Advances in EAGO.jl: Updates, Dynamics, and Parallelism

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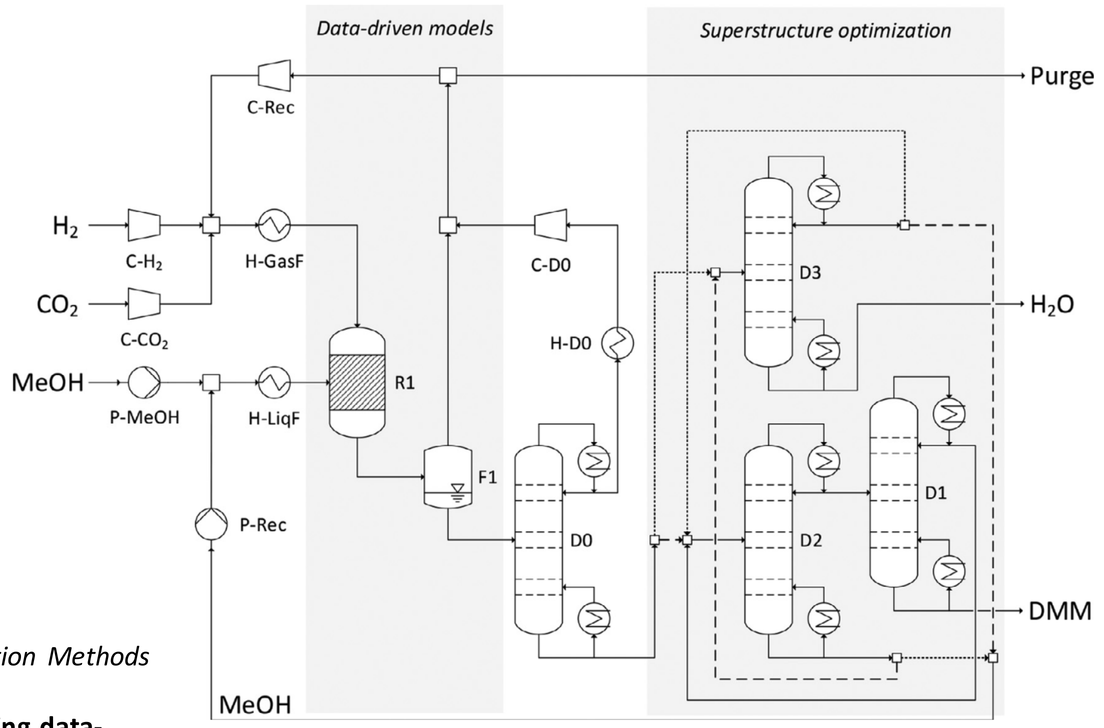
Process Systems and Operations Research Laboratory

EAGO Philosophy

Easy Advanced Global Optimization[1]

Deterministic global optimizer

- High performance
- Easy to formulate complicated problems
- Open-source and free for non-commercial use



1. Wilhelm, M.E., and Stuber, M.D. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, (2022) **37**(2): 425-450.
2. Burre, J., *et al*. **Global flowsheet optimization for reductive dimethoxymethane production using data-driven thermodynamic models.** *Computers & Chemical Engineering*, (2022): 107806.

EAGO Philosophy

Easy Advanced Global Optimization[1]

Research Platform

- Focus on **unsolved problems**
- Designed for **user-defined functions** and custom routines
  - **Anyone** can implement and test new ideas

```julia
import EAGO: Optimizer, GlobalOptimizer

function αBB_relax(Q::Matrix{T},c::Vector{T},xL::Vector{T},xU::Vector{T},x::Real...) where {T<:Float64}
    α=max(0,-minimum(eigvals(Q))/2)
    y = [x[1];x[2]]
    cv = 1/2*y'*Q*y+c'*y+α*(xL-y)'*(xU-y)
    return cv
end

struct αBB_Convex <: EAGO.ExtensionType end
import EAGO: lower_problem!
function EAGO.lower_problem!(t::αBB_Convex, opt::GlobalOptimizer)···
end
```

