

Qi Chen and Braulio Brunaud

Pyomo and JuMP – Modeling environments for the 21st century

EWO Seminar
Carnegie Mellon University
March 10, 2017

Disclaimer

1. All the information provided is coming from the standpoint of two somewhat expert users in Pyomo and JuMP, former GAMS users
2. All the content is presented to the best of our knowledge

Data Input

Data
Manipulation

Optimization

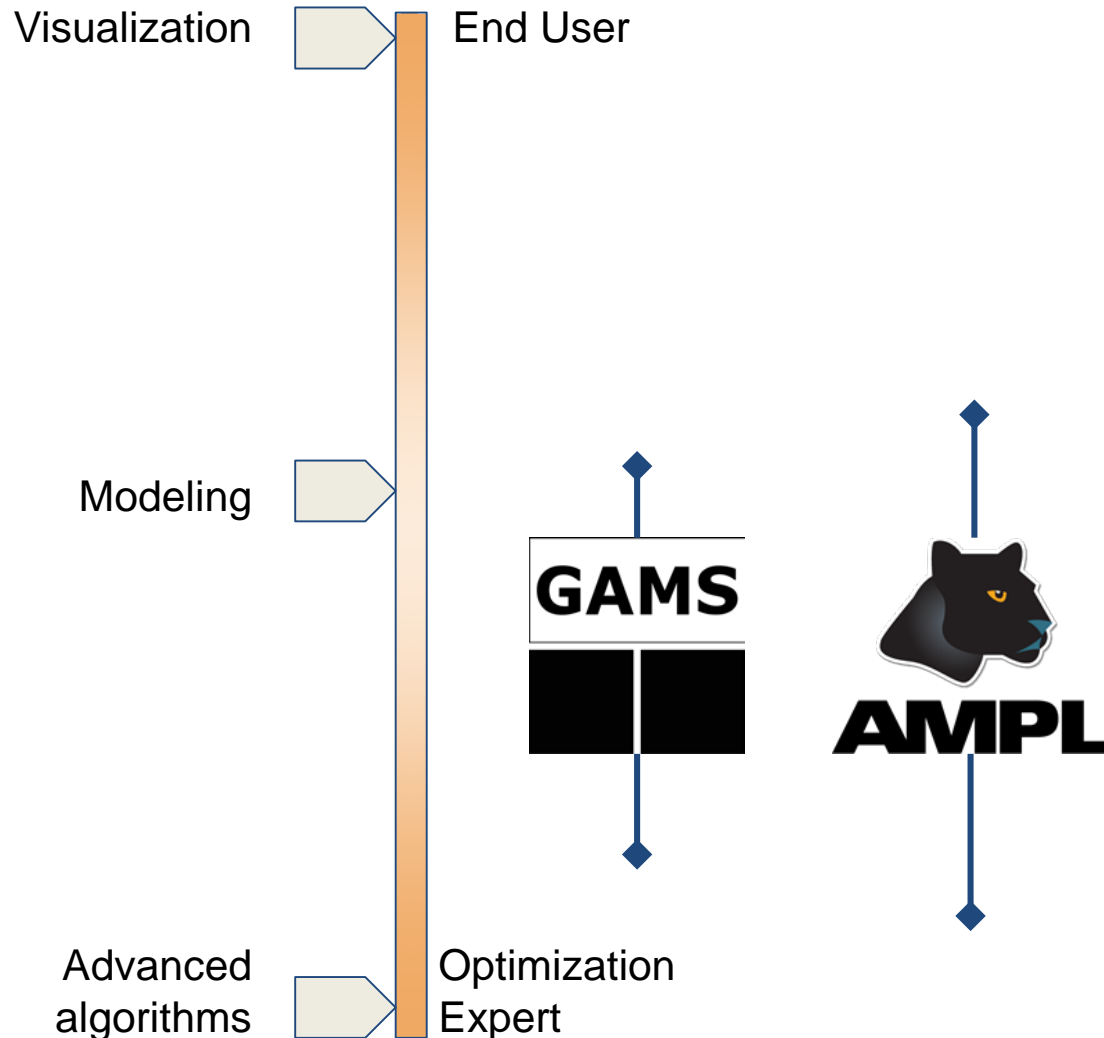
Analysis

Visualization

- These tasks usually involve many tools:
 - Databases
 - Excel
 - GAMS/AMPL/AIMMS/CPLEX
 - Tableau

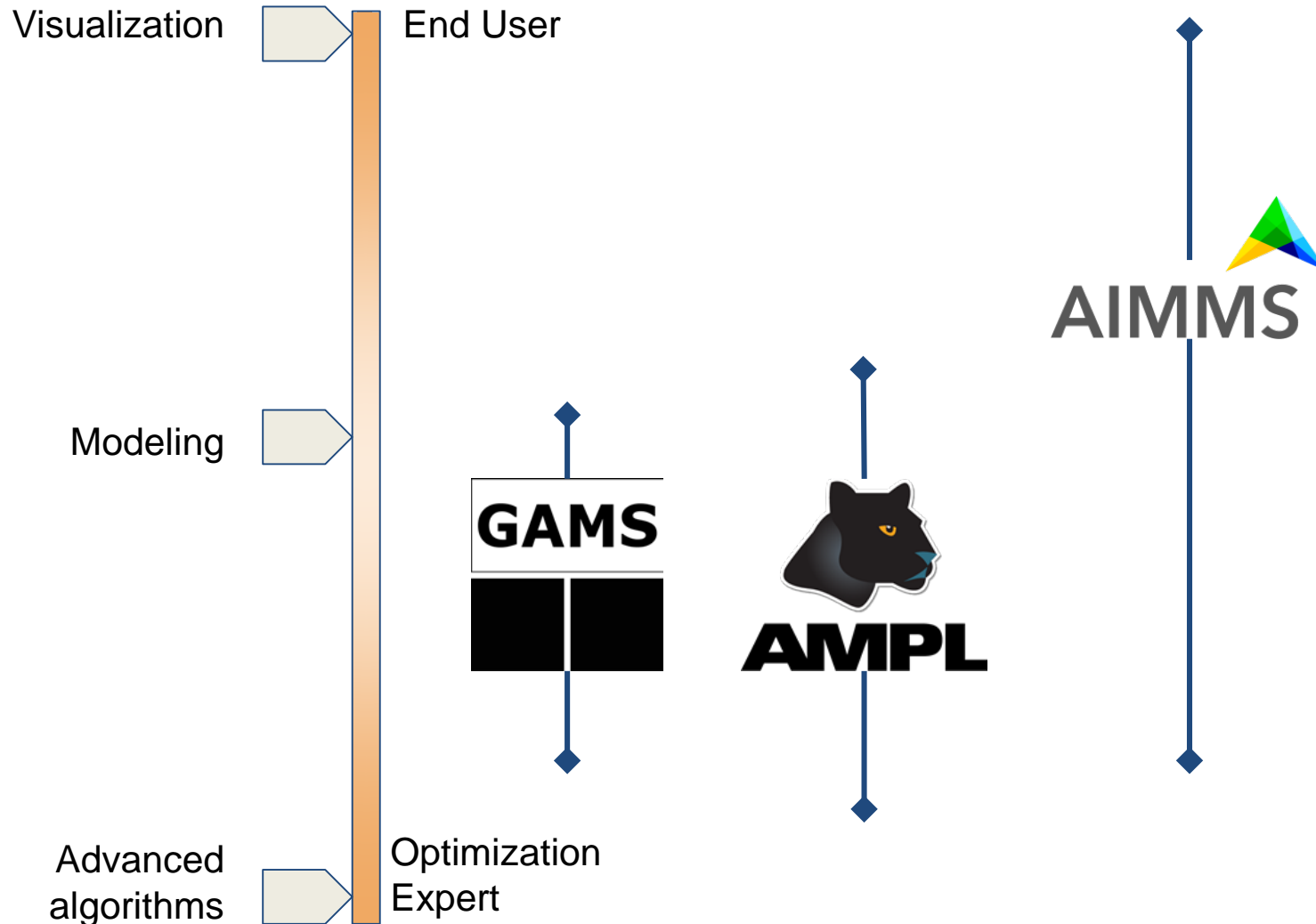
- Can a single tool be used to complete the entire workflow?

Optimization Environments Overview



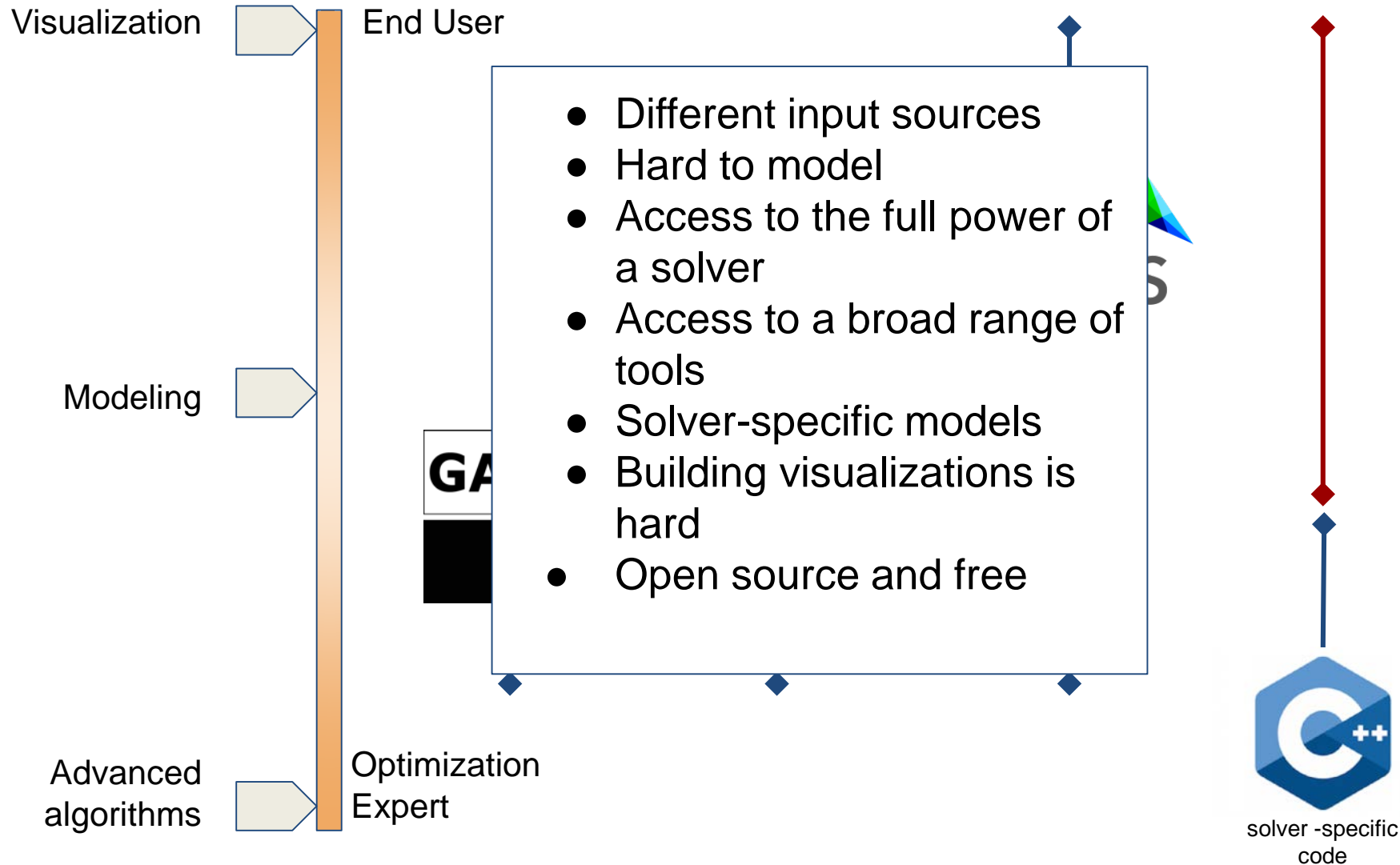
- Different input sources
- Easy to model
- AMPL: Specific modeling constructs
 - Piecewise
 - Complementarity conditions
 - Logical Implications
- Solver independent models
- Developing complex algorithms can be challenging
- Large number of solvers available
- Commercial

Optimization Environments Overview

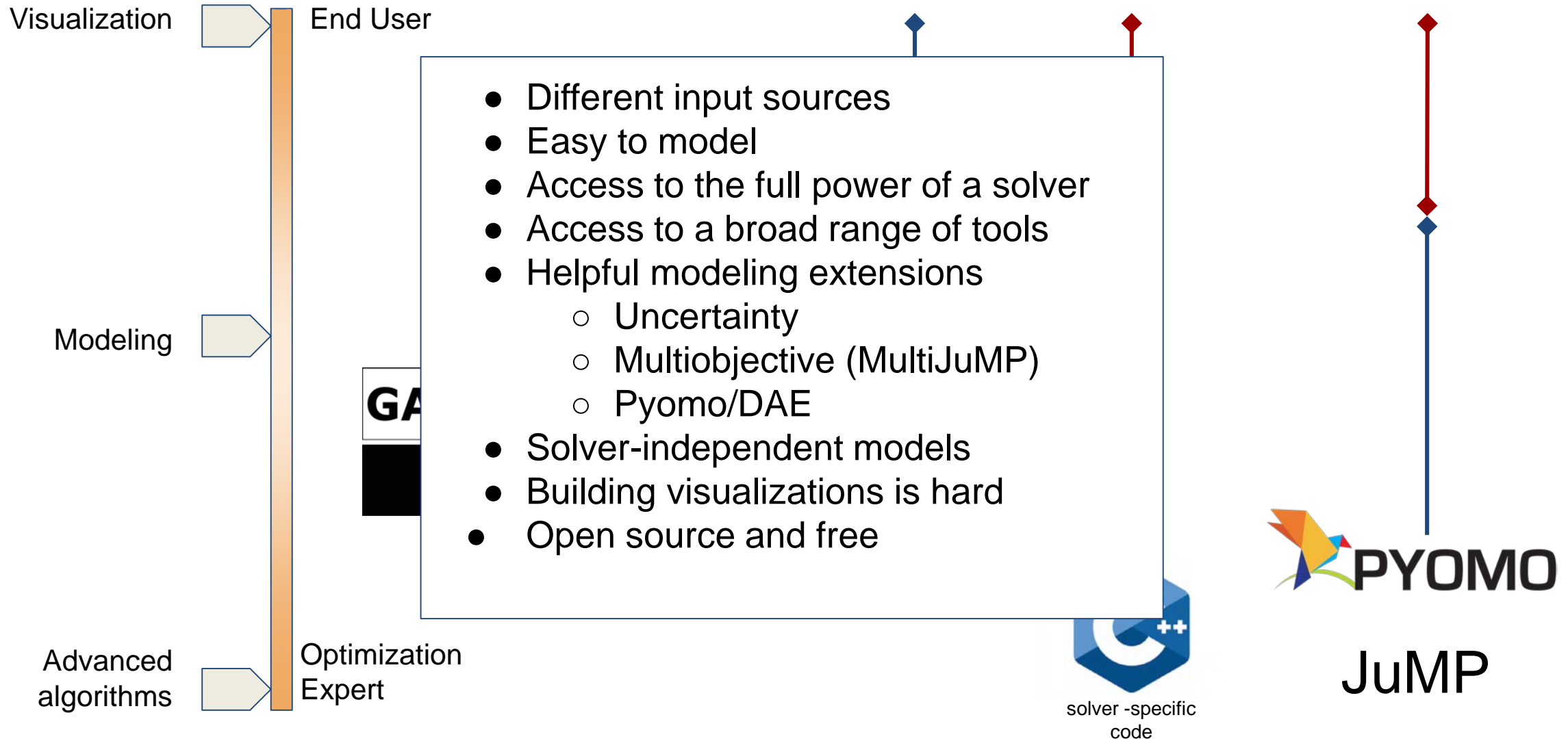


- Different input sources
- Build input forms
- Easy to model
- Multiplatform:
 - Standalone
 - Web
 - Mobile
- Solver independent models
- Build visualizations
- Commercial

