

On the interaction of VANESA, PNLlib, and OpenModelica

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MoRitS is a cooperation between:



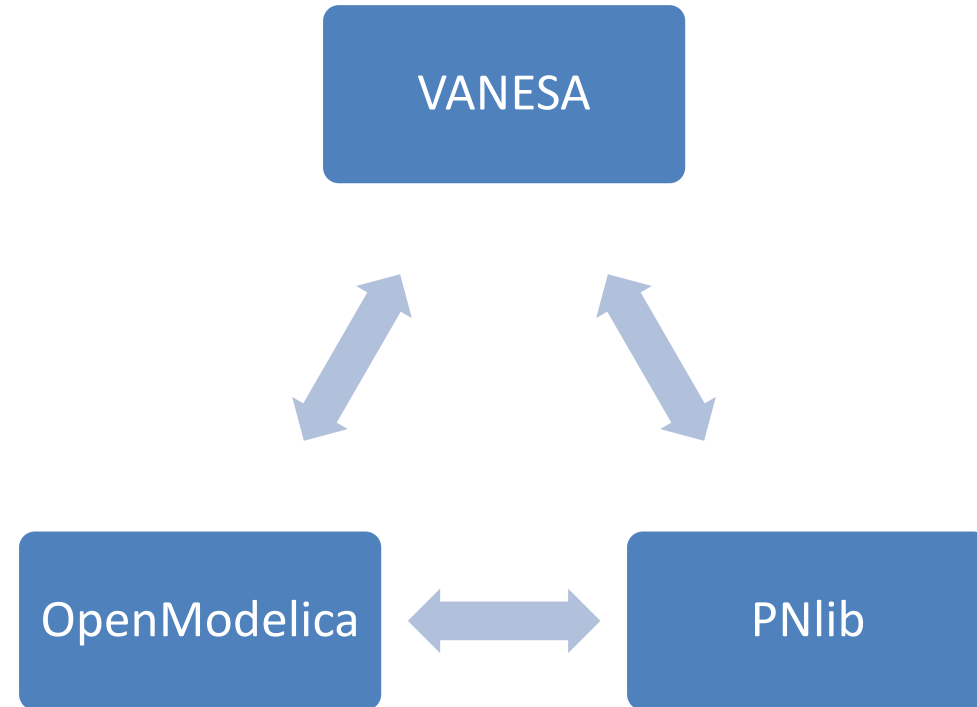
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Ministerium für Innovation,
Wissenschaft und Forschung
des Landes Nordrhein-Westfalen



Outline

- **VANESA**
- PNlib
- OpenModelica
- Summary



VANESA in a Nutshell

- Department of Bioinformatics (Prof. Hofestädt), Bielefeld University
- Development since 2009
- Graph-based editor for Systems biology applications
 - Modeling of Cell-to-Cell Communication Processes with Petri Nets Using the Example of Quorum Sensing
 - Hydrogen production in *Chlamydomonas reinhardtii*
- Binding to in-house data warehouse DAWIS-M.D.
 - Integration of several microbiological databases, e.g. KEGG and BRENDA
- Java based, open-source, and free-of-charge

→ <http://agbi.techfak.uni-bielefeld.de/vanesa/>

VANESA in a Nutshell

- Simulation of biological systems using Petri nets
 - Biological network → Petri net → Modelica model
- Visualizing of simulation results
 - On-the-fly
 - Tokens, token flow, firing speed mapped on nodes and edges
- Applying algorithms on networks
 - Discrete PN: reachability and coverability
 - Calculation of centrality measurements
 - ...

VANESA in a Nutshell

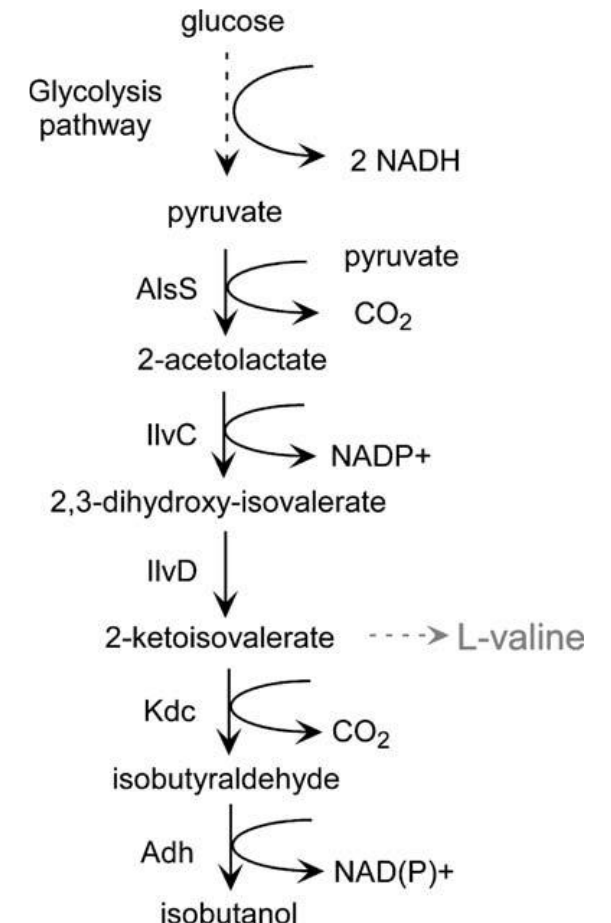
The screenshot displays the VANESA 2.0 software interface, titled "VANESA 2.0 - Visualization and Analysis of Networks in Systems Biology Applications". The main window shows a network graph with 264 nodes and 301 edges, with 3 nodes picked. The graph is a complex network of interconnected nodes, with several nodes highlighted in yellow. The interface includes several panels:

