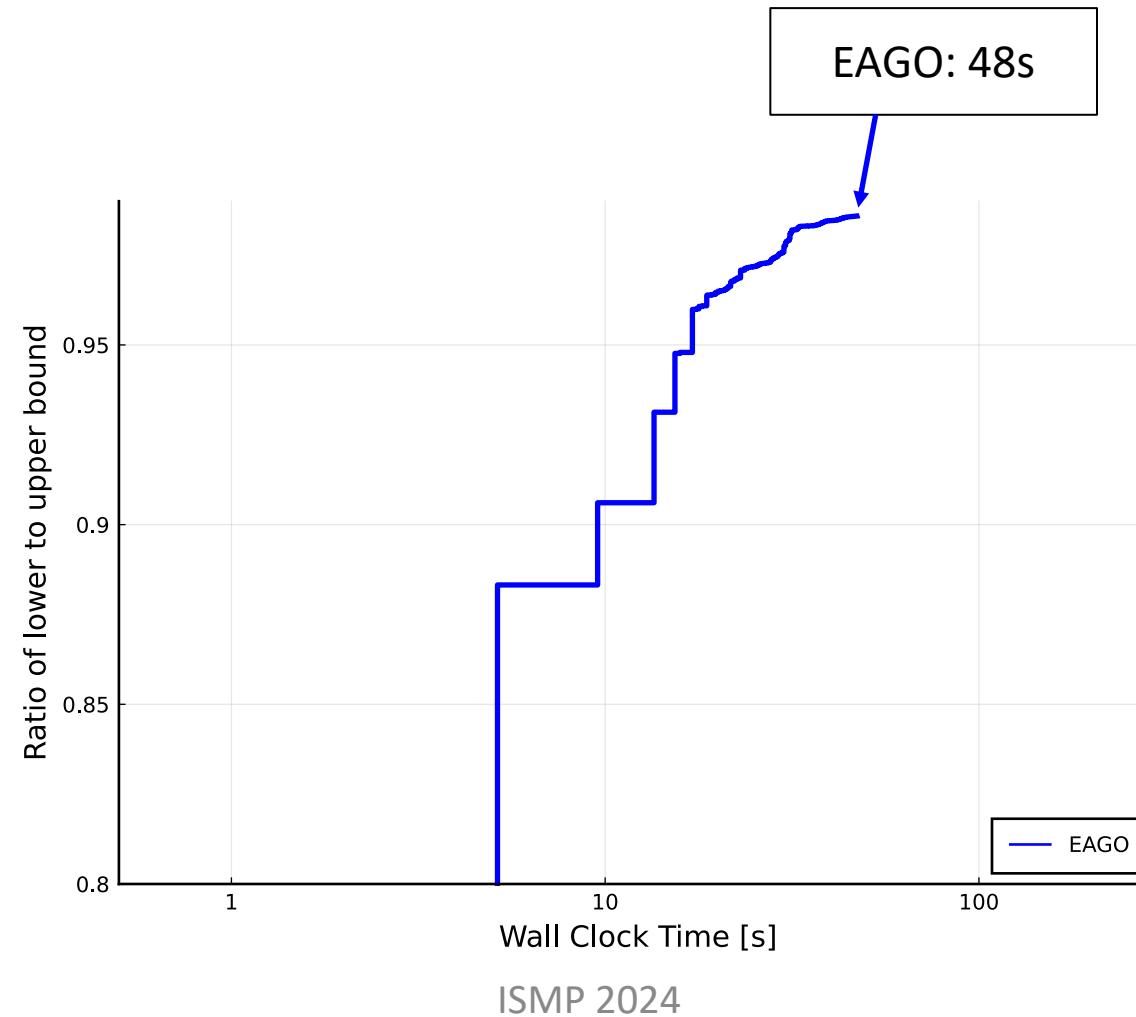
a_0/kPa	8.7369
a_1/kPa	27.0375
a_2/kPa	-21.4172
$b_0/\text{kPa}\cdot\text{K}$	-2432.1378
$b_1/\text{kPa}\cdot\text{K}$	-6955.3785
$b_2/\text{kPa}\cdot\text{K}$	4525.9568

Davidson and Erickson ² working pair			
LiNO ₃ + KNO ₃ + NaNO ₃ (53:28:19)			
p/kPa	w	p/kPa	w
$T = 333.15 \text{ K}$		$T = 353.15 \text{ K}$	
12.38	0.4992	28.33	0.4994
10.40	0.5997	24.17	0.6000
6.31	0.6997	18.00	0.7000
		12.38	0.7493
$T = 373.15 \text{ K}$		$T = 393.15 \text{ K}$	
60.13	0.4997	118.57	0.5004
48.49	0.6006	92.90	0.6015
36.46	0.7003	70.48	0.7008
26.54	0.7495	53.49	0.7500
20.32	0.8000	40.23	0.8004
13.61	0.8503	27.84	0.8506
$T = 413.15 \text{ K}$		$T = 433.15 \text{ K}$	
215.95	0.5014	377.13	0.5030
179.25	0.6033	292.92	0.6054
126.59	0.7017	220.38	0.7031
100.39	0.7508	175.32	0.7520
78.16	0.8011	140.91	0.8022
52.82	0.8511	93.25	0.8519
33.67	0.8998	59.32	0.9003
		38.36	0.9501
$T = 453.15 \text{ K}$		$T = 473.15 \text{ K}$	
596.57	0.5050	920.02	0.5079
496.87	0.6092	789.60	0.6145
361.58	0.7051	564.39	0.7078
288.22	0.7537	451.19	0.7560
229.18	0.8036	357.82	0.8056
159.01	0.8531	249.55	0.8547
101.20	0.9011	162.51	0.9022
63.43	0.9506	99.24	0.9512

8. Álvarez, M.E., et al., **Vapor-liquid equilibrium of aqueous alkaline nitrate and nitrite solutions for absorption refrigeration cycles with high-temperature driving heat**, *Journal of Chemical & Engineering Data* 56 (2011), pp. 491–496.



