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# Reduced-Space Optimization of Data-Driven Hybrid Models in EAGO.jl


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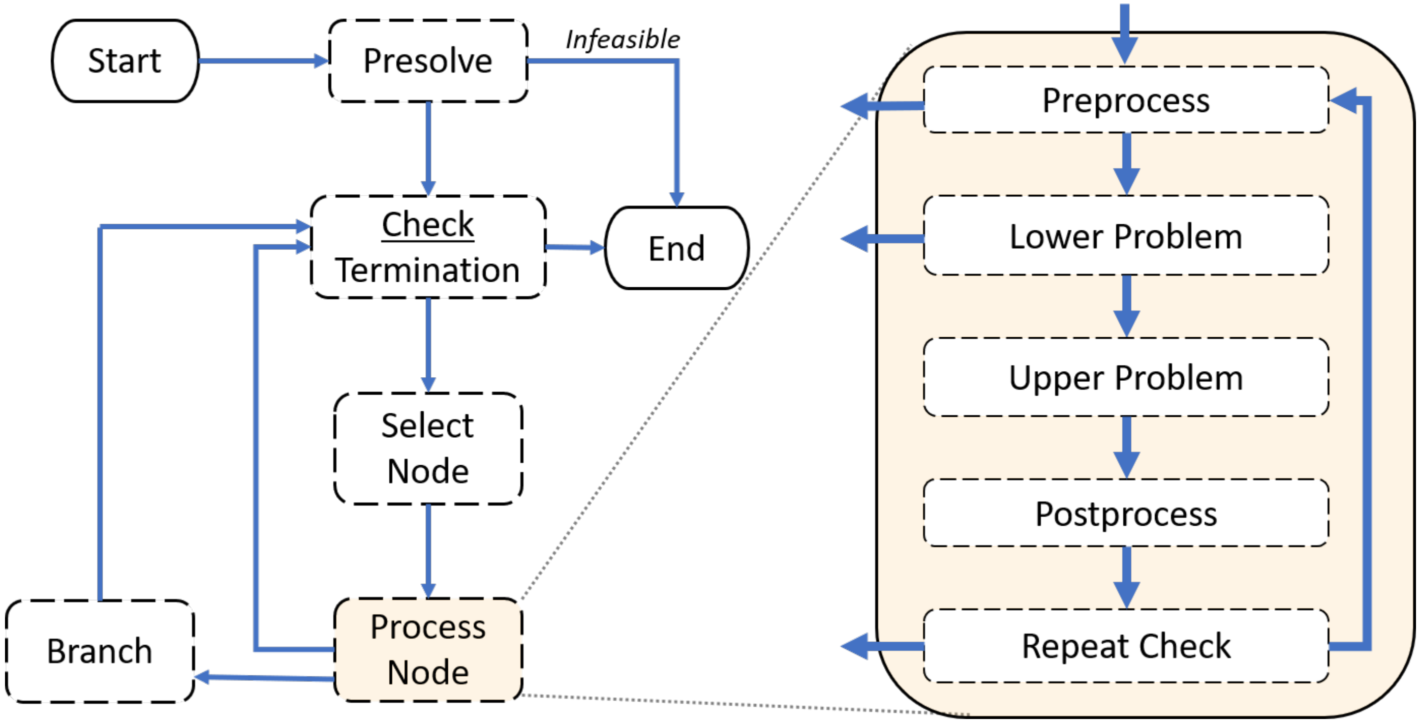
Process Systems and Operations Research Laboratory

# EAGO.jl: Global Deterministic Optimization of Simulations

- EAGO.jl: A deterministic global optimizer in JuMP/Julia (for nonconvex MINLP via branch-and-cut)