- Database Search:** Features search options for KEGG, PPI, BRENDA, miRNA, and UNID. The BRENDA Search Window is active, showing search criteria: EC-Number (4.2.1.9), Name, Substrat, Product, and Organism (coli). Buttons for "headless", "reset", and "search" are present.
- Petri Net Simulation:** A panel for simulating Petri nets.
- Graph Analysis:** A panel for analyzing graph properties.
- Element Properties:** A panel showing details for the selected enzyme: EC: 2.2.1.6, Name: acetolactate synthase, Reference: Choose Reference / Show Labels, Compartment: Cytoplasma, and other identifiers.
- Network Modelling:** The main graph area, showing a zoom of 0.68x. The graph contains numerous nodes and edges, with some nodes highlighted in yellow. The status bar at the bottom of the graph area shows "Nodes: 264 Edges: 301 Picked nodes: 3".

The interface also includes a menu bar (File, Graph, Petri Net, Transformation, Layout, Tools, Settings, Help) and a toolbar on the right side with various icons for navigation and manipulation.

VANESA: Introductory Example

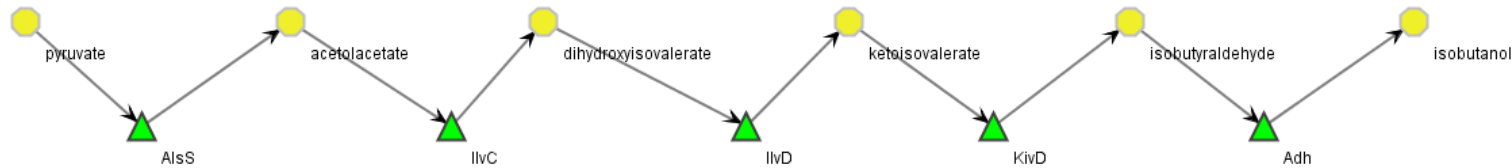
- Production of isobutanol in *Escherichia coli*
 - Isobutanol is renewable bio fuel
- Database connection
 - Exploration of pathways
 - Database-supported modeling of pathways
- Network simulation
 - Automatic transformation to Petri net formalism
 - Modelica-based simulation



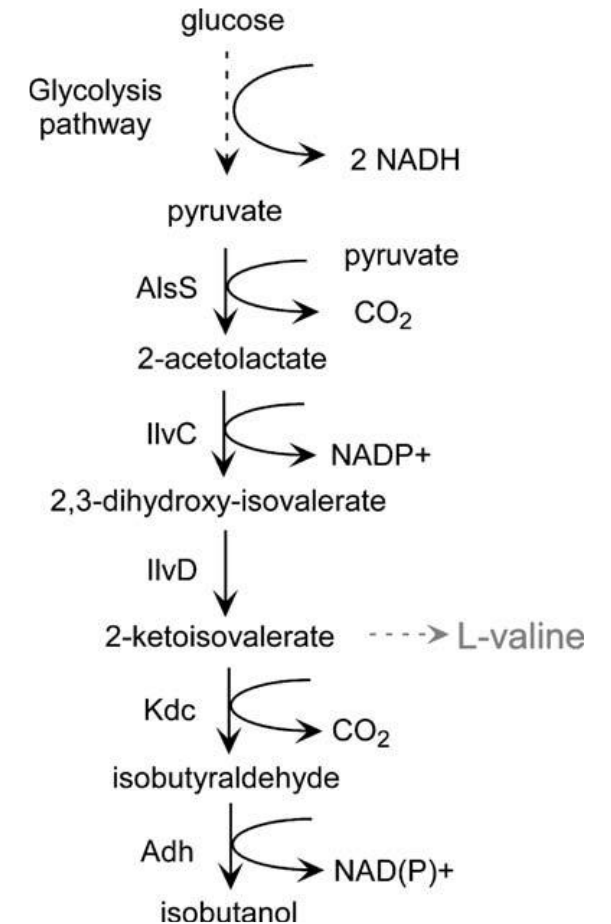
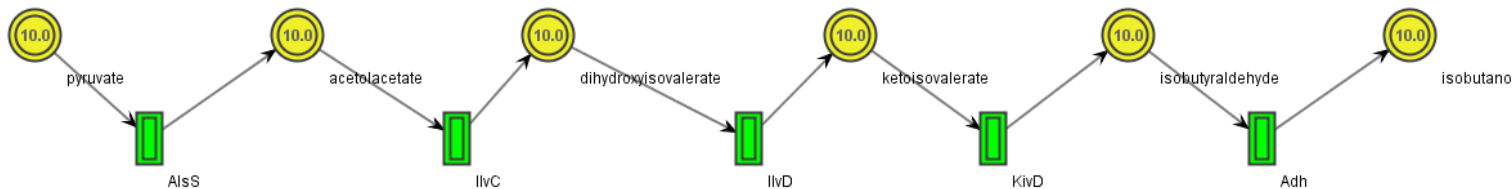
VANESA: Introductory Example

