FERN

Framework for Evaluation of chemical Reaction Networks

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Overview

What is FERN?

A fast, extensible and comprehensive framework for simulation and analysis of chemical reaction networks.

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Overview

What is FERN?
A fast, extensible and comprehensive framework for simulation and analysis of chemical reaction networks.

What is FERN not?
A second Dizzy / Copasy / Stocks. You cannot do simulations by mouseclick but by a very few lines of code.

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Overview

What is FERN?
A fast, extensible and comprehensive framework for simulation and analysis of chemical reaction networks.

What is FERN not?
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Advantage
If you are able to write many reasonable lines of code, you can do arbitrarily complex simulations.

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Elementary Example

```
1  Network net = new RNMLNetwork(new
       File("some_net.xml"));
2  Simulator sim = new GibsonBruckSimulator(net);
3  Observer obs = sim.addObserver(new
       AmountIntervalObserver(sim,1,X));
4  sim.start(50);
5  System.out.println(obs);
```

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Complexity

Complicated?

- ▶ 100 classes / interfaces
- ▶ with 12906 lines

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But...

- ▶ only 3 central classes
- ▶ half of the lines are javadoc
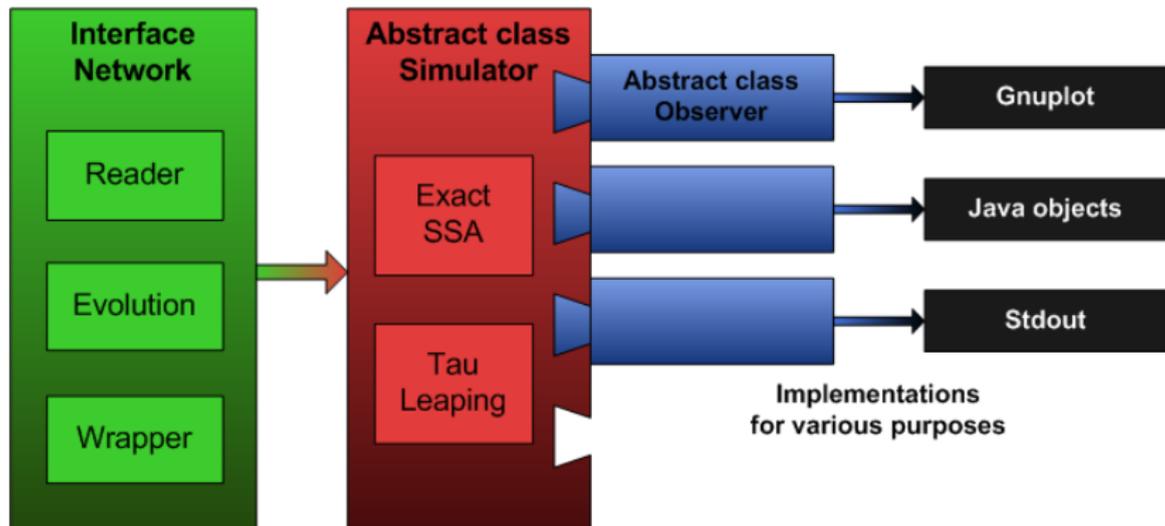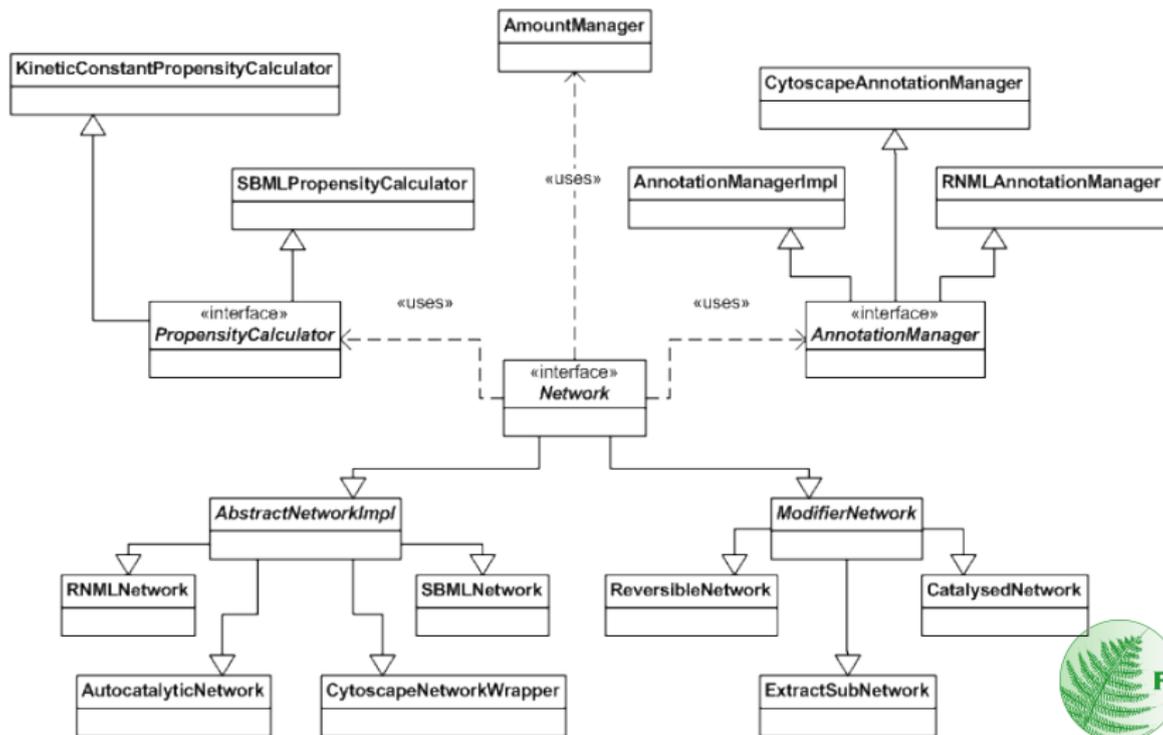
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Main classes / interfaces
UML of Network related classes
Observer system

