Recent Advances in EAGO.jl and Its Use With JuMP.jl

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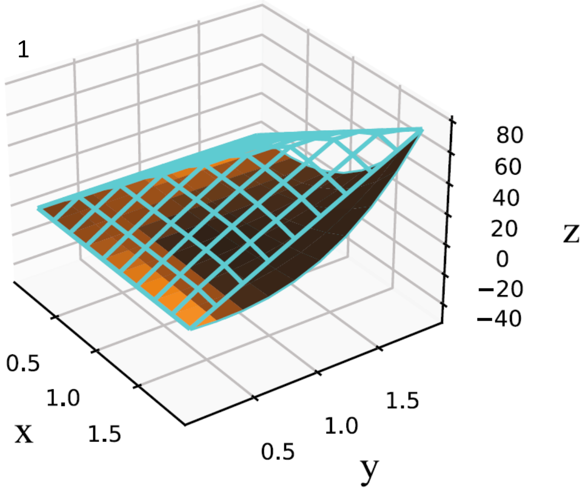
UCONN
UNIVERSITY OF CONNECTICUT

Process Systems and Operations Research Laboratory

Easy Advanced Global Optimization

- Open-source deterministic global solver for nonconvex MINLPs
  - Semi-infinite programs (SIPs)
  - Dynamic optimization
  - User-defined functions
- Uses branch-and-bound (B&B) to guarantee global optimality or infeasibility
- Applies McCormick-based relaxations for convex lower-bounding problems
- Designed in conjunction with JuMP



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

Parameter Estimation Example

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

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

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

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

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

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

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

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$$x_A^{i+1} = x_A^i + \Delta t\left(k_1 x_Z^i x_Y^i - c_{O_2}(k_{2f} + k_{3f})x_A^i + \frac{k_{2f}}{K_2}x_D^i + \frac{k_{3f}}{K_3}x_B^i - k_5 (x_A^i)^2 \right)$$

$$x_B^{i+1} = x_B^i + \Delta t\left(c_{O_2} k_{3f} x_A^i - \left(\frac{k_{3f}}{K_3} + k_4 \right) x_B^i \right)$$

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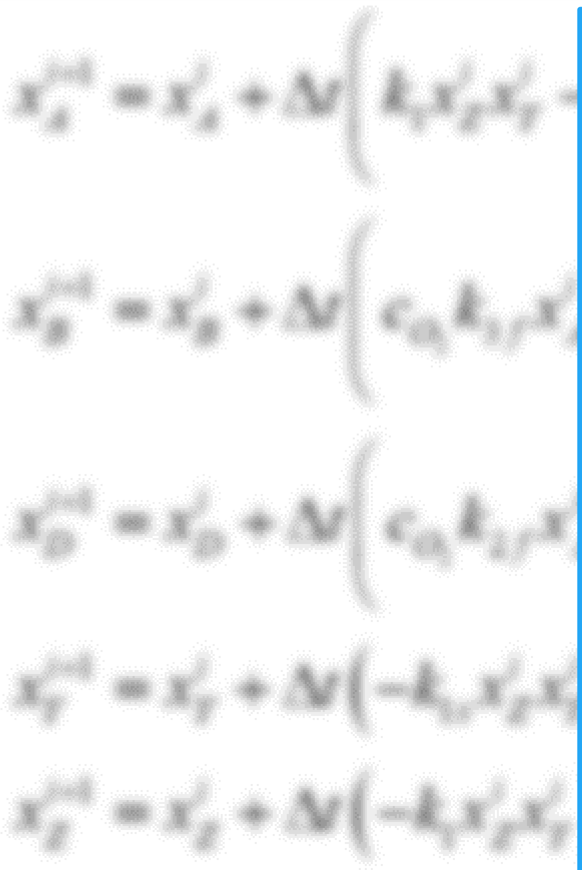