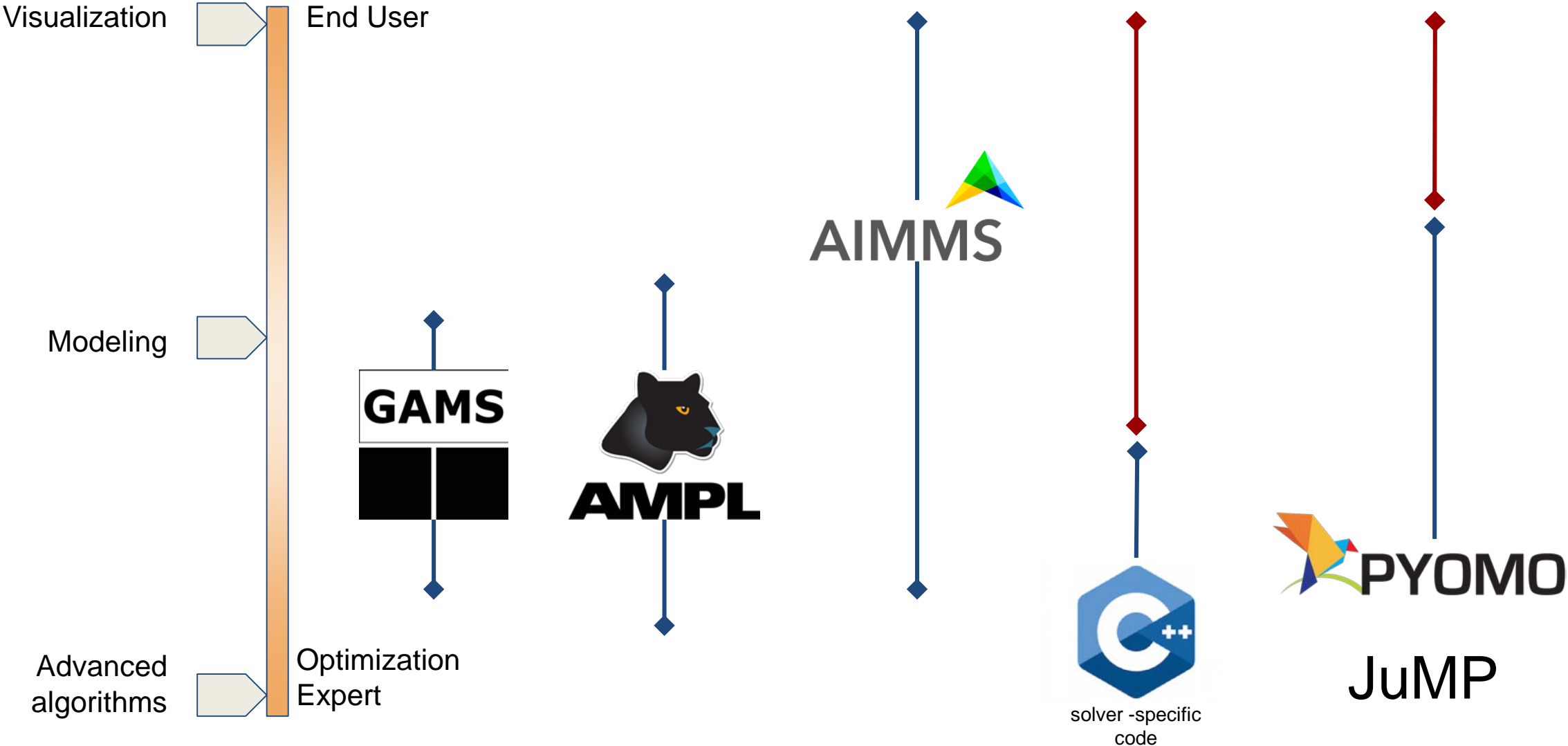
Optimization Environments Overview








Optimization Environments Overview



Optimization Environments Overview



Optimization Environments Overview

						JuMP
Data Input	hard	hard	✓	✓	✓	✓
Data Manipulation	✗	✗	✓	✓	✓	✓
Modeling	✓	✓	✓	hard	✓	✓
Advanced Algorithms	hard	hard	✓	✓	✓	✓
Solvers Availabilty	✓	✓	limited	✗	limited	limited
Visualization	✗	✗	✓	hard	hard	hard
License	\$	\$	\$\$	free	free	free



version 0.5.1

<http://julialang.org/>

- New programming language for scientific computing
- Aims to combine
 - Flexibility from Python
 - Math power from Matlab and R
 - High performance from C++
- Designed with performance in mind
- Designed for parallel computing
- Metaprogramming
 - Code that generates code
- Very easy to code

Learn:

<https://learnxinyminutes.com/docs/julia/>

- Julia module for **M**athematical **P**rogramming
- Provides objects for Model, Variables, Constraints and Expressions
- Easy implementation of callbacks
- Supports Unicode characters
- Supports:
 - MINLP
 - Second order conic programming
 - Semi-definite programming
- @ sign means a macro (metaprogramming)

In [9]: `using JuMP`

```
m = Model()
@variable(m, x[1:2] >= 0)
@variable(m, α == 5)

@constraint(m, con[i in 1:2], x[i] <= α)
@objective(m, Max, sum(x[i] for i in 1:2))

@show m
```

m = Maximization problem with:
* 2 linear constraints
* 3 variables
Solver is default solver

Out[9]:

$$\begin{aligned} & \max && x_1 + x_2 \\ \text{Subject to} &&& x_1 - \alpha \leq 0 \\ &&& x_2 - \alpha \leq 0 \\ &&& x_i \geq 0 \quad \forall i \in \{1, 2\} \\ &&& \alpha = 5 \end{aligned}$$

1. Database

```
In [ ]: using MySQL

con = mysql_connect("localhost", "bbrunaud", "****", "DFLdata")

# Get Demands
query = """
        SELECT Customer, Product, Period, Demand
        FROM Demands
        WHERE
            (ProductNumber BETWEEN $firstP AND $lastP)
            AND
            (Period BETWEEN $t1 AND $tN)
            AND
            (SiteCode BETWEEN $firstCcode AND $lastCcode)
        """

demands = mysql_execute(con, query)
```

For other databases check [JuliaDB](#)

2. Excel

```
In [2]: using ExcelReaders
        using DataFrames

        demand = readxl(DataFrame, "demand.xlsx", "Sheet1!A1:D5")
```

Out[2]:

	Customer	Product	Period	Demand
1	CUS1	A	1.0	36.0
2	CUS1	B	1.0	57.0
3	CUS2	A	1.0	30.0
4	CUS2	B	1.0	44.0

3. Julia Code

Use dictionaries

```
In [4]: demand = Dict(  
    ("CUS1", "A", 1) => 36.0,  
    ("CUS1", "B", 1) => 57.0,  
    ("CUS2", "A", 1) => 30.0,  
    ("CUS2", "B", 1) => 44.0  
)
```

Use matrices

```
In [5]: TransportationCost = [ 100 1.5; 1.7 100]
```

```
Out[5]: 2×2 Array{Float64,2}:  
 100.0  1.5  
  1.7 100.0
```

```
In [6]: TransportationCost[1,2]
```

```
Out[6]: 1.5
```

In this case, indices are restricted to be integers

JuMP - A simple example

Solve the following problem using CPLEX

In [22]: `@show m`

```
m = Minimization problem with:  
  * 3 linear constraints  
  * 5 variables  
Solver is Cplex
```

Out [22]:

$$\begin{aligned} \min \quad & x \\ \text{Subject to} \quad & x + 16y_1 + 19y_2 + 23y_3 + 28y_4 = 0 \\ & 2y_1 + 3y_2 + 4y_3 + 5y_4 \leq 9 \\ & 6y_1 + y_2 + 3y_3 + 2y_4 \leq 2 \\ & y_i \geq 0 \quad \forall i \in \{1, 2, 3, 4\} \\ & x \text{ free} \end{aligned}$$

Load Packages

In [17]: `using JuMP`
`using CPLEX`

Declare model

Solver options go inside the parenthesis of `CplexSolver()`

In [18]: `m = Model(solver=CplexSolver())`

Out [18]:

$$\begin{aligned} \min \quad & 0 \\ \text{Subject to} \end{aligned}$$

Declare variables and constraints

```
In [19]: @variable(m, x)
@variable(m, y[1:4] >= 0)

@constraints m begin
    x + 16y[1] + 19y[2] + 23y[3] + 28y[4] == 0
    2y[1] + 3y[2] + 4y[3] + 5y[4] <= 9
    6y[1] + 1y[2] + 3y[3] + 2y[4] <= 2
end
```

Declare objective and solve

```
In [20]: @objective(m, Min, x)

solve(m)
```

Tried aggregator 1 time.
LP Presolve eliminated 1 rows and 1 columns.
Reduced LP has 2 rows, 4 columns, and 8 nonzeros.
Presolve time = 0.00 sec. (0.00 ticks)

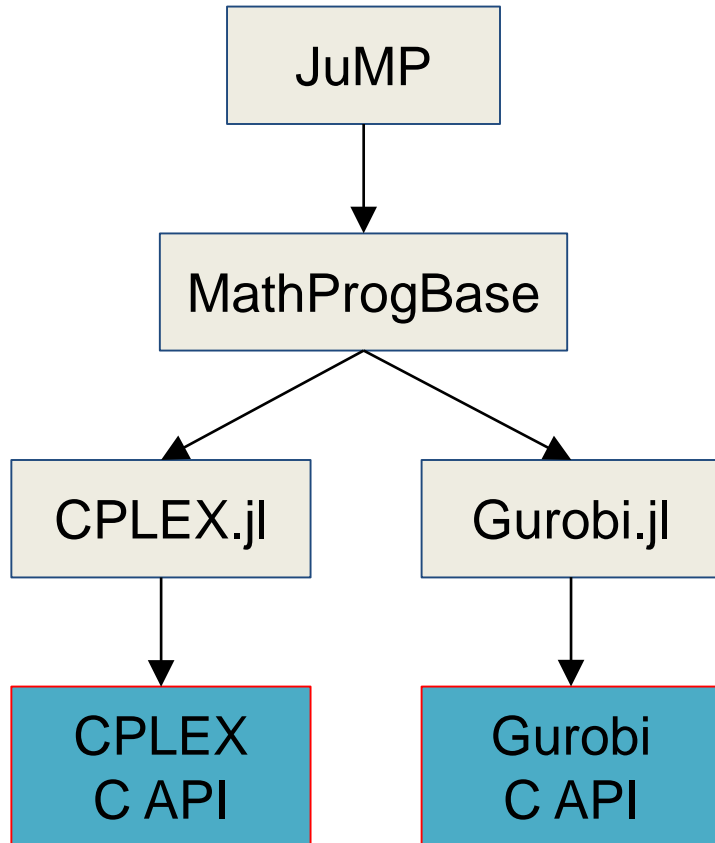
```
Iteration log . . .
Iteration:    1    Dual infeasibility =          0.000000
Iteration:    2    Dual objective    =         -56.375000
```

```
Out[20]: :Optimal
```

Save the solution vector

```
In [7]: using JLD

save("solution.jld", "sol", m.colVal)
```

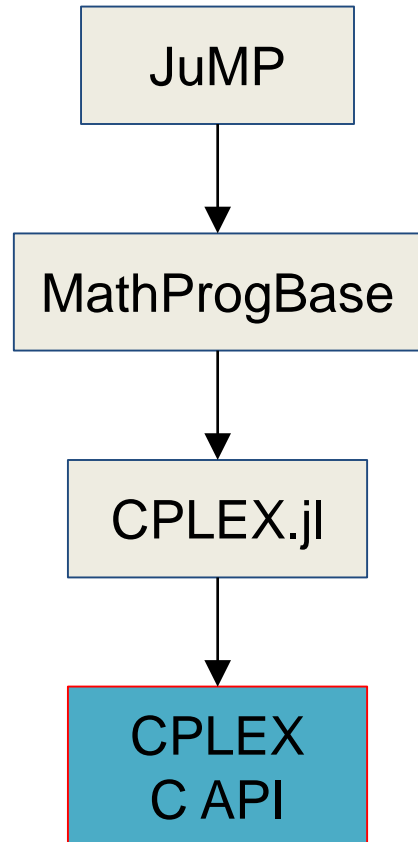
JuMP objects

Interface

Solvers interface

C libraries

- All the layers are very thin. This is why creating and manipulating models is very fast.
- Julia is designed to make efficient calls to C or Fortran



JuMP objects

@variable(m, x >=0)

Interface

addvar!

Solvers interface

addvar!