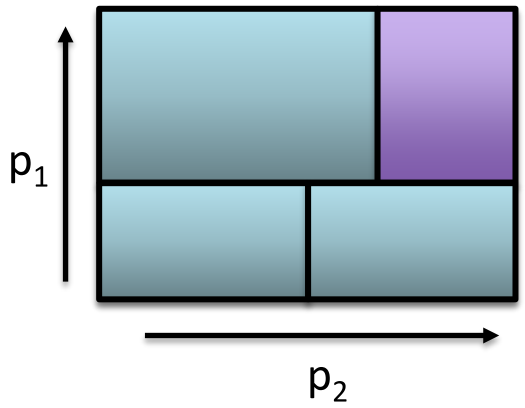



1. Wilhelm, M.E., and Stuber, M.D.. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, 1-26.

# EAGO.jl: Global Deterministic Optimization of Simulations

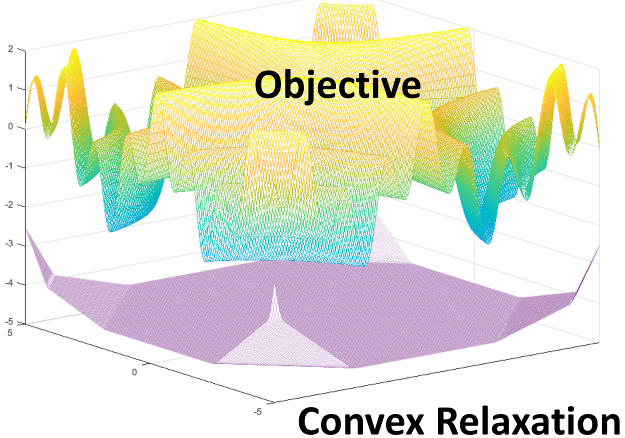
- EAGO.jl: A deterministic global optimizer in JuMP/Julia (for nonconvex MINLP via branch-and-cut)
- Can solve formulations with **user-defined expressions (simulations, etc.)**
- Uses composite relaxation framework which enables expansion to an esoteric set of problems

*(Domain of Active Node)*




Generalized McCormick Operator Arithmetic[2,3]

*(Relaxation of Objective and Constraints)*




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

# EAGO.jl: McCormick Relaxations

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

**Relaxations of g(x) at x in X**

**…**

**Relaxations of h(x) at x in X**

*Apply* **f** *composite relaxation rules*

**Relaxations of f(x) at x in X**

## Akin to automatic differentiation but computes relaxations instead of derivatives

- **EAGO generates relaxations of complicated nonlinear expressions using a McCormick relaxation methodology**[2,3]
- **Intrinsic library of relaxations**
- **Hybrid source-code transformation approach**
  - Method overloading for basic functions.
  - Store and analyze graph structure as well.

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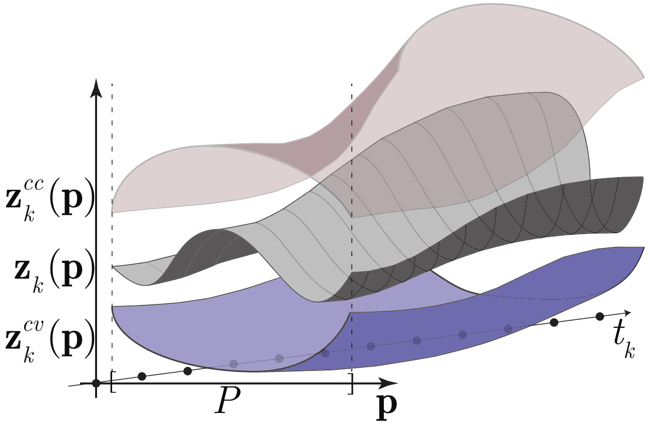
# New Applications