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using CSV, DataFrames, JuMP, EAGO, Gurobi

data = CSV.read("kinetic_intensity_data.csv", DataFrame)
bounds = CSV.read("implicit_variable_bounds.csv", DataFrame)

pL = [10.0, 10.0, 0.001]
pU = [1200.0, 1200.0, 40.0];

intensity(xA, xB, xD) = xA + (2/21)*xB + (2/21)*xD

function objective(p...)
    x = explicit_euler_integration(p)
    SSE = 0.0
    for i=1:200
        SSE += (intensity(x[5i-4],x[5i-3],x[5i-2]) - data[!, :intensity][i])^2
    end
    return SSE
end

factory = () -> EAGO.Optimizer(SubSolvers(; r = Gurobi.Optimizer()))
model = JuMP.Model(factory)
@variable(model, pL[i] <= p[i=1:3] <= pU[i])
fobj(p...) = objective(p...)
JuMP.register(model, :fobj, 3, fobj, autodiff=true)
@NLobjective(model, Min, fobj(p...))
JuMP.optimize!(model)
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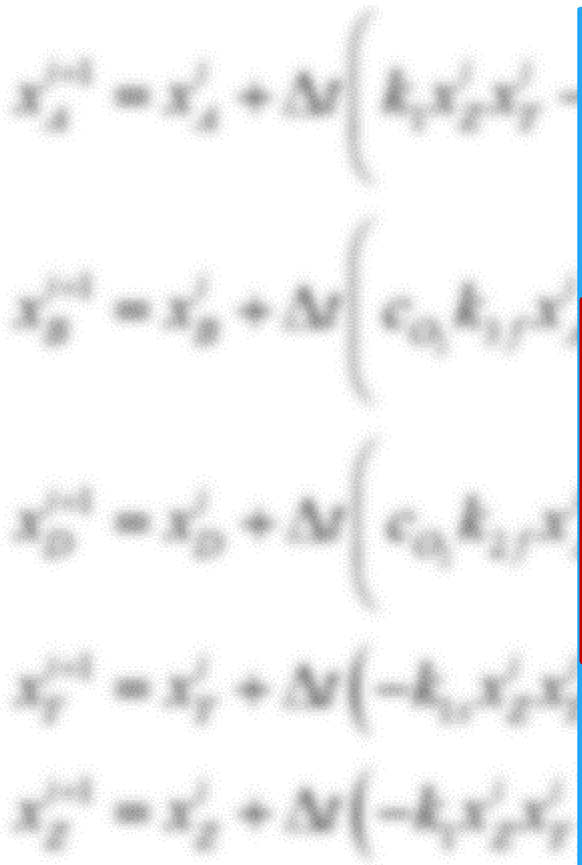

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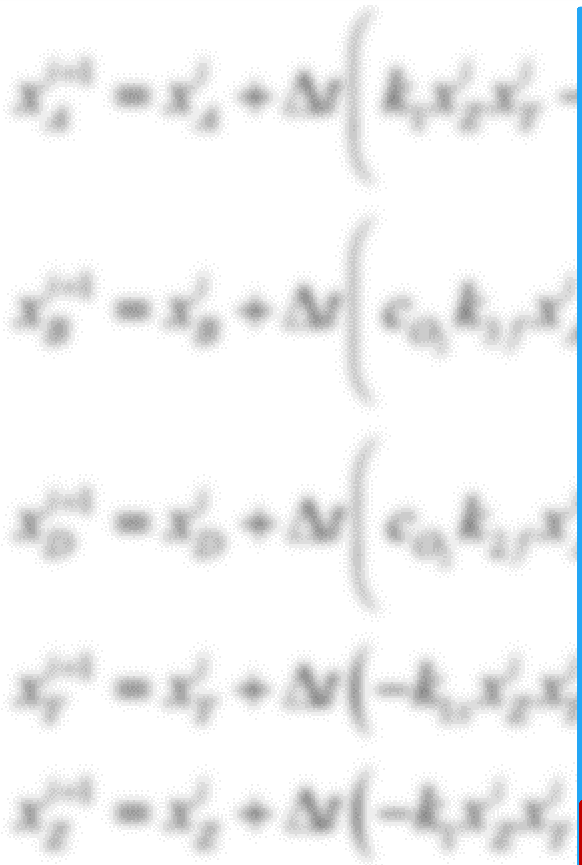

