The Sellar Problem - Coupled Disciplinary Problem

This tutorial illustrates how to set up a coupled disciplinary problem in OpenMDAO and prepare it for optimization, using the Sellar Problem consisting of two disciplines as follows:

$$\begin{gathered}\text{minimize } x_1^2 + z_2 + y1 + e^{-y_2} \\ \text{with respect to } z_1, z_2, x_1 \\ \text{subject to:} \\ \frac{y_1}{3.16} - 1 \geq 0 \\ 1 - \frac{y_2}{24} \geq 0 \\ -10 \leq z_1 \leq 10 \\ 0 \leq z_2 \leq 10 \\ 0 \leq x_1 \leq 10\end{gathered}$$

$$\begin{gathered}\text{Discipline 1: } y_1(z_1, z_2, x_1, y_2) = z_1^2 + x_1 + z_2 - 0.2y_2 \\ \text{Discipline 2: } y_2(z_1, z_2, y_1) = \sqrt{y_1} + z_1 + z_2\end{gathered}$$

[SELLAR] Sellar, R. S., Batill, S. M., and Renaud, J. E., “Response Surface Based, Concurrent Subspace Optimization for Multidisciplinary System Design”, 34th Aerospace Sciences Meeting and Exhibit, Aerospace Sciences Meetings, ().

Variables *z1, z2,* and *x1* are the design variables. Both disciplines are functions of *z1* and *z2,* so they are called the *global* design variables, while only the first discipline is a function of *x1,* so it is called the *local* design variable. The two disciplines are coupled by the coupling variables *y1* and *y2.* Discipline 1 takes *y2* as an input, and computes *y1* as an output, while Discipline 2 takes *y1* as an input and computes *y2* as an output. This coupling creates a non-linear system of equations which must be satisfied for valid solutions.

First, disciplines 1 and 2 were implemented in OpenMDAO as components.

```
# For printing, use this import if you are running Python 2.x
from __future__ import print_function


import numpy as np

from openmdao.api import Component


class SellarDis1(Component):
    """Component containing Discipline 1."""

    def __init__(self):
        super(SellarDis1, self).__init__()

        # Global Design Variable
        self.add_param('z', val=np.zeros(2))

        # Local Design Variable
        self.add_param('x', val=0.)

        # Coupling parameter
        self.add_param('y2', val=1.0)

        # Coupling output
        self.add_output('y1', val=1.0)

    def solve_nonlinear(self, params, unknowns, resids):
        """Evaluates the equation
        y1 = z1**2 + z2 + x1 - 0.2*y2"""

        z1 = params['z'][0]
        z2 = params['z'][1]
        x1 = params['x']
        y2 = params['y2']

        unknowns['y1'] = z1**2 + z2 + x1 - 0.2*y2

    def linearize(self, params, unknowns, resids):
```

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```
        """ Jacobian for Sellar discipline 1."""
        J = {}

        J['y1','y2'] = -0.2
        J['y1','z'] = np.array([[2*params['z'][0], 1.0]])
        J['y1','x'] = 1.0

        return J


class SellarDis2(Component):
    """Component containing Discipline 2."""

    def __init__(self):
        super(SellarDis2, self).__init__()

        # Global Design Variable
        self.add_param('z', val=np.zeros(2))

        # Coupling parameter
        self.add_param('y1', val=1.0)

        # Coupling output
        self.add_output('y2', val=1.0)

    def solve_nonlinear(self, params, unknowns, resids):
        """Evaluates the equation
        y2 = y1**(.5) + z1 + z2"""

        z1 = params['z'][0]
        z2 = params['z'][1]
        y1 = params['y1']

        # Note: this may cause some issues. However, y1 is constrained to be
        # above 3.16, so lets just let it converge, and the optimizer will
        # throw it out
        y1 = abs(y1)

        unknowns['y2'] = y1**.5 + z1 + z2

    def linearize(self, params, unknowns, resids):
        """ Jacobian for Sellar discipline 2."""
        J = {}

