

Recent updates of the E-Cell Software developments

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E-Cell Project

E-Cell software developments (1996~present)



- E-Cell 1 (1996~2001)
- E-Cell 2 (2000~2002)
- E-Cell 3 (2001~)
 - E-Cell Simulation Environment (ver. 3.2 is under preparing with Molecuizer integration)
 - E-Cell3D (2006~2007, 3-D graphical simulation viewer prototype)
 - E-Cell IDE (2004~, Integrated Development Environment for modeling/simulation/analysis with SBML support)
- E-Cell 4 (under planning, implementing test code)

E-Cell IDE Overview



QuorumSensing2 - E-Cell IDE

File Edit Setup Layout View Simulation Tools Help

DefaultSets Time: 39.18999999 sec 1 Step 60%

Project Explorer

- QuorumSensing2
 - Analysis
 - DMs
 - Log archives
 - Models
 - QuorumSensing2
 - Cell1

Property

Variable/Cell1:c1

Name	Value
ModeID	QuorumSensing2
ID	c1
ClassName	Variable
DiffusionCoeff	0
Fixed	0
MolarConc	1.29002807658518
Name	CI transcripts
NumberConc	7.76872542403399E+23
Value	776872542.403399

Spreadsheet

	A	B	C	D	E	F	G
6	Variable	/AHL	QuorumSensing2	Variable		1031829753711.81	0.0171339477184...
7	Variable	/CellNum	QuorumSensing2	Variable	cellnum	10	1.6605401866749...
8	Variable	/Cell1:c1	QuorumSensing2	Variable	CI transcripts	776872542.403399	1.29002807658518
9	Variable	/Cell1:CI	QuorumSensing2	Variable	CI protein	942742968.59728	1.56546258506101
10	Variable	/Cell1:lacI	QuorumSensing2	Variable	LacI transcripts	3574231476.50937	5.93515500322232
11	Variable	/Cell1:LacI	QuorumSensing2	Variable	LacI protein	2735721160.60779	4.54277492672623
12	Variable	/Cell1:luxI	QuorumSensing2	Variable		3266688899.43987	5.42446819488482

Graph plotter1

LoggerWindow

Show	FULLPN	Color	Line	Y2
<input checked="" type="checkbox"/>	Variable:/AHL:NumberConc	Red	—	<input type="checkbox"/>
<input checked="" type="checkbox"/>	Variable:/AHL:MolarConc	Green	—	<input type="checkbox"/>

Console Output Errors Spreadsheet

/Cell1:c1

X:0000, Y:0009

E-Cell IDE Overview



- Purposes

- Provide useful integrated software for cell modeling/analysis between newbie and professionals.