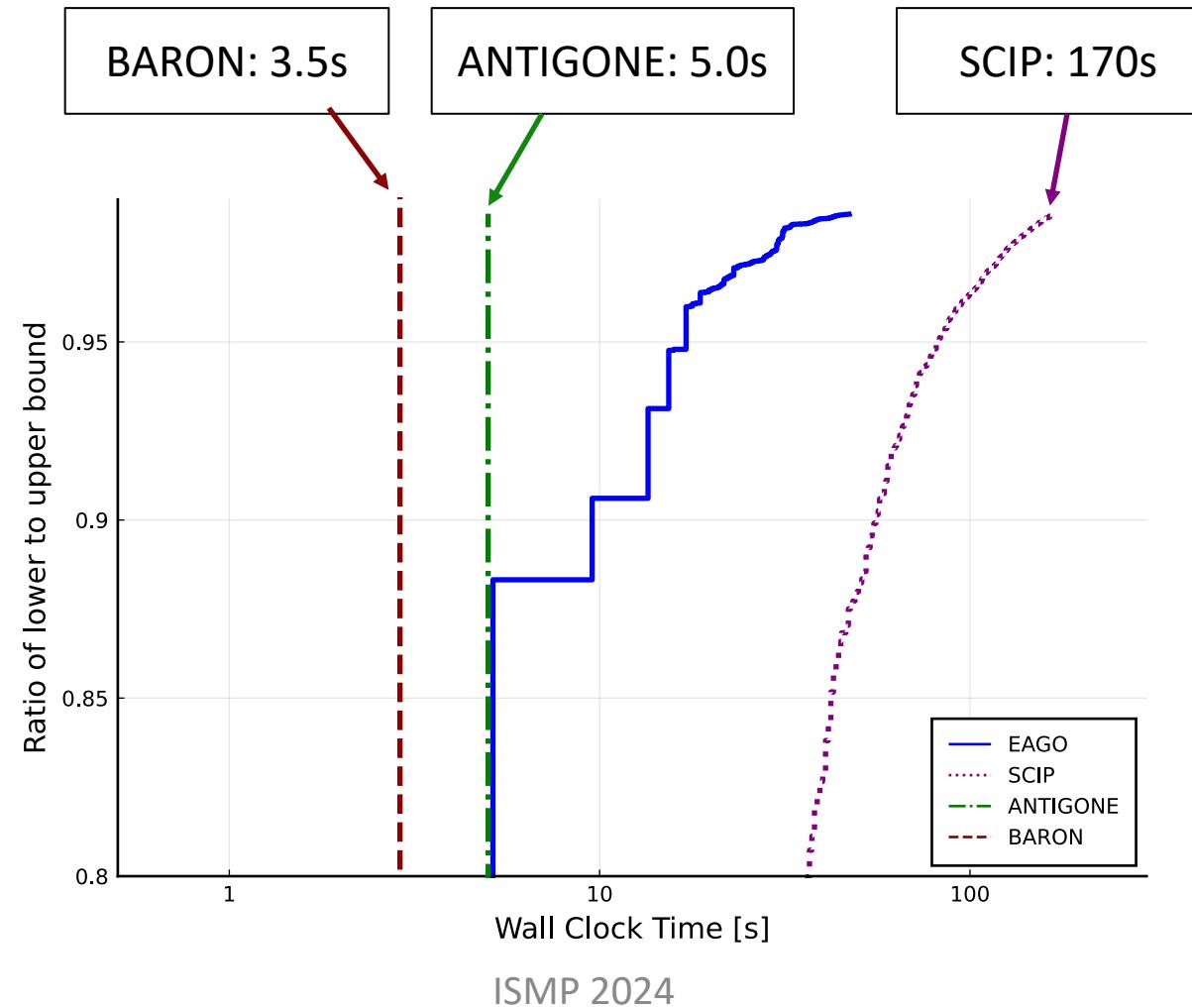
Convergence Plot



*All examples run on an Intel Xeon W-2195 2.30/4.0 GHz (base/turbo) processor, with an NVIDIA Quadro GV100 GPU