        J['y2', 'y1'] = .5*params['y1']**-.5

        #Extra set of brackets below ensure we have a 2D array instead of a 1D array
        # for the Jacobian;  Note that Jacobian is 2D (num outputs x num inputs).
        J['y2', 'z'] = np.array([[1.0, 1.0]])

        return J
```

For the most part, construction of these *Components* builds on what you learned in previous tutorials. In building these disciplines, we gave default values to all of the *params* and *unknowns* so that OpenMDAO can allocate the correct size in the vectors. The global design variables *z1* and *z2* were combined into a 2-element *ndarray*.

Note

`Discipline2` contains a square root of variable *y1* in its calculation. For negative values of *y1*, the result would be imaginary, so the absolute value is taken before the square root is applied. This component is clearly not valid for `y1 < 0`, but some solvers could occasionally force *y1* to go slightly negative while trying to converge the two disciplines . The inclusion of the absolute value solves the problem without impacting the final converged solution.

We have written two (very simple) analysis components. If you were working on a real problem, your components could be more complex, or could potentially be wrappers for external analysis components. But keep in mind that from an optimization point of view, whether they are simple tools or wrappers for real analyses, OpenMDAO still views them as components with *params*, *unknowns*, *resids* and a *solve_nonlinear* function, and optionally a *linearize* function.

At this point we've written the components, but we haven't combined them together into any kind of model. That's what we'll get to next!

Building the Sellar Model

Next we will set up the Sellar *Problem* and optimize it. First we will take the *Components* that we just created and assemble them into a *Group*. We will also add the objective and the multivariable constraints to the problem using a utility *Component* that can be used when you have simple equations for things like objectives and constraints.

```
from openmdao.api import ExecComp, IndepVarComp, Group, NLGaussSeidel, \
                         ScipyGMRES
```

```
class SellarDerivatives(Group):
    """ Group containing the Sellar MDA. This version uses the disciplines
    with derivatives."""

    def __init__(self):
        super(SellarDerivatives, self).__init__()

        self.add('px', IndepVarComp('x', 1.0), promotes=['x'])
        self.add('pz', IndepVarComp('z', np.array([5.0, 2.0])), promotes=['z'])

        self.add('d1', SellarDis1(), promotes=['z', 'x', 'y1', 'y2'])
        self.add('d2', SellarDis2(), promotes=['z', 'y1', 'y2'])

        self.add('obj_cmp', ExecComp('obj = x**2 + z[1] + y1 + exp(-y2)',
                                     z=np.array([0.0, 0.0]), x=0.0, y1=0.0, y2=0.0),
                 promotes=['obj', 'z', 'x', 'y1', 'y2'])

        self.add('con_cmp1', ExecComp('con1 = 3.16 - y1'), promotes=['y1', 'con1'])
        self.add('con_cmp2', ExecComp('con2 = y2 - 24.0'), promotes=['con2', 'y2'])

        self.nl_solver = NLGaussSeidel()
        self.nl_solver.options['atol'] = 1.0e-12

        self.ln_solver = ScipyGMRES()
```

We use *add* to add *Components* or *Systems* to a *Group*. The order you add them to your *Group* is the order they will execute, so it is important to add them in the correct order. Here, this means starting with the IndepVarComps, then adding our disciplines, and finishing with the objective and constraints. In the statements that add *x* and *z* to groups, note that the args *1.0* and *np.array([5.0, 2.0])* are simply initial user-defined starting values that were arbitrarily chosen in this case.

We have also decided to declare all of our connections to be implicit by using the *promotes* argument when we added any component. When you promote a variable, that means that it is available in the parent system. Thus, if you wanted to connect something to variable *y1*, you would address it with the string *y1* instead of *dis1.y1*.

In this case, our two disciplines both promote *y1* and *y2*. Discipline 1 provides *y1* as a source and discipline 2 needs it as a *param*, so when both of them promote *y1*, the connection is made for you, implicitly.

Due to the implicit connections, we now have a cycle between the two disciplines. This is fine because a nonlinear solver can converge the cycle to arrive at values of *y1* and *y2* that satisfy the equations in both disciplines. We have selected the *NLGaussSeidel* solver (i.e., fixed point iteration), which will converge the model in our *Group*. We also specify a tighter tolerance in the solver's *options* dictionary, overriding the 1e-6 default. Note that we had to change our linear solver to ScipyGMRES instead of using the default LinearGaussSeidel solver because we have a cycle.

The objective and constraints are defined with the *ExecComp*, which is really a shortcut for creating a *Component* that is a simple function of other variables in the model. *ExecComp* is just there as a convenience for users. You don't have to use it, if for example you wrote your own component that already outputs objective and constraint variables.