- Production of isobutanol in *Escherichia coli*

Biological network

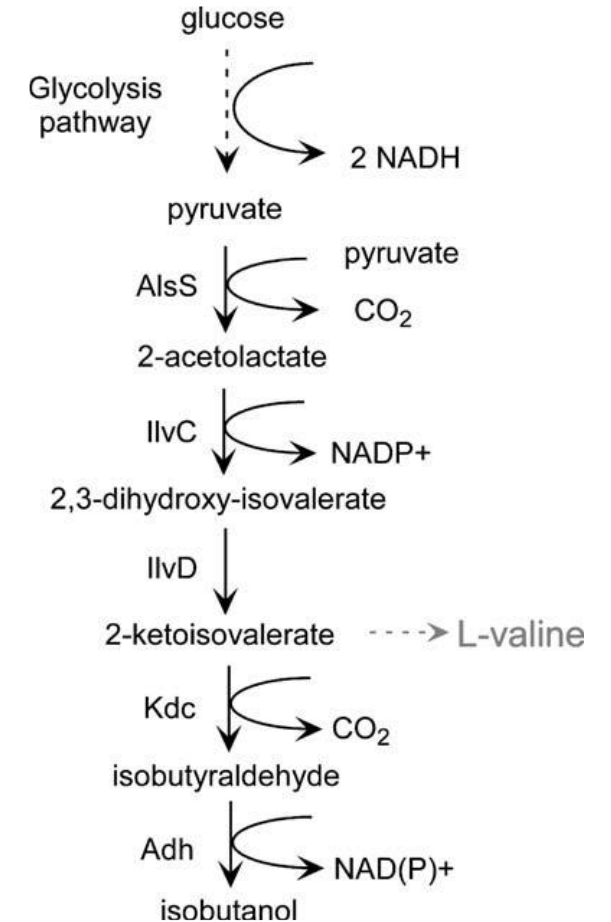
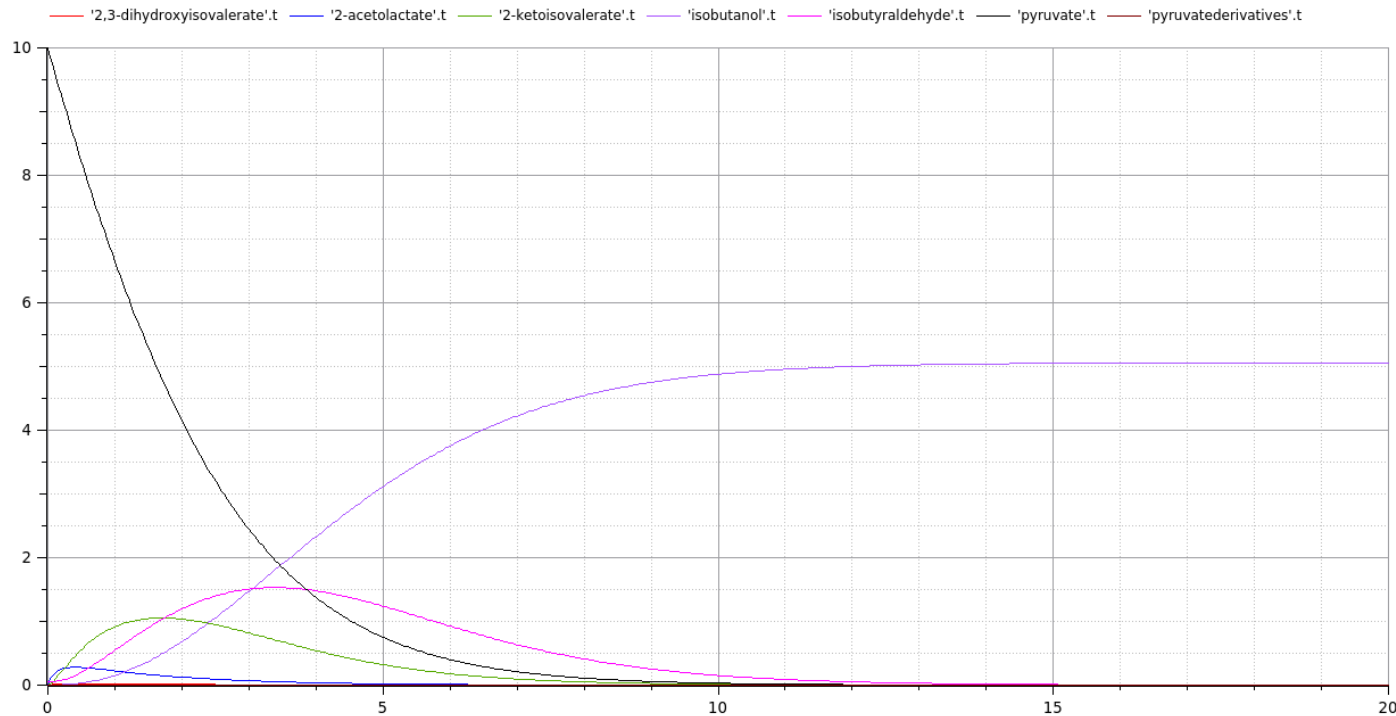