C libraries

addcols

**Example:
Adding a
variable**

JuMP - Accessing the low level objects

- Let's get the simplex tableau of the simplex example

```
In [24]: mpb = m.internalModel # MathProgBase Model
         cpx = mpb.inner       # CPLEX Model

         tableau = zeros(length(m.linconstr),m.numCols)

         for k in 1:length(m.linconstr)
             row = CPLEX.get_tableau_row(cpx,k-1)
             tableau[k,:] = row'
         end

         tableau
```

```
Out[24]: 3x5 Array{Float64,2}:
          1.0  -98.0  0.0  -34.0  -10.0
          0.0   6.0  1.0   3.0   2.0
          0.0 -16.0  0.0  -5.0  -1.0
```

JuMP - Accessing the low level objects

- Let's get the simplex tableau of the simplex example

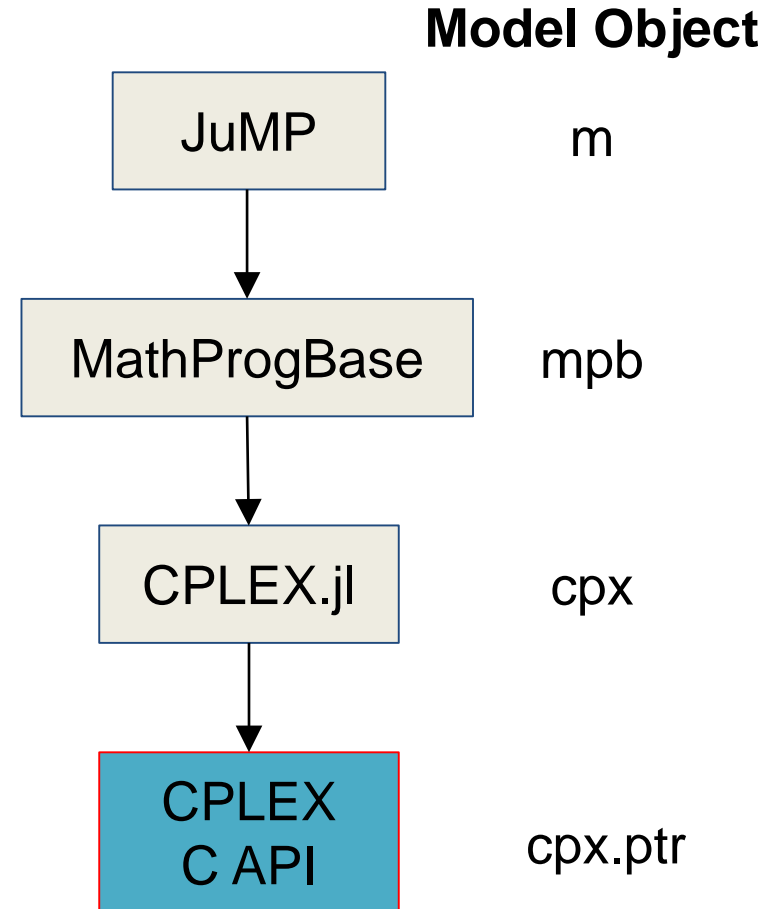
```
In [24]: mpb = m.internalModel # MathProgBase Model
         cpx = mpb.inner       # CPLEX Model

         tableau = zeros(length(m.linconstr),m.numCols)

         for k in 1:length(m.linconstr)
             row = CPLEX.get_tableau_row(cpx,k-1)
             tableau[k,:] = row'
         end

         tableau
```

```
Out[24]: 3x5 Array{Float64,2}:
          1.0  -98.0  0.0  -34.0  -10.0
          0.0   6.0  1.0   3.0   2.0
          0.0 -16.0  0.0  -5.0  -1.0
```



JuMP - Accessing the low level objects

- Let's get the simplex tableau of the simplex example

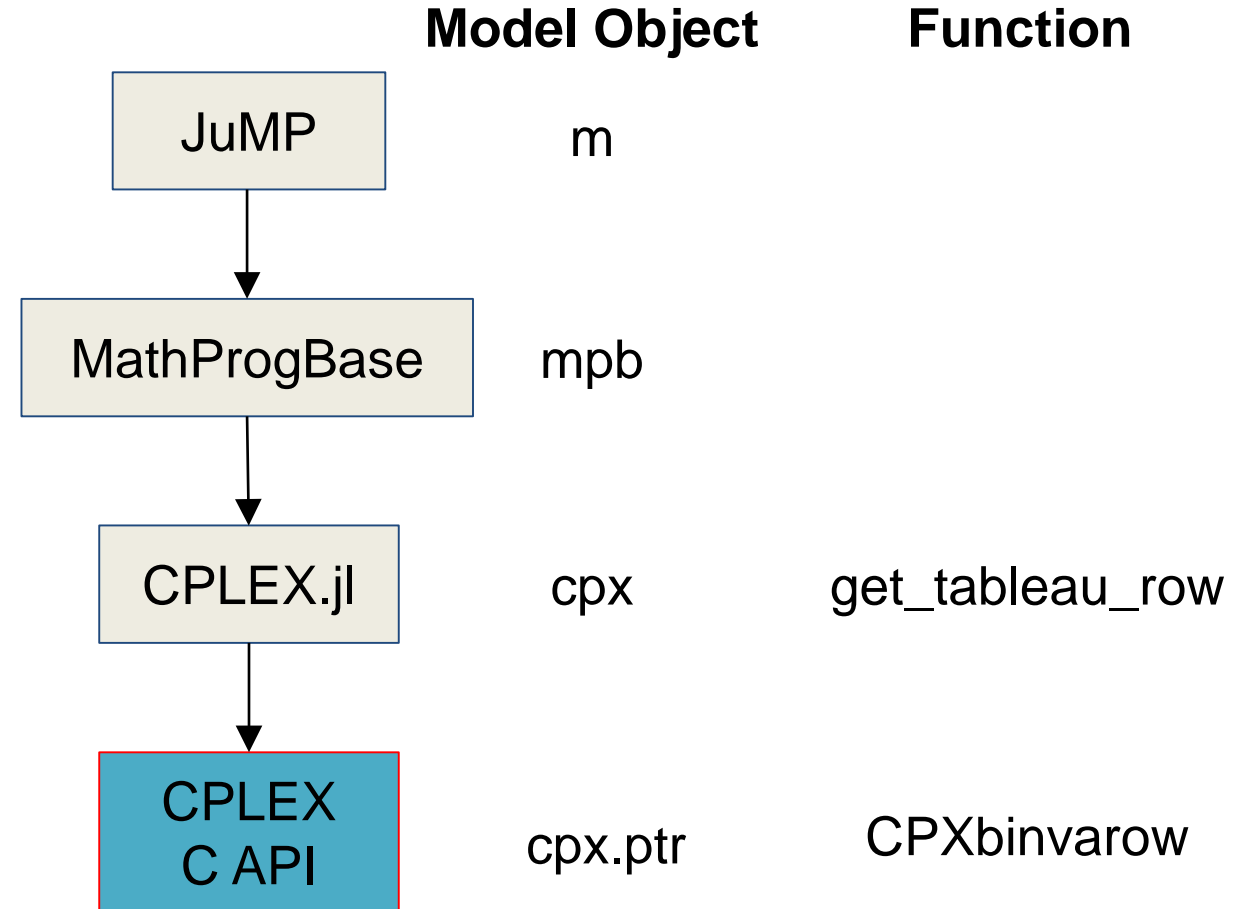
```
In [24]: mpb = m.internalModel # MathProgBase Model
         cpx = mpb.inner       # CPLEX Model

         tableau = zeros(length(m.linconstr),m.numCols)

         for k in 1:length(m.linconstr)
             row = CPLEX.get_tableau_row(cpx,k-1)
             tableau[k,:] = row'
         end

         tableau
```

```
Out[24]: 3x5 Array{Float64,2}:
          1.0  -98.0  0.0  -34.0  -10.0
          0.0   6.0  1.0   3.0   2.0
          0.0 -16.0  0.0  -5.0  -1.0
```



JuMP - Accessing the low level objects

- Let's get the simplex tableau of the simplex example

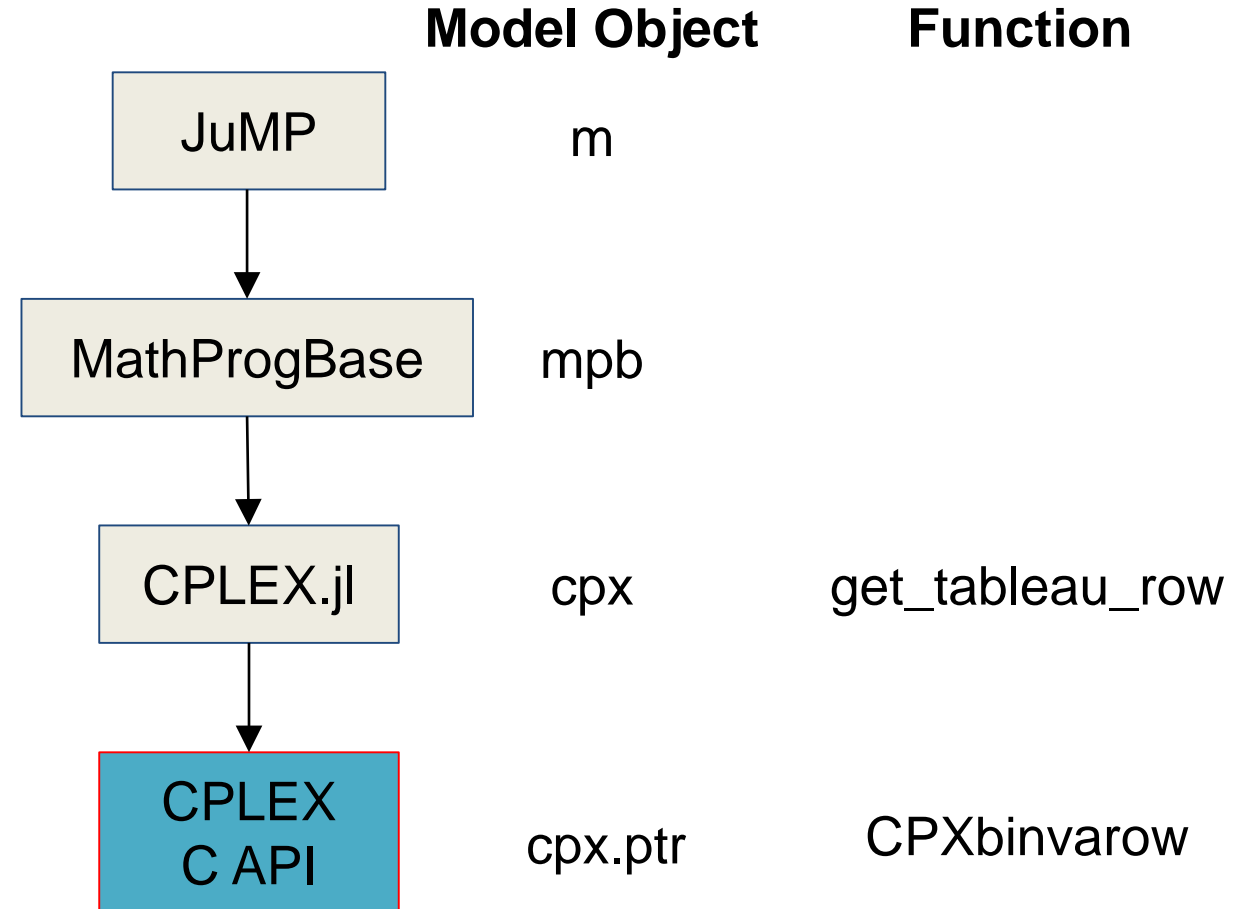
```
In [24]: mpb = m.internalModel # MathProgBase Model
         cpx = mpb.inner       # CPLEX Model

         tableau = zeros(length(m.linconstr),m.numCols)

         for k in 1:length(m.linconstr)
             row = CPLEX.get_tableau_row(cpx,k-1)
             tableau[k,:] = row'
         end

         tableau
```

```
Out[24]: 3x5 Array{Float64,2}:
          1.0  -98.0  0.0  -34.0  -10.0
          0.0   6.0  1.0   3.0   2.0
          0.0 -16.0  0.0  -5.0  -1.0
```



When declaring a model in JuMP it is possible to access every single function in the C API

- JuMP is written in very few lines of code (9,000) and it is very simple to understand
- It is not difficult to write extensions
 - [JuMPeR.jl](#): for robust optimization
 - [MultiJuMP.jl](#): for multi-objective optimization
 - [JuMPChance.jl](#): for probabilistic chance constraints
 - [StochDynamicProgramming.jl](#): for discrete-time stochastic optimal control problems
 - [PolyJuMP.jl](#): for polynomial optimization
 - [StructJuMP.jl](#): for block-structured optimization
 - [NLOptControl.jl](#): for formulating and solving nonlinear optimal control problems
 - [Complementarity.jl](#): for complementarity problems
 - DSP, Argonne National Lab: Implements decomposition methods for stochastic mixed-integer programs

<http://www.juliaopt.org/packages/>

Pros

- ✓ It's new
- ✓ Fast
- ✓ Free
- ✓ Easy and simple source code
- ✓ Access to low level objects
- ✓ Built with performance in mind
- ✓ Support through an active community at the Julia forums
- ✓ Plenty of libraries to support your workflow
 - ✓ Data analysis
 - ✓ Plotting
 - ✓ Statistics
 - ✓ It is also possible to call libraries from other languages within Julia: Python, C++, Fortran, R, Matlab, Java, etc

Pros

- ✓ It's new
- ✓ Fast
- ✓ Free
- ✓ Easy and simple source code
- ✓ Access to low level objects
- ✓ Built with performance in mind
- ✓ Support through an active community at the Julia forums
- ✓ Plenty of libraries to support your workflow
 - ✓ Data analysis
 - ✓ Plotting
 - ✓ Statistics
 - ✓ It is also possible to call libraries from other languages within Julia: Python, C++, Fortran, R, Matlab, Java, etc

Cons

- ☐ It's new
 - ☐ The platform and the supporting packages are not mature enough
 - ☐ JuMP version 0.16
- ☐ No standard solution report
- ☐ Lack of modeling features
 - ☐ Piecewise (SOS are supported though)
 - ☐ Disjunctions
 - ☐ Indicator Constraints



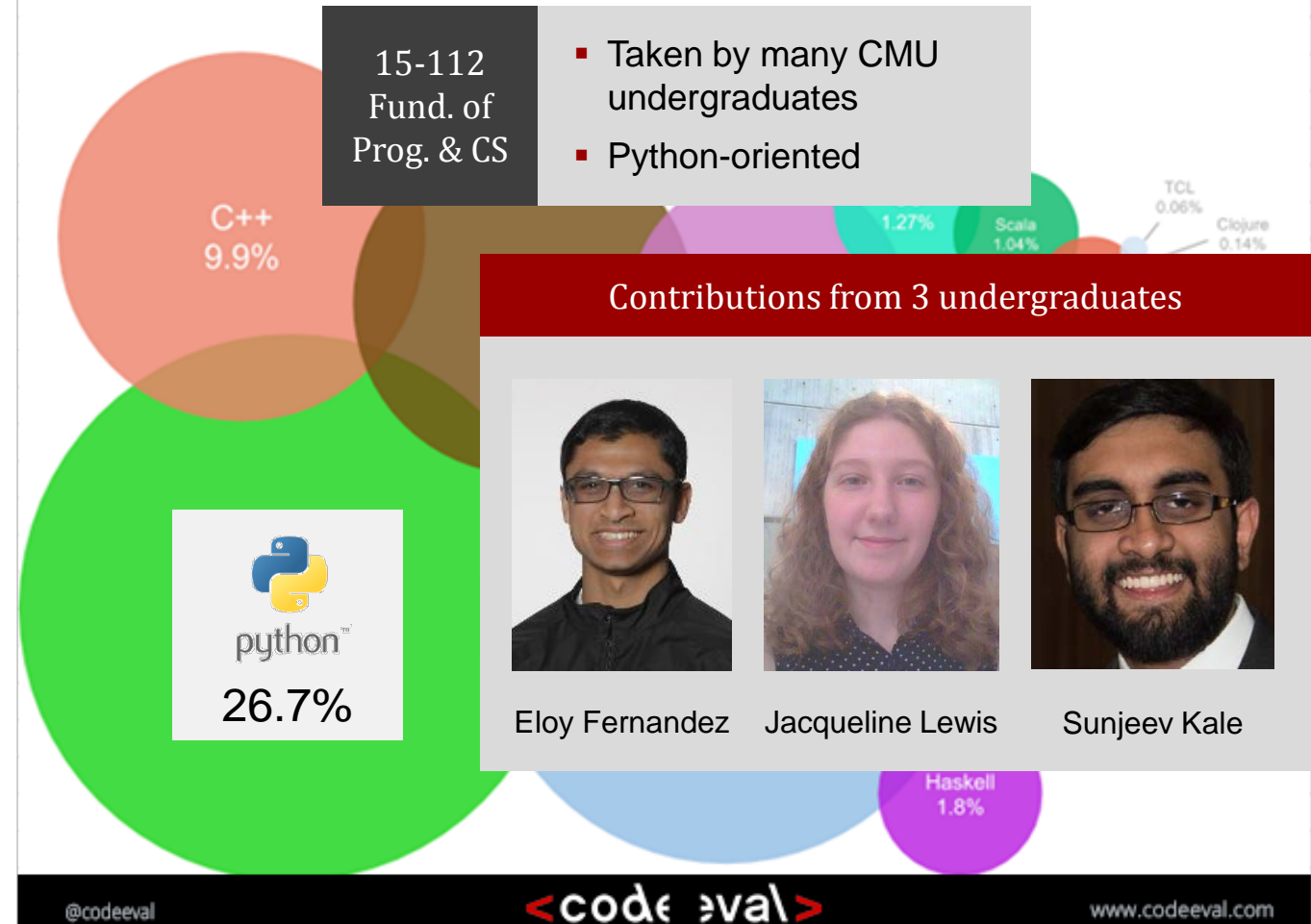
<http://python.org/>

Mathematical Modeling in Python

Why Python?