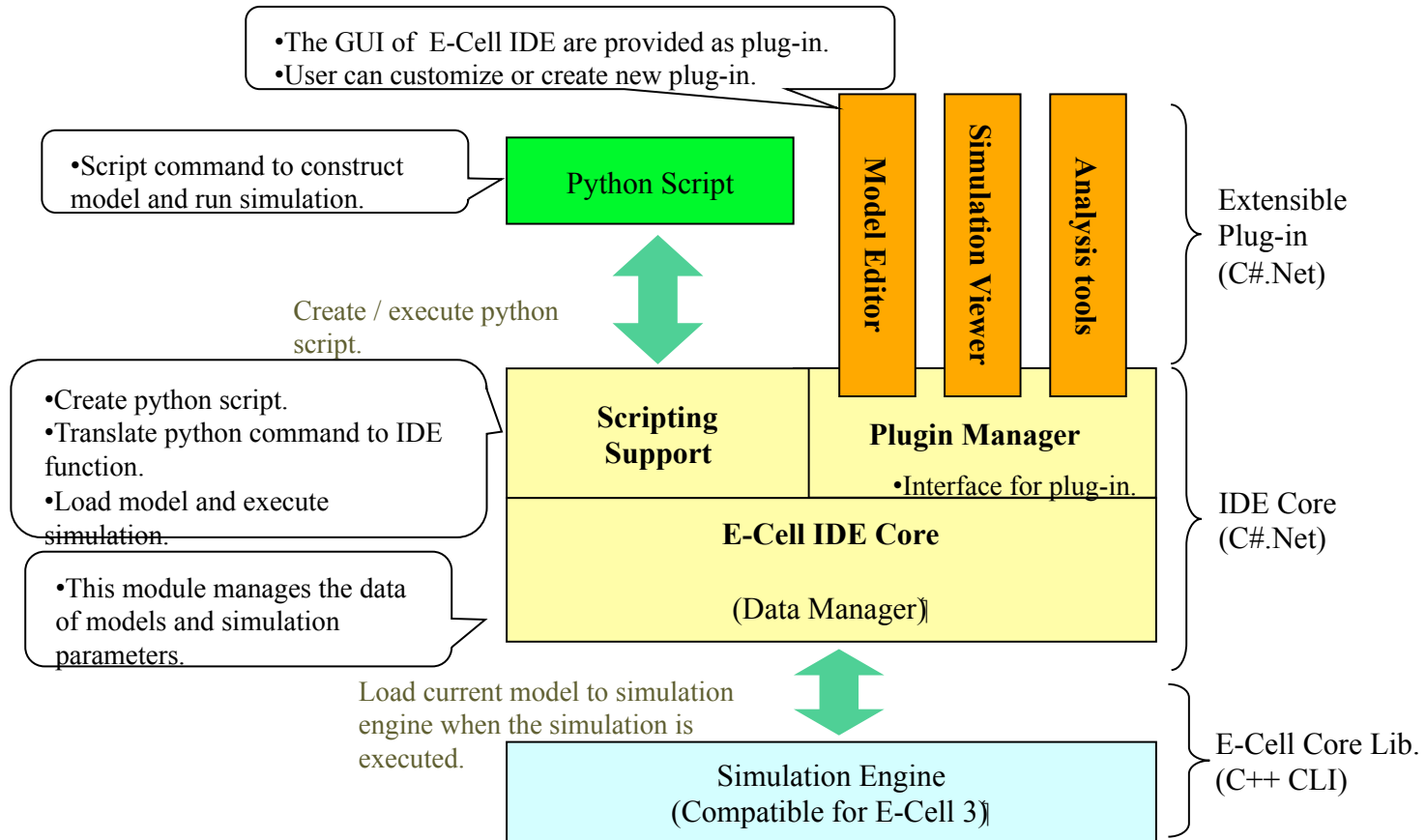
- Implementation

- Simulation core(Numerical computation)
 - Using E-Cell ver. 3.2 core libs wrapped by C++/CLI
- Frontend(GUI)
 - C#.Net Framework 2.0

- Current development status

- RC2 (Release candidate) released on Aug. 24.
 - 32bit/64bit Windows XP and later version are supported.
- 1.0 stable release will be out by Oct. 2009.

E-Cell IDE Application framework structure



E-Cell IDE with SBML support



- libSBML

- E-Cell 3 provides SBML import/export program which uses libSBML and Python binding.

- E-Cell IDE has re-implemented converter uses libSBML and C# binding.

- Current implementation is experimental but we're testing our code by SBML TestSuite.



A result of SBML importer

- 100 sample data of SBML Lv.2 was retrieved and tested by SBML TestSuite
 - 97% models could be loaded and automatically converted to E-Cell model objects.
 - 38% models could run the simulation without modifications manually
 - 31% models need small tweaking to adopt the E-Cell's model data ontology.
- Total: 69% models could be run on the E-Cell IDE



Future work

- Improve the convertor which can load SBML models automatically.
- Make a report website of compatibility results of the E-Cell IDE using SBML model

E-Cell IDE website
<http://www.e-cell.org/ide/>