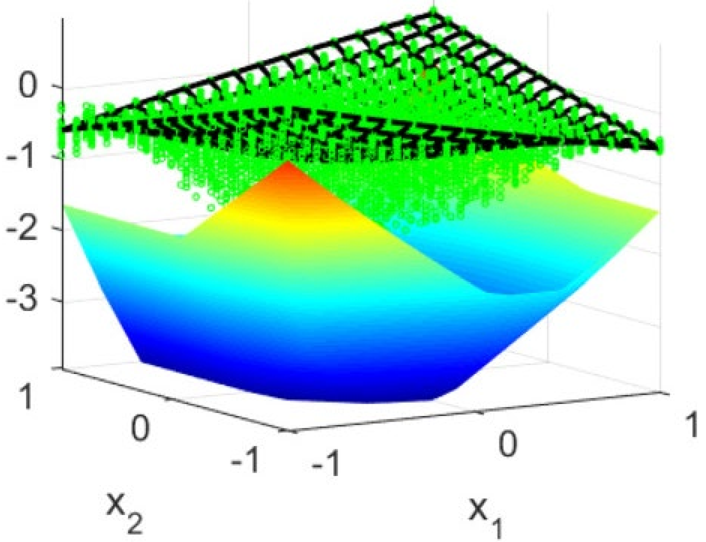
### Implicit Functions[4]

$$\mathbf{x}(\mathbf{p}) \mid \mathbf{h}(\mathbf{x}(\mathbf{p}), \mathbf{p}) = \mathbf{0}$$

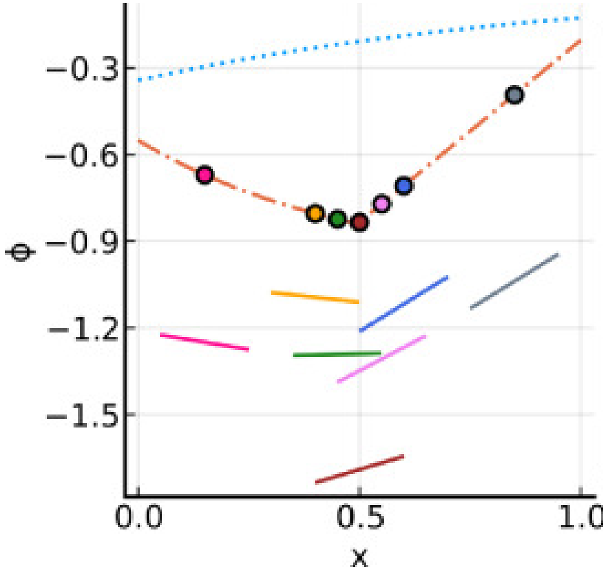
### ODEs and DAEs[5]




### Continuous Random Variables[6]




### Blackbox Functions[7]





4. Stuber, MD et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
5. Wilhelm, ME; Le, AV; and Stuber. MD. **Global Optimization of Stiff Dynamical Systems.** *AIChE Journal: Futures Issue,* 65 (12), *2019*
6. Shao, Y and Scott JK. **Convex relaxations for global optimization under uncertainty described by continuous random variables**, *AIChE Journal*, (2018): 3023 – 3033.
7. Song, Y; Cao, H; Mehta, C; and Khan KA. **Bounding Convex Relaxations of Process Models from Below by Tractable Black-Box Sampling**, *Computers & Chemical Engineering*, In Press, (2021).

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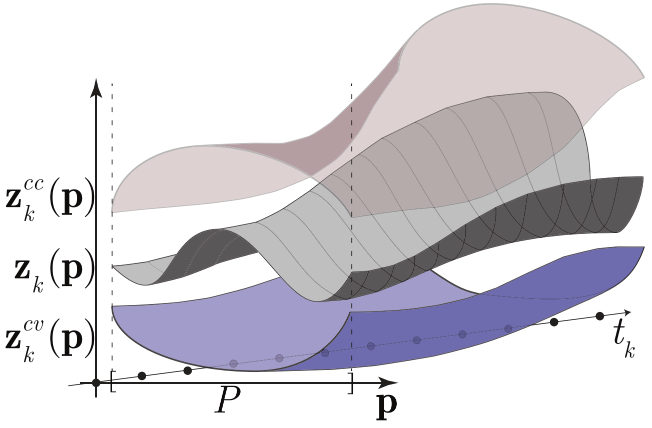


