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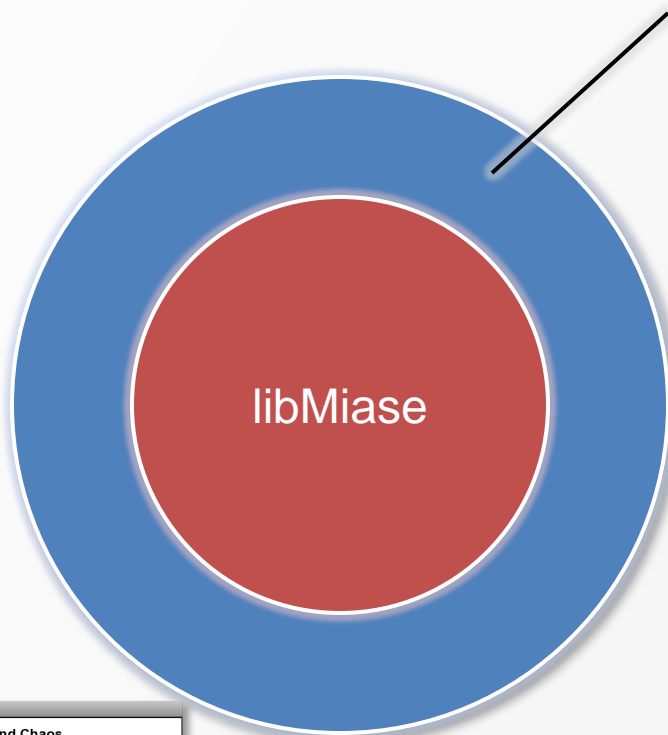
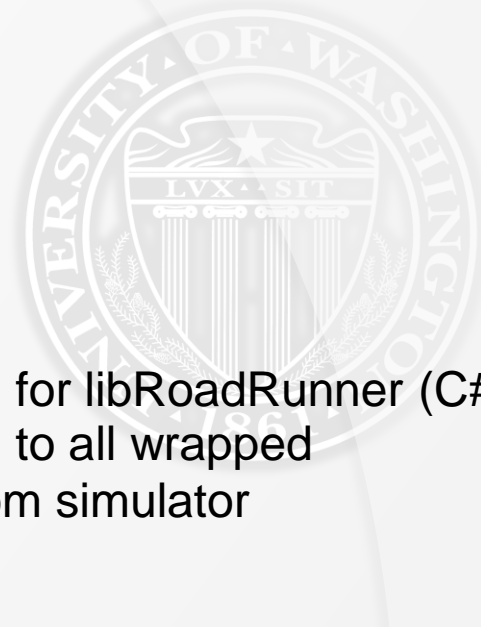
of Applied Life Sciences



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# AN IMPLEMENTATION OF SED-ML

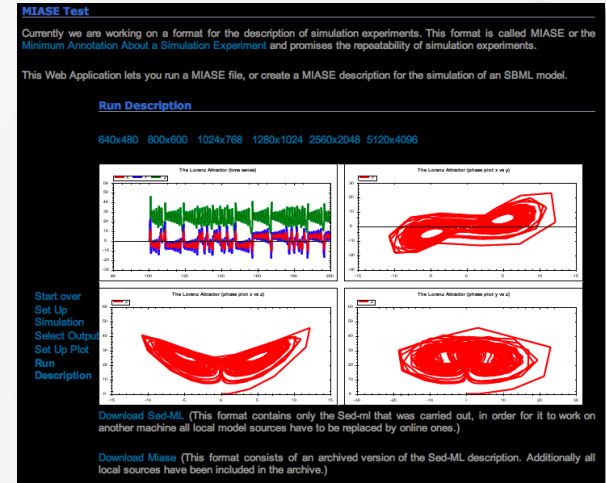
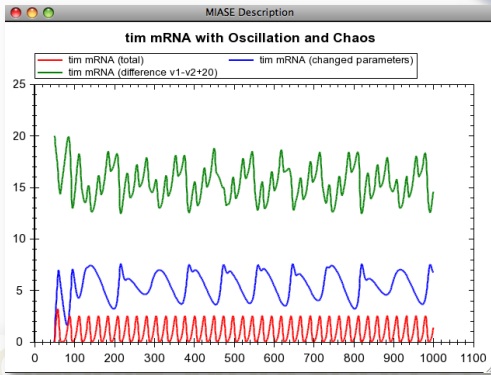
# Current Implementation



libMiaseRunner

Implementation for libRoadRunner (C#)  
{ generalization to all wrapped  
simulators, from simulator  
comparison }