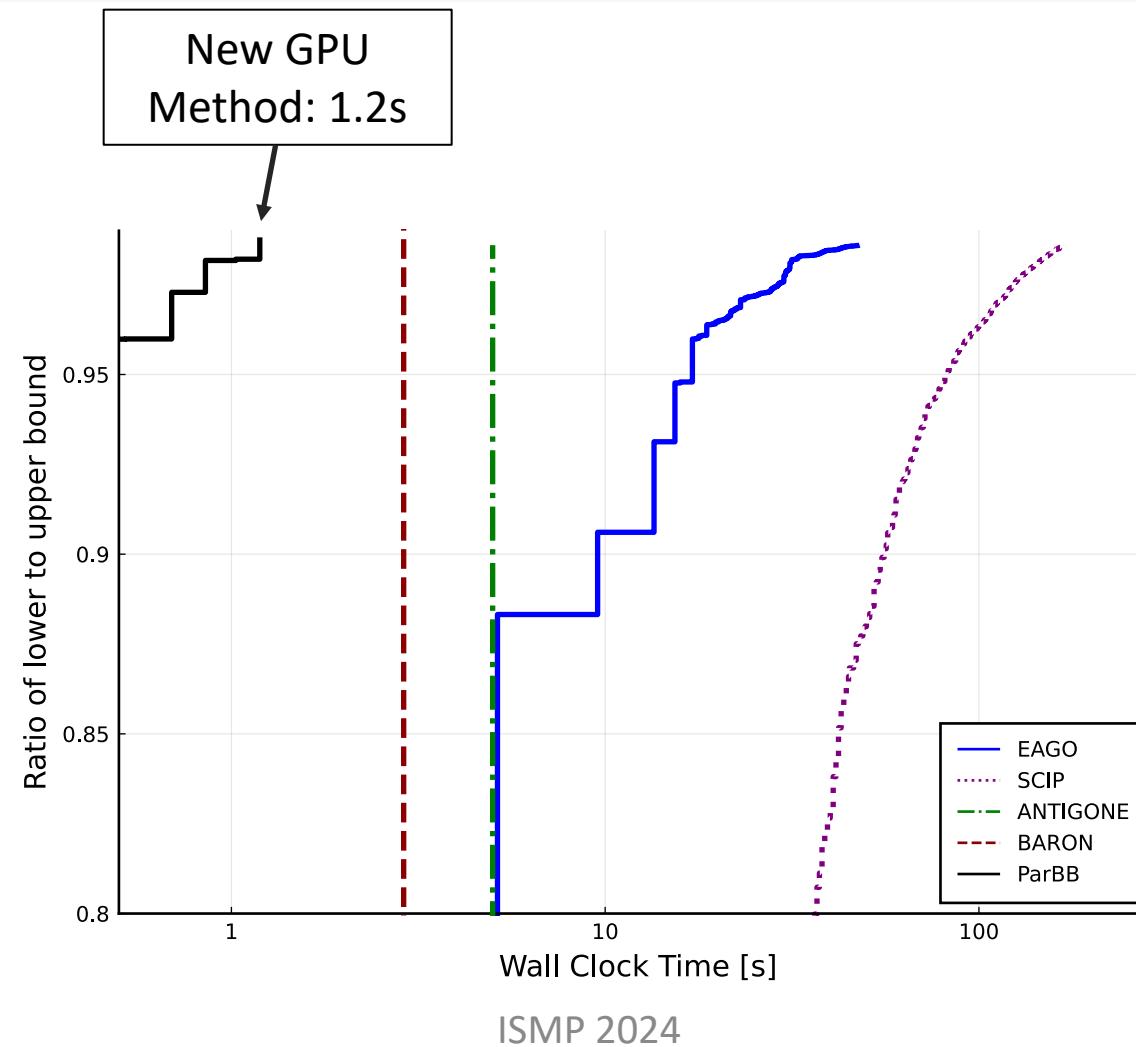
Convergence Plot



*All examples run on an Intel Xeon W-2195 2.30/4.0 GHz (base/turbo) processor, with an NVIDIA Quadro GV100 GPU

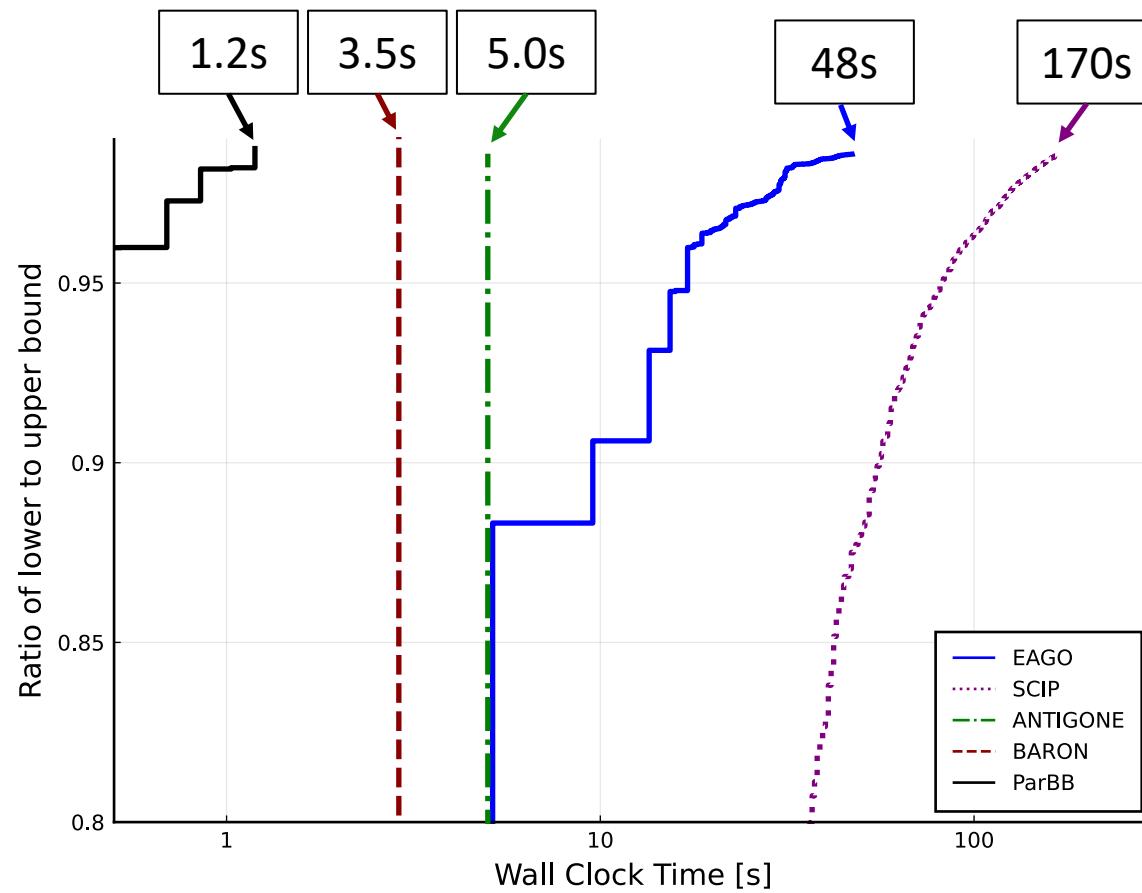


Convergence Plot



*All examples run on an Intel Xeon W-2195 2.30/4.0 GHz (base/turbo) processor, with an NVIDIA Quadro GV100 GPU