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Observer

Observer

Observers can be registered at the Simulator and record various
data about the simulation runs. Some are able to handle repeated
runs (and yield average data), some are not (refer to the javadoc).

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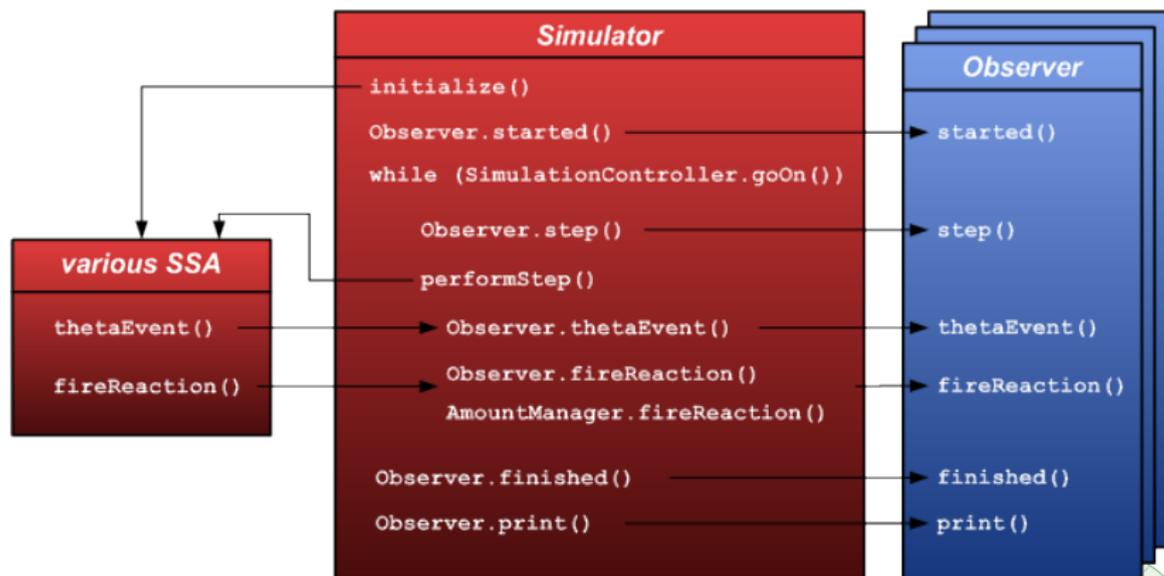
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Observer
Observers can be registered at the Simulator and record various data about the simulation runs. Some are able to handle repeated runs (and yield average data), some are not (refer to the javadoc).

Data
Depending on what kind of data observers record, they provide different kind of data (plain text, gnuplot, histograms,...).

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Gnuplot

A class GnuPlot is included in FERN which enables you to

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A class GnuPlot is included in FERN which enables you to

- retrieve the gnuplot data as String or save it to a file

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- retrieve the gnuplot data as String or save it to a file
- get the plot command

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- ▶ retrieve the gnuplot data as String or save it to a file
- ▶ get the plot command
- ▶ plot the data by calling gnuplot from java

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- ▶ get the plot command
- ▶ plot the data by calling gnuplot from java
- ▶ retrieve the plot as image object or save it to a png file

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A class GnuPlot is included in FERN which enables you to

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- ▶ get the plot command
- ▶ plot the data by calling gnuplot from java
- ▶ retrieve the plot as image object or save it to a png file
- ▶ show the plot in a JFrame

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Analysis

The AnalysisBase class provides

- additional index structures
- generic bfs / dfs

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Analysis

The AnalysisBase class provides

- ▶ additional index structures
- ▶ generic bfs / dfs

Used by included algorithms

- ▶ ShortestPaths
- ▶ AutocatalyticNetworkDetection

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Random number generation

is handled in one central Stochastics class

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► easy replacement of the random number generator

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▶ easy replacement of the random number generator

▶ make simulations deterministic by explicitly setting the seed value

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Stochastics

Random number generation

is handled in one central Stochastics class

- ▶ easy replacement of the random number generator
- ▶ make simulations deterministic by explicitly setting the seed value
- ▶ count number of random numbers generated from various distributions

Documentation

javadoc

comprehensive documentation of each class and method

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comprehensive documentation of each class and method

Technical overview

A detailed technical overview about FERN's implementation is
accessible as pdf document.

Examples

Maybe most important...

There are many examples included in the package fern.example
which demonstrate different aspects of FERN.