- High level coding language: **mature** + **stable**
 - Used in production by Google, Facebook, IBM, Nasdaq, etc.
 - Deep pool of **experienced developers**
- Enables **fast prototyping** and **integrated** work process
- Many useful **libraries**:
 - Numpy – linear algebra
 - Pandas – Data input/output + parsing
 - Networkx – Network graph analysis + display
 - PyQt – Graphical User Interface
 - Matplotlib – plotting results
 - Python interfaces common for external tools
- Ability to **aggregate data** from multiple sources

Most Popular Coding Languages of 2016



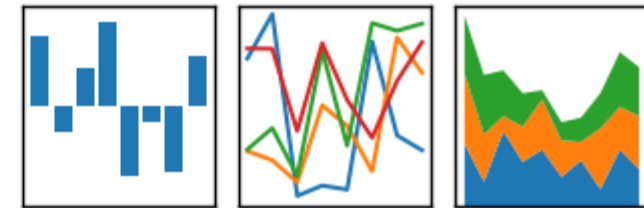
Mathematical Modeling in Python

Why Python?

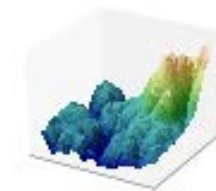
- High level coding language: **mature** + **stable**
 - Used in production by Google, Facebook, IBM, Nasdaq, etc.
 - Deep pool of **experienced developers**
- Enables **fast prototyping** and **integrated** work process
- Many useful **libraries**:
 - Numpy – linear algebra
 - Pandas – Data input/output + parsing
 - Networkx – Network graph analysis + display
 - PyQt – Graphical User Interfaces
 - Matplotlib – plotting results
 - Python interfaces common for external tools
- Ability to **aggregate data** from multiple sources



pandas
 $y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$



matplotlib



PyQt tool for model visualization

Pyomo Model Viewer

Model		Solver						
Name	Value	L.B.	U.B.	Type	Fixed	Active	Stale	Doc
▼ _SimpleMeaSheet				MeaSheet		true		
links				Block		true		
▶ absorb				Absorber		true		C02 abso
▶ regen				Regenerator		true		Solvent r
▶ xhx				General		true		Lean/Rich
▶ reboiler				General		true		Regenera
▶ mumix				General		true		Makeup s
s1				Constraint		false		
s2				Constraint		false		
s3				Constraint		false		
s4				Constraint		false		
s5				Constraint		false		
s6				Constraint		false		
s7				Constraint		false		
▶ s1.expanded				IndexedCons...		true		
▶ s2.expanded				IndexedCons...		true		
▶ s3.expanded				IndexedCons...		true		
▶ s4.expanded				IndexedCons...		true		
▶ s5.expanded				IndexedCons...		true		
▶ s6.expanded				IndexedCons...		true		
▶ s7.expanded				IndexedCons...		true		
mea_h2o_ratio	0.1124			Var	true	true	true	
eq_mea_h2o_ratio				Constraint		true		
eq_mumix_y				Constraint		true		
int_cuts				IndexedCons...		true		
tmp_int_cuts				IndexedCons...		true		

Courtesy of John Eslick, NETL

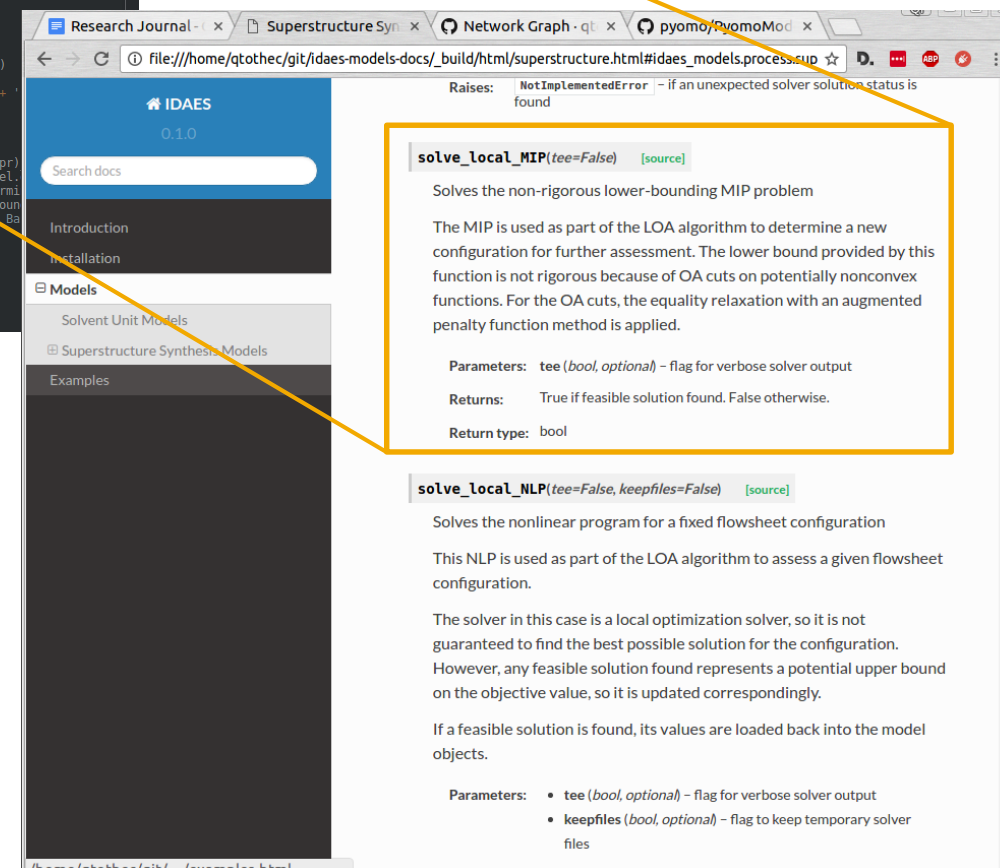
Solve Load Save OK

Why Python? (cont.)

Tools for effective model stewardship

- Programmatic **documentation** generation
 - Easily generate webpage with code and model documentation
- Standardized code style guide (PEP8)
 - **Automatic code formatting**
 - Makes models more consistently readable to multiple users
- Software version control (Git)
- **Automatic testing**
 - Ensures that future changes do not silently break existing functionality
 - Identifies affected code
 - Automatically executed when changes made to code
- Facilitates **management of change** from user to user

```
432 def solve_local_MIP(self, tee=False):
433     """Solves the non-rigorous lower-bounding MIP problem
434
435     The MIP is used as part of the LOA algorithm to determine a new
436     configuration for further assessment. The lower bound provided by
437     this function is not rigorous because of OA cuts on potentially
438     nonconvex functions. For the OA cuts, the equality relaxation with
439     an augmented penalty function method is applied.
440
441     Args:
442         tee (bool, optional): flag for verbose solver output
443
444     Returns:
445         bool: True if feasible solution found. False otherwise.
446     """
447     self.activate_standard_objective()
448     self.activate_penalized_oa_objective()
449     for intervals(self.units):
450         get_str(o, 'apply MIP', doNothing())
451         results = self.solve_local_MIP(self.model, tee=tee)
452         self.solver.time_tot += get_time(results)
453         print('MIP took ' + str(round(get_time(results), 2)) + 's')
454         if results.solver.termination_condition is TerminationCondition.optimal:
455             self.local_LB = max([self.local_LB,
456                                value(self.model.oa.obj.expr)
457                                + str(round(self.local_LB, 2)) + ' U: ' + str(round(self.global_UB, 2)) + ' B: ' + str(round(value(self.model.oa.obj.expr), 2))])
458             print('MIP proposes a configuration of:')
459             self.print_active_units()
460             return True
461         else:
462             print('MIP infeasible')
463             return False
```



Research Journal - x Superstructure Syn - Network Graph - qt x pyomo/PyomoMod x

file:///home/qtothec/git/daes-models-docs/_build/html/superstructure.html#daes_models.process.supp

IDAES 0.1.0

Search docs

- Introduction
- Installation
- Models
 - Solvent Unit Models
 - Superstructure Synthesis Models
- Examples

Raises: **NotImplementedError** - if an unexpected solver solution status is found

`solve_local_MIP(tee=False)` [\[source\]](#)

Solves the non-rigorous lower-bounding MIP problem

The MIP is used as part of the LOA algorithm to determine a new configuration for further assessment. The lower bound provided by this function is not rigorous because of OA cuts on potentially nonconvex functions. For the OA cuts, the equality relaxation with an augmented penalty function method is applied.

Parameters: `tee (bool, optional)` - flag for verbose solver output

Returns: `True` if feasible solution found. `False` otherwise.

Return type: `bool`

`solve_local_NLP(tee=False, keepfiles=False)` [\[source\]](#)

Solves the nonlinear program for a fixed flowsheet configuration

This NLP is used as part of the LOA algorithm to assess a given flowsheet configuration.

The solver in this case is a local optimization solver, so it is not guaranteed to find the best possible solution for the configuration. However, any feasible solution found represents a potential upper bound on the objective value, so it is updated correspondingly.

If a feasible solution is found, its values are loaded back into the model objects.

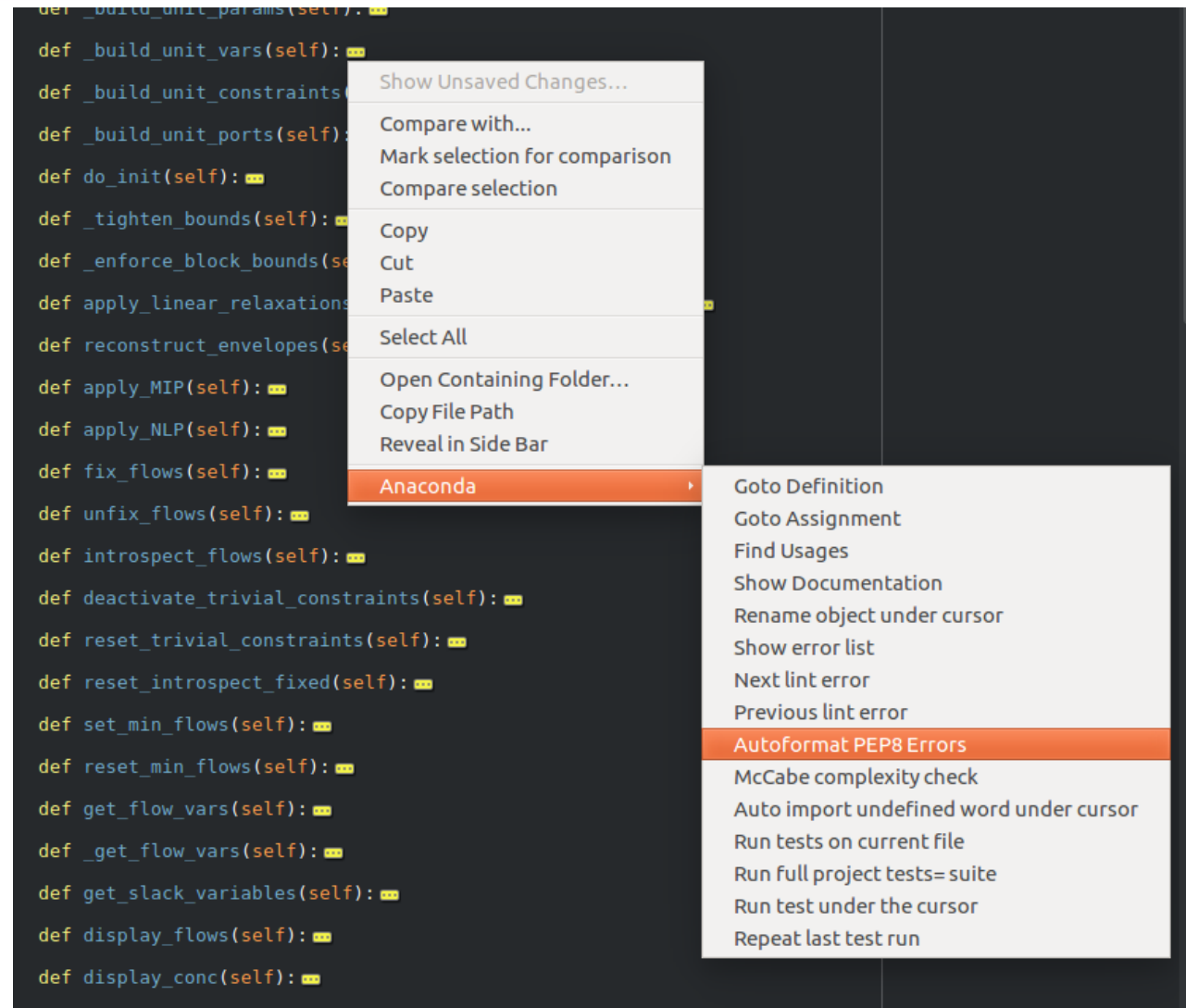
Parameters:

- `tee (bool, optional)` - flag for verbose solver output
- `keepfiles (bool, optional)` - flag to keep temporary solver files

Why Python? (cont.)

Tools for effective model stewardship

- Programmatic **documentation** generation
 - Easily generate webpage with code and model documentation
- Standardized code style guide (PEP8)
 - **Automatic code formatting**
 - Makes models more consistently readable to multiple users
- Software version control (Git)
- **Automatic testing**
 - Ensures that future changes do not silently break existing functionality
 - Identifies affected code
 - Automatically executed when changes made to code
- Facilitates **management of change** from user to user



Why Python? (cont.)