Understanding Comparisons



BARON/ANTIGONE

- Problem solved during preprocessing

SCIP

- Evaluated 28161 B&B nodes

EAGO

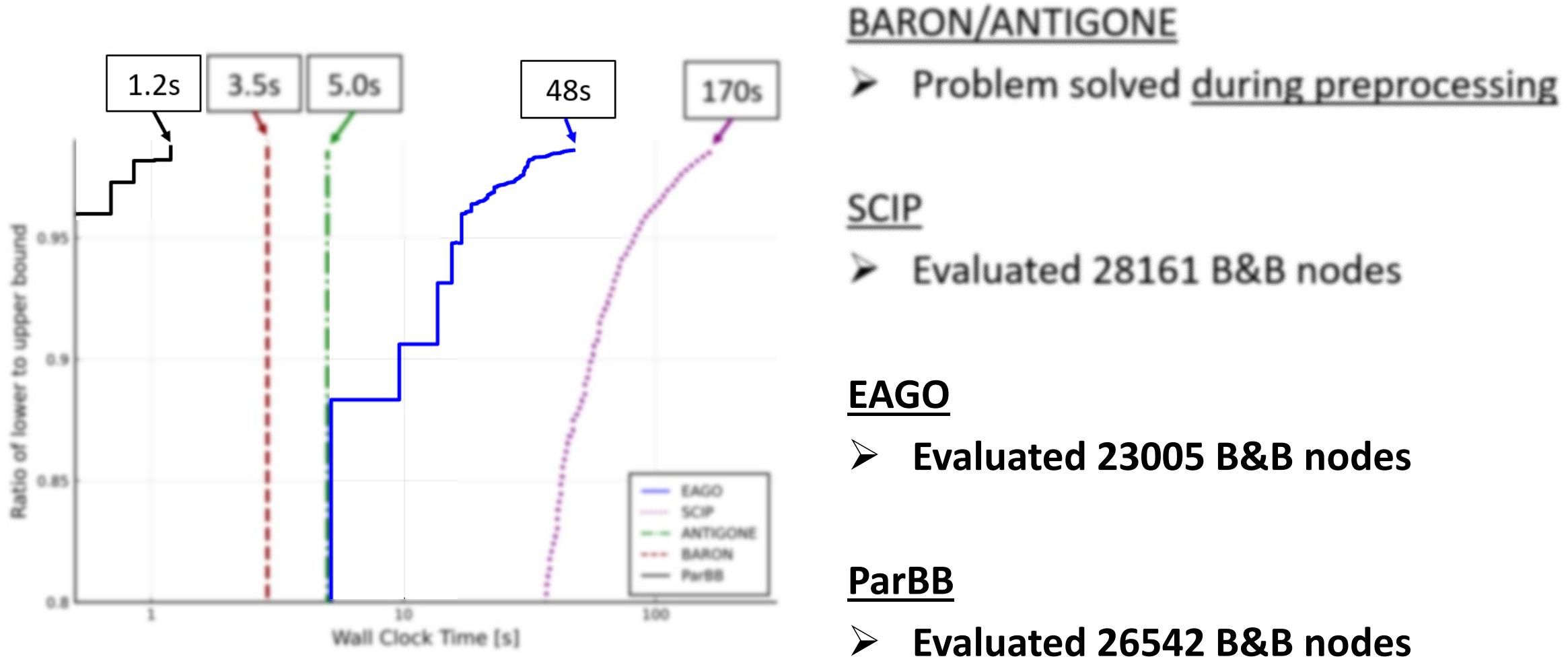
- Evaluated 23005 B&B nodes

ParBB

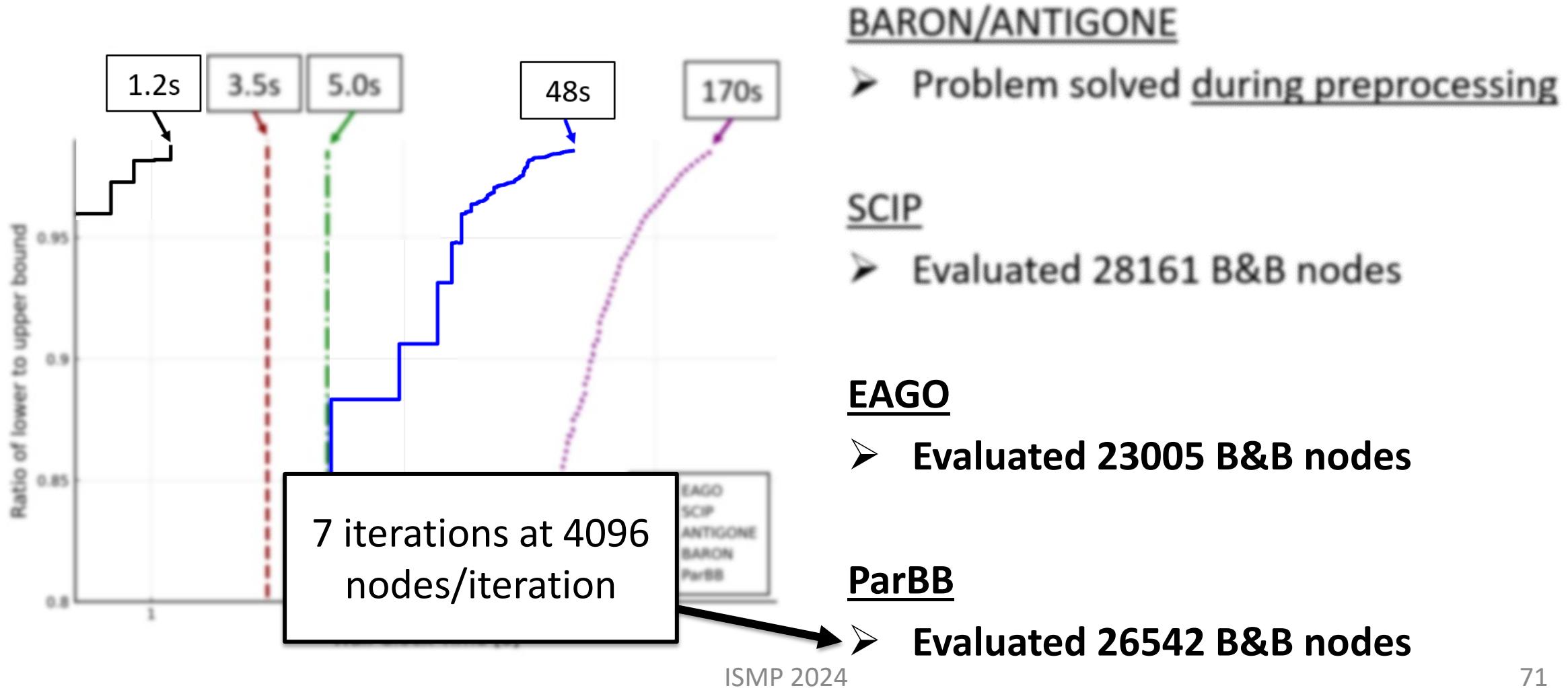