Petri net



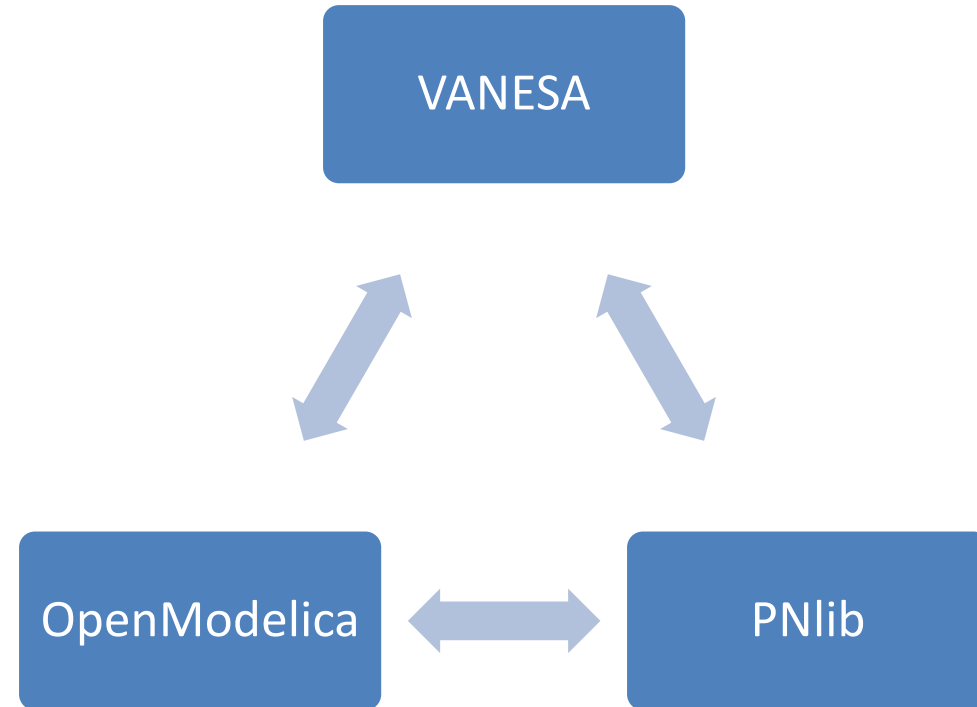
VANESA: Introductory Example

- Production of isobutanol in *Escherichia coli*



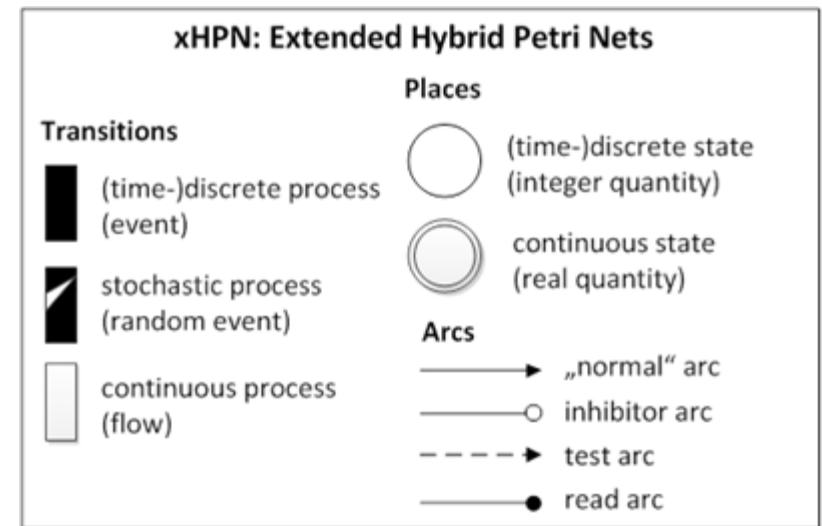
Outline

- VANESA
- **PNlib**
- OpenModelica
- Summary



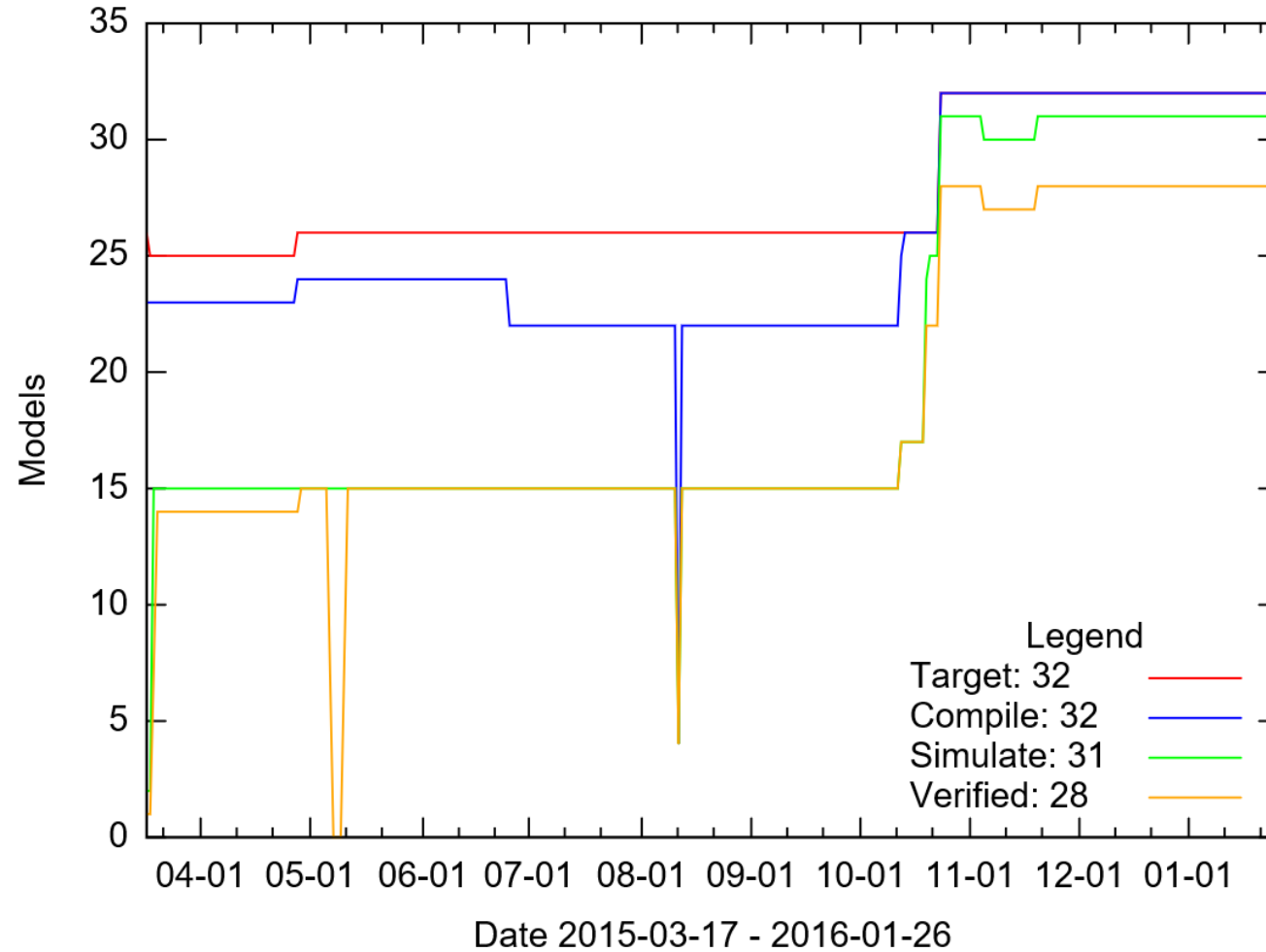
PNlib

- Implementation of extended hybrid Petri Nets (xHPN) formalism
 - Discrete and continuous places