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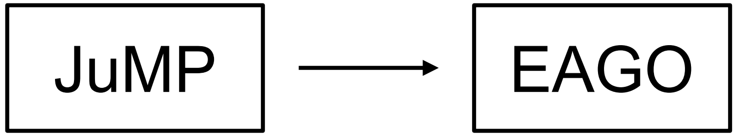
Integration with JuMP

- EAGO parses a JuMP model and sends information to bounding subroutines



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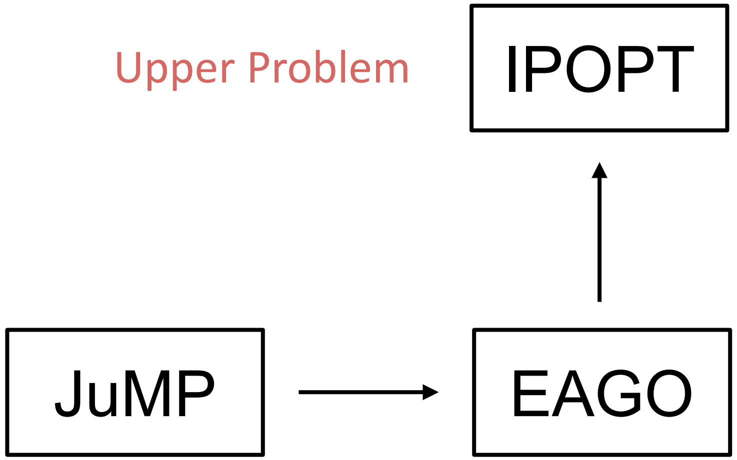
  - Original problem is sent to IPOPT to generate an upper bound



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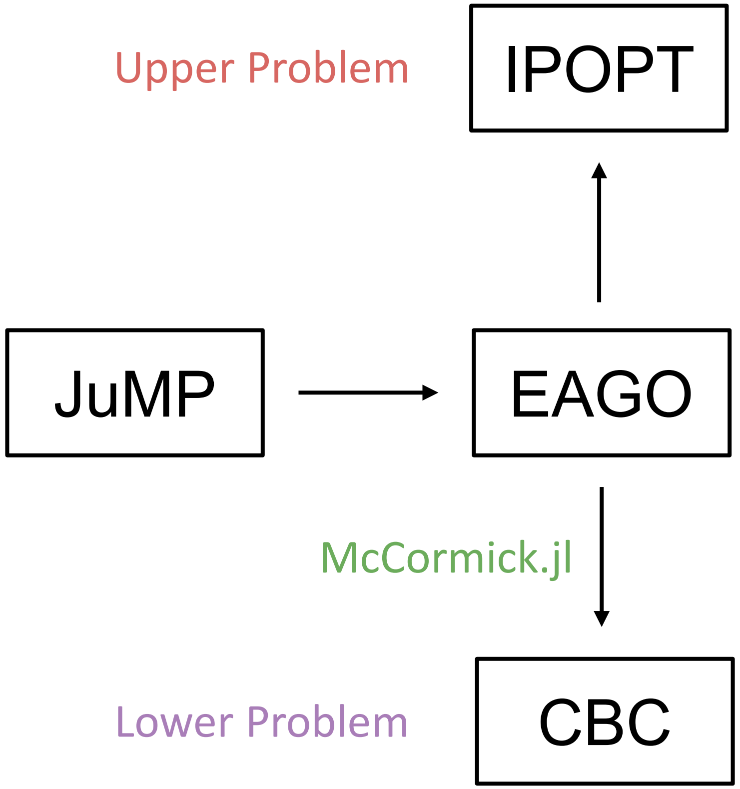