1. Wilhelm, M.E., and Stuber, M.D. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, (2022) **37**(2): 425-450.

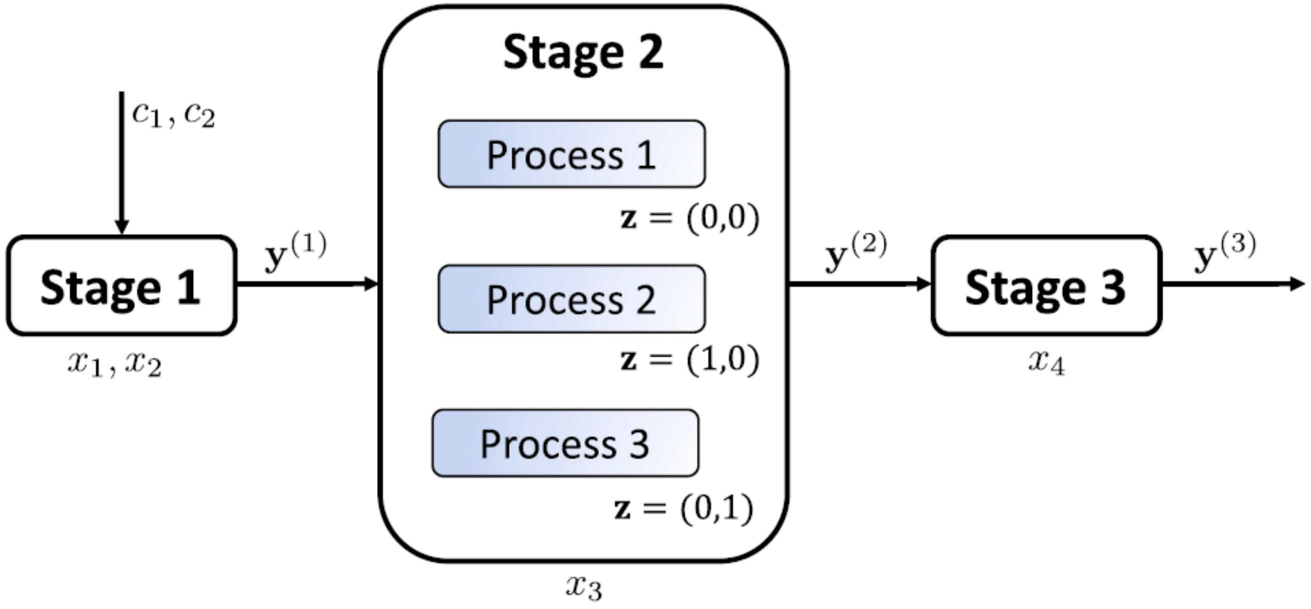
MINLP Example

Process parameters:

$$\hat{y}_1^{(1)}(\mathbf{x}) = 3.55 + 0.27c_1 + 0.58c_2 + 60.6x_2 - 2.8c_1x_2 - 2.3c_2x_2,$$

$$\hat{y}_1^{(2)}(\mathbf{x},\mathbf{z}) = 126586.5 - 21466.8\hat{y}_1^{(1)}(\mathbf{x}) + 520.43x_3 + 56.29z_1 + 315.95z_2 - 43.72x_3\hat{y}_1^{(1)}(\mathbf{x}) + 3.74x_3^2 + 910.1\hat{y}_1^{(1)}(\mathbf{x})^2 - 30.6\hat{y}_1^{(1)}(\mathbf{x})z_1 - 173.17\hat{y}_1^{(1)}(\mathbf{x})z_2,$$

$$\hat{y}_1^{(3)}(\mathbf{x},\mathbf{z}) = 9.16 + 0.092x_3 + 0.73x_4 + 0.64x_3x_4 - 0.49x_4^2 - 0.13x_4\hat{y}_1^{(2)}(\mathbf{x},\mathbf{z}) + 0.0019\hat{y}_1^{(2)}(\mathbf{x},\mathbf{z})^2 + 0.018\hat{y}_1^{(2)}(\mathbf{x},\mathbf{z}),$$



Reduced space formulation:

$$f^* = \min_{\mathbf{x}\in X, \mathbf{z}\in Z} \left(\hat{y}_1^{(3)}(\mathbf{x},\mathbf{z}) - \eta\right)^2$$

$$\text{s.t.} \quad z_1 + z_2 \leq 1$$

$$X = [7, 10] \times [0.1, 0.3] \times [-1.078, 1.078] \times [-1.078, 1.078]$$

$$c_1 = 0.001, \quad c_2 = 0.03$$

2. Wilhelm, M.E., & Stuber, M.D. **Improved Convex and Concave Relaxations of Composite Bilinear Forms**. *Journal of Optimization Theory and Applications*, **197** (2023): 174-204.