 - Discrete, stochastic, and continuous transitions
 - Test, inhibitor, and read arcs
- Updated to latest Modelica version
- Latest release: v1.2
 - Added support for 64bit systems
 - Revised some internal algorithms to archive less complex equation systems structure
 - Minor bug fixes



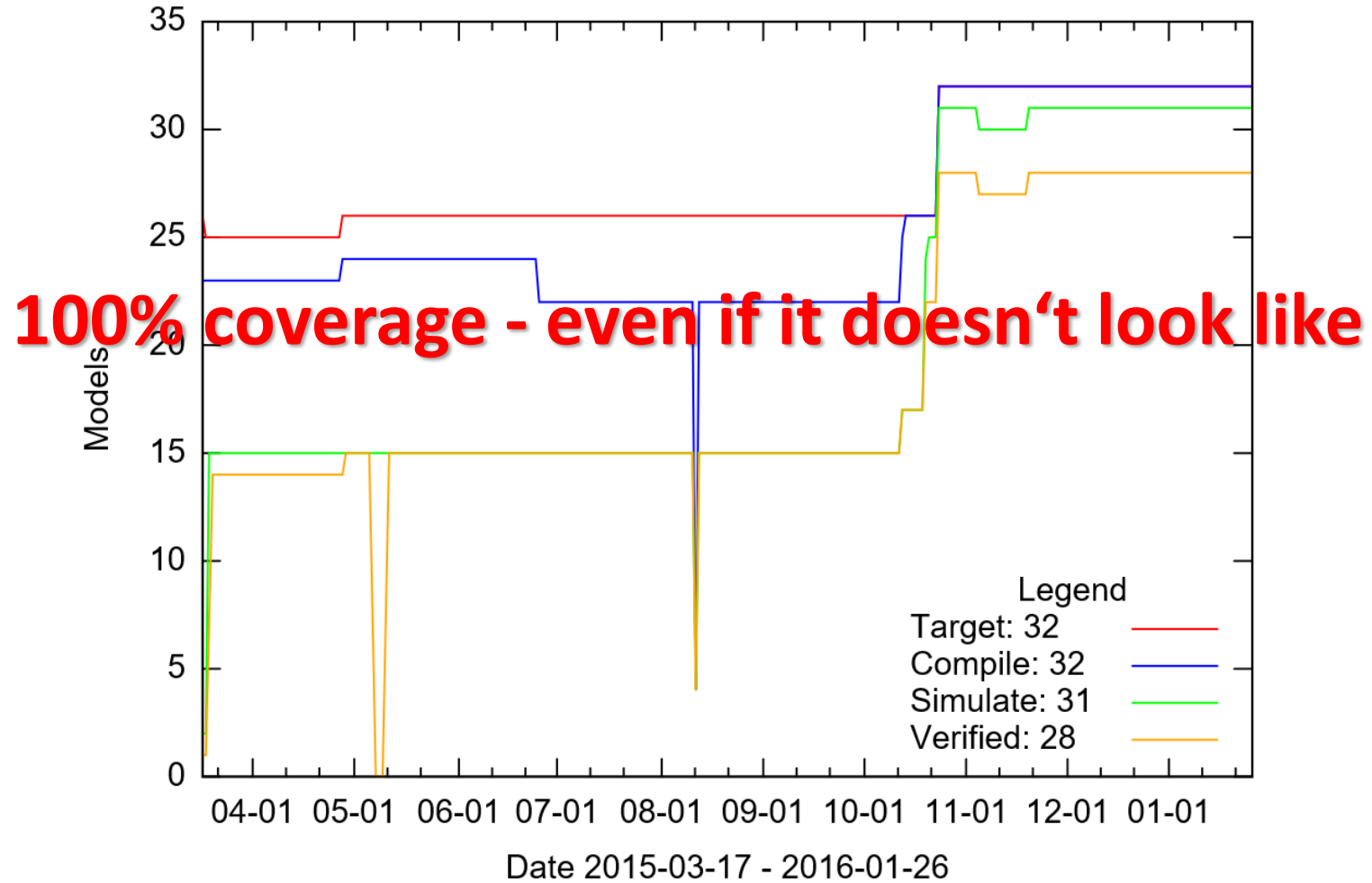
→ <https://github.com/modelica-3rdparty/PNlib>