- Evaluated 26542 B&B nodes



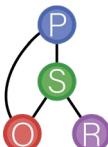
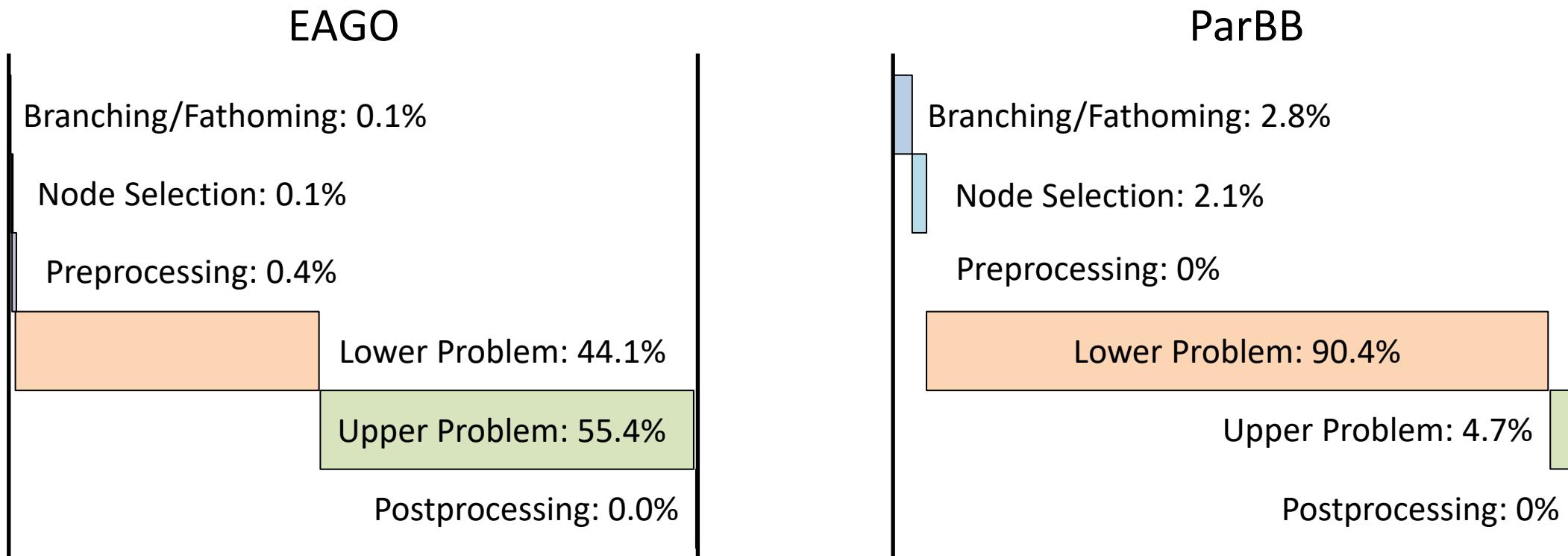
Understanding Comparisons



Understanding Comparisons

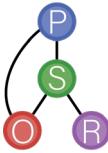
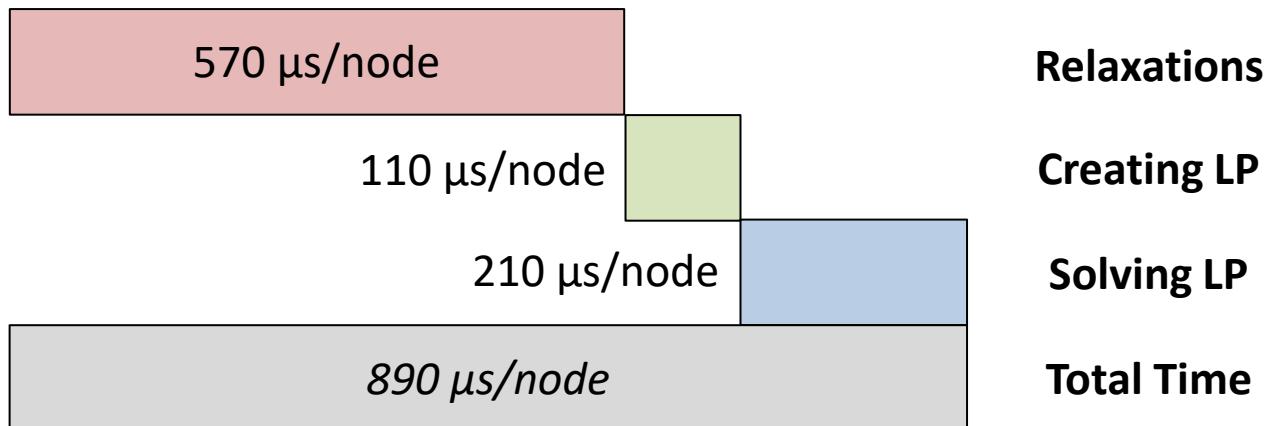


