Easy Advanced Global Optimization (EAGO)

An Open-Source Platform for Robust and Global Optimization in Julia

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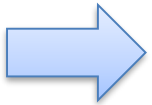
UCONN

Motivation

- Advanced optimization formulations emerge naturally from common system design problems

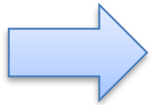
Design Specification

Worst-case constraint satisfaction[1]



Logical Statement[4]

$$\forall \mathbf{p} \in P, \quad \exists \mathbf{u} \in U:$$
$$g(\mathbf{u}, \mathbf{x}, \mathbf{p}) \leq 0$$
$$\mathbf{h}(\mathbf{u}, \mathbf{x}, \mathbf{p}) = \mathbf{0}$$



Semi-infinite Program[4]

$$f^* = \min_{\mathbf{x} \in X} f(\mathbf{x})$$
$$\text{s.t.} \quad g(\mathbf{u}, \mathbf{x}, \mathbf{p}) \leq 0, \forall \mathbf{p} \in P$$
$$\mathbf{h}(\mathbf{u}, \mathbf{x}, \mathbf{p}) = \mathbf{0}, \quad \forall \mathbf{p} \in P$$

- Implementations for recent theoretical advances aren't readily accessible.
  - No publicly available library for differentiable McCormick relaxations[2]
  - No publicly available library for implicit McCormick relaxations[3,4]
  - Prior implementations have an high barrier to usage.

[1] **Worst-case design of subsea production facilities using semi-infinite programming.** Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524
[2] **Differentiable McCormick relaxations.** Khan, K. et al. (2017) *Journal Global Optimization*, 67(4), 687-729
[3] **Convex and concave relaxations of implicit functions.** Stuber, M.D. et al. (2015) *Optimization Methods and Software*, 30, 424-460
[4] **Semi-Infinite Optimization with Implicit Functions.** Stuber, M.D., Barton, P.I. (2015) *Industrial & Engineering Chemistry Research*, 54, 307-317

Progression of the Talk

- ☐ Julia Capabilities
- ☐ Developing Robust Optimization for Julia
- ☐ Illustrative Examples
- ☐ Future Directions

Why Julia?

Overview

Ease of Use

- Simplistic Syntax
- Package Management
- Cloud Computing
- Notebook Support

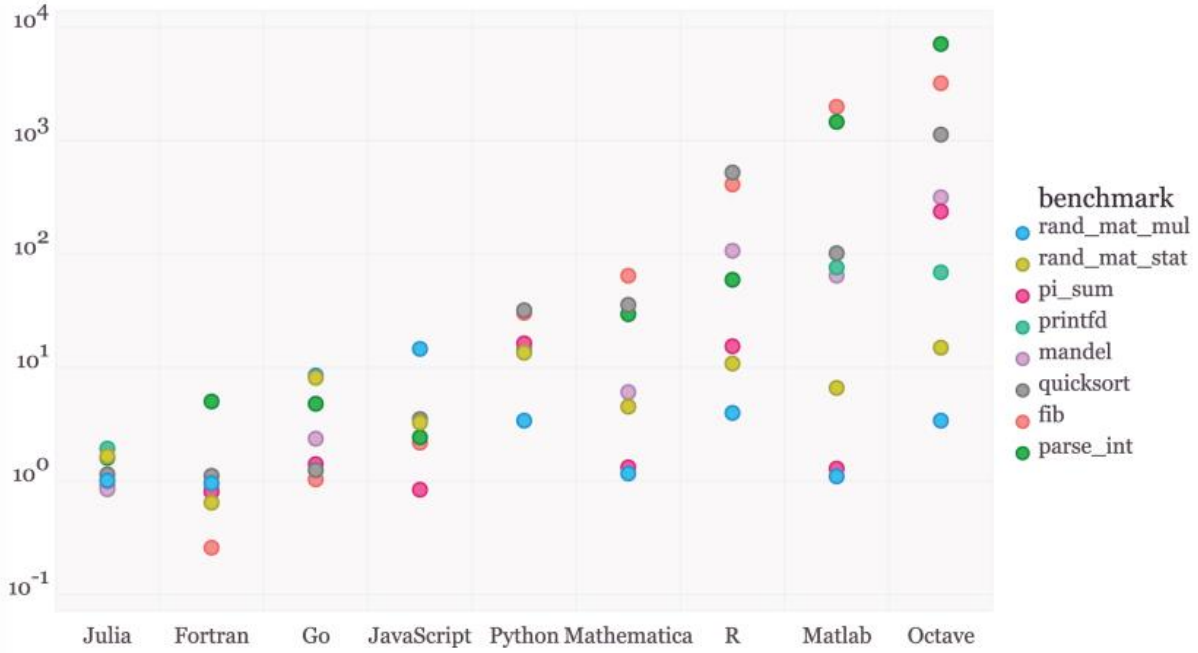
Performance

- Speed of C/Fortran
- Parallelism
- JIT Optimization

Example Julia Code of Solving ODE[4]

```julia
# add packages to library
Pkg.add("DifferentialEquations")
Pkg.add("Plots")
# import packages from library
using DifferentialEquations
using Plots
# setup problem
function lorenz(t,u,du)
 du[1] = 10.0(u[2]-u[1])
 du[2] = u[1]*(28.0-u[3]) - u[2]
 du[3] = u[1]*u[2] - (8/3)*u[3]
end
u0 = [1.0;0.0;0.0]
tspan = (0.0,100.0)
prob = ODEProblem(lorenz,u0,tspan)
# solve problem
sol = solve(prob)
# plot problem
plot(sol,vars=(1,2,3))
```

- Run-time benchmark comparison[5]



Performance comparison of various languages performing simple microbenchmarks. Benchmark execution time relative to C. (Smaller is better; C performance = 1.0.)

[4] DifferentialEquations.jl – A Performant and Feature-Rich Ecosystem for Solving Differential Equations in Julia. Rackauckas, C. & Nie, Q. (2017). *Journal of Open Research Software,* 5(1), p.15

[5] Julia: A Fresh Approach to Numerical Computing. Jeff Bezanson, Alan Edelman, Stefan Karpinski and Viral B. Shah (2017) *SIAM Review*, 59: 65–98.

Why Julia?

