Webinar: Migration of acslX Model Code to Magnolia

SOT BMSS

January 18, 2019

Webinar Outline

- Overview of Magnolia UI and workflow
- Migration of model (CSL) code
- Summary of command scripting language (CMD) differences between acslX and Magnolia
- Advanced scripting using Python

What's Magnolia?

- *Magnolia is an environment for modeling systems whose behavior can be described by systems of differential equations. Magnolia provides the tools for developing models using an equation-based modeling language, scripting the execution of simulations using either the Python programming language or a simple command-based language, and for interactively exploring model behavior using an intuitive user interface.*
- Modeling language heavily influenced by ACSL/acslX
- http://www.magnoliasci.com, team@magnoliasci.com

Overview of Magnolia UI and workflow

- Workspaces/projects are no longer used; all files are organized using filesystem folders according to user's preferences
- Models are translated and compiled silently and automatically as needed (this usually takes only a fraction of a second, even for large models)
- Running a loaded model automatically creates a default plot from which the model behavior may be interactively explored
- A command prompt is provided, but uses the Python language instead of the M language
- Multiple models may be loaded and active simultaneously
- Scripts may be developed using either the CMD language or the Python language

Magnolia UI and Workflow Demo

ACSL/acslX Model Code Migration

Why change the language?

- Simplify language by unifying syntax constructs which all do the same thing
  - E.g., code block delimiters: “end” vs “end if” versus “label:continue”
- Remove legacy syntax constructs which would interfere with planned future language extensions
  - E.g., planned object-orientation makes use of “dot” token in things like “.AT.” and “.GT.” problematic
- Make the language more consistent with modern, popular programming languages
  - MATLAB, C/C++, Java, Python
- Replace syntax constructs which could lead to ambiguities
  - E.g., function call versus array notation

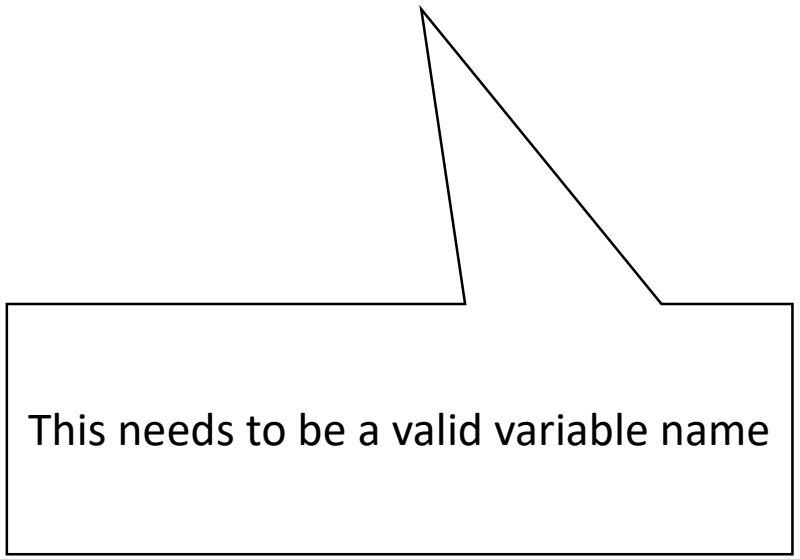
Replace the PROGRAM keyword

Old Syntax

```
program This is a model
```

New Syntax

```
model butadiene
```



Replace old-style comment delimiters

Old Syntax	New Syntax
`'This is a comment'`	`! This is a comment`
`$This is a comment`	

Combine datatype declarations and DIMENSION statements

- Datatype specification (REAL, INTEGER, LOGICAL, CHARACTER) is now included in the DIMENSION statement and array declaration uses square brackets. CHARACTER variables no longer have to be assigned a size.

Old Syntax

```
dimension x(2, 3)
dimension flag(4)
logical flag
character*25 title
```

New Syntax

```
dimension x[2, 3]
dimension logical flag(4)
character title
dimension Exponential m1
```

Update array declarations and references

- Array elements are now addressed using square bracket notation.