EAGO vs. ParBB Comparison



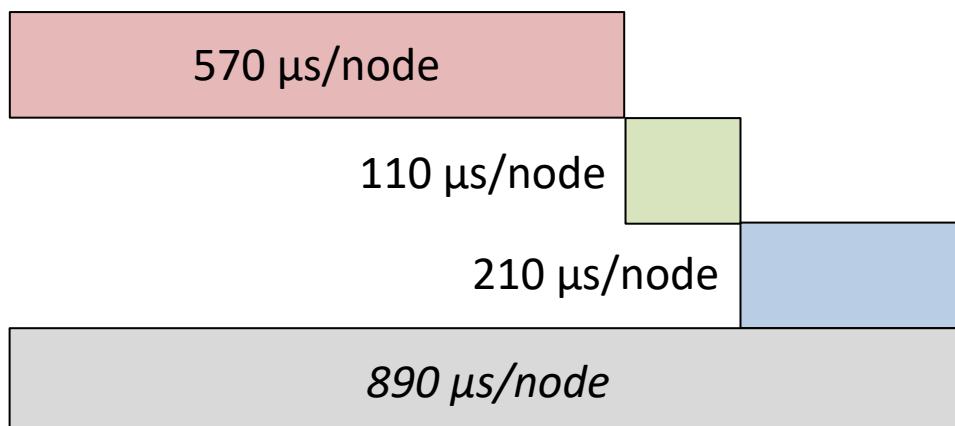
EAGO vs. ParBB Comparison

EAGO's Lower Problem

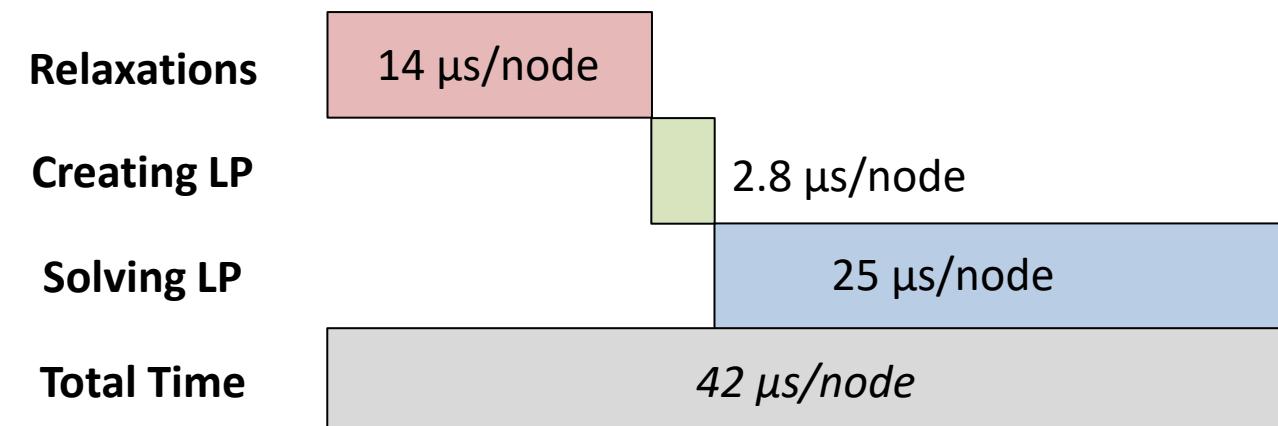


EAGO vs. ParBB Comparison

EAGO's Lower Problem