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- EAGO parses a JuMP model and sends information to bounding subroutines
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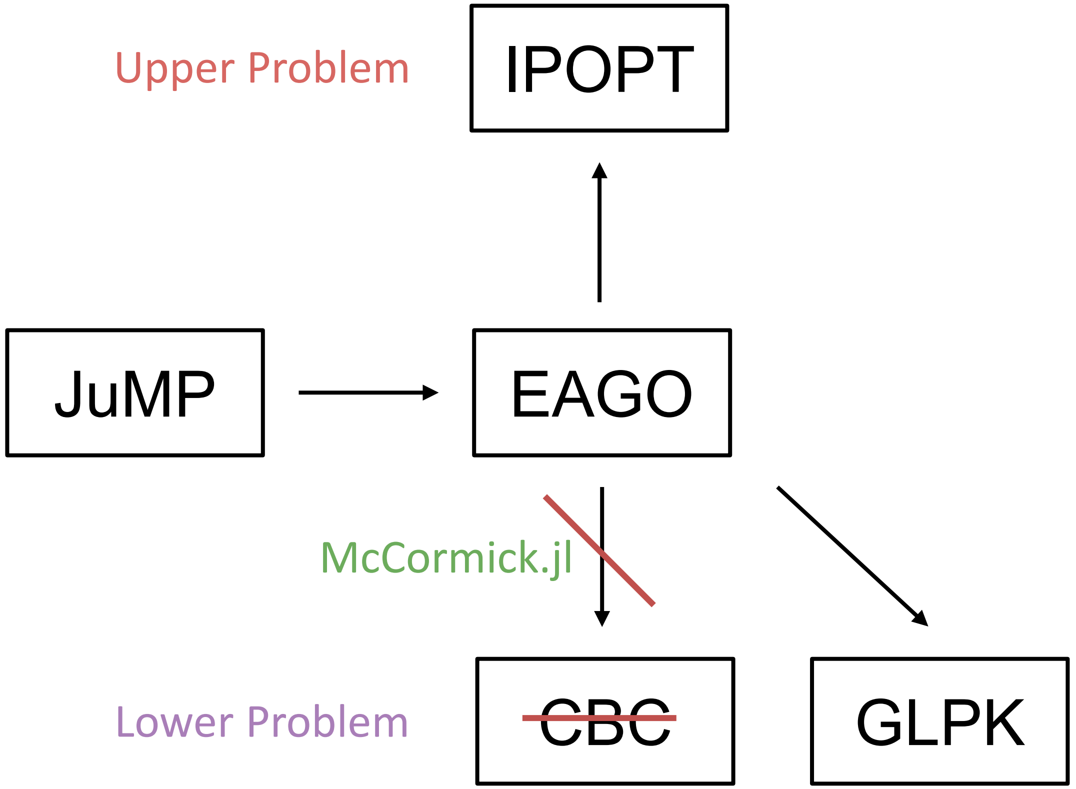
  - Subsolvers can be any appropriate MOI.AbstractOptimizer




```julia
using JuMP, EAGO, GLPK

factory = () -> EAGO.Optimizer(SubSolvers(; r = GLPK.Optimizer()))
model = JuMP.Model(optimizer_with_attributes(factory))
```