OpenModelica - PNlib Coverage Trend



→ <https://test.openmodelica.org/libraries/PNlib/BuildModelRecursive.html>

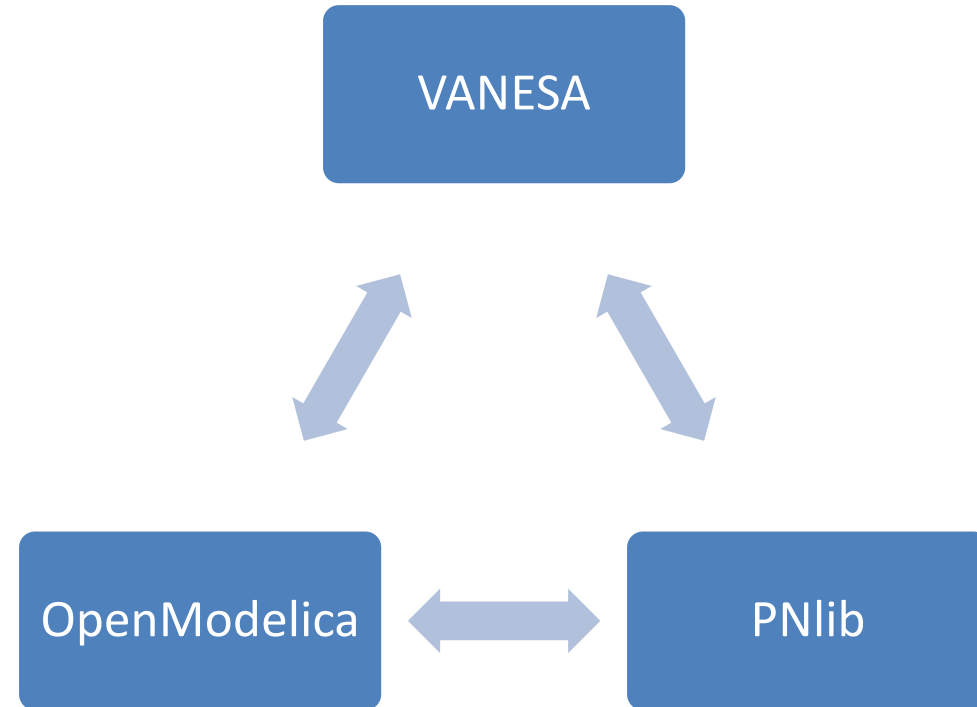