```
self.add('obj_cmp', ExecComp('obj = x**2 + z[1] + y1 + exp(-y2)',
                             z=np.array([0.0, 0.0]), x=0.0, y1=0.0, y2=0.0),
         promotes=['z', 'x', 'y1', 'y2'])
```

This creates a component named 'obj_comp' with inputs 'x', 'z', 'y1', and 'y2', and with output 'obj'. The first argument is a string expression that contains the function. OpenMDAO can parse this expression so that the *solve_nonlinear* and *linearize* methods are taken care of for you. Notice that standard math functions like *exp* are available to use. Because we promote every variable in our call to *add*, all of the input variables are automatically connected to sources in the model. We also specify our default initial values as the remaining arguments for the ExecComp. You are not required to do this for scalars, but you must always allocate the array inputs ('z' in this case). The output of the objective equation is stored in the promoted output 'obj'.

So that's three *ExecComp* instances, one each for the objective and two constraints. Now, that we are done creating the *Group* for the Sellar problem, let's hook it up to an optimizer.

Setting up the Optimization Problem

Any analysis or optimization in OpenMDAO always happens in a *Problem* instance, with a Group at the root. Here we set our Sellar group as root. Then we set the driver to be the ScipyOptimizer, which wraps scipy's minimize function.

Note

Scipy offers a number of different optimizers, but COBYLA and SLSQP are the only two choices that support constrained optimization. SLSQP is the only gradient based method of the two. If you want a broader selection of optimizers, you
install the pyopt_sparse library, which we also have a wrapper for.

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Note

All optimizers in OpenMDAO try to minimize the value of the objective, so to maximize a variable, you will have to place a minus sign in the expression you give to the objective ExecComp.

```
from openmdao.api import Problem, ScipyOptimizer

top = Problem()
top.root = SellarDerivatives()

top.driver = ScipyOptimizer()
top.driver.options['optimizer'] = 'SLSQP'
top.driver.options['tol'] = 1.0e-8

top.driver.add_desvar('z', lower=np.array([-10.0, 0.0]),
                     upper=np.array([10.0, 10.0]))
top.driver.add_desvar('x', lower=0.0, upper=10.0)

top.driver.add_objective('obj')
top.driver.add_constraint('con1', upper=0.0)
top.driver.add_constraint('con2', upper=0.0)

top.setup()

# Setting initial values for design variables
top['x'] = 1.0
top['z'] = np.array([5.0, 2.0])

top.run()