MINLP Example

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```julia
# Set up the model
m = Model(EAGO.Optimizer(SubSolvers(; r = GLPK.Optimizer())))

# Write out process parameters
c = [0.001; 0.03]
η = 5.0
y1ex = :(3.55 + 0.27*$(c[1]) + 0.58*$(c[2]) + 60.6*$(x[2]) - 2.8*$(c[1])*$(x[2]) -
            2.3*$(c[2])*$(x[2]))
y2ex = :(126585.5 - 21466*$y1ex + 520.43*$(x[3]) + 56.29*$(z[1]) + 315.95*$(z[2]) -
            43.72*$(x[3])*$(y1ex) + 3.74*$(x[3])^2 + 910.1*$y1ex^2 - 30.6*$y1ex*$(z[1]) -
            173.17*$y1ex*$(z[2]))
y3ex = :(9.16 + 0.092*$(x[3]) + 0.73*$(x[4]) + 0.64*$(x[3])*$(x[4]) - 0.49*$(x[4])^2 -
            0.13*$(x[4])*$y2ex + 0.0019*$y2ex^2 + 0.018*$y2ex)

# Define optimization problem variables
xL = [7.0; 0.1; -1.078; -1.078]
xU = [10.0; 0.3; 1.078; 1.078]
@variable(m, xL[i] <= x[i=1:4] <= xU[i])
@variable(m, z[i=1:2], Bin)