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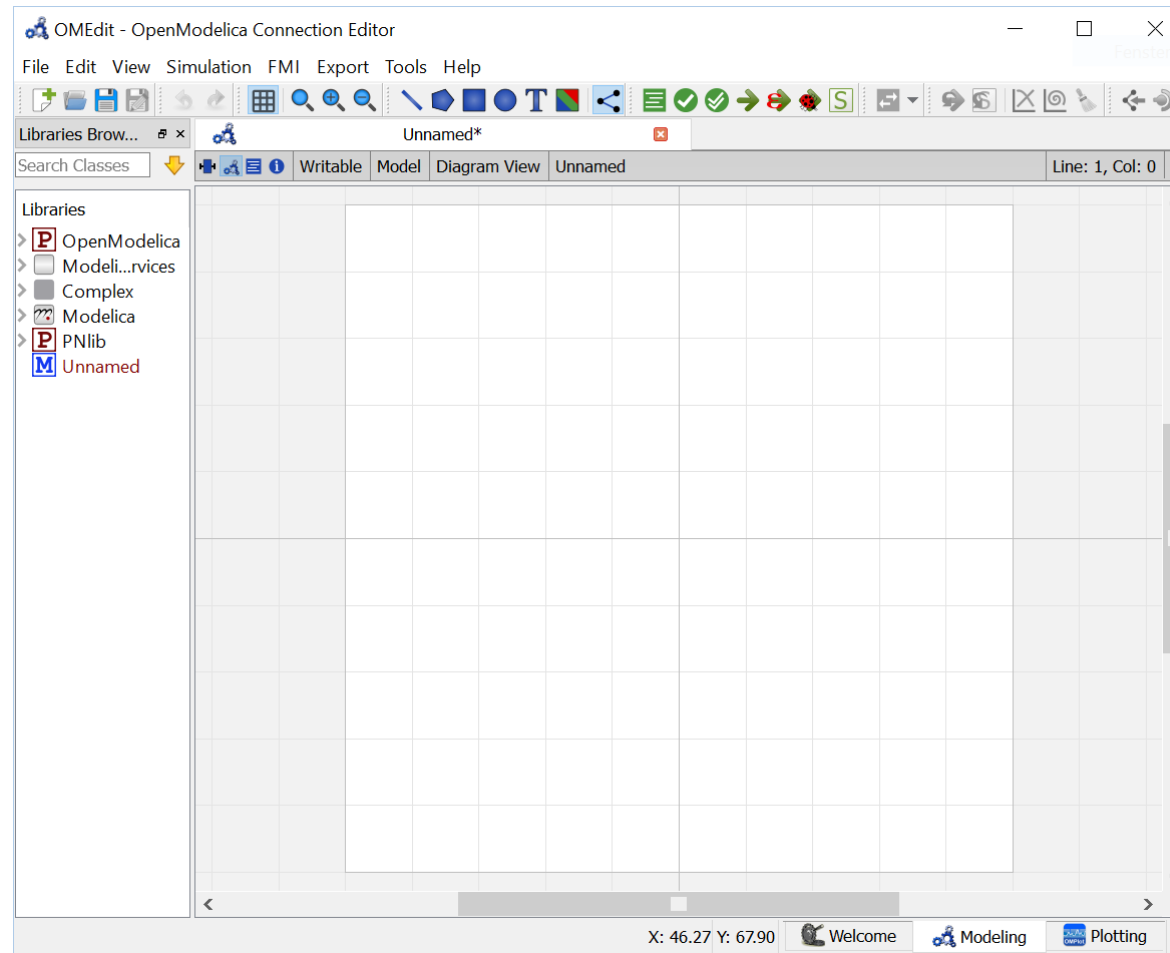
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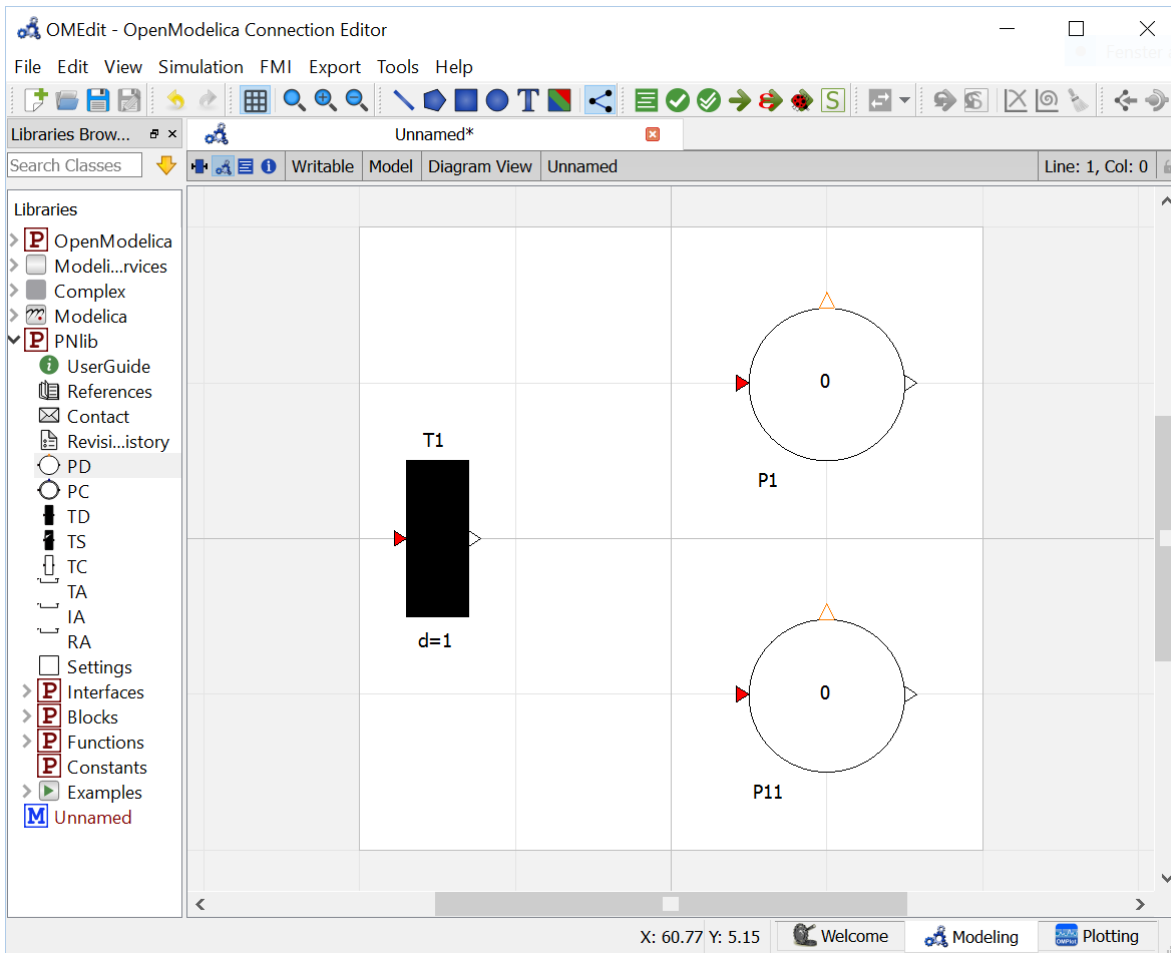
OpenModelica