Tools for effective model stewardship

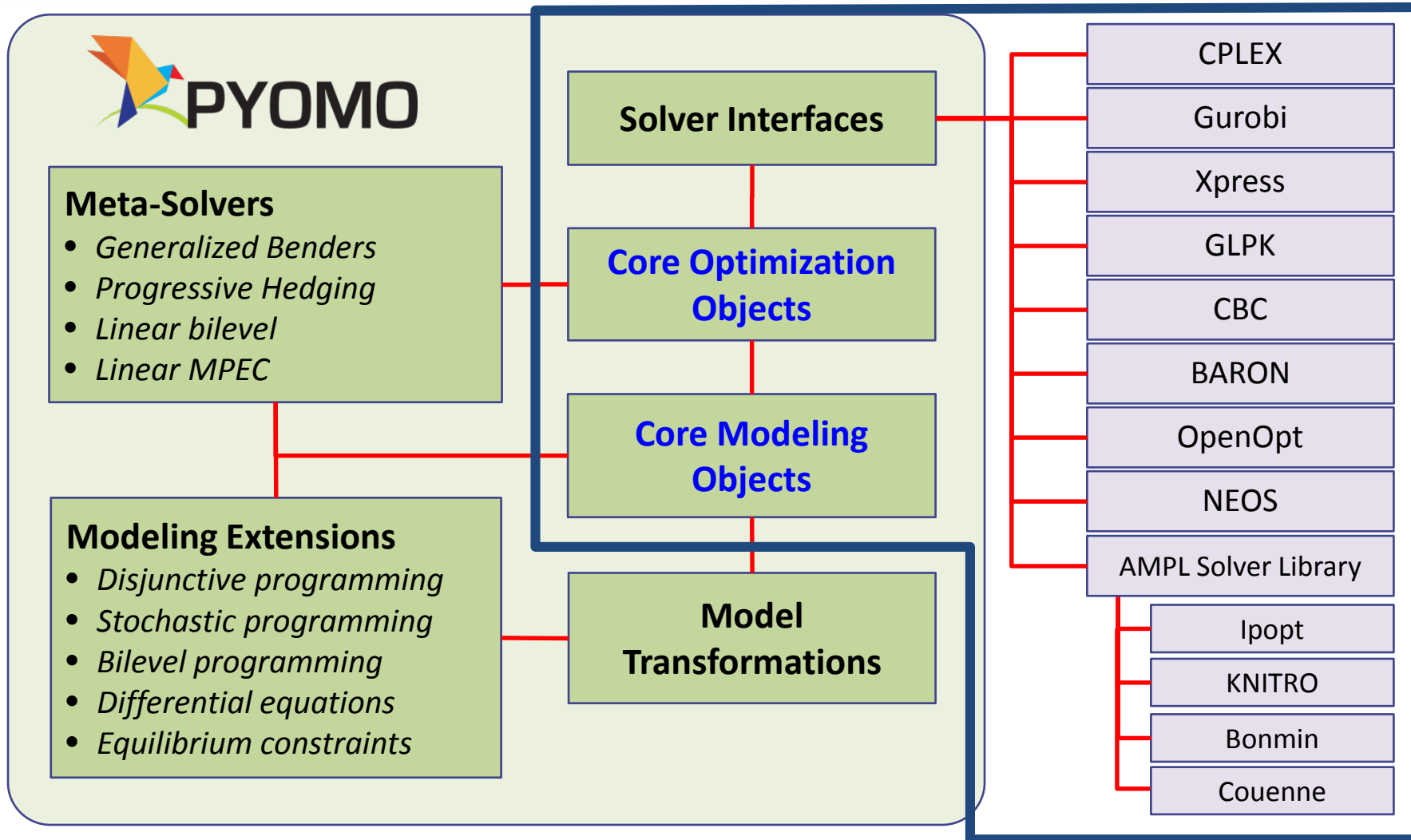
- Programmatic **documentation** generation
 - Easily generate webpage with code and model documentation
- Standardized code style guide (PEP8)
 - **Automatic code formatting**
 - Makes models more consistently readable to multiple users
- Software version control (Git)
- **Automatic testing**
 - Ensures that future changes do not silently break existing functionality
 - Identifies affected code
 - Automatically executed when changes made to code
- Facilitates **management of change** from user to user

```
qichen@QC-CMU-Tower:~/git/super$ nosetests > ~/test.log
nose.config: INFO: Ignoring files matching ['^\\.\\.py$']
test_case_1 (idaes_models.process.superstructure_synthesis.methanol.blocks.tests.test_compressor.TestCompressor) ... ok
test_case_2 (idaes_models.process.superstructure_synthesis.methanol.blocks.tests.test_compressor.TestCompressor) ... ok
test_case_1 (idaes_models.process.superstructure_synthesis.methanol.blocks.tests.test_flash.TestFlash) ... ok
test_case_2 (idaes_models.process.superstructure_synthesis.methanol.blocks.tests.test_flash.TestFlash) ... ok
test_case_1 (idaes_models.process.superstructure_synthesis.methanol.blocks.tests.test_reactor.TestReactor) ... ok
test_LOA (idaes_models.process.superstructure_synthesis.methanol.test_main.TestMethanol) ... ok
test_case_pb (idaes_models.process.superstructure_synthesis.rpb.blocks.tests.test_packed_bed.TestPackedBed) ... ok
test_case_rpb (idaes_models.process.superstructure_synthesis.rpb.blocks.tests.test_packed_bed.TestPackedBed) ... ok
test_0rpb_1pb (idaes_models.process.superstructure_synthesis.rpb.test_rpb_main.TestPackedBed) ... ok
test_1rpb_0pb (idaes_models.process.superstructure_synthesis.rpb.test_rpb_main.TestPackedBed) ... ok
test_1rpb_1pb (idaes_models.process.superstructure_synthesis.rpb.test_rpb_main.TestPackedBed) ... ok
test_2rpb_2pb (idaes_models.process.superstructure_synthesis.rpb.test_rpb_main.TestPackedBed) ... ok
test_default_LOA (idaes_models.process.superstructure_synthesis.ruiz_water.test_main.TestWater) ... ok
test_trial01_LOA (idaes_models.process.superstructure_synthesis.ruiz_water.test_main.TestWater) ... ok

-----
Ran 14 tests in 7.828s

OK
qichen@QC-CMU-Tower:~/git/super$
```


Pyomo: *Python Optimization Modeling Objects*



Python library for optimization

- Key optimization objects
 - Sets
 - Variables
 - Parameters
 - Constraints
 - Objective
 - Model
 - Solvers
- Able to manipulate core modeling and optimization objects

Pyomo features

- Pyomo library offers algebraic modeling language (like AMPL and GAMS) and solver interfaces in Python
- Allows programmatic access to modeling objects (sets, variables, constraints, etc.)
 - **Enables advanced model design**

```
# simple.py
from pyomo.environ import *

M = ConcreteModel()
M.x1 = Var()
M.x2 = Var(bounds=(-1,1))
M.x3 = Var(bounds=(1,2))
M.c1 = Constraint(expr=M.x1 == M.x2 + M.x3)
M.o = Objective(
    expr=M.x1**2 + (M.x2*M.x3)**4 + \
        M.x1*M.x3 + \
        M.x2*sin(M.x1+M.x3) + M.x2)

opt_result = SolverFactory('ipopt').solve(M)
opt_model = M
```

Features

- Open source + free to use/modify commercially
- Modeling extensions
 - Pyomo.GDP
 - Pyomo.DAE
 - PySP (stochastic)
 - Bilevel programming
- Strong support for modular modeling
- Ability to perform programmatic model transformations
- Allows use of advanced solution algorithms

Modeling extensions

- GDP automatic reformulations
- Express DAE in terms of differential equations
- PySP: support for scenario generation and progressive hedging algorithm
- Ability to build models at **high level of abstraction**

GDP

MINLP big-M

MINLP Hull Reform.

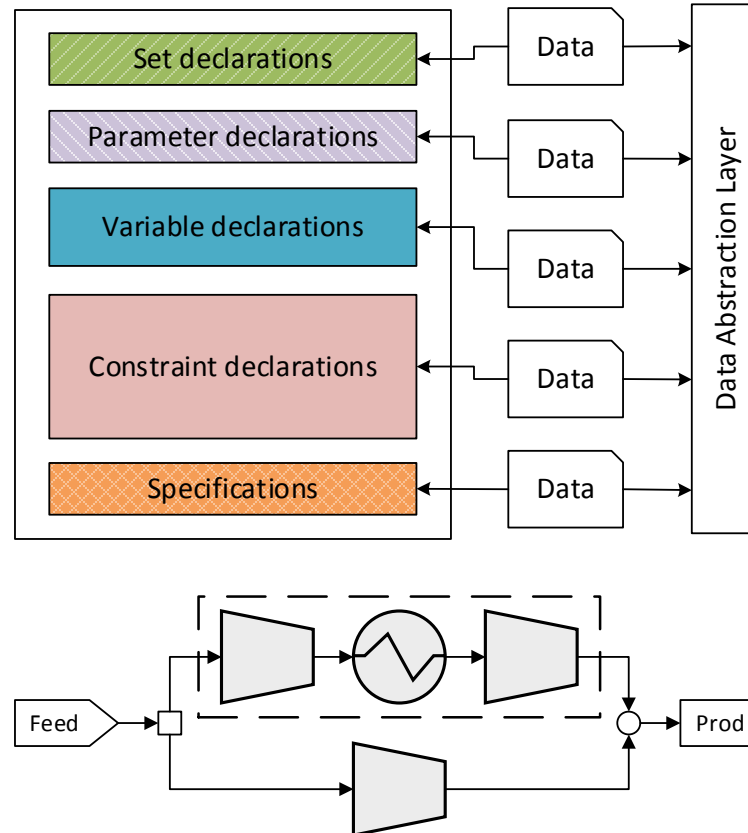
DAE

NLP

Advantages of modularity

- Ability to create **nested** unit models
- Each unit model has its own namespace
 - No need to keep track of T1, T2, T3...
 - Instead: reactor.T, flash.T
- **Easier maintenance** of unit models
- Ability to test models independently

Traditional modeling approach



Object-oriented modeling

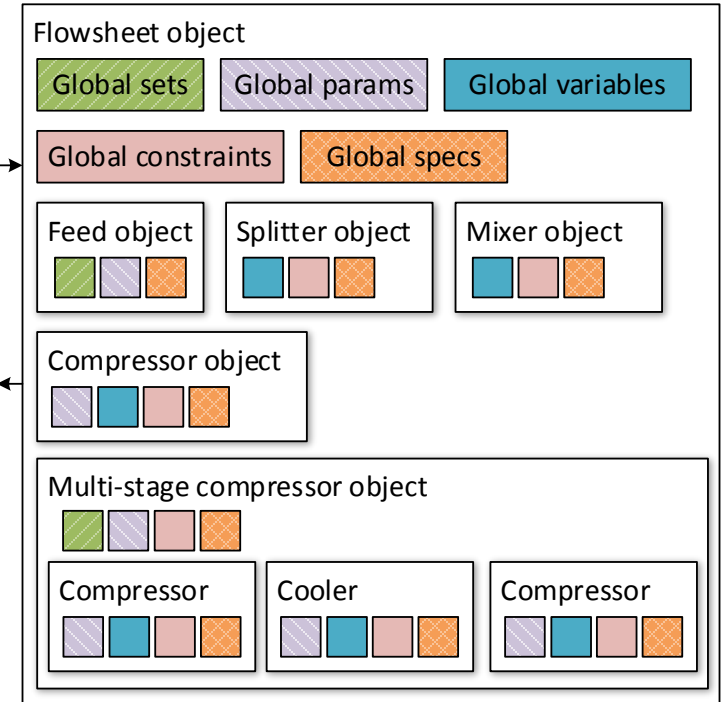


Figure from

Chen, Qi; Grossmann, IE. "Recent Developments and Challenges in Optimization-Based Flowsheet Synthesis." *Annual Review of Chemical and Biomolecular Engineering*. In press, expected July 2017.

Dynamic model transformations

- Utility functions to add linear relaxations
- Dynamic activation or deactivation of nonlinear expressions
- Automatic generation and addition of linearizations
- Model state introspection
 - Propagation of fixed variables
 - Deactivation of redundant constraints



Code

```
for s in streams:  
    for c in components:  
        add_mccormick_relaxation(mc_flow_block,  
                                z=fc[comp, s], x=F, y=mole_frac[c, s], nsegs=5, (s, c))
```



Result

Automatically adds variables and equations for a 5-segment **piecewise McCormick** relaxation for the bilinear relation $f_{c,s} = F_s x_s$ for each component c and stream s

Dynamic model transformations

- Utility functions to add linear relaxations
- Dynamic activation or deactivation of nonlinear expressions
- Automatic generation and addition of linearizations
- Model state introspection
 - Propagation of fixed variables
 - Deactivation of redundant constraints



Nonlinear constraint deactivation/reactivation

```
Model.deactivate_nonlinear_constraints()  
Model.reactivate_nonlinear_constraints()
```



Implication

- Required in order to switch between linearized and nonlinear forms of model for LOA
- **Dynamically detects** which equations are nonlinear (vs. linear due to fixed variables)
- Ability to remember which equations need to be reactivated

Dynamic model transformations

- Utility functions to add linear relaxations
- Dynamic activation or deactivation of nonlinear expressions
- Automatic generation and addition of linearizations
- Model state introspection
 - Propagation of fixed variables
 - Deactivation of redundant constraints



Code

```
Model.apply_OA_strategy()  
Model.add_oa_cuts()
```



Result

- Analyzes nonlinear expressions and computes Jacobians
- Evaluates the Jacobians at the current variable values when `add_oa_cuts` is called in order to construct the outer approximation constraints
- Automatically adds the OA constraints to the model

Dynamic model transformations

- Utility functions to add linear relaxations
- Dynamic activation or deactivation of nonlinear expressions
- Automatic generation and addition of linearizations
- Model state introspection
 - Propagation of fixed variables
 - Deactivation of redundant constraints