# Define constraints
@constraint(m, z[1] + z[2] <= 1)

# Define the objective function
@NLobjective(m, Min, (y3ex - η)^2)

# Optimize
optimize!(m)
```

2. Wilhelm, M.E., & Stuber, M.D. **Improved Convex and Concave Relaxations of Composite Bilinear Forms**. *Journal of Optimization Theory and Applications*, **197** (2023): 174-204.

Anaerobic Digestion

- U.S. wastewater treatment:
  - ~2% of energy consumption[3]
  - ~0.7% of greenhouse gas emissions[4]
- Both costs can be offset by utilizing **anaerobic digestion (AnD)** and a **combined heat and power (CHP)** system
- Common models of AnD are **complicated**
  - High-dimensional
  - Dynamic
  - Challenging to optimize

Photo credit: https://glsd.org

3. EPA. Energy efficiency for water utilities, March 2022. URL https://www.epa.gov/sustainable-water-infrastructure/energy-efficiency-water-utilities.
4. EPA. Inventory of U.S. greenhouse gas emissions and sinks: 1990-2020. Technical Report EPA 430-R-22-003, U.S. Environmental Protection Agency, 2022. URL https://www.epa.gov/ghgemissions/draft-inventory-us-greenhouse-gas-emissions-and-sinks-1990-2020.

McCormick Relaxations of Factorable Functions

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

Auxiliary Variable Method

$$\mathbf{z}_1 = \mathbf{g}(\mathbf{x})$$

$$\vdots$$

$$\mathbf{z}_n = \mathbf{h}(\mathbf{x})$$

$$\mathbf{y} = \mathbf{f}(\mathbf{z}_1, \ldots, \mathbf{z}_n)$$

→ **Relaxations of *f at (x, z) on (X, Z)***