- Best Open Source Modelica Compiler on the planet
- Full support of PNlib library
- Simulation results on-the-fly
- Useful feedback, e.g. unit checking

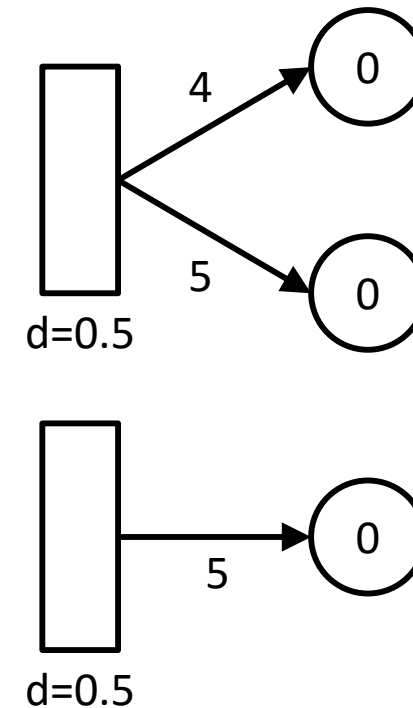
Why not just using OMEdit?



Why not just using OMEdit?

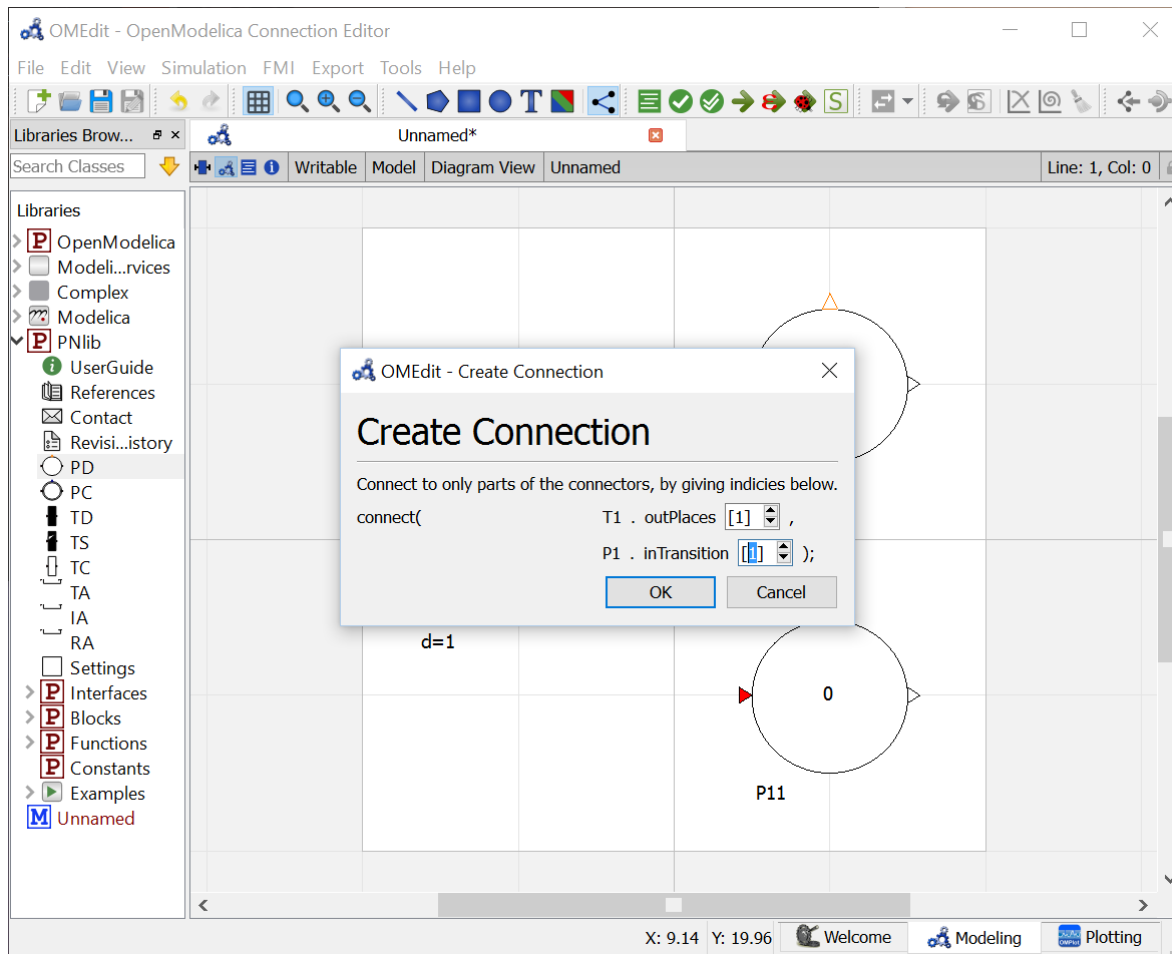


Demonstration of modelling simple Petri nets using PNlib and OpenModelica/OMEdit