Abstract Syntax Tree

- *Syntactic macros*[5]
  - Work on Abstract Syntax Tree
  - Preserve lexical structure reliably
  - Increased capability relative to text substitution macros in C++
- *Multiple Dispatch Capable*
- *AST representation allows for graph level optimization and modification as alternative to operator overloading*
- *Allows for "overdubbing" instead of overloading to generate context unaware code with context dependent behavior*

Code Generating Smooth McCormick Objects

```
# Generate SMC objects for increasing concave functions
CC_List = [:acosh,:log,:log2,:log10,:sqrt]
for j in CC_List
    eval(quote
          @inline $j(x,xL,xU;relax="cv") = line_seg($j,x,xL,xU)
          @inline $j(x,xL,xU;relax="cc") = $j(x)
          function $j(x::SMC)
            cc = $j(mid(x.cc,x.cv,x.Intv.hi),x.Intv.lo,x.Intv.hi;relax="cc")
            cv = $j(mid(x.cc,x.cv,x.Intv.lo),x.Intv.lo,x.Intv.hi;relax="cv")
            return SMC(cc,cv,$j(x.Intv))
          end
        end)
end
```

Compiler Interaction via Macros

```
x = [1:100]; y = [2:2:200]
# Devectorization of Array Operations
@devec r = exp(x + y) .* sum(x)
# SIMD & Eliminate Bound Checking
@simd for i=1:length(x)
    @inbounds s += x[i]*y[i]+x[i]
end
```

[5] Julia: A Fresh Approach to Numerical Computing. Jeff Bezanson, Alan Edelman, Stefan Karpinski and Viral B. Shah (2017) *SIAM Review*, 59: 65–98.

Why Julia?
Design Objectives

Current Capabilities:

- Native use of LAPACK, SuiteSparse
- JuMP/JuMPeR[6] (Julia AML)
  - Low syntax, User Defined Functions
  - Automatic Derivative Calculations
  - Callback Support
- ValidatedNumerics.jl (Interval Library)
- ForwardDiff.jl[8] (Automatic Differentiation)

Future Capabilities:

- Future Compatibility for Overdubbing Approaches to Source-Code Transformation

Objective: *Open-Source*

Create a toolbox of modules that end-users can modify

Objective: *Intuitive User Interface*

Provide a graphical interface and interface to AMPL

Objective: *Easily Accessible Routines*

Provide pre-built routines for that can be used without advanced subject area knowledge

[6] **JuMP: A Modeling Language for Mathematical Optimization** Iain Dunning and Joey Huchette and Miles Lubin (2017) *SIAM Review*, 59: 295–320.
[7] **ValidatedNumerics.jl** [Computer Software]. Retrieved from https://github.com/JuliaIntervals/ValidatedNumerics.jl.
[8] **Forward-Mode Automatic Differentiation in Julia.** (2016) Revels, J., Lubin, M., Paramarkou, T. arXiv:1607.07892

Progression of the Talk

☑ Julia Capabilities

☐ Developing Robust Optimization for Julia

Build global solver*

- **Nonconvex Semi-Infinite Programming**
- **Branch-and-Bound Library**
- **Smooth McCormick Relaxation Library**
- **Implicit Function Bounding Routine**
- **Constraint Propagation via DAG**
- **Global Solver**

Analytic Tools

- **Directed Graph Toolbox**
- Parametric Interval Methods

User Interface

- Flow-sheeting Interface
- Solution Visualization
- Data Import/Export/Storage
- AML Integration

☐ Illustrative Examples

☐ Future Directions

* Support for validated calculations
* Special routines for imbedded implicit functions

SIP Solvers

- **EAGOSemiInfinite** implements implicit and explicit meta-algorithms

Explicit SIP

$$f^* = \min_{\mathbf{x}\in X} f(\mathbf{x})$$

$$\text{s.t. } g(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) \le 0, \forall (\mathbf{y}, \mathbf{p}) \in Y \times P$$

$$\mathbf{h}(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) = \mathbf{0}, \ \forall (\mathbf{y}, \mathbf{p}) \in Y \times P$$

Implicit SIP

$$f^* = \min_{\mathbf{x}\in X} f(\mathbf{x})$$

$$\text{s.t. } g(\mathbf{y}(\mathbf{x}, \mathbf{p}), \mathbf{x}, \mathbf{p}) \le 0, \quad \forall \mathbf{p} \in P$$

- Solved generally via restriction of right-hand side method[9,4]
  - *Discretization of uncertainty set for upper/lower bounds.*
  - *Finite convergence (if Slater point arbitrarily near minimizer).*

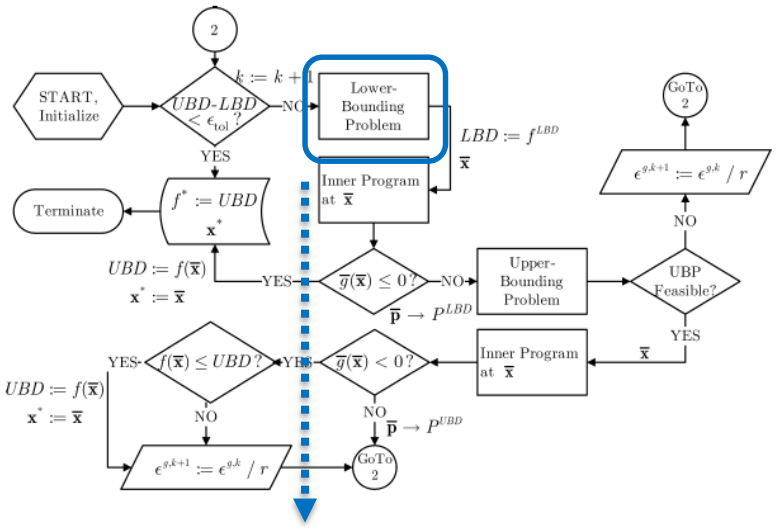
- Problem size and complexity dramatically increased with equality constraints[4,9,10]

[9] **Global optimization of semi-infinite programs via restriction of the right-hand side**. Mitsos, A. (2011). *Optimization* 60:10-11, 1291-1308

[4] **Semi-Infinite Optimization with Implicit Functions.** Stuber, M.D., Barton, P.I. (2015) *Industrial & Engineering Chemistry Research*, 54, 307-317

[10] **Evaluation of process systems operating envelopes.** Stuber, M.D., (2013) Ph.D Thesis.