McCormick-Based Relaxations[5,6]

Relaxations of g at x on X

⋮

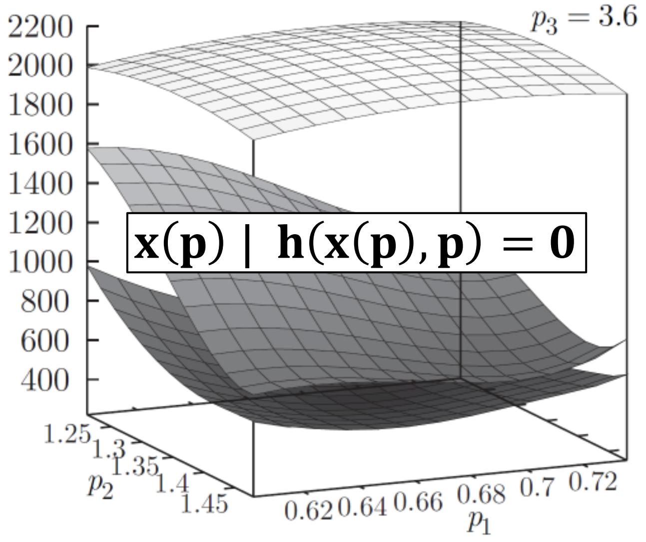
Relaxations of h at x on X

→ *Apply composite relaxation rules* → **Relaxations of *f at x on X***

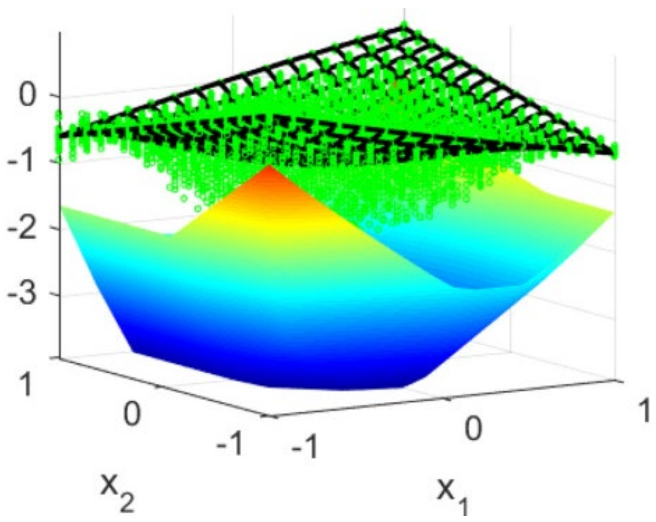
5. Mitsos, A., et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
6. Scott, J.K., et al. **Generalized McCormick relaxations.** *Journal of Global Optimization* 51.4 (2011): 569-606.

Reduced Space Relaxations

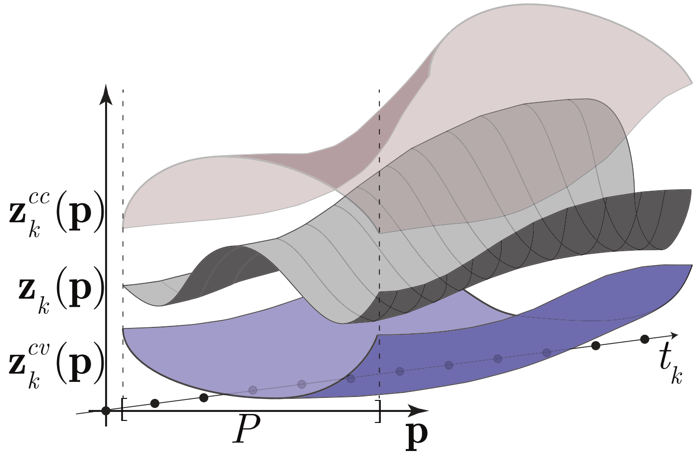
Implicit Functions[7]



Continuous Random Variables[8]



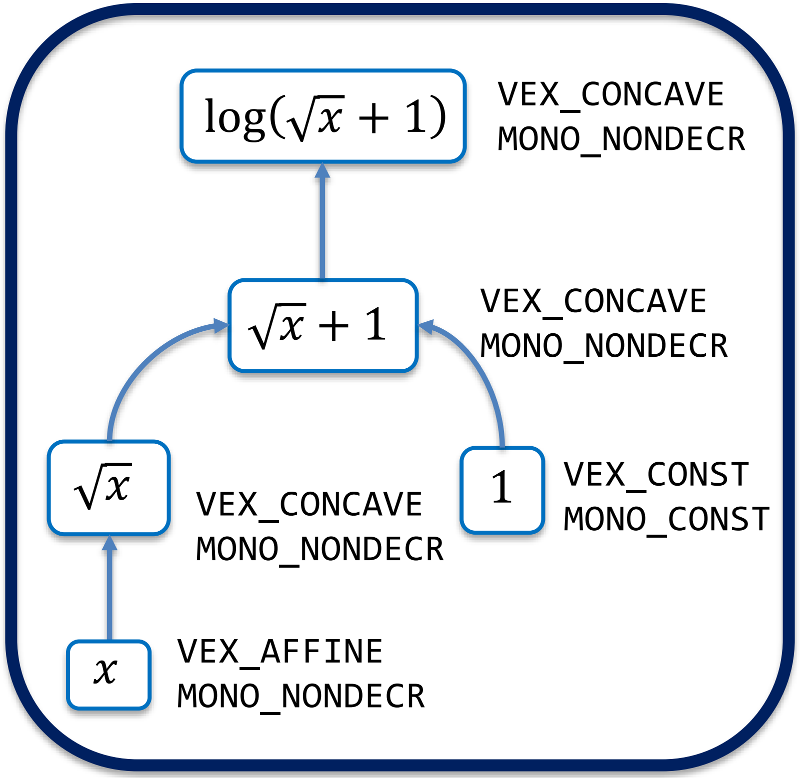
ODEs and DAEs[9]



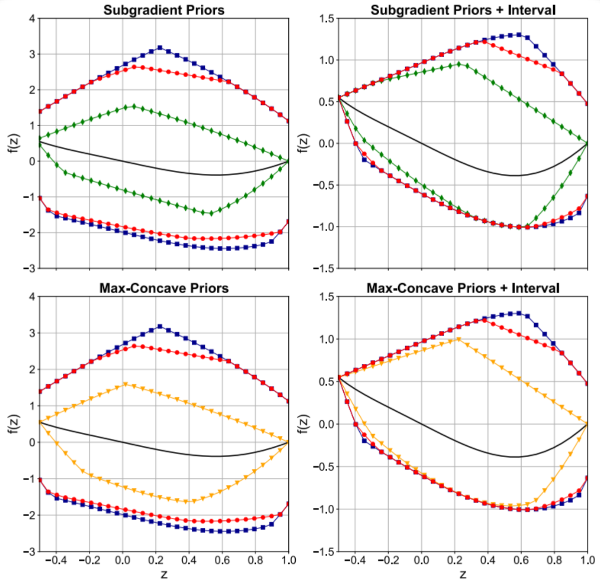
7. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* 30, (2015), 424-460
8. Shao, Y. and Scott J.K. **Convex relaxations for global optimization under uncertainty described by continuous random variables**, *AIChE Journal*, (2018): 3023 – 3033.
9. Wilhelm, M.E.; Le, A.V.; and Stuber, M.D. **Global Optimization of Stiff Dynamical Systems.** *AIChE Journal: Futures Issue,* 65 (12), (2019).

Additional Features

Built-in Convexity Detection (Disciplined Convex Programming[10], etc.)



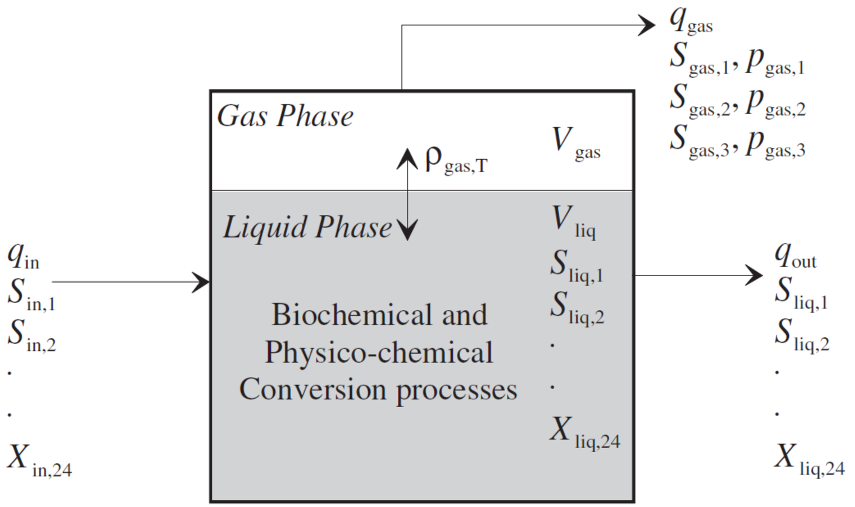
Improved Composite Bilinear Relaxations[2]



2. Wilhelm, M.E., & Stuber, M.D. **Improved Convex and Concave Relaxations of Composite Bilinear Forms**. *Journal of Optimization Theory and Applications*, **197** (2023): 174-204.
5. Mitsos, A., et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