print("\n")
print( "Minimum found at (%f, %f, %f)" % (top['z'][0], \
                                         top['z'][1], \
                                         top['x']))
print("Coupling vars: %f, %f" % (top['y1'], top['y2']))
print("Minimum objective: ", top['obj'])
```

Next we add the parameter for ‘z’. Recall that the first argument for *add_desvar* is a string containing the name of a variable declared in a *IndepVarComp*. Since we are promoting the output of this pcomp, we use the promoted name, which is ‘z’ (and likewise we use ‘x’ for the other parameter.) Variable ‘z’ is a 2-element array, and each element has a different set of bounds defined in the problem, so we specify the *low* and *high* attributes as numpy arrays. If you are ok with the same *low* or *high* for all elements of your design variable array, you could also give a scalar for those arguments.

Next, we add the objective by calling *add_objective* on the *driver* giving it the promoted path of the quantity we wish to minimize. All optimizers in OpenMDAO try to minimize the value of the objective, so to maximize a variable, you will have to place a minus sign in the expression you give to the objective *ExecComp*.

Finally we add the constraints using the *add_constraint* method, which takes any valid *unknown* in the model as the first argument. We want to constrain the unknowns “con1” and “con2” to be less than zero, so we set an upper bound of zero on both constraints.

Don’t forget to call *setup* on your *Problem* before calling *run*. Also, we are using the Python 3.x print function to print results. To keep compatibility with both Python 2.x and 3.x, don’t forget the following import at the top of your python file:

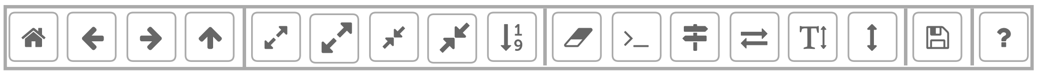
```
from __future__ import print_function
```

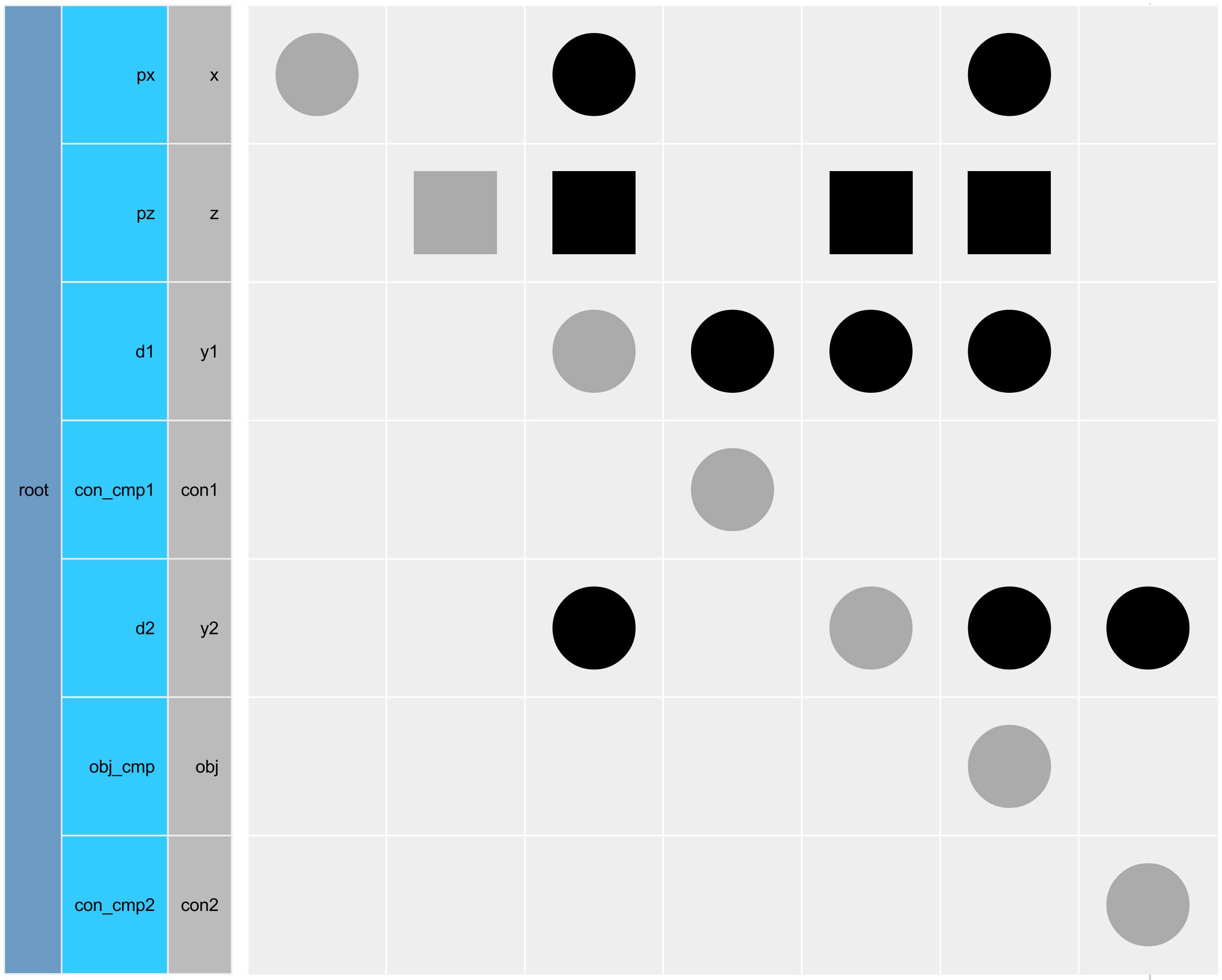
If we take all of the code we have written in this tutorial and place it into a file called *sellar_MDF_optimization.py* and run it, the final output will look something like:

```
$ python sellar_MDF_optimization.py
.
.
.
Minimum found at (1.977639, ...0.000000, ...0.000000)
Coupling vars: 3.160000, 3.755278
Minimum objective:  3.18339395045
```

Depending on print settings, there may be some additional optimizer output where the ellipses are. This is the expected minimum for the Sellar problem.

Visualizing the Model





Sellar with an Implicit Component

We have just built an implementation of the Sellar problem where the two disciplines are connected with a cycle. We could also sever the direct connection and close the gap with an implicit component. The purpose of this component is to express as a residual the difference between the output side and the input side of the connection that we are replacing.

In Sellar, we will leave the *y1* connection and replace the *y2* connection. First we need to write the component to replace the connection:

```
class StateConnection(Component):
    """ Define connection with an explicit equation"""

    def __init__(self):
        super(StateConnection, self).__init__()

        # Inputs
        self.add_param('y2_actual', 1.0)

        # States
        self.add_state('y2_command', val=1.0)

    def apply_nonlinear(self, params, unknowns, resids):
        """ Don't solve; just calculate the residual."""

        y2_actual = params['y2_actual']
        y2_command = unknowns['y2_command']

        resids['y2_command'] = y2_actual - y2_command

    def solve_nonlinear(self, params, unknowns, resids):
        """ This is a dummy comp that doesn't modify its state."""
        pass

    def linearize(self, params, unknowns, resids):
        """Analytical derivatives."""