Flowchart for restriction of RHS method[4]



Lower Bounding Problem (explicit) for restriction of RHS method[4]

$$f^{LBD} = \min_{\mathbf{x}\in X} f(\mathbf{x})$$

$$\text{s.t. } g_{SIP}(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) \le 0 \quad \forall (\mathbf{y}, \mathbf{p}) \in Y^{LBD} \times P^{LBD}$$

$$\mathbf{h}(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) = \mathbf{0} \quad \forall (\mathbf{y}, \mathbf{p}) \in Y^{LBD} \times P^{LBD}$$

Branch & Bound Library

- **Configuration**
  - BNB type (option storage)
  - BNBObject type (node storage)
- **Fully customizable**
- **Natively for common schemes**
  - Best-first, depth-first, breadth-first search
  - Absolute/relative midpoint bisection

Install Packages

```
using EAGOBranchBound
using ValidatedNumerics
```

Initialize B&B Objects

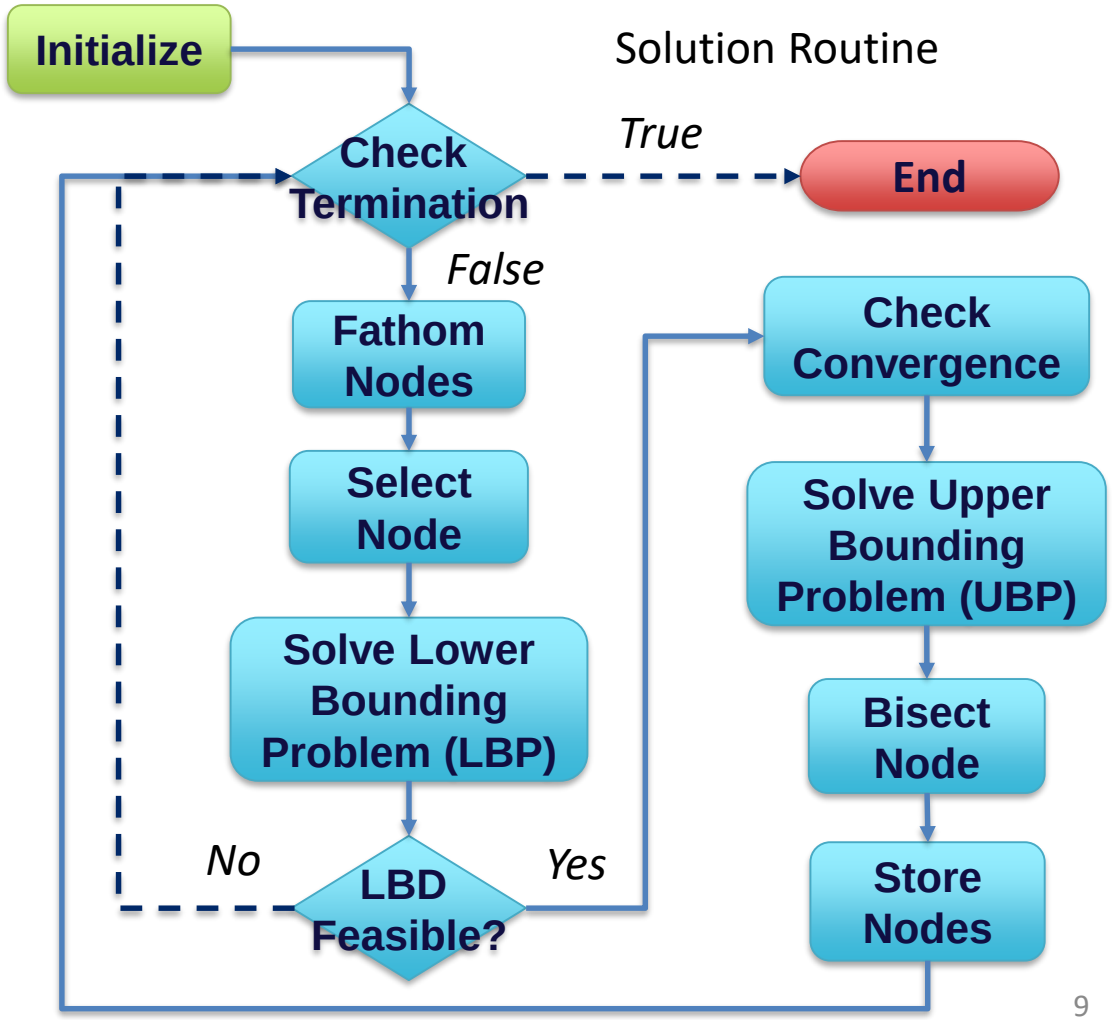
```
b = IntervalBox(-1..1,2..9)
a = EAGOBranchBound.BnB(b)
C = EAGOBranchBound.BnBObject(b)
EAGOBranchBound.set_to_default!(a)
```

Define and Set UBP/LBP

```
function ex_LBP(X::IntervalBox,k,opt)
  ex_LBP_int = @interval X[1]+X[2]^2
  return ex_LBP_int.lo, mid.(X), true
end
function ex_UBP(X::IntervalBox,k,opt)
  ex_UBP_int = @interval X[1]+X[2]^2
  return ex_UBP_int.hi, mid.(X), true
end
a.Lower_Prob = ex_LBP
a.Upper_Prob = ex_UBP
```

Solve Problem

```
outy = EAGOBranchBound.solve(a,C)
```



McCormick Relaxations

Implementation

Smooth McCormick Object[11]

```
struct SMC <: AbstractMC
  cc
  cv
  Intv
  function SMC(a,b,c)
    if ~(typeof(c)<:Interval)
      error("SMC of form SMC($a,$b,$c) not allowed.
             Last argument must be an interval.")
    elseif (a<b)
      error("SMC of form SMC($a,$b,$c) not allowed.
             Must have cv <= cc.")
    end
    new SMC(a,b,c)
end
```

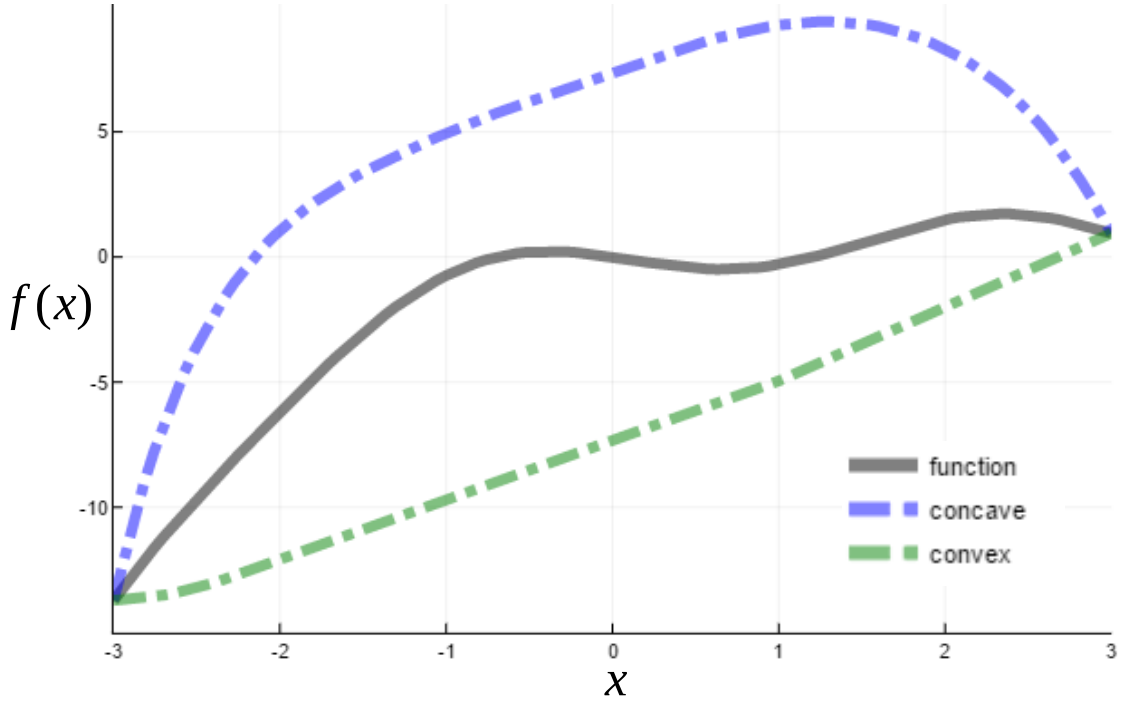
Expressions Supported:

+, -, /, *, ^, exp, exp2, exp10, log, log2, log10, sqrt, pow, sin, cos, tan, asin, acos, atan, sinh, cosh, tanh, asinh, acosh, atanh, min, max, abs, step, sign

Gradients of Relaxations:

- Absent from SMC to allow for flexibility
- Can be readily calculated via automatic differentiation
- Existing packages (JuMP[6], ForwardDiff[8]) outperform naïve implementation

$$f(x) = \exp(-x/2)x - \sin(2x)$$



Performance:

Comparable in speed to MC++ library[11] +/-30% runtime in benchmarks

[2] **Differentiable McCormick relaxations.** Khan, K. et al. (2017) *Journal Global Optimization*, 67(4), 687-729
[6] **JuMP: A Modeling Language for Mathematical Optimization.** Dunning, I. Huchette, J. and Lubin, M. (2017) *SIAM Review*, 59, 295–320.
[8] **Forward-Mode Automatic Differentiation in Julia.** (2016) Revels, J., Lubin, M., Paramarkou, T. arXiv:1607.07892
[11 **MC++: A versatile library for McCormick relaxations and Taylor models**. B. Chachuat. http://www3.imperial.ac.uk/people/b.chachuat/research
[12] **McCormick-based relaxations of algorithms.** Mitsos et al. (2009) *SIAM Journal on Optimization*, SIAM, 2009, 20, 73-601

Abstract Syntax Tree

Directed Graphs & Interval Constraint Propagation

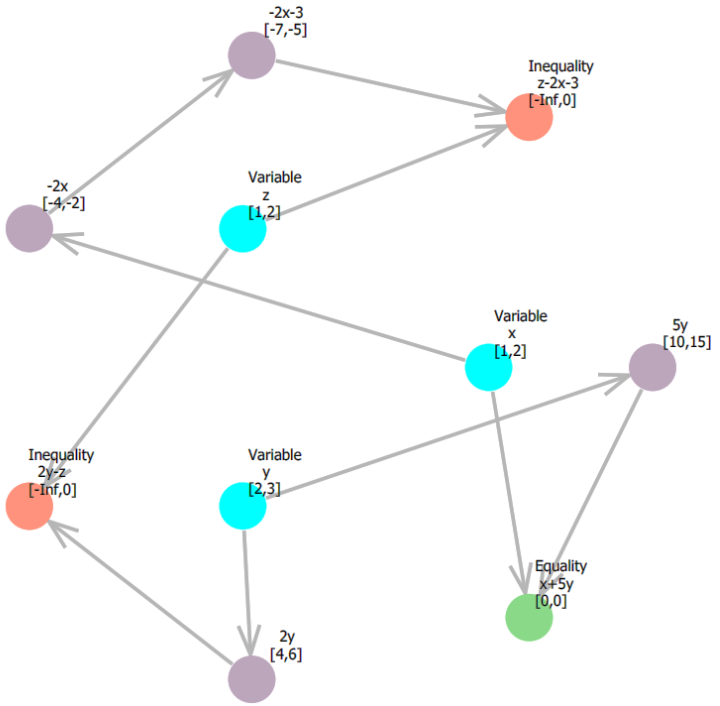
EAGODAGContractor Package

- Methods for interval constraint propagation via natural interval extensions and interval contractors[1]
- Supports visualization of directed acyclic graphs (DAG) via Gladfly integration
- Integrates with common-subexpression reduction routines (@cse) in Julia

Expressions Supported:

+, -, /, *, ^, exp, exp2, exp10, log, log2, log10, sqrt, pow, sin, cos, tan, asin, acos, atan, sinh, cosh, tanh, asinh, acosh, atanh, min, max, abs, step, sign

DAG Visualization



[1] **Worst-case design of subsea production facilities using semi-infinite programming.** Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524

[7] **ValidatedNumerics.jl** [Computer Software]. Retrieved from https://github.com/JuliaIntervals/ValidatedNumerics.jl.

Global Solver[2,3]

Solver Options

- **IPOPT is standard solver for LBP/UBP**
  - Open-source
  - Compiled version via Package manager
  - Sparsity Pattern Detected Automatically
  - Forward-Mode AD Calculation of Hessian/Jacobian/Gradients Used
- **Alternative LBD Solver:**
  - SNOPT
  - Proximal-Bundle
- **Alternative UBP Solver:**
  - Any JuMP NLP solver
- **Affine Relaxations Also Available**
  - JuMP LP solvers

Global Solution Scheme

- **Default settings:**
  - Best-first search
  - Relative-width bisection
  - Validated interval calculations
- **Preprocessing Step**
  - Forward-Reverse Interval Constraint Propagation
  - (Optional): Interval Parametric Tests

- **Lower Bounding Problem***

$$f^{LBD} = \min_{\mathbf{p}\in P} f^{cv}(\mathbf{x}(\mathbf{p}),\mathbf{p})$$

$$\text{s.t. } g^{cv}(\mathbf{x}(\mathbf{p}),\mathbf{p}) \le 0$$

**Bounds calculated via implicit-function based fixed point iteration[3] using smooth McCormick relaxations[2].*

- **Upper Bounding Problem**

$$f^{UBD} = \min_{\mathbf{z}\in Z,\mathbf{p}\in P} f(\mathbf{z},\mathbf{p})$$

$$\text{s.t. } g(\mathbf{z},\mathbf{p}) \le 0$$

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

[2] **Differentiable McCormick relaxations.** Khan, K. et al. (2017) *Journal Global Optimization*, 67(4), 687-729
[3] **Convex and concave relaxations of implicit functions.** Stuber, M.D. et al. (2015) *Optimization Methods and Software*, 30, 424-460

Progression of the Talk

- ☑ Julia Capabilities
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- ☐ Illustrative Examples
- ☐ Future Directions

Case Study I

Kinetic Parameter Estimation[3,12,13,14]

Problem Statement

- Determine the forward rate constants (k_{2f}, k_{3f}, k_4) of oxygen addition to cyclohexadienyl radicals from transient flash photolysis data.
- Mass-balance ODEs system discretized via implicit Euler.
- Minimize residual sum-of-squares for intensity.