Old Syntax

```
dimension x(2, 3)
x(i, j) = 10.0*k(i)*y(j)
```

New Syntax

```
dimension x[2, 3]
X[i, j] = 10.0*k[i]*y[j]
```

Update TABLE statements

- The data used to populate a TABLE statement is now specified in two or more CONSTANT arrays.

Old Syntax

```
table Bodywieght, 1, 10 /0, 1, …
                  15, 20/
```

New Syntax

```
constant ageData = 0, 1, 2…
constant bwData  = 0.1, 0.13…
table Bodyweight = ageData, bwData
```

Update SCHEDULE statements

- The AT/XZ/XP/XN qualifiers are no longer delimited by periods.

Old Syntax

```
schedule on .at. t + 0.5
schedule Bounce .xn. x
```

New Syntax

```
schedule on at t + 0.5
schedule Bounce xn x
```

Migrate old-style DO loops

- DO loops are replaced with FOR loops, which are delimited by an END statement, not a CONTINUE statement.

Old Syntax

```
do 10 i = 1, 2
  do 20 j = 1, 3
    dx(i, j) = -k(i, j)*x(i, j)
  20: continue
10: continue
```

New Syntax

```
for i = 1, 2
  for j = 1, 3
    dx[i, j] = -k[i, j]*x[i, j]
  end
end
```

Migrate IF/THEN/ELSE statements

- Conditionals no longer use the THEN keyword, and the end block is delimited by END, not ENDIF.

Old Syntax

```
if (t .LT. 1.0) then
  x = t^2
else if ( t .LT. 1.35) then
  x = exp(t)
else
  x = sqrt(t)
end if
```

New Syntax

```
if (t < 1.0)
  x = t^2
else if ( t < 1.35)
  x = exp(t)
else
  x = sqrt(t)
end
```

Update relational and logical Operators

- FORTRAN-style relational and logical operators have been replaced by the C- and Java-style counterparts: ==, <, >, <=, >=, &, |. The only exception is the logical negation operator, which uses the MATLAB-style ~ instead of ! to avoid conflicts with CSL comments.

Old Syntax

```
termt(t .GE. tstop)
if(a .LT. 0.0 .OR. a .GT. 1.0)
```

New Syntax

```
termt(t >= tstop)
if(a < 0.0 || a > 1.0)
```

Remove (comment) ALGORITHM

- Presently, the default ODE solver in Magnolia is a fast solver which is appropriate for stiff systems
- Other solvers may be added in the future, at which point the ALGORITHM statement will be reintroduced

```
! algorithm ialg = 2
```

Example Ported CSL Model

Command Scripting Language (CMD)

General Differences

- Command abbreviation not presently supported
  - E.g., “d” cannot be used instead of “display”
- Command flags are now denoted with an “@” symbol instead of a “/”
  - E.g., “display @all” instead of “display /all”
- CMD scripts are now compiled instead of interpreted
  - Python is now used as the interactive scripting language
- Commands have been extended/added for parameter estimation, Monte Carlo analysis, and MCMC
- The “start” command no longer requires the /nocallback flag

Commands for which syntax has not changed

- DISPLAY
- OUTPUT
- PREPARE
- PROCEDURE
- PRINT

DATA

- Tabular data is no longer specified inline using the DATA command. Instead, data is imported from a CSV file and the DATA command is used to map columns to model variables
- The DATA command is also used to assign descriptor variable values for use in parameter estimation
- Example

```
data @file='butadiene.csv' ds1e1 t='T' c_exh='S1E1' ...
     tstop=60 BDW=86.2600 height=1.7400 Sex=1 Age=28
```