Timeline

Apr 2018 – Initial EAGO Release

Jun 2018 – JuMP-dev 2018

[3]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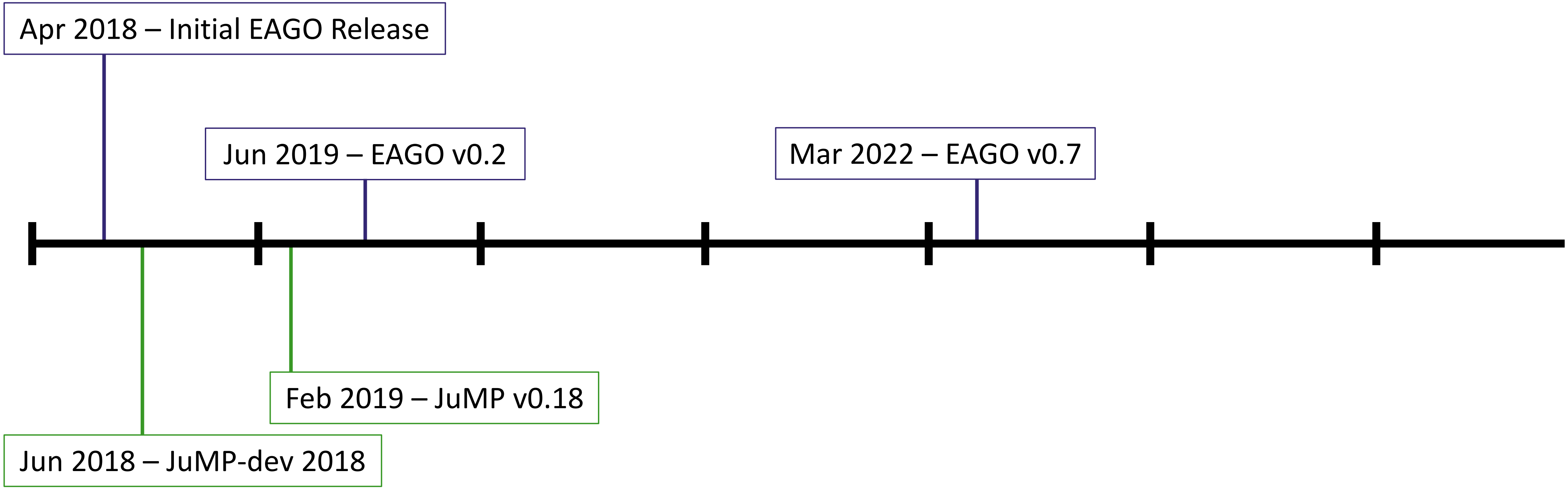

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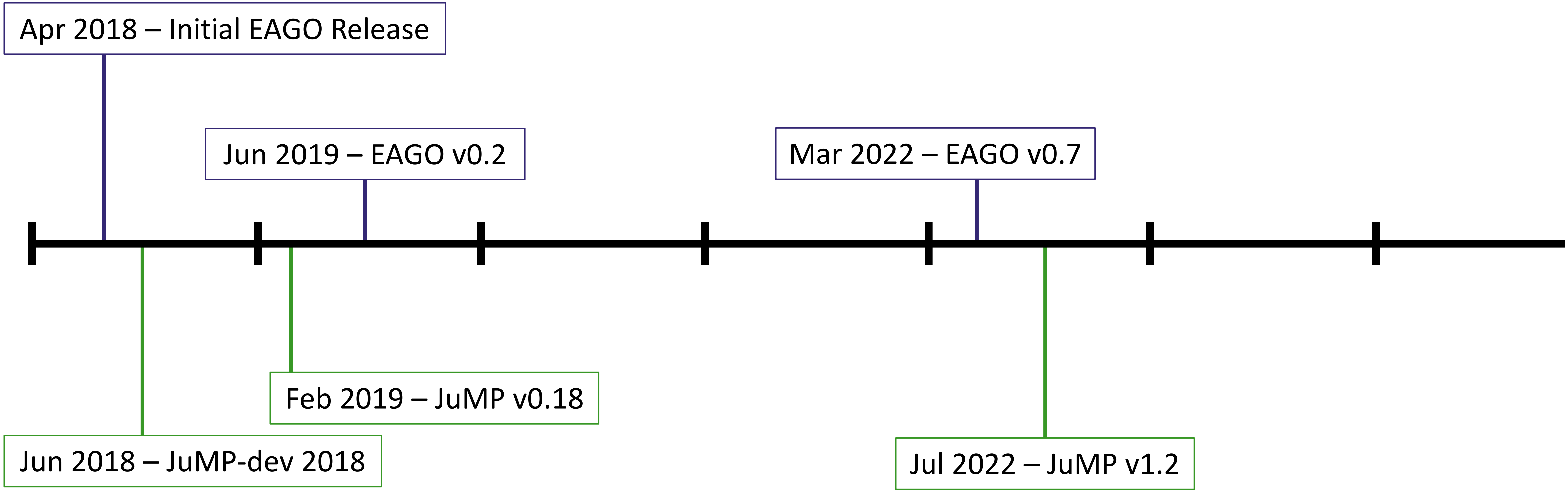