Equality Constraints

$$\boldsymbol{h}(\boldsymbol{z},\boldsymbol{p}) = \begin{cases} \boldsymbol{c}_{\boldsymbol{A}}^{i-1} - \boldsymbol{c}_{\boldsymbol{A}}^{i} + \Delta t\left(k_1 \boldsymbol{c}_{\boldsymbol{Y}}^{i}\boldsymbol{c}_{\boldsymbol{Z}}^{i} - C_{O_2}(k_{2f}+k_{3f})\boldsymbol{c}_{\boldsymbol{A}}^{i} + \frac{k_{2f}}{K_2}\boldsymbol{c}_{\boldsymbol{D}}^{i} + \frac{k_{3f}}{K_3}\boldsymbol{c}_{\boldsymbol{B}}^{i} - k_5 \boldsymbol{c}_{\boldsymbol{A}}^{i\,2}\right) = 0 \\ \boldsymbol{c}_{\boldsymbol{B}}^{i-1} - \boldsymbol{c}_{\boldsymbol{B}}^{i} + \Delta t\left(k_{3f}\boldsymbol{c}_{\boldsymbol{A}}^{i} C_{O_2} - \left(\frac{k_{3f}}{K_3} + k_4\right)\boldsymbol{c}_{\boldsymbol{B}}^{i}\right) = 0 \\ \boldsymbol{c}_{\boldsymbol{D}}^{i-1} - \boldsymbol{c}_{\boldsymbol{D}}^{i} + \Delta t\left(k_{2f}\boldsymbol{c}_{\boldsymbol{A}}^{i} C_{O_2} - \frac{k_{2f}}{K_2}\boldsymbol{c}_{\boldsymbol{D}}^{i}\right) = 0 \\ \boldsymbol{c}_{\boldsymbol{Y}}^{i-1} - \boldsymbol{c}_{\boldsymbol{Y}}^{i} + \Delta t\left(-k_{1s}\boldsymbol{c}_{\boldsymbol{Y}}^{i}\boldsymbol{c}_{\boldsymbol{Z}}^{i}\right) = 0 \\ \boldsymbol{c}_{\boldsymbol{Z}}^{i-1} - \boldsymbol{c}_{\boldsymbol{Z}}^{i} + \Delta t\left(-k_1 \boldsymbol{c}_{\boldsymbol{Y}}^{i}\boldsymbol{c}_{\boldsymbol{Z}}^{i}\right) = 0 \end{cases}$$

Objective Function

$$\min_{\boldsymbol{p}\in P} \sum_{i=1}^{n} \left(\boldsymbol{I}^{i} - \boldsymbol{I}_{\boldsymbol{data}}^{i}\right)^2$$

$$s.t. \quad \boldsymbol{I}^{i} = \boldsymbol{c}_{A}^{i} + \tfrac{2}{21}\boldsymbol{c}_{B}^{i} + \tfrac{2}{21}\boldsymbol{c}_{D}^{i}$$

Uncertain Variables

$$\boldsymbol{p} = (k_{2f}, k_{3f}, k_4)$$

State Variables

$$\boldsymbol{z} = (\ldots, \boldsymbol{c}_{\boldsymbol{A}}^{i}, \boldsymbol{c}_{\boldsymbol{B}}^{i}, \boldsymbol{c}_{\boldsymbol{D}}^{i}, \boldsymbol{c}_{\boldsymbol{Y}}^{i}, \boldsymbol{c}_{\boldsymbol{Z}}^{i}, \ldots)$$

$$s.t. \quad i = 1 \ldots n$$

Parameters

$$k_1, k_{1s}, k_5, K_2, K_3, c_{O2}, \Delta t, n$$

[3] **Convex and concave relaxations of implicit functions.** Stuber, M.D. et al. (2015) *Optimization Methods and Software*, 30, 424-460
[12] **McCormick-based relaxations of algorithms.** Mitsos et al. (2009) *SIAM Journal on Optimization*, SIAM, 2009, 20, 73-601
[13] **Direct measurement of the fast, reversible addition of oxygen to cyclohexadienyl radicals in nonpolar solvents**, J. W. Taylor, et al. *Phys. Chem. A*, 108 (2004), pp. 7193–7203.
[14] **Global dynamic optimization for parameter estimation in chemical kinetics** A. B. Singer et al., *J. Phys. Chem. A*, 110 (2006), pp. 971–976.

Case Study II

Kinetic Parameter Estimation

Read Data in Julia

```
using ExcelReaders, DataFrames, IntervalArithmetic, EAGOGlobalSolver

xls_data = readxl("C:/Users/matt/Desktop/KineticParameterData.xlsx",
                  "Sheet1!A1:B5")
data = convert(Array{Float64},xls_data[:,2])
```

Define objective

```
eval( quote function f(x,p)
                I_calc = x[1:5:996]+(2/21)*x[2:5:997]+(2/21)*x[3:5:998]
                return sum((I_calc-data).^2) end end)
```

Define equality constraints

```
delt = 0.01; T = 273; k1 = 53; k1s = k1*1E-6; k5 = 1.2E-3
K2 = 46*exp(6500/T-18); K3 = 2*K2; cO2 = 2E-3; n = 200
eval( quote function h(z,p)
  h = zeros(typeof(z),n*5)
  for i=0:($n-1)
    h[5*i+1] = z[5*(i+1)+1] - z[5*i+1] + $delt*($k1*z[5*i+4]*z[5*i+5]
             - (p[1]+p[2])*z[5*i+1]*$cO2  + (p[1]/$K2)*z[5*i+4]
             + (p[2]/$K3)*z[5*i+4] - $k5*z[5*i+1]^2)
    h[5*i+2] = z[5*(i+1)+2] - z[5*i+2] + $delt*(p[2]*z[5*i+1]*$cO2
             - (p[2]/$K3+p[3])*z[5*i+2])
    h[5*i+3] = z[5*(i+1)+3] - z[5*i+3] + $delt*(p[1]*z[5*i+1]*$cO2
             - (p[1]/$K2))
    h[5*i+4] = z[5*(i+1)+4] - z[5*i+4] + $delt*(-$k1s*z[5*i+4]*z[5*i+5])
    h[5*i+5] = z[5*(i+1)+5] - z[5*i+5] + $delt*(-$k1*z[5*i+4]*z[5*i+5])
  end
return h
end end)
```

Setup Box Constraints for Problem

```
# creates intervalboxes
Xt = []
for i=1:1000
  mod(i,4)==0 ? push!(Xt,Interval(0,140)) : push!(Xt,Interval(0,0.4))
end
X = IntervalBox(tuple(Xt)...)
P = IntervalBox(10..1200,10..1200,(0.001)..40)
```