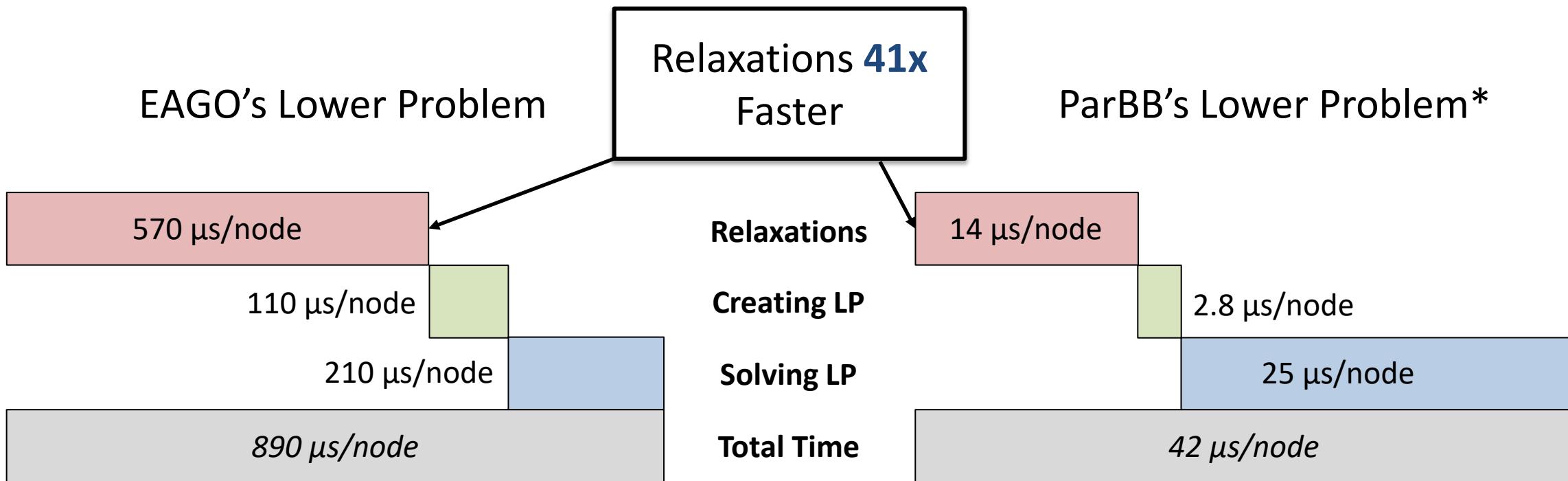
ParBB's Lower Problem*



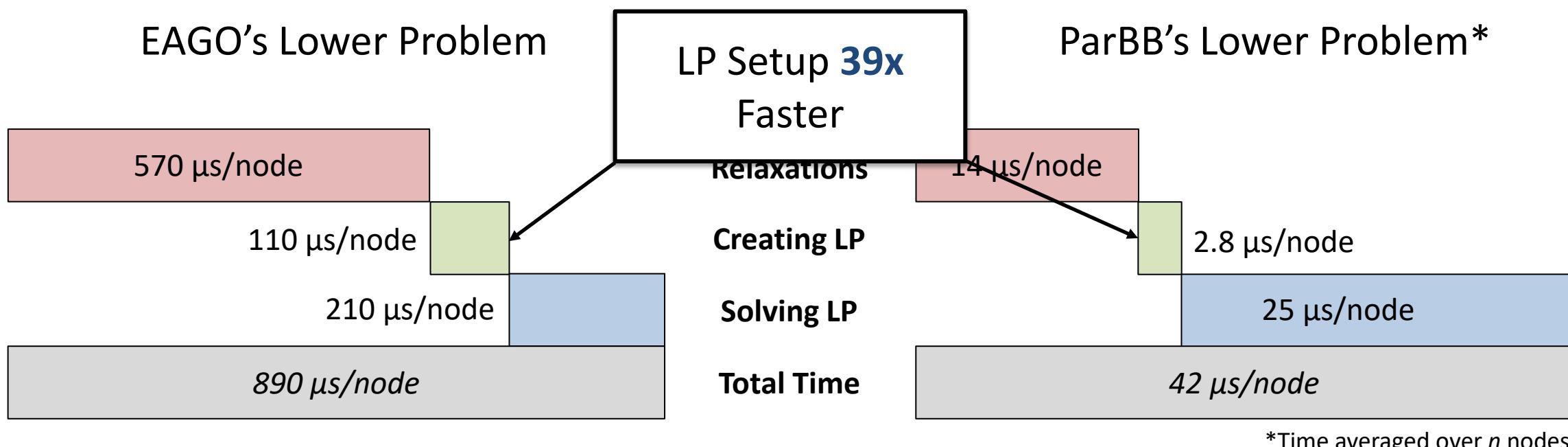
*Time averaged over n nodes



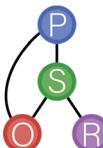
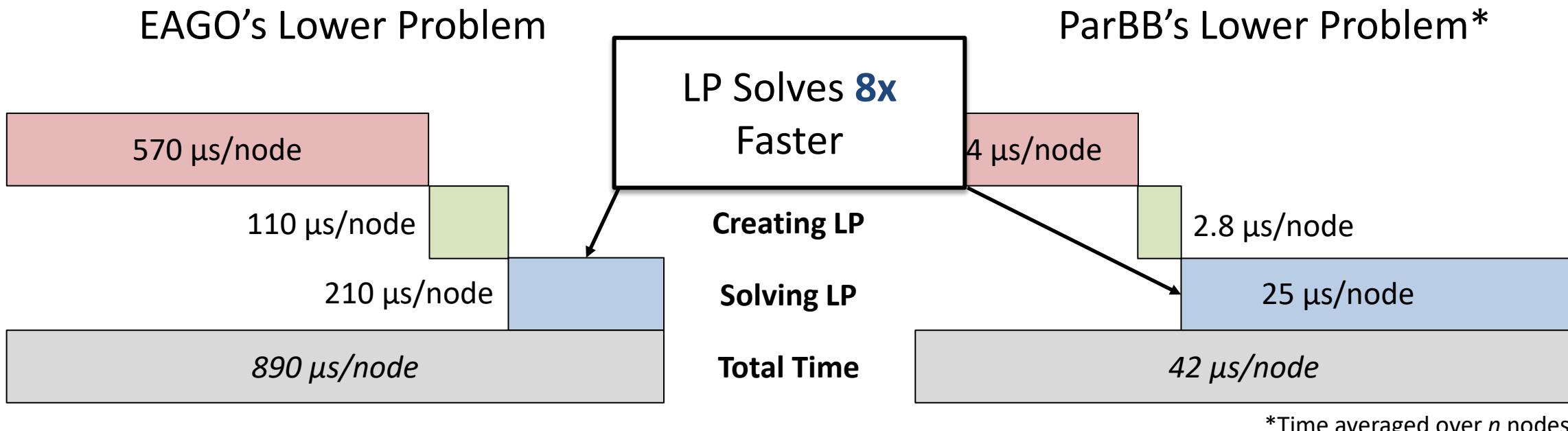
EAGO vs. ParBB Comparison