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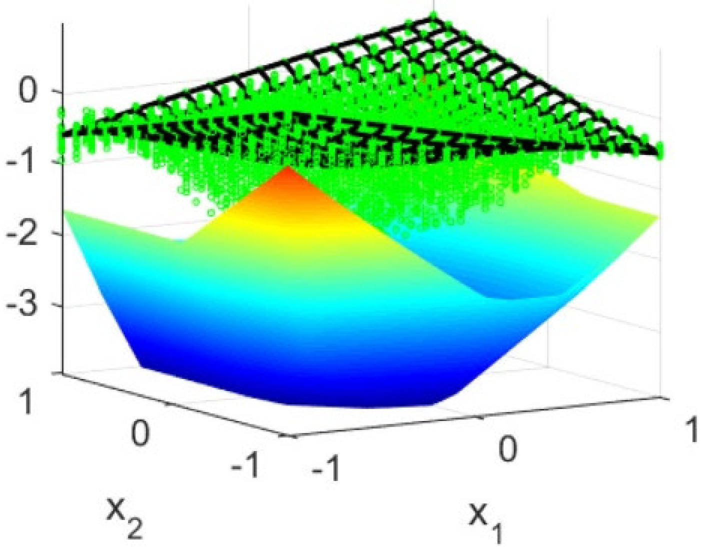


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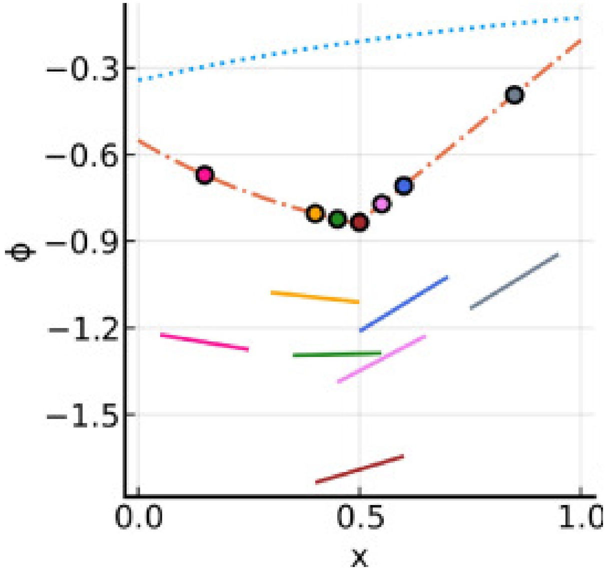


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# EAGO.jl: Extended Nonlinear

**New multi-graph representation:**

- Extends JuMP + EAGO backend to introduce auxiliary variables

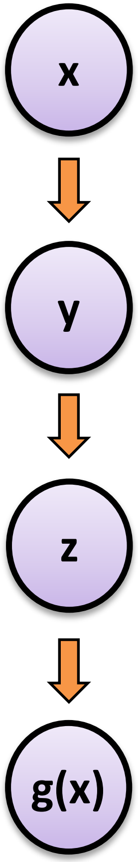
```julia
m = EAGOModel()
@variable(m, -2 <= x[i=1:2] <= 2)
@auxiliary_variable(m, z[i=1:2])
```

- Support for multiple-output subexpressions using new multigraph backend representation.

```julia
function f!(d, y)
    d[1] = y[1]^2 + y[2]
    d[2] = y[2]^2 + y[1]
end
@mimo_expression(m, f!, z, x)
@constraint(m, sum(z) <= 0.0)
```

**Composability of Nonlinear Functions (via JuMP extension):**

- Facilities chaining blocks of general nonlinear expressions (such as implicitly defined functions).