Call EAGO to Solve Problem

```
# creates initial interval box, #4 = [0,140], #1-3,5 = [0,0.4]
solution = EAGO_Global_Implicit(f,[],h,X,P,[],hbox,[])
```

Finishes with certificate of global optimality

- *Optimal point:* (789.02, 423.85,12.969)
- *Optimal value:* 16796.04
- Solution consistent with the literature

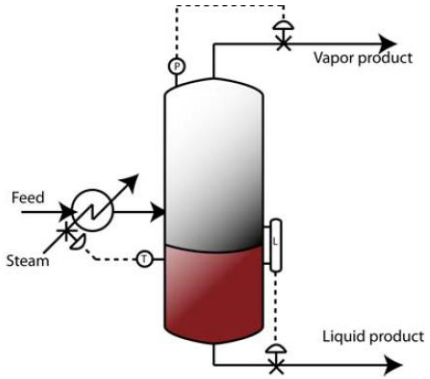
Case Study II

Flash Separation of Benzene and Toluene[14]

Problem Statement

We wish to ensure a cut-fraction, α, of less than or equal to 0.7 in the flash separation of a benzene-toluene mixture subject to uncertain temperature, T, by controlling the pressure, P.

Flash Separator



SIP Formulation

$$\max_{\tau \in T,\, p \in P} \eta$$

$$s.t. \quad \eta \le \alpha(\tau, p) - 0.7, \quad \forall p \in P$$

$$\tau \in T = [80,110]$$

$$p \in P = [90,100]$$

$$\alpha \in A = [0,1]$$

Process Model

$$h(\alpha,\tau,p) = \sum_{i=1}^{2} \frac{z_i(K_i(\tau,p)-1)}{(K_i(\tau,p)-1)\alpha+1}, \quad K_i(\tau,p) = \frac{p_i^{sat}(\tau)}{p}, \quad \log(p_i^{sat}(\tau)) = A_i - \frac{B_i}{C_i+\tau}$$

JuMP/Julia Code for Formulating/Solving Model

```
# specifies model and variables
m = RobustModel()
@uncertain(m, 90.0 <= P <= 100) @variable(m, 80.0 <= T <= 110)
@variable(m, nu) @variable(m, 0<= alpha <= 1)
# sets parameters
@NLparameter(m, z == 0.5)
n = 2 # number of species
data = [6.95087 6.87987; 1342.31 1936.01; 219.187 258.451]
for j in [[A,1],[B,2],[C,3]]
  @NLparameter(m, j[i,1][i=1:n] == data[i,j[i,2]])
end
# defines constraints
Psat = @NLexpression(m,[i=1:n],10^(A[i]-B[i]/(C[i]+tau)))
K = @NLexpression(m,[i=1:n],Psat[i]/P)
summand = @NLexpression(m,[i=1:n],z*(K[i]-1)/((K[i]*alpha-1)))
@NLconstraint(m, sum(summand[i] for i=1:n) == 0.0)
@NLconstraint(m, nu <= alpha-0.7)
@NLobjective(m, Max, nu)
value,point,info = SolveSIP(m)
```

Solving the SIP, we find that no pressure setting exists which is robust to the full range of temperature variation.

[14] **Robust simulation and design using semi-infinite programs with implicit functions.** Stuber, M. D. & Barton, P. I. (2011) *International Journal of Reliability and Safety*, 5, 378-397

Recap

- ☑ Julia Capabilities
- ☑ Developing Robust Optimization for Julia
- ☑ Illustrative Examples
- ☐ Future Directions

Case Study III

Worst-Case Subsea Separator Design[1]

Problem Statement (Original)

For any inlet gas fraction (*stream 1*) within typical bounds, is there a control setting that will prevent the effluent gas fraction of the liquid-liquid separator (*stream 7*) from exceeding the specification and damaging the pump.

Problem Statement (Semi-infinite Program)

$$\mathbf{h}(\mathbf{z},\mathbf{u},\mathbf{p})=\mathbf{0}\longrightarrow\mathbf{z}=\mathbf{x}(\mathbf{u},\mathbf{p})$$

$$\eta^{*}=\max_{\mathbf{p}\in P,\mathbf{u}\in U}\eta$$

$$\eta\le g(\mathbf{x}(\mathbf{u},\mathbf{p}),\mathbf{u},\mathbf{p}),\forall\mathbf{u}\in U$$

Equality constraints specified by mass balances, energy balances, and unit operation relations from previous flowsheet.

Semi-infinite constraint:

$$g(\mathbf{x}(\mathbf{u},\mathbf{p}),\mathbf{u},\mathbf{p})\equiv x_{G7}(\mathbf{u},\mathbf{p})-0.05$$

Uncertain Parameter (Inlet Gas Fraction)

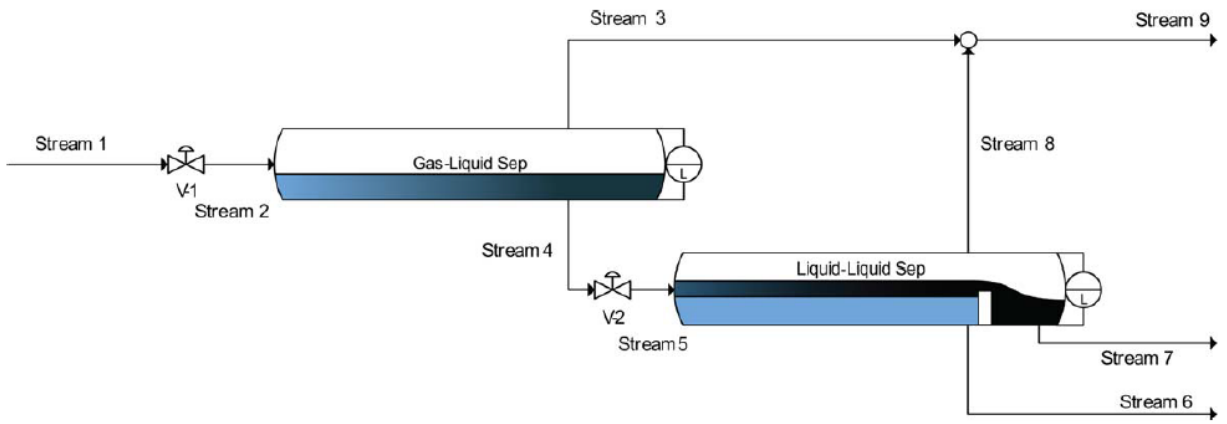
$$\mathbf{p}=(\xi_{G1})\in[0.35,0.5]$$

Control Settings (Valve Position)

$$\mathbf{u}=(u_1,u_2)\in[0,1]\times[0,1]$$

State Variables

$$\mathbf{z}=\left(\xi_{G4},\xi_{W4},\xi_{O4},\xi_{G7},\xi_{O7},H_{GLS},\dot{m}_3,\dot{m}_4,\dot{m}_6,\dot{m}_7,\dot{m}_8\right)$$