FIT

- The FIT command is used to execute parameter estimation runs from within a CMD file
- Used in conjunction with DATA and SET commands
- Example

```
data @file='observed.csv' dataset1 t='T' x='X' tstop=60 c=12.0
set k1 = 0.2 @min=0.1 @max=0.35
set k2 = 0.4 @min=0.23 @max=0.45
set k3 = 0.05 @min=0.03 @max=0.09
fit k1 k2 k3
```

LOAD

- Loads a model for use with the enclosing CMD script
- Must use the exact file name of the corresponding CSL file (case-sensitive)
- Example

```
load 'butadiene.csl'
```

PLOT

- Used to create plots, similar to legacy syntax
- Additional syntax for creating “interactive” plots
- Additional syntax for plotting observed data specified in DATA statement
- Examples

```
plot @interactive @xvar=vtheta vthetadot rdot r theta ...
    @param=k @param=l
plot x 'obsdata:xobs'
```

SET

- Used to set model constants, similar to legacy syntax
- Additional syntax for assigning upper and lower limits to constants for use in parameter estimation
- Additional syntax for assigning distributions to constants for use in Monte Carlo analyses
- Examples

```
set k1 = 0.0  k2 = 0.3  k3 = 1.5
set pc_pp=1.4 @dist=norm @mean=1.4 @std=0.3
```

START

- Used to start a simulation run, similar to legacy syntax
- Additional syntax for performing Monte Carlo iterations: @hold, @nruns
- Example

```
prepare t c_ven
set sc_vmax=0.0026 @dist=norm @mean=0.0026 @std=0.0008
start @hold @nruns=20
print @file='temp.csv' t c_ven
```

Example Magnolia-Compatible CMD Script

Advanced Scripting using Python

General Comments

- Python is a full-featured general programming language with a huge number of libraries. The Python website (python.org) is a good starting point to find language and library documentation, tutorials, examples, videos, etc.
- A few specific scripting tasks are presented here for guidance:
  - Loading and running a model
  - Setting the values of model constants
  - Getting the value of model variables or time histories following a run
  - Loading tabulated data from a file
  - Plotting from Python script code within Magnolia

Loading and running a model

- Models are represented as Python objects. Magnolia allows multiple models to be open and loaded into memory simultaneously. Use the models.get() method to assign a reference to an open model to a Python variable.
- Use the run() function of the model object to run a simulation
- Example

```
mdl = models.get("butadiene.csl")
mdl.run()
```

Setting model constants

- Model constants (and variables) are referenced as Python object fields in using the “dot” notation
- Examples

```
mdl.xic = 0.0
mdl.k[0][1] = 3.0
```

Getting model variables and time histories

- Again, use the “dot” notation to reference model variables
- Use the prepae() function of the model object to add a variable to the prepare list
- Time histories are accessed using the history() function of the model object
- Examples

```
mdl.prepare("x")
mdl.run()
yval = mdl.y
xvals = mdl.history("x")
```

Loading tabulated data

- Tabulated data can be loaded from a CSV file using the Python “csv” library
- Example

```
csvreader = csv.reader(open('obsdata.csv'),
     delimiter=',')
next(csvreader) # Skip header row
for row in csvreader:
     mdl.x = row[0] # Col 1 value
     mdl.y = row[1] # Col 2 value
     # Etc...
```

Plotting from Python code

- Magnolia provides multiple methods for generating plots from Python using the “plot” Python object interface
- The handle-based plotting methods are similar to those used in acslX M language scripts
- Example

```
a = array(range(0, 100))/10.0
b = sin(a)
c = cos(a)

h = plot.line(a, b, ".R")
plot.append(h, a, c, "*B")

names = ["sine", "cosine"]

plot.legend(h, names)
plot.title(h, "Sin and Cos")
plot.xlabel(h, "Theta (radians)")
plot.ylabel(h, "Sin/Cos")

plot.xmin(h, -1.0)
plot.xmax(h, 11.0)
plot.ymin(h, -2.0)
plot.ymax(h, 2.0)
```

Example Magnolia-Compatible Python Script