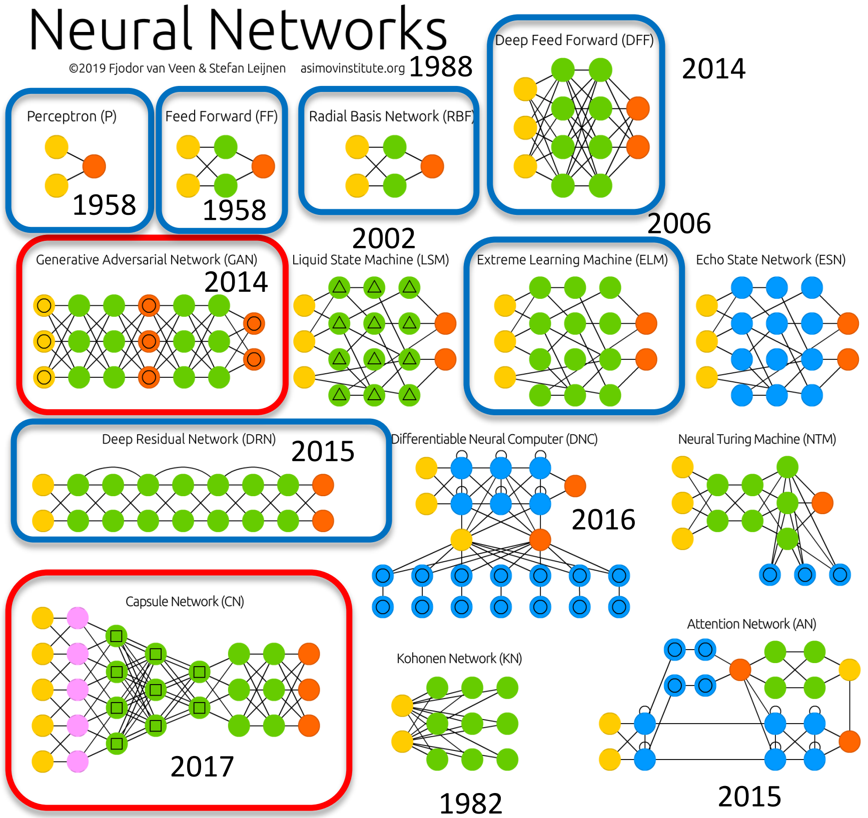

$$\mathbf{h}_1(\mathbf{y},\mathbf{x}) = \mathbf{0}$$
$$\mathbf{y} = \mathbf{y}(\mathbf{x})$$
$$\mathbf{h}_2(\mathbf{z},\mathbf{y}) = \mathbf{0}$$
$$\mathbf{z} = \mathbf{z}(\mathbf{y})$$
$$\mathbf{g}(\mathbf{x}) = \mathbf{f}(\mathbf{z}(\mathbf{y}(\mathbf{x})))$$

# EAGO.jl: Embedded ML

- Currently, EAGO.jl supports ML-models that are embedded with have a factorable representation.
- Additional work underway to natively support embedded Flux.jl models.
- Future support for more complex ML model structures
  - Layers with implicit functions evaluated via fixed-point methods (i.e. deep equilibrium networks).

$$\hat{y}\,(u) = Cx + Du$$
$$x = \phi(Ax + Bu)$$


8. L.E. Ghaoui et al. **Implicit Deep Learning.** https://arxiv.org/pdf/1908.06315.pdf.
9. S. Bai, J.Z. Kolter, and V. Koltun. **Deep Equilibrium Models.** https://arxiv.org/abs/1909.01377.pdf


*Adapted from https://www.asimovinstitute.org/neural-network-zoo/*

# Simple Surrogate Model

***Peaks Function***

$$f(x,y) = 3(1-x)^2 e^{-x^2-(y+1)^2} - 10\left(\frac{x}{5} - x^3 - y^5\right) e^{-x^2-y^2} - \frac{e^{-(x+1)^2-y^2}}{3}$$

```
function f(x,y)
    3*exp(-x^2-(y+1)^2)*(1-x)^2 - 10*(x/5-x^3-y^5)*exp(-x^2-y^2) - exp(-(x+1)^2-y^2)/3
end
```

