

# The E-Cell Simulation Environment

Nathan Addy

SBML Forum

October 13th, 2007

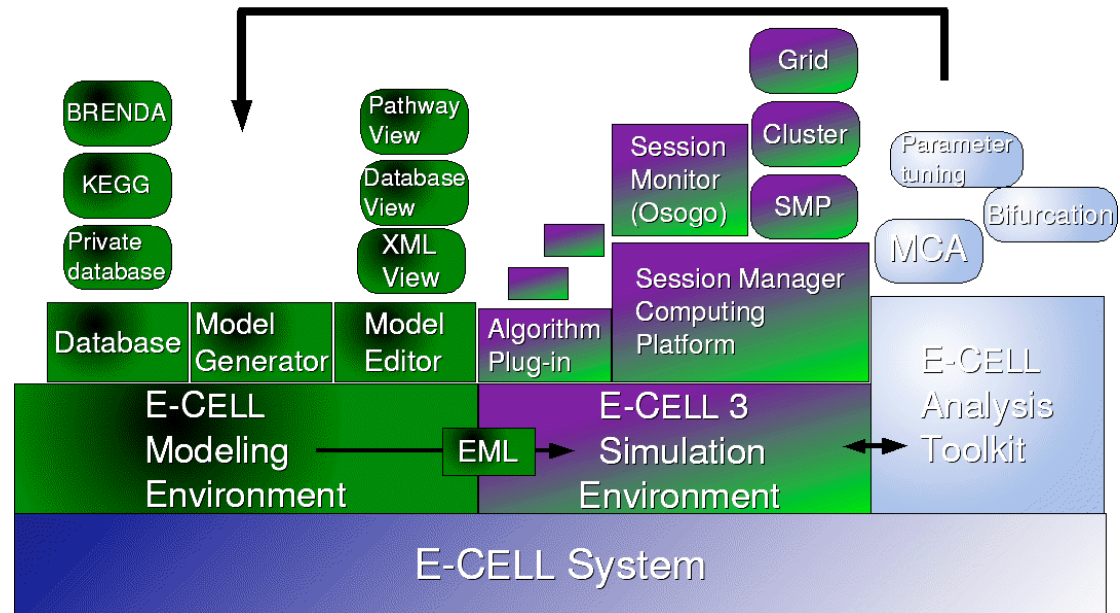
# The E-Cell System

The E-Cell System is a complete environment for the creation, simulation, and analysis of models.

There are three components:

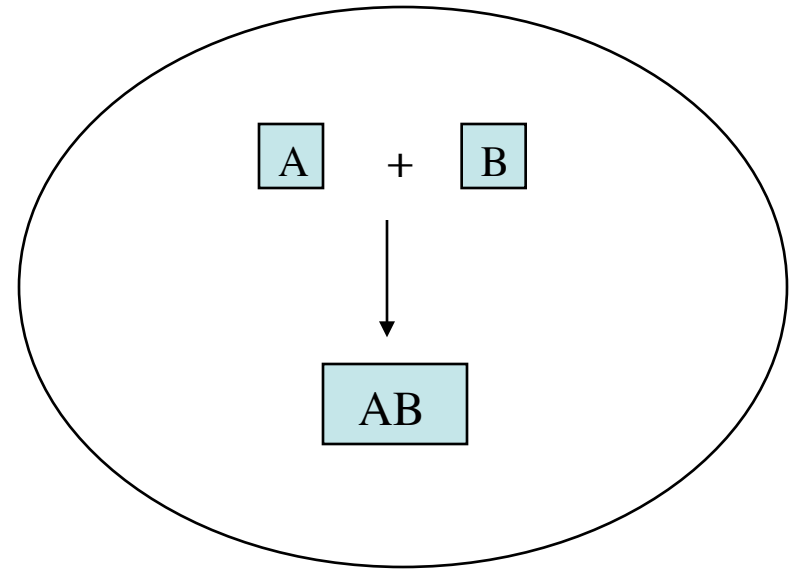
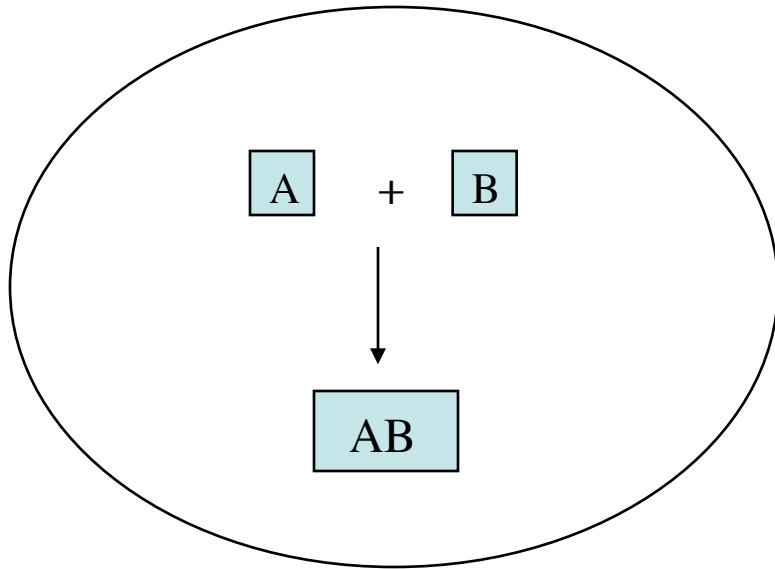
- Modeling Environment
- Simulation Environment
- Analysis Toolkit