Code

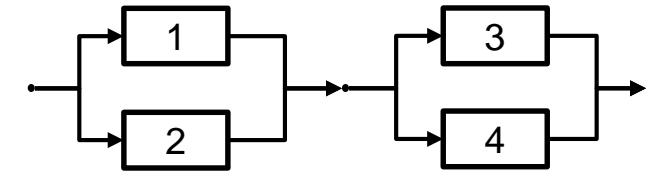
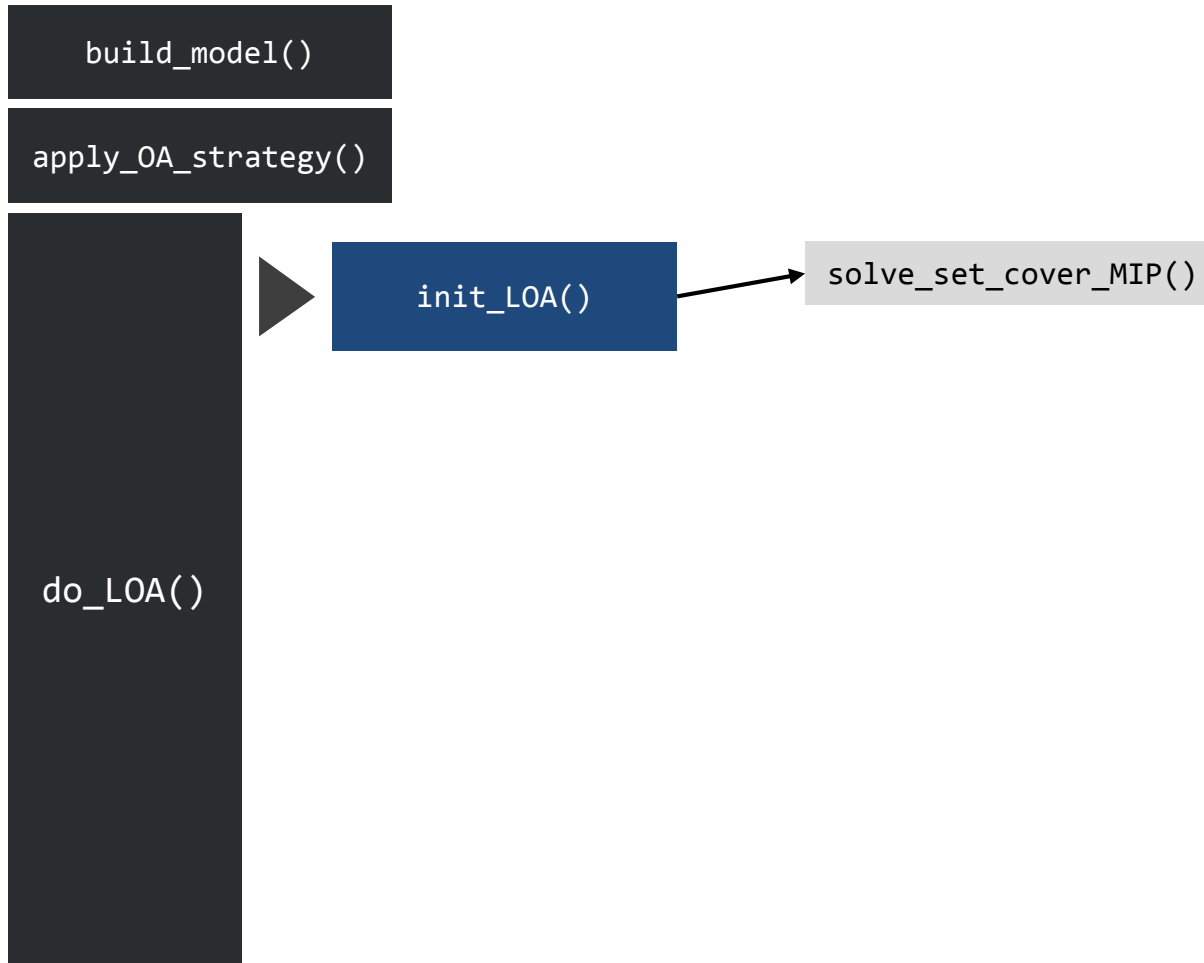
```
Model.propagate_var_fix(tmp=True)
Model.introspect_flows()
```



Result

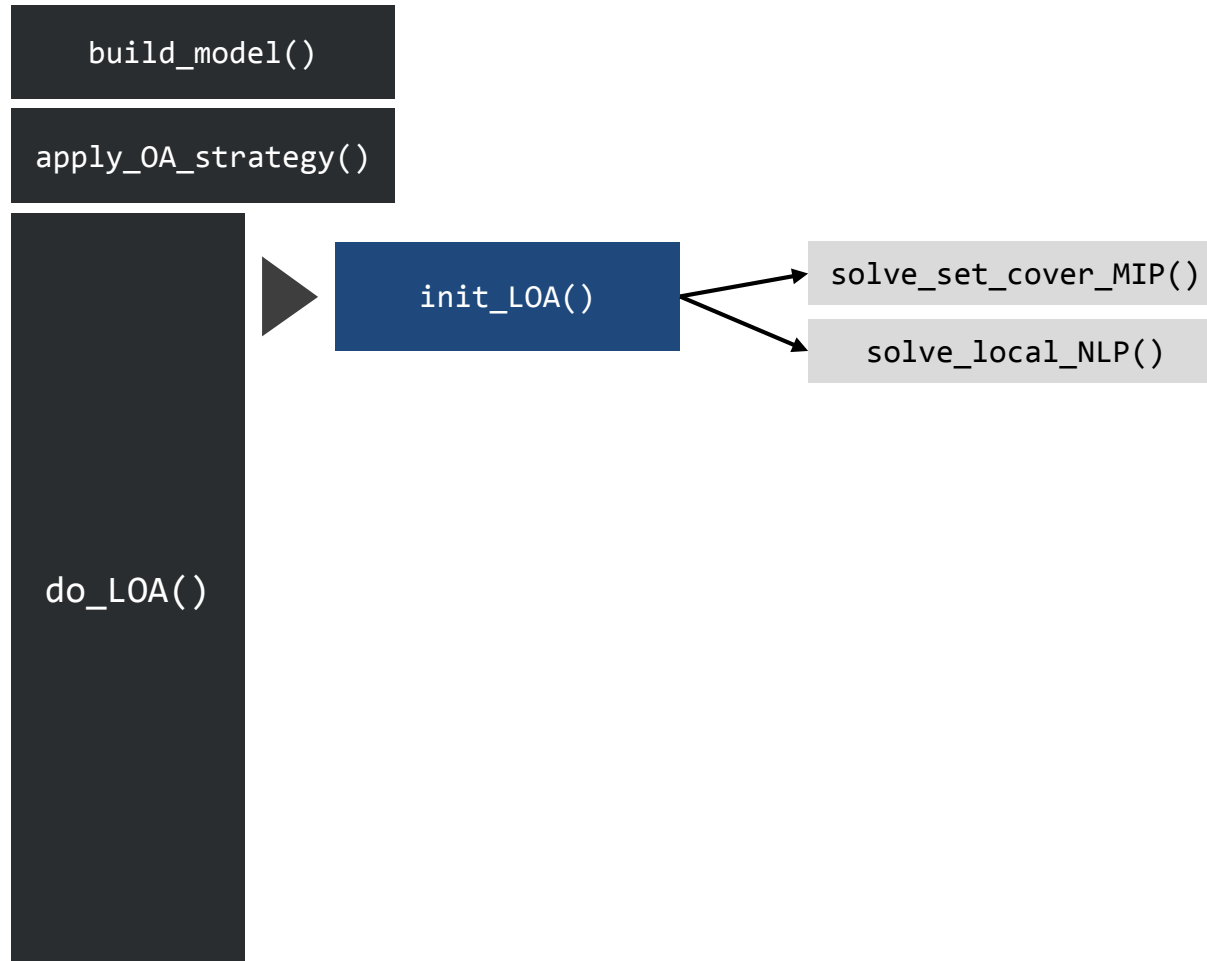
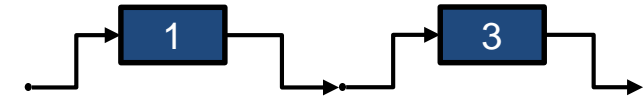
- Looks for simple constraints of form $A = B$. If A or B is fixed, then fix the other variable to the same value. Propagates for all members of the equality set
- Looks to see if a stream has all of its flow variables deactivated. If so, deactivates the constraints associated with the stream.
 - Avoids redundant equations, making NLP solver more **robust**

Implementation of logic-based outer approximation (LOA)



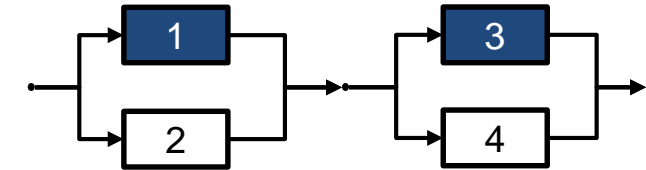
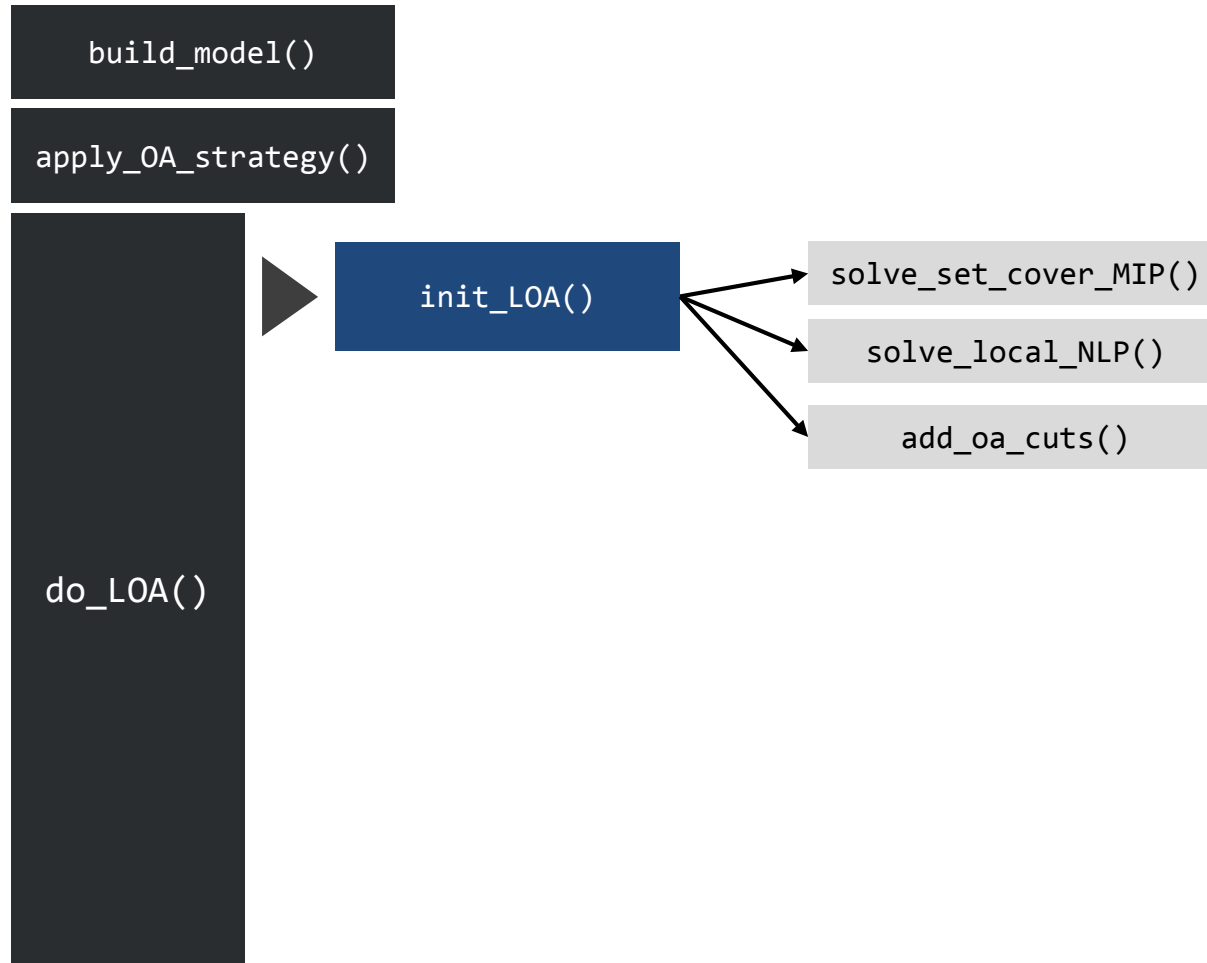
- Compute + activate set covering objective
- Activate linearizations
- Deactivate nonlinear constraints
- Deactivate fathomed units
- Deactivate OA cuts
- Solve MIP
- Reactivate OA cuts

Implementation of logic-based outer approximation (LOA)



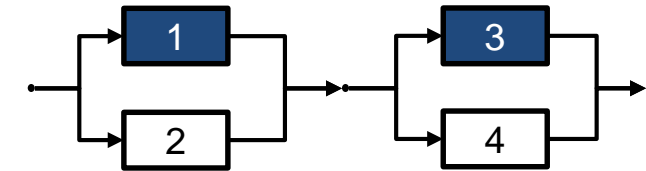
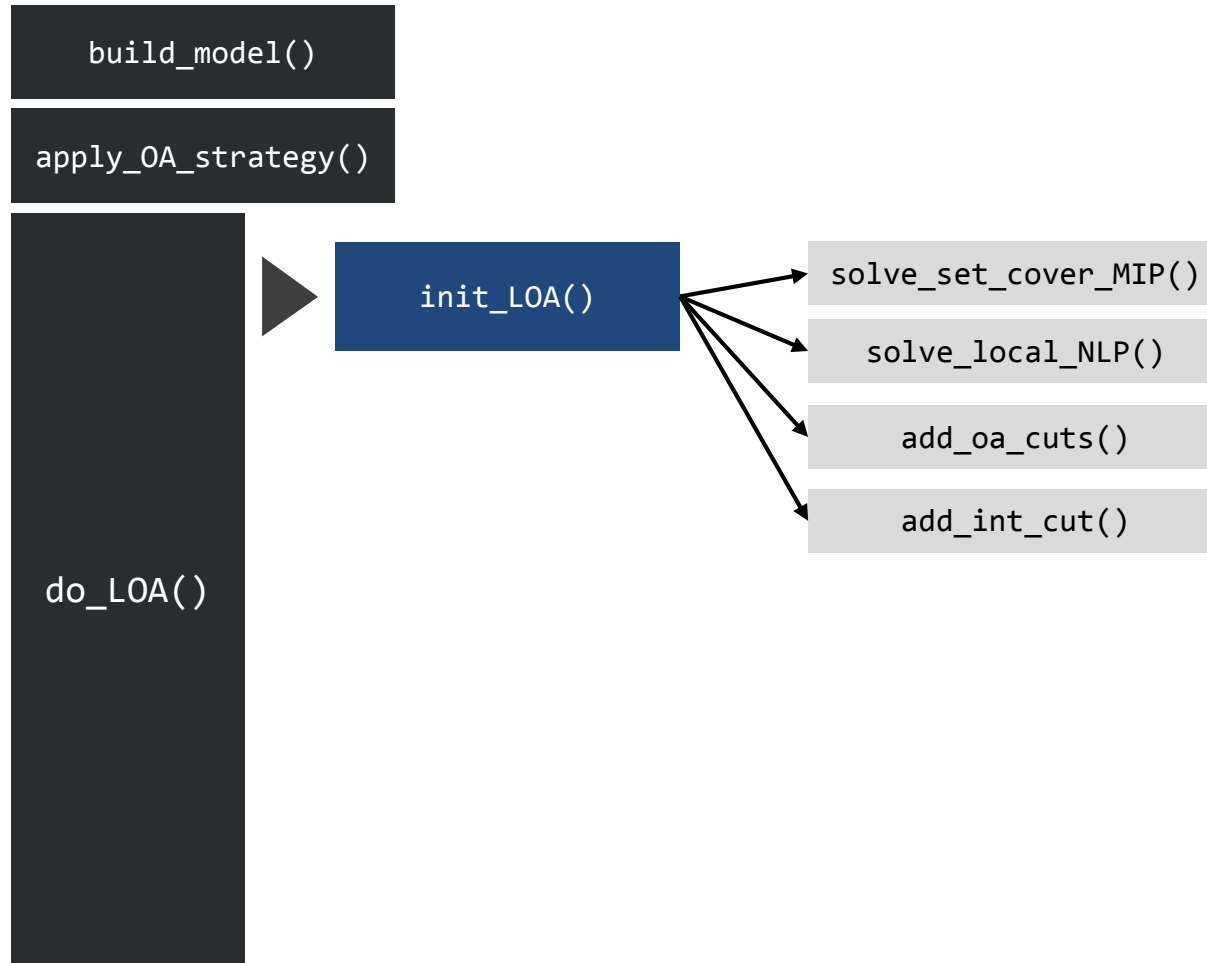
- Activate normal objective
- Activate relevant nonlinear constraints
- Deactivate linearizations
- Deactivate OA cuts
- Apply NLP initialization strategy
- Propagate fixed variables
- Introspect flows
- Deactivate trivial constraints
- Set minimum flows
- Solve NLP
- Unset minimum flows
- Undo pre-solve model transformations
- Update upper bound
- Save values if best so far
- If not optimal, reinitialize + try again