10. Grant, M., Boyd, S., & Ye, Y. (2006). **Disciplined convex programming.** In *Global optimization* (pp. 155-210). Springer, Boston, MA.
11. Tsoukalas, A., and Mitsos, A. **Multivariate McCormick relaxations**. *Journal of Global Optimization*, 59.2-3 (2014): 633-662.

Addressing AnD Optimization

- Optimization of a **dynamical system**
- **Hybrid modeling** approach
  - Complex mechanistic model
  - Integrated machine learning elements
- **Higher dimensionality** than typical solvable global optimization problems



$$\frac{dS_{gas,i}}{dt} = \frac{V_{liq}\rho_{i,T}}{V_{gas}} - \frac{q_{gas}S_{gas,i}}{V_{gas}}$$

$$\frac{dS_{liq,i}}{dt} = \frac{q_{in}S_{in,i}}{V_{liq}} - \frac{q_{out}S_{liq,i}}{V_{liq}} - \rho_{i,T} + \sum_{j=1-19} \rho_j \nu_{i,j}$$

$$\frac{dX_{liq,i}}{dt} = \frac{q_{in}X_{in,i}}{V_{liq}} - \frac{q_{out}X_{liq,i}}{V_{liq}} + \sum_{j=1-19} \rho_j \nu_{i,j}$$

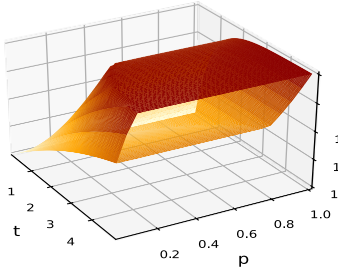
Addressing AnD Optimization

Global Dynamic Optimization

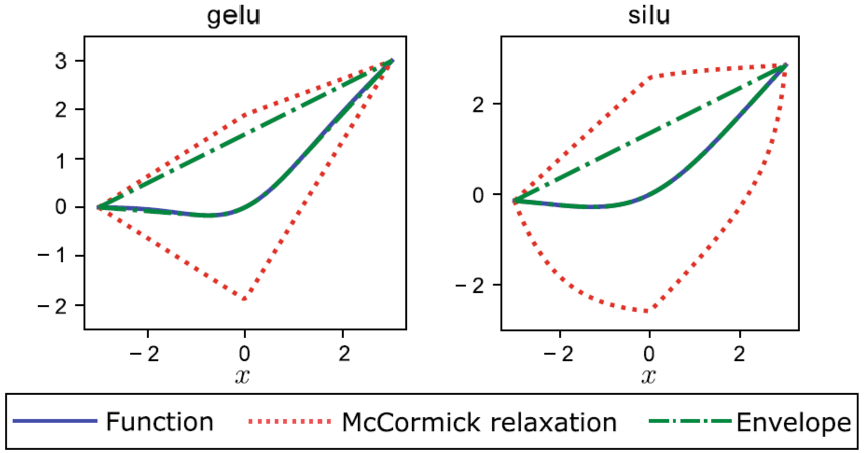
DynamicBounds.jl[12]

$$\frac{dx}{dt} = \exp(p)\sin(x)(2 - x),$$

$$x(0) = 1, \quad p \in [0.01,1], \quad t \in [0,5]$$



Activation Function Envelopes[13]



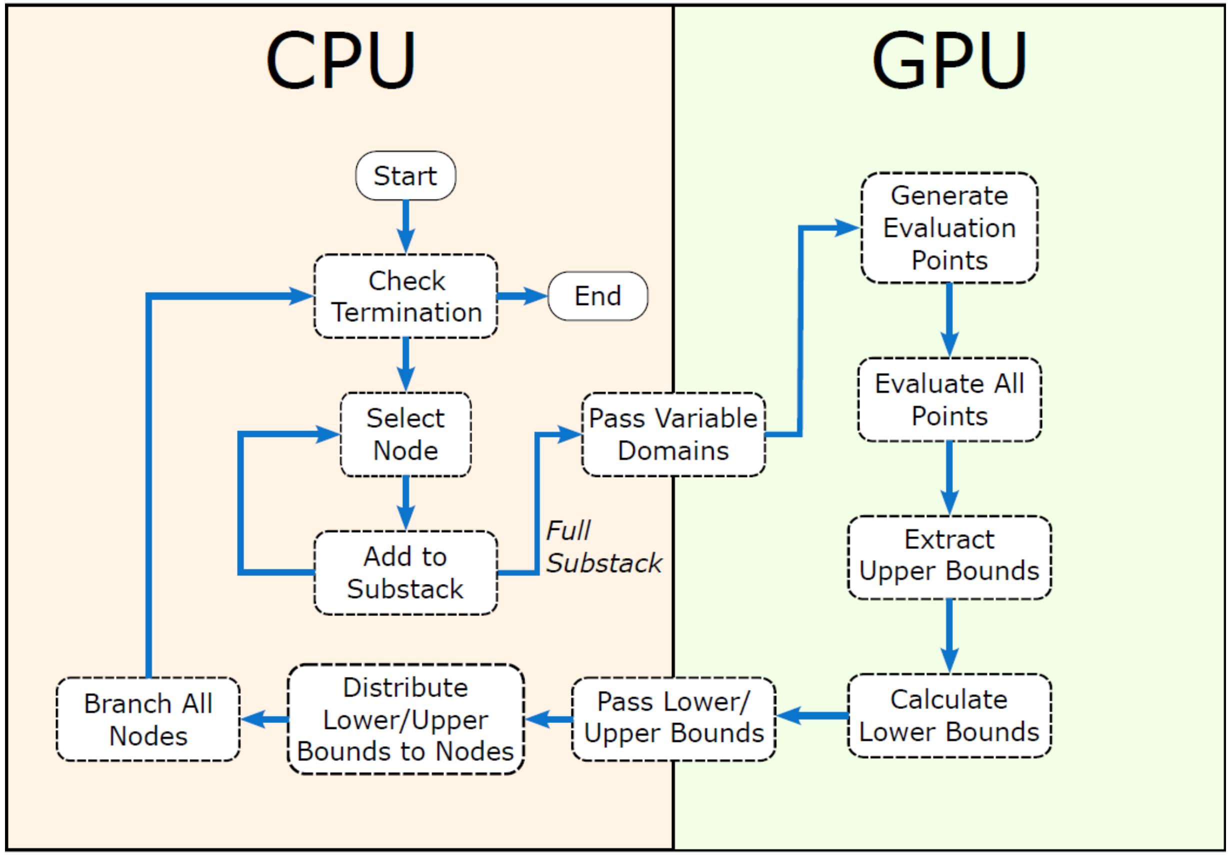
- Enables global optimization with embedded ANN surrogate models

12. Wilhelm, M. E., **DynamicBounds.jl**, (2020), GitHub repository, https://github.com/PSORLab/DynamicBounds.jl
13. Wilhelm, M.E., Wang, C., Stuber, M.D. **Convex and concave envelopes of artificial neural network activation functions for deterministic global optimization.** *Journal of Global Optimization* (2022)

Parallelism

Working GPU-based algorithm

- **SourceCodeMcCormick.jl**[14]
- EAGO will soon incorporate **GPU acceleration** option
- Will also add **multi-core CPU** support at solver level rather than only subsolvers



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

Other Notable Updates

EAGO v0.8

- **Fully compatible** with latest version of JuMP
  - Major changes to backend nonlinear expression handling
- Additional **use-case examples**
- **Improved formatting** for outputs, docstrings, and comments

On the horizon:

- Migrating features into "extensions"
  - More consistent user experience
- Documentation website overhaul

JUMP v1.16.0

EAGO-notebooks

Conclusions

EAGO — An extensible deterministic global optimizer

- **High performance solver**
- **Open-source and free** for non-commercial use
- Designed for **user-defined functions** and routines

Future Outlook

- Parallel computing capability (GPU/CPU)
- Improvements to user-friendliness
- Updates to documentation

Process Systems and Operations Research Laboratory

EAGO

julia

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Questions?

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EAGO

https://www.psor.uconn.edu

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