***Domain***

$$-3 \leq x, y \leq 3$$

```
l = [-3; -3]
u = [3; 3]
```

# Simple Surrogate Model

**Surrogates.jl**
Workflow for Model Development

1. Generate Data

```
xd = sample(n, l, u, SobolSample())
yd = f.(xd)
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m = Chain(Dense(2,6,tanh), Dense(6,1))
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2. Specify Model

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m = Chain(Dense(2,6,tanh), Dense(6,1))
```

3. Train Model

```
ns = NeuralSurrogate(xd, yd, l, u, model = m)
surrogate_optimize(f, SRBF(), l, u, ns, SobolSample())
```

# Optimize Surrogate Model

**JuMP + EAGO.jl**
Workflow for Optimization

4. Create Model

```julia
using JuMP, EAGO

m = Model(EAGO.Optimizer)
@variable(m, l[i] <= x[i=1:2] <= u[i])
```

5. Register Function, Specify Problem

```julia
@register(m, :f, 2, f)
@NLobjective(m, Min, f(x[1], x[2]))
```

6. Optimize the problem

```julia
optimize!(m)
```

# Optimize Surrogate Model

- ❑ Dispatch to improved relaxations for a large library of activation functions automatically
- ❑ Some support for "cleaning" script defined models  for compatibility.
- ❑ Compatible with standard global optimization methods

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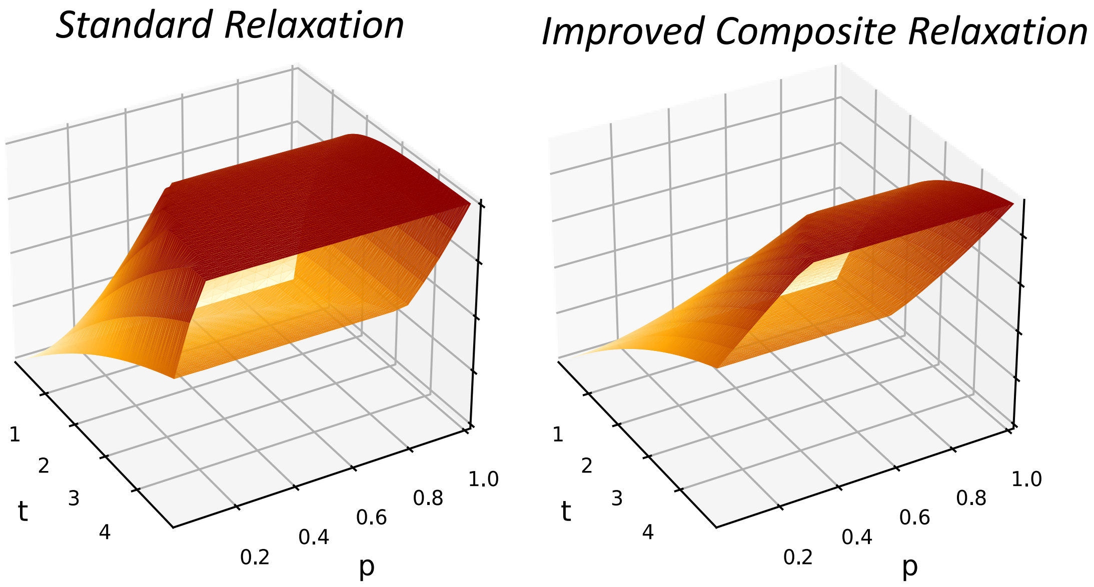
# Next Steps

- **Support for neural-ODE models.**
- **Improvements to composite relaxation forms (faster global optimization of surrogate models).**
- **Continually add support for additional ML forms.**
    - Relaxation of implicit functions[10]
    - Reverse propagation of relaxations[11]




10. Stuber, MD et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
11. Wechsung, Achim, et al. **Reverse propagation of McCormick relaxations.** *Journal of Global Optimization* 63.1 (2015): 1-36.

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# Questions?

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EAGO

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