Implementation of logic-based outer approximation (LOA)



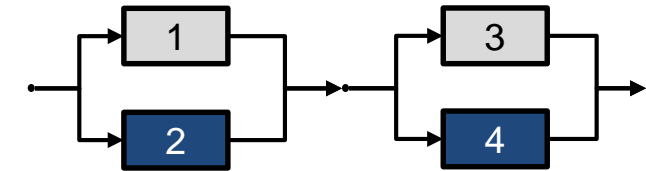
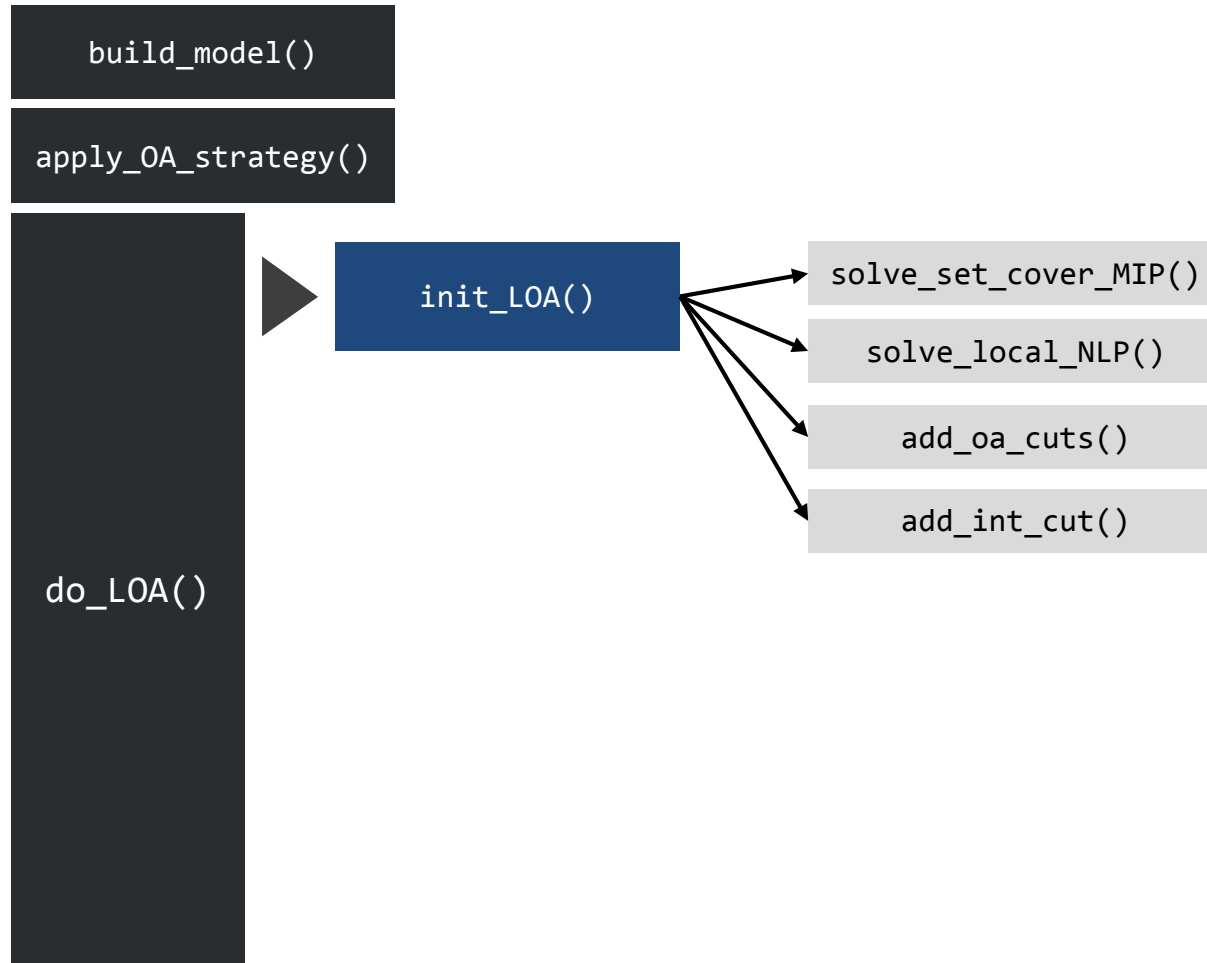
- Evaluate Jacobians
- Generate + add outer approximation (OA) constraints corresponding to all nonlinear constraints

Implementation of logic-based outer approximation (LOA)



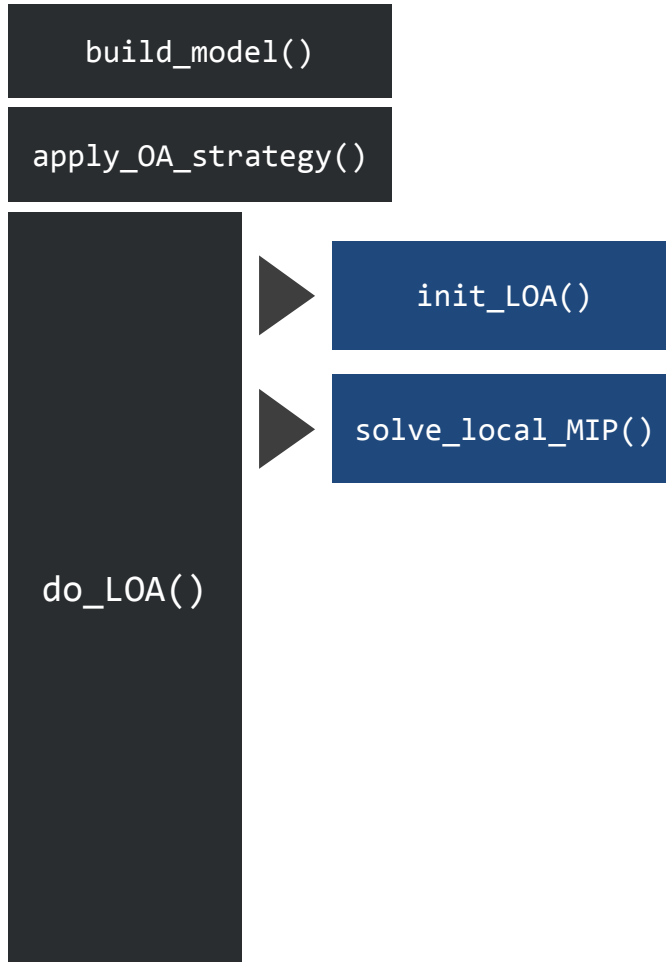
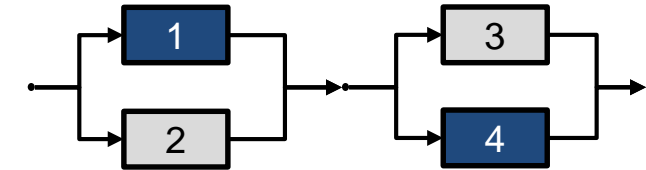
- Generate + add integer cut

Implementation of logic-based outer approximation (LOA)



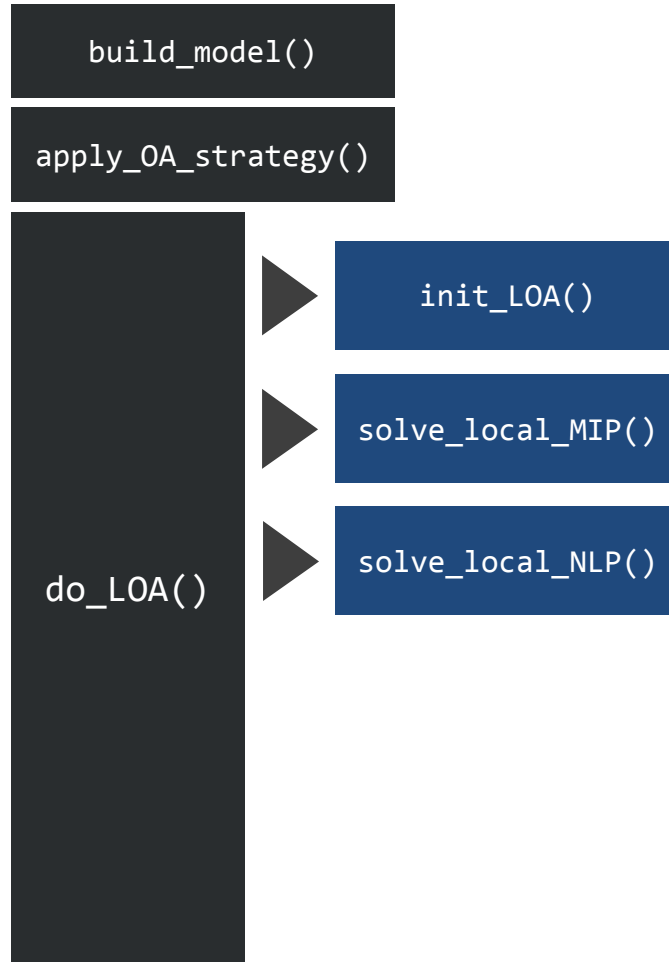
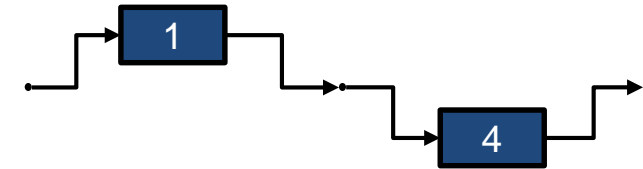
- Loop until all units covered

Implementation of logic-based outer approximation (LOA)



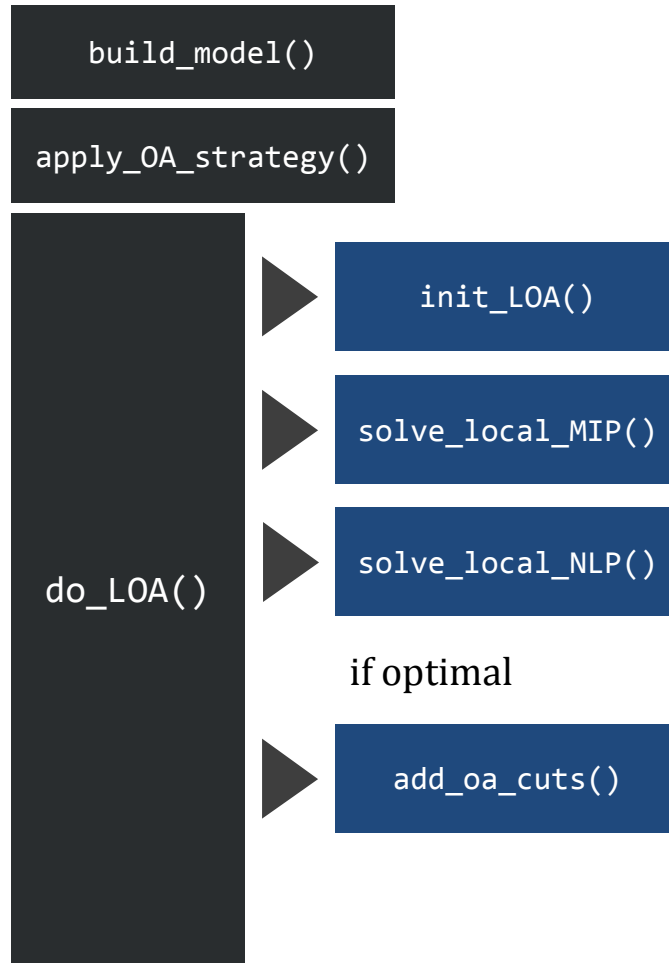
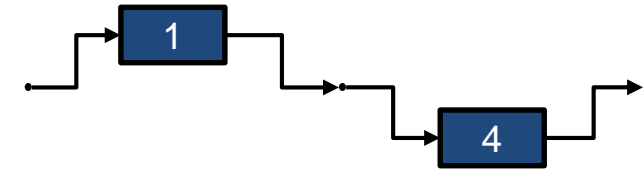
- Activate augmented Lagrangian OA objective
- Activate linearizations
- Deactivate nonlinear constraints
- Deactivate fathomed units
- Activate OA cuts
- Solve MIP
- Update lower bound

Implementation of logic-based outer approximation (LOA)