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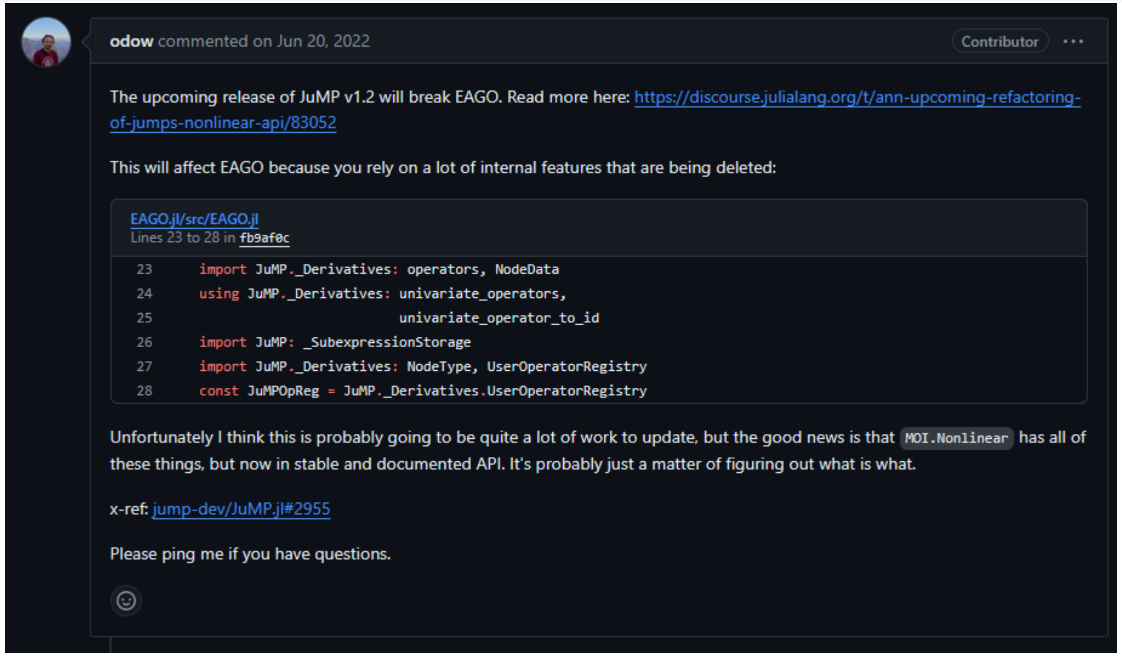
Nonlinear Refactor

- Nonlinearity moved from JuMP to MOI
- Relatively low impact for EAGO
  - JuMP._Derivates → MOI.Nonlinear
  - Other minor name changes
  - Changes to EAGO's internal operator registry



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odow commented on Jun 20, 2022 Contributor

The upcoming release of JuMP v1.2 will break EAGO. Read more here: https://discourse.julialang.org/t/ann-upcoming-refactoring-of-jumps-nonlinear-api/83052

This will affect EAGO because you rely on a lot of internal features that are being deleted:

EAGO.jl/src/EAGO.jl
Lines 23 to 28 in fb9af0c

```julia
import JuMP._Derivatives: operators, NodeData
using JuMP._Derivatives: univariate_operators,
                         univariate_operator_to_id
import JuMP: _SubexpressionStorage
import JuMP._Derivatives: NodeType, UserOperatorRegistry
const JuMPOpReg = JuMP._Derivatives.UserOperatorRegistry
```

Unfortunately I think this is probably going to be quite a lot of work to update, but the good news is that `MOI.Nonlinear` has all of these things, but now in stable and documented API. It's probably just a matter of figuring out what is what.

x-ref: jump-dev/JuMP.jl#2955

Please ping me if you have questions.

```diff
-    for n in d.nd
-        if n.nodetype == JuMP._Derivatives.VARIABLE
             if !haskey(variable_dict, n.index)
                 variable_dict[n.index] = true
             end
         end
```

```diff
+    for n in d.nodes
+        if n.type == MOINL.NODE_VARIABLE
             if !haskey(variable_dict, n.index)
                 variable_dict[n.index] = true
             end
         end
```

EAGO's Directed Acyclic Graph

- MOI nodes converted to EAGO nodes
  - Forward pass: relaxations
  - Reverse pass: constraint propagation

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→

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EAGO.Node(EAGO.EXPRESSION, EAGO.PLUS, 0, 0, 2, [2, 6])
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  - Rewrite EAGO's internal routines?
  - Convert symbolic tree into a node tree?