EAGO vs. ParBB Comparison

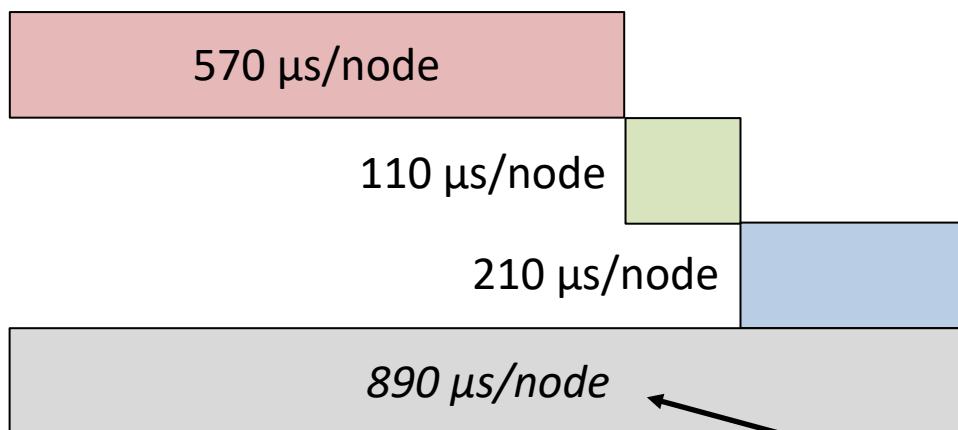


EAGO vs. ParBB Comparison

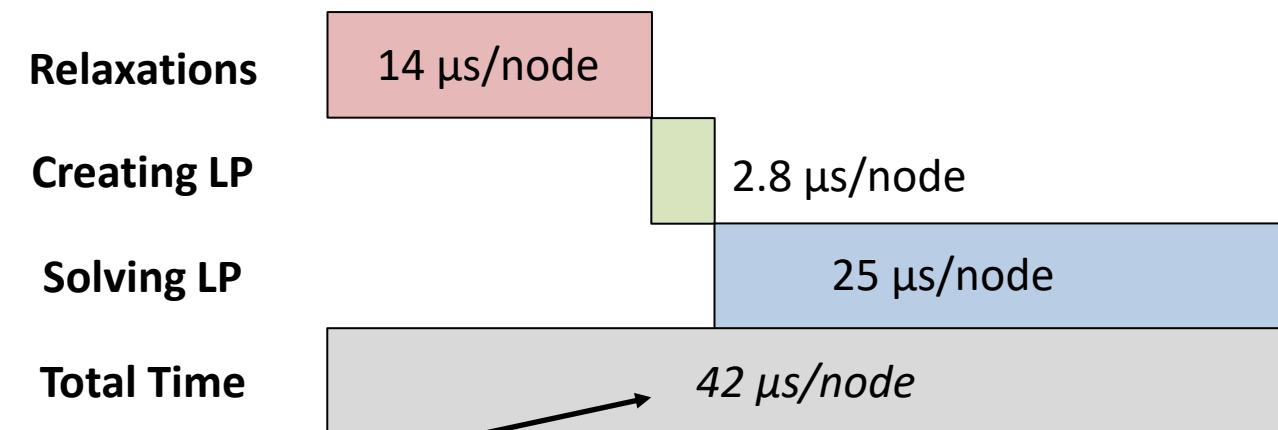


EAGO vs. ParBB Comparison

EAGO's Lower Problem



ParBB's Lower Problem*

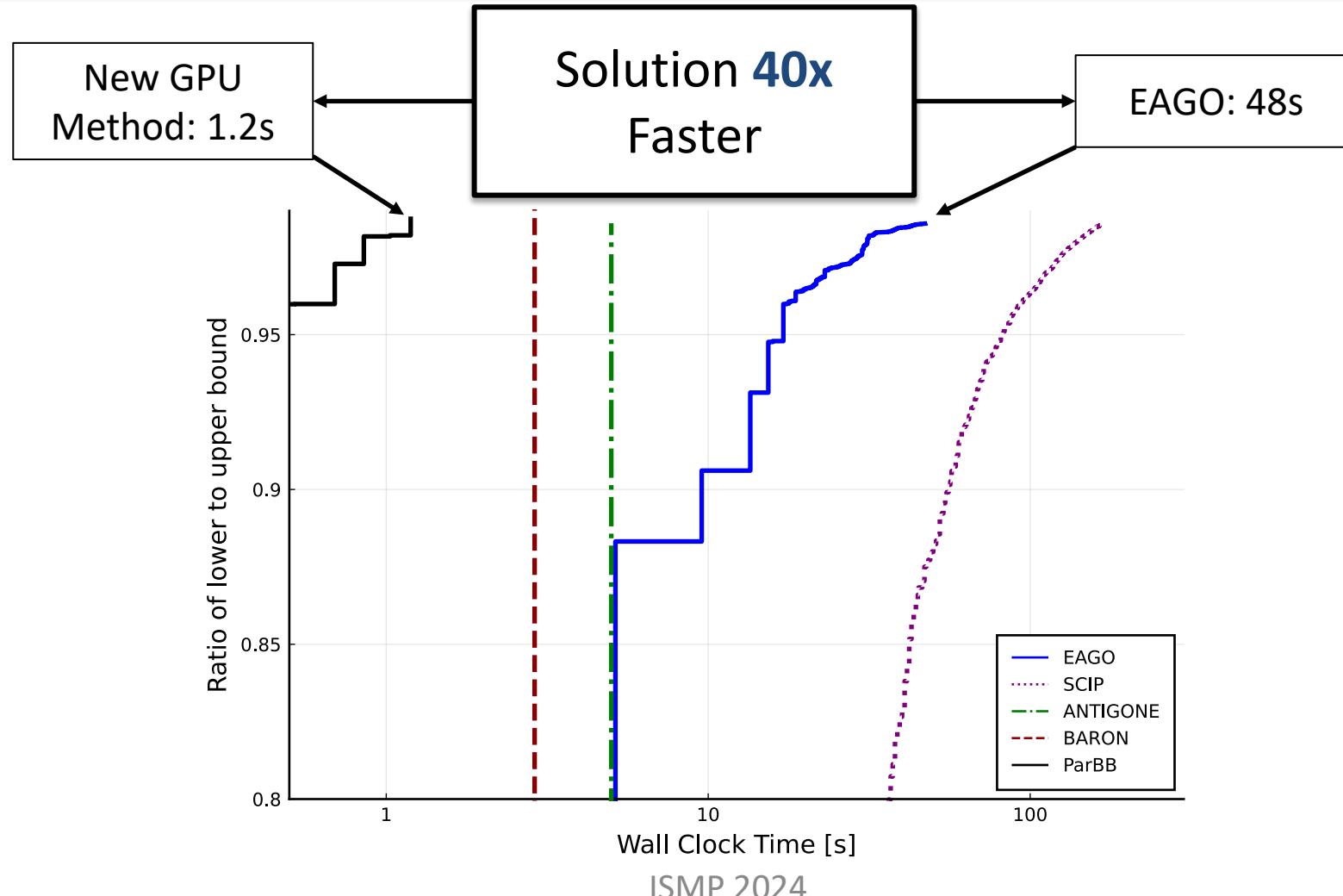


*Time averaged over n nodes

Overall Lower
Problem **21x**
Faster



Convergence Plot



Future Steps

Many avenues of future research

GPU Relaxations

- Automatic subexpression detection and replacement
- Algorithmic CUDA kernel generation

GPU Simplex

- Hot/warm starting after adding cuts
- Adding cycling detection to use faster heuristic than Bland's rule

GPU B&B

- Support for nontrivial constraints*
- MINLP handling
- Parallelized preprocessing (OBBT, FBBT)
- (Long term) Integration with EAGO/JuMP

*Almost there! Coded up, but more testing needed



Acknowledgements

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



Funding:

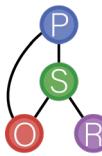
National Science Foundation, Award No.: **1932723**

National Science Foundation, Award No.: **2330054**

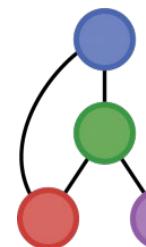
Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation or the United States Government.



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2024 }

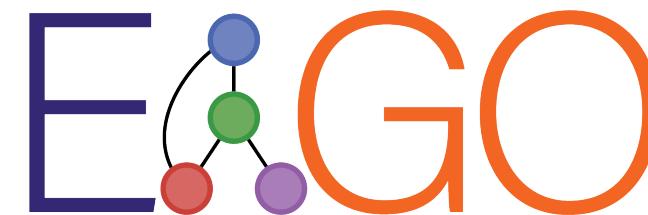


Questions?



Process Systems and
Operations Research
Laboratory

<https://www.psor.uconn.edu>



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