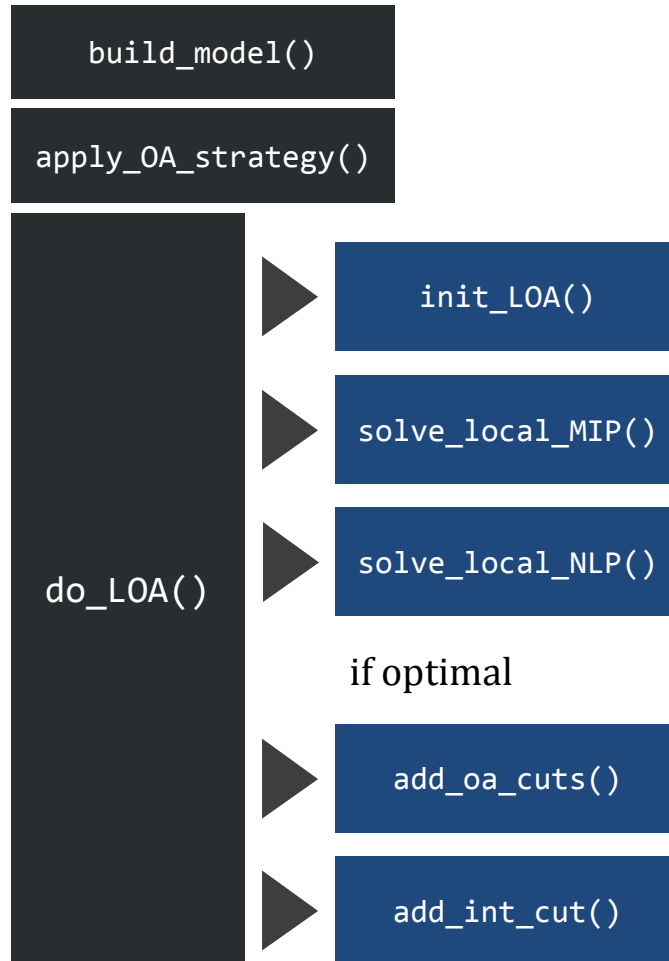
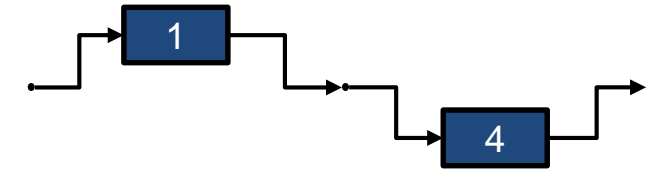
- Activate normal objective
- Activate relevant nonlinear constraints
- Deactivate linearizations
- Deactivate OA cuts
- Apply NLP initialization strategy
- Propagate fixed variables
- Introspect flows
- Deactivate trivial constraints
- Set minimum flows
- Solve NLP
- Unset minimum flows
- Undo pre-solve model transformations
- Update upper bound
- Save values if best so far
- If not optimal, reinitialize + try again

Implementation of logic-based outer approximation (LOA)



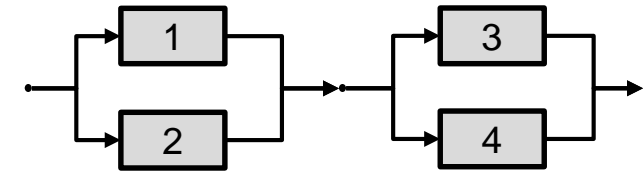
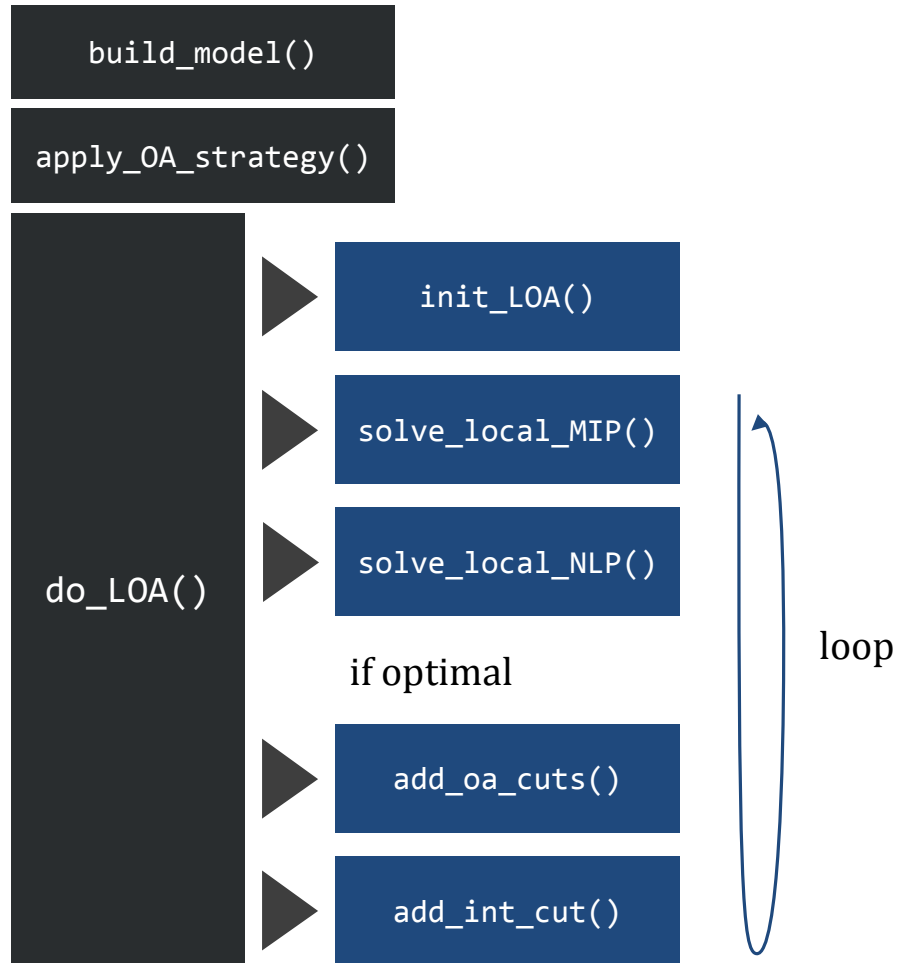
- Evaluate Jacobians
- Generate + add outer approximation (OA) constraints corresponding to all nonlinear constraints

Implementation of logic-based outer approximation (LOA)



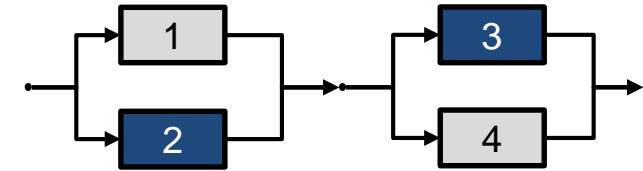
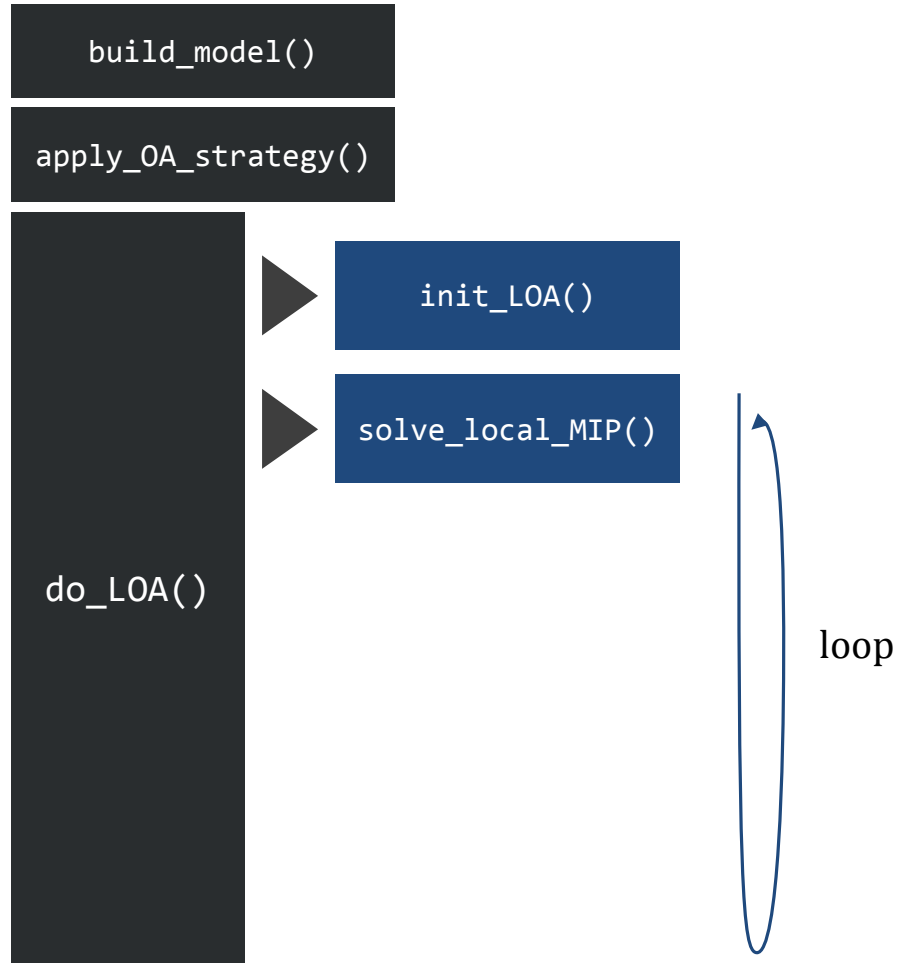
- Generate + add integer cut

Implementation of logic-based outer approximation (LOA)



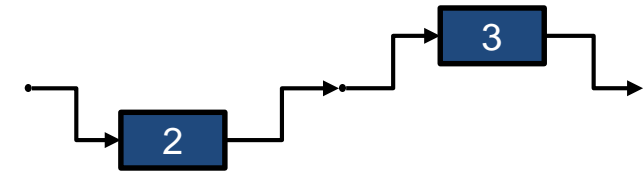
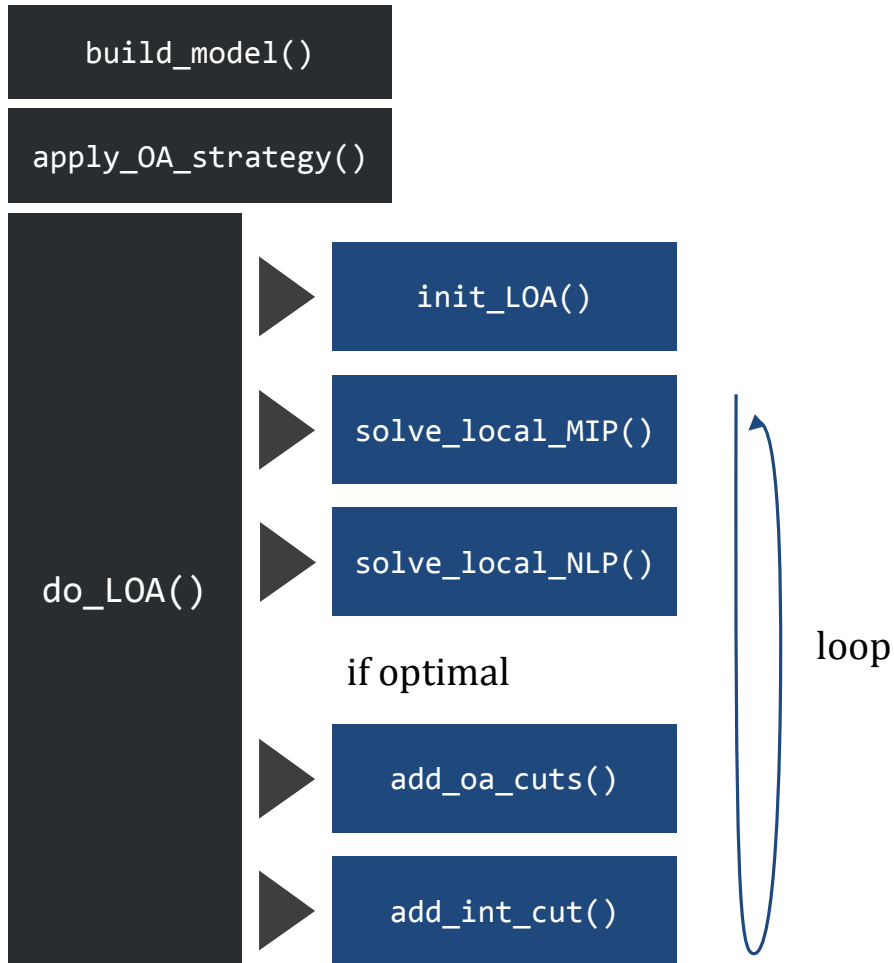
- Loop until upper bound and lower bound converge

Implementation of logic-based outer approximation (LOA)



- Loop until upper bound and lower bound converge

Implementation of logic-based outer approximation (LOA)



- Loop until upper bound and lower bound converge

Conclusion

- Pyomo allows for advanced algorithm development

Opportunities for growth

- Does not ship with solvers
 - Can be difficult for novice users to install solvers and set up solver licensing
- Lack of pre-processor [active development]
- Documentation is sparse for advanced usage and modeling extensions: difficult learning curve past basic modeling
 - Plugin system is complex: difficult to figure out how to contribute new plugins
- Best practices for saving/loading of model state currently unclear
 - Would be useful in some multiprocessing applications
- Backwards compatibility of new releases not guaranteed
 - Old release will remain usable, but without newer features

When to use Pyomo

- Perform data input, cleaning, problem formulation, optimization, analysis, and visualization in integrated workflow
- Construct models at a high level with advanced concepts and apply custom transformations into algebraic forms (GDP, DAE, stochastic, bilevel)
- Development or prototyping of advanced multi-step solution algorithms
- Second layer to traditional AMLs

When not to use Pyomo

- Model solution time in deployment is dominated by model compilation time
- Require access to certain unavailable solvers, e.g. DICOPT
- Individual solver licensing and deployment is a headache
- Onerous conversion cost

This work was conducted as part of the Institute for the Design of Advanced Energy Systems (IDAES) with funding from the Office of Fossil Energy, Cross-Cutting Research, U.S. Department of Energy.

Disclaimer: This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.



IDAES
Institute for the Design of
Advanced Energy Systems

Conclusion

Pyomo and JuMP are excellent open source modeling environments embedded in fully featured programming languages, suitable for users at all levels

Appendix

JuMP - Quick Installation Guide

1. Download and install Julia
 - a. <http://julialang.org/downloads/>
 - b. You can also try it without installing it at JuliaBox.com
2. Install JuMP
 - a. `julia> Pkg.add("JuMP")`
3. Install your favorite solver (example CPLEX)
 - a. <http://www-03.ibm.com/software/products/en/ibmilogcpleoptistud>
 - b. You need to get your license
4. Install the julia package for your solver
 - a. `julia> Pkg.add("CPLEX")`

A screenshot of a terminal window titled "/bin/bash" with a cityscape background. The prompt is "[RapaNui ~]\$ julia". The Julia logo is displayed on the left. On the right, a welcome message reads: "A fresh approach to technical computing", "Documentation: http://docs.julialang.org", "Type '?help' for help.", "Version 0.5.1 (2017-03-05 13:25 UTC)", "Official http://julialang.org/ release", and "x86_64-pc-linux-gnu". The prompt has changed to "julia> Pkg.add("JuMP")".

```
[RapaNui ~]$ julia
A fresh approach to technical computing
Documentation: http://docs.julialang.org
Type "?help" for help.

Version 0.5.1 (2017-03-05 13:25 UTC)
Official http://julialang.org/ release
x86_64-pc-linux-gnu

julia> Pkg.add("JuMP")
```

Pyomo – Installation and References



Install Python

- <https://www.python.org/downloads/>
- Alternative implementations also popular, especially Anaconda: <https://www.python.org/download/alternatives/>

Install Pyomo

- <http://www.pyomo.org/installation>
- `pip install pyomo`

Install Solvers

- IPOPT: <https://www.coin-or.org/Ipopt/documentation/node10.html>
- Gurobi: <http://www.gurobi.com/registration/download-reg>

References

- Pyomo docs: <http://www.pyomo.org/documentation>
- Help forum: <https://groups.google.com/forum/#!forum/pyomo-forum>