        J = {}

        # State equation
        J[('y2_command', 'y2_command')] = -1.0
        J[('y2_command', 'y2_actual')] = 1.0
        return J
```

So this *Component* has one *state* and one *param*. The *StateConnection* component will bridge the gap between the output of *y2* from Discipline2 and the input for *y2* in Discipline1. The solver sets the new value of y2 based on the model's residuals, which now include the difference between 'y2' leaving Discipline2 and the 'y2' entering Discipline1. So the *solve_nonlinear* method does nothing, but we need to define *apply_nonlinear* to return this residual. Residuals live in the *resids* vector, so we set:

```
resids['y2_command'] = y2_actual - y2_command
```

We also define the *linearize* method, and the derivatives are trivial to compute.

Next, we need to modify the model that we defined in *SellarDerivatives* to break the connection and use the *StateConnection* component.

```
from openmdao.api import Newton, ScipyGMRES

class SellarStateConnection(Group):
    """ Group containing the Sellar MDA. This version uses the disciplines
    with derivatives."""

    def __init__(self):
        super(SellarStateConnection, self).__init__()

        self.add('px', IndepVarComp('x', 1.0), promotes=['x'])
        self.add('pz', IndepVarComp('z', np.array([5.0, 2.0])), promotes=['z'])

        self.add('state_eq', StateConnection())
        self.add('d1', SellarDis1(), promotes=['x', 'z', 'y1'])
        self.add('d2', SellarDis2(), promotes=['z', 'y1'])
        self.connect('state_eq.y2_command', 'd1.y2')
        self.connect('d2.y2', 'state_eq.y2_actual')

        self.add('obj_cmp', ExecComp('obj = x**2 + z[1] + y1 + exp(-y2)',
                                     z=np.array([0.0, 0.0]), x=0.0, y1=0.0, y2=0.0),
                 promotes=['x', 'z', 'y1', 'obj'])
        self.connect('d2.y2', 'obj_cmp.y2')

        self.add('con_cmp1', ExecComp('con1 = 3.16 - y1'), promotes=['con1', 'y1'])
        self.add('con_cmp2', ExecComp('con2 = y2 - 24.0'), promotes=['con2'])
        self.connect('d2.y2', 'con_cmp2.y2')

        self.nl_solver = Newton()
        self.ln_solver = ScipyGMRES()
```

The first thing to notice is that we no longer promote the variable *y2* up to the group level. We need to add the connections manually because we really have two different variables: 'd1.y2' and 'd2.y2'. In addition to the two connections to the 'state_eq' component, we also need to manually connect *y2* to the objective and one of the constraints.

We have also switched the solver to the Newton solver, since we no longer are iterating around a loop. Don't forget to change your import. The default settings should be fine for Sellar.

Also, because we have states, we have switched the linear solver to ScipyGMRES instead of using the default LinearGaussSeidel solver.

Otherwise, there are no other differences in the model, and the remaining optimization set up is the same as before. However, a small change in printing our results is required because 'y2' no longer exists in the group. We must print either 'state_eq.y2_command' or 'd2.y2' instead. It doesn't matter which one, since they should only differ by the solver tolerance at most.

```
from openmdao.api import Problem, ScipyOptimizer

top = Problem()
top.root = SellarStateConnection()

top.driver = ScipyOptimizer()
top.driver.options['optimizer'] = 'SLSQP'
top.driver.options['tol'] = 1.0e-8

top.driver.add_desvar('z', lower=np.array([-10.0, 0.0]),
                     upper=np.array([10.0, 10.0]))
top.driver.add_desvar('x', lower=0.0, upper=10.0)

top.driver.add_objective('obj')
top.driver.add_constraint('con1', upper=0.0)
top.driver.add_constraint('con2', upper=0.0)

top.setup()
top.run()
```

```
print("\n")
print( "Minimum found at (%f, %f, %f)" % (top['z'][0], \
                                        top['z'][1], \
                                        top['x']))
print("Coupling vars: %f, %f" % (top['y1'], top['d2.y2']))
print("Minimum objective: ", top['obj'])
```

You can verify that the new model arrives at the same optimum as the old one.

Tags

Tutorials , Coupling , Multi-Component , Optimization