## E-CELL Development Overview



# E-Cell Simulation Environment

- Unlike traditional models and simulators, E-Cell models include information about the algorithms required to simulate them.
- E-Cell simulates a model by coordinating the various algorithms and data involved with a meta-algorithm.
- Since the algorithms involved are specified by the the model, this provides a great deal of flexibility in how a physical system is simulated.



```
Stepper ODEStepper( theStepper )
{ #no properties
}
```

```
System System( / )
{
  StepperID theStepper;
  Variable Variable (SIZE) { Value 1e-18; #Liters}
  Variable Variable( A ) { Value 1000; }
  Variable Variable(B) { Value 1000; }
  Variable Variable( AB ){ Value 0; }
```

```
Process MassActionFluxProcess( OnReaction )
{
  k 1.0;
  VariableReferenceList [SO Variable:/:A -1]
                      [S1 :::B -1]
                      [PO :::AB 1];
}
```

```
Stepper DiscreteEventStepper( theStepper )
{ #no properties
}
```

```
System System( / )
{
  StepperID theStepper;
  Variable Variable (SIZE) { Value 1e-18; #Liters}
  Variable Variable( A ) { Value 1000; }
  Variable Variable(B) { Value 1000; }
  Variable Variable( AB ){ Value 0; }
```

```
Process GillespieProcess( OnReaction )
{
  k 1.0;
  VariableReferenceList [SO Variable:/:A -1]
                      [S1 :::B -1]
                      [PO :::AB 1];
}
```

# E-Cell Processes

- DecayFluxProcess
- MassActionProcess
- MichelisUniUniProcess
- PingPongBiBiFluxProcess
- ContantFluxProcess
- DecayFluxProcess
- ExpressionAlgebraicProcess
- ExpressionFluxProcess
- GMAProcess
- ESSYNSystemProcess
- TauLeapProcess
- SSystemProcess
- QuasiDynamicFluxProcess

# Extendibility with Pluggable Simulation Algorithms

- E-cell allows new simulation algorithms to be written and used in models as Processes.
- The meta-algorithm can then automatically use these new algorithms in coordination with pre-existing algorithms.
- Processes are written in C++ and must specify what happens when they “fire”. Compiling is made easy with a special compiling tool provided by E-Cell.

# SBML Support

The E-Cell SE currently imports and exports models in SBML format.

SBML Level 1	-- Yes
SBML Level 2 Version 1	-- Yes
SBML Level 2 Version 2	-- In Progress

Models are currently imported as systems of ODEs.

# Future E-Cell Developments

- Spatial support for molecular interactions using any number of different spatial representations.
- Dynamic model structure, including dynamic species and reaction generation (based on Molecuizer).

These features will be released in E-Cell Version 4, which we expect to be out this time next year.