[1] **Worst-case design of subsea production facilities using semi-infinite programming.** Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524

Case Study III

Worst-Case Subsea Separator Design[1]

$$SG_O = \frac{141.5}{131.5 + API}$$

Inlet Specification

$$SG_{mix} = (\xi_{G1}/SG_G + \xi_{W1}/SG_W + \xi_{O1}/SG_O)^{-1}$$

$$\xi_{G1} + \xi_{W1} + \xi_{O1} = 1$$

Gas Mixer

$$\xi_4 = \xi_5$$

$$\dot{m}_9 = \dot{m}_3 + \dot{m}_8$$

$$P_9 = \min(P_3, P_8)$$

$$P_5 = P_{LLS}$$

$$\xi_4 = \xi_5$$

Valve 2

$$\dot{m}_4 = \dot{m}_5 = u_2 C_{v2} \sqrt{\frac{P_4 - P_5}{\rho_4 / \rho_W{}^o}}$$

$$\xi_6 = (0,1,0), \quad \xi_8 = (1,0,0), \quad \xi_{G7} + \xi_{O7} = 1$$

$$\dot{m}_5 = \dot{m}_6 + \dot{m}_7 + \dot{m}_8, \quad \xi_{G5}\dot{m}_5 = \xi_{G8}\dot{m}_8 + \xi_{G7}\dot{m}_7, \quad \xi_{W5}\dot{m}_5 = \xi_{W6}\dot{m}_6$$

$$\xi_{G7} = \xi_{G5} \exp\left[-k_{LLS} \frac{V_{oil}}{\dot{m}_7 / \rho_7}\right]$$

$$\rho_7 = \rho_W{}^o (\xi_{G7} / SG_G + \xi_{O7} / SG_O)^{-1}, \quad P_8 = P_{LLS}$$

Liquid-Liquid Separator

$$V_{oil} = V_{LLS}\left(\frac{\dot{m}_7}{\rho_7}\frac{\rho_5}{\dot{m}_5}\right)$$

$$V_{LLS} = L_{LLS}\left((H_{LLS} - R_{LLS})\sqrt{2R_{LLS}H_{LLS} - H_{LLS}{}^2} + R_{LLS}{}^2 \cos^{-1}\left[1 - \frac{H_{LLS}}{R_{LLS}}\right]\right)$$

$$P_1 = P_{well}$$

$$P_2 = P_{GLS}$$

$$\xi_1 = \xi_2$$

Valve 1

$$\dot{m}_1 = \dot{m}_2 = u_1 C_{v1} \sqrt{\frac{P_1 - P_2}{SG_{mix}}}$$

$$\xi_3 = (1,0,0), \quad \xi_{G4} + \xi_{O4} + \xi_{W4} = 1$$

$$\dot{m}_2 = \dot{m}_3 + \dot{m}_4, \quad \xi_{G2}\dot{m}_2 = \xi_{G3}\dot{m}_3 + \xi_{G4}\dot{m}_4, \quad \xi_{W2}\dot{m}_2 = \xi_{W4}\dot{m}_4$$

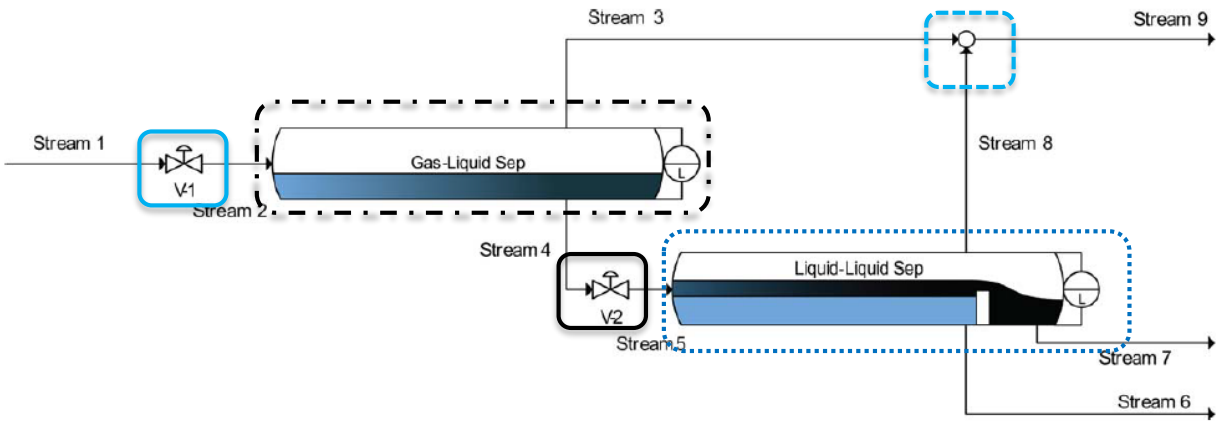
$$\xi_{G4} = \xi_{G2} \exp\left[-k_{GLS} \frac{V_{GLS}}{\dot{m}_4 / \rho_4}\right]$$

Gas-Liquid Separator

$$\rho_4 = \rho_W{}^o (\xi_{G4} / SG_G + \xi_{W4} / SG_W + \xi_{O4} / SG_O)^{-1}, \quad P_3 = P_2, \quad P_4 = P_3 + \rho_4 g_a H_{GLS}$$

$$V_{GLS} = L_{GLS}\left((H_{GLS} - R_{GLS})\sqrt{2R_{GLS}H_{GLS} - H_{GLS}{}^2} + R_{GLS}{}^2 \cos^{-1}\left[1 - \frac{H_{GLS}}{R_{GLS}}\right]\right)$$

$\dot{m}_2$ & ξ_2 *wellhead – specification*



Case Study III

Worst-Case Subsea Separator Design[1]

$$P_5 = P_{LLS}$$
$$\xi_4 = \xi_5$$
$$\dot{m}_4 = \dot{m}_5 = u_2 C_{v2} \sqrt{\frac{P_4 - P_5}{\rho_4 / \rho_W^{\,o}}}$$

- **Each of the four design case in the literature were run for Subsea Separator Design**
- **Good agreement with published results in all cases.**

```
using EAGOSemiInfinite
using EAGOFlowsheet
m = Flowsheet()
@define_parameters(m,
Cv2 = 1.67E-2,
PLLS = 4E6)
@define_equality(
$P5-$PLLS,
$x1-$x51,
$x2-$x52,
$x3-$x53,
$x7-$u2*$Cv2*sqrt(($P4-$PLLS)/($rho4/$pwo))
)
@define_state(x1,x2,x3,x7)
@define_internal(P5,rho4,pwo)
@define_control(u2)
@define_uncertain(u2)

###### INPUT FOR OTHER BLOCKS FOR PROCESS MODEL
###### ....

model = @generate_model(m)
value,point,info = SolveSIP(model)
```