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Future Work

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\begin{aligned}
f^* &= \min_{\mathbf{x}} f(\mathbf{x}) \\
&\text{s.t. } 0 \geq \max g(\mathbf{x}, \tilde{\mathbf{y}}, \mathbf{p}) \\
&\text{s.t. } \mathbf{h}(\mathbf{x}, \tilde{\mathbf{y}}, \mathbf{p}) = \mathbf{0} \\
&\mathbf{x} \in X = \{\mathbf{x} \in \mathbb{R}^{n_x} : \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U\} \\
&\mathbf{p} \in \mathbf{P} = \{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^L \leq \mathbf{p} \leq \mathbf{p}^U\} \\
&\tilde{\mathbf{y}} \in D_y \subset \mathbb{R}^{n_y}
\end{aligned}
$$

$$\rightarrow$$

$$
\begin{aligned}
f^* &= \min_{\mathbf{x}} f(\mathbf{x}) \\
&\text{s.t. } g(\mathbf{x}, \mathbf{y}(\mathbf{x}, \mathbf{p}), \mathbf{p}) \leq 0, \quad \forall \mathbf{p} \in P \\
&\mathbf{x} \in X = \{\mathbf{x} \in \mathbb{R}^{n_x} : \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U\} \\
&P = \{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^L \leq \mathbf{p} \leq \mathbf{p}^U\}
\end{aligned}
$$

Future Work

- Add support for MOI.ScalarNonlinearFunction
- Update EAGO's use of JuMP for advanced problem formulations
  - **SIPs**
  - Implicit functions

```julia
using EAGO

f(x) = (1/3)*x[1]^2 + x[2]^2 + x[1]/2
gSIP(x, p) = (1.0 - (x[1]^2)*(p[1]^2))^2 - x[1]*p[1]^2 - x[2]^2 + x[2]
x_l = Float64[-1000.0, -1000.0]
x_u = Float64[1000.0, 1000.0]
p_l = Float64[0.0]
p_u = Float64[1.0]
EAGO.sip_solve(EAGO.SIPRes(), x_l, x_u, p_l, p_u, f, [gSIP], res_sip_absolute_tolerance = 1E-3, verbosity = 3);
```

$$\mathbf{p} \in \mathbf{P} = \{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^L \leq \mathbf{p} \leq \mathbf{p}^U\}$$

$$\tilde{\mathbf{y}} \in D_y \subset \mathbb{R}^{n_y}$$

Future Work

- Add support for MOI.ScalarNonlinearFunction
- Update EAGO's use of JuMP for advanced problem formulations
  - **SIPs**
  - Implicit functions

```julia
using JuMP, EAGO

factory = () -> EAGO.Optimizer(SubSolvers(; t = SIPOptimizer(SIPRes(), 2, 1)))
model = JuMP.Model(optimizer_with_attributes(factory))
@variable(model, -1000.0 <= x[i=1:2] <= 1000.0)
@variable(model, 0.0 <= p <= 1.0)
@constraint(model, (1.0 - (x[1]^2)*(p^2))^2 - x[1]*p^2 - x[2]^2 + x[2] <= 0.0)
@objective(model, Min, (1/3)*x[1]^2 + x[2]^2 + x[1]/2)
JuMP.optimize!(model)
```

$$\mathbf{p} \in \mathbf{P} = \{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^L \le \mathbf{p} \le \mathbf{p}^U\}$$

$$\tilde{\mathbf{y}} \in D_y \subset \mathbb{R}^{n_y}$$

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Questions?

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Process Systems and Operations Research Laboratory

EAGO

GPU-Accelerated Deterministic Global Optimization
Robert Gottlieb
Tuesday, July 23rd, 2024, 8:30 AM

https://www.psor.uconn.edu

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