Standalone  
Runner

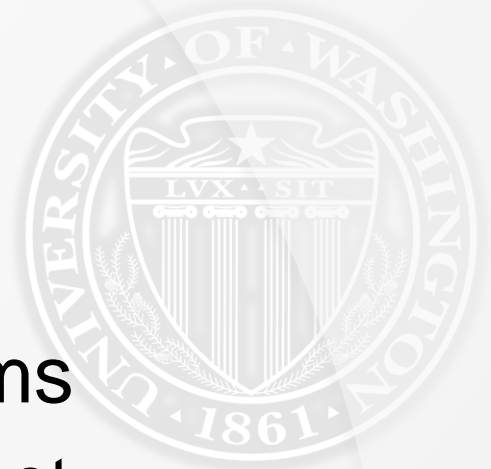


WebSite

\* Implementation was completed before the renaming of miase-ml to sed-ml

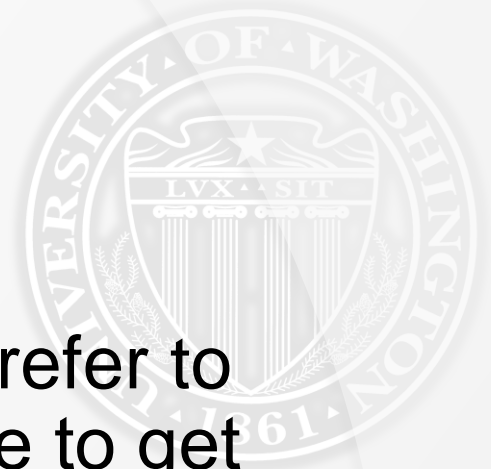
# Implementation

- Based on agreed on UML Diagrams
  - Library implemented in C#, as such not meant as general purpose library, same as pure Java should not be seen as general purpose library
  - Implemented:
    - UniformTimeCourse, ChangeAttribute, Tasks, DataGenerators, Plots



# Archive Type

- SED-ML descriptions will frequently refer to 'local' files, those references are sure to get stale / out of sync.
- A simple archive file, with/without manifest that contains SED-ML + (local) models (+ data files), will solve that issue.
- Proposal: Submit RFC for MIME sub-type registration for application/miase+xml



# Going forward



## ⦿ New Simulation Types:

- Parameter Scan

```
<parameterScan id="scan" start="0.0" end="1.0"  
stepSize="0.1" />
```

- Frequency Analysis

```
<frequencyResponse id="freq" startFrequency="1E-  
4" numDecades="6" numPoints="40" />
```

- Bifurcation Search ...

## ⦿ Those Simulation Types should operate on a designated variable, that has been tagged through a `<csymbol 'target'>`

# Implied Task Value

- It might be nice to think about multivariate types for tasks:
  - Currently for example a task running a `uniformTimeCourse` yields the time series data
  - One could envision additional channels to be returned, such as information when events fire, or constraints are violated ...
  - This would be helpful for bifurcation searches, where we would be interested in obtaining stable / unstable regions, as well as bifurcation points (and information about them).



# Clarification

- Need to precisely formulate which subset of MathML to support, with respect to aggregates like means/std dev, sums ... if we want them
- Reports: should they have a fixed format? If so it needs to be stated.
- Referencing Data, again the issue with data formats
- Elements: changeMath / changeXml



# Problems



## ○ Symbols Missing:

- As soon as we start thinking about new simulation/analysis Types, we need ways to access:
  - Eigenvalues, Flux / Concentration Control Coefficients, scaled / unscaled Elasticities, Rate of Change vs. Flux ...
- Other types might define:
  - Stable / Unstable regions, Bifurcation points
  - Gain / Phase for Frequency Analysis
- Or even simpler:
  - Refer to Amounts instead of Concentrations



# Problems

## ⦿ KISAO:

- Currently a nice description of available Integration methods (i.e: CVODE, Euler, Runge Kutta ...) however the methods do not really describe the differences between simulation packages
- Stochastic methods even more troublesome: If we want to repeat simulation experiments need way to specify how to draw random numbers, along with seeds...
- Missing: Generalized way to attach parameters to the simulation tasks, such as tolerances if needed.





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# Questions ?

# Funding