Accessing EAGO & Future Plans

An intuitive graphical user interface - *EAGOFlowsheet*

- Equation-Oriented Flow-sheeting
- Graphical Manipulation of Directed Graphs
- Template Registration of New Relaxations
- AMPL Compatibility for Benchmarking

Explore and Contribute to the EAGO Package Library at

https://github.com/MatthewStuber/EAGO

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- David Saunders

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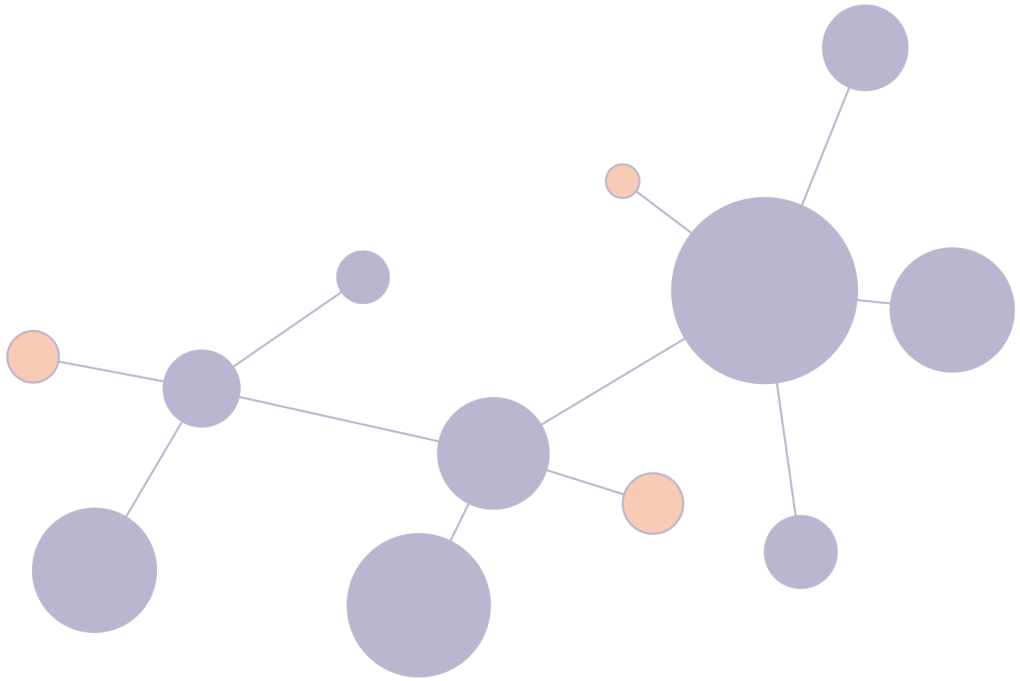
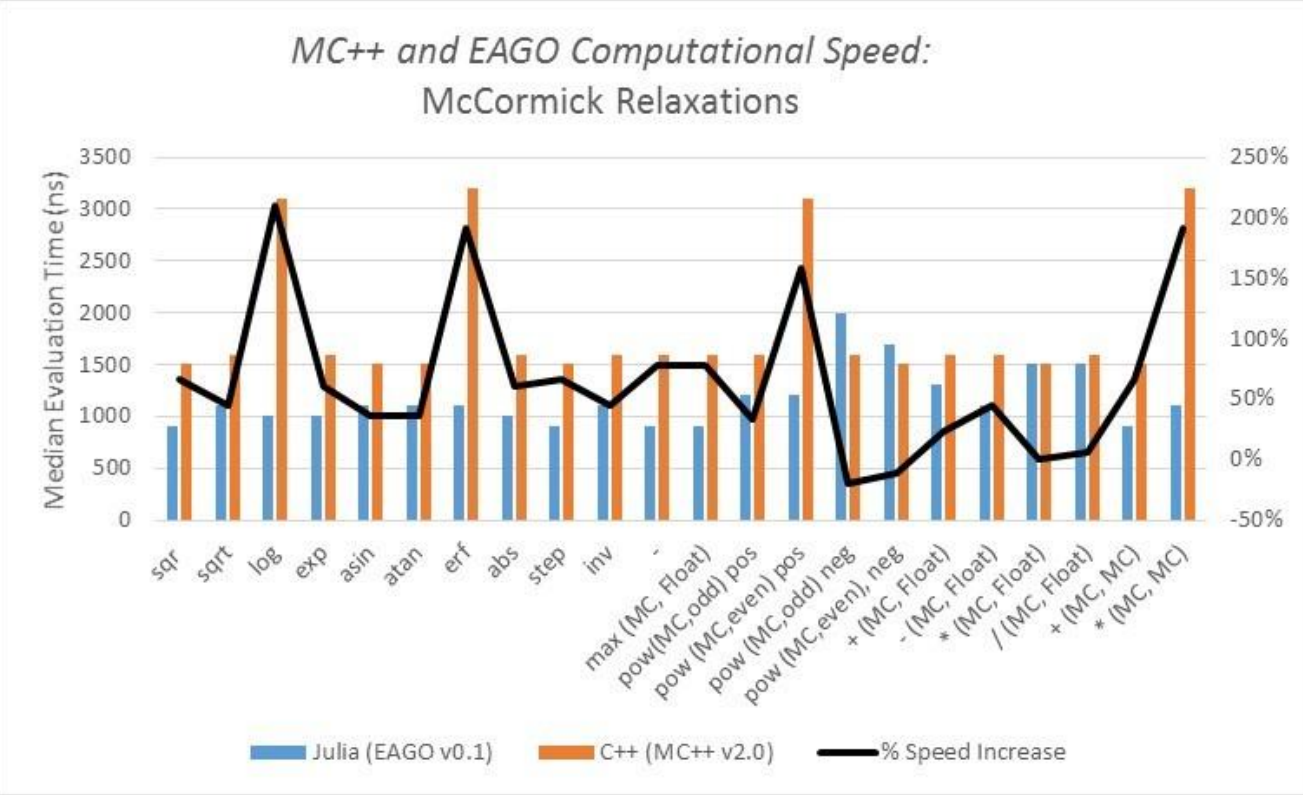


The End

Julia MC vs. MC++



- Using 64bit, Intel Xeon E3-1270 v5 @ 3.60 GHz, 32GB RAM
- Non-validated interval calculations
- Ubuntu/Linux 16.04 LTS and Julia v0.6
- Profiling 10,000 evaluations with recommend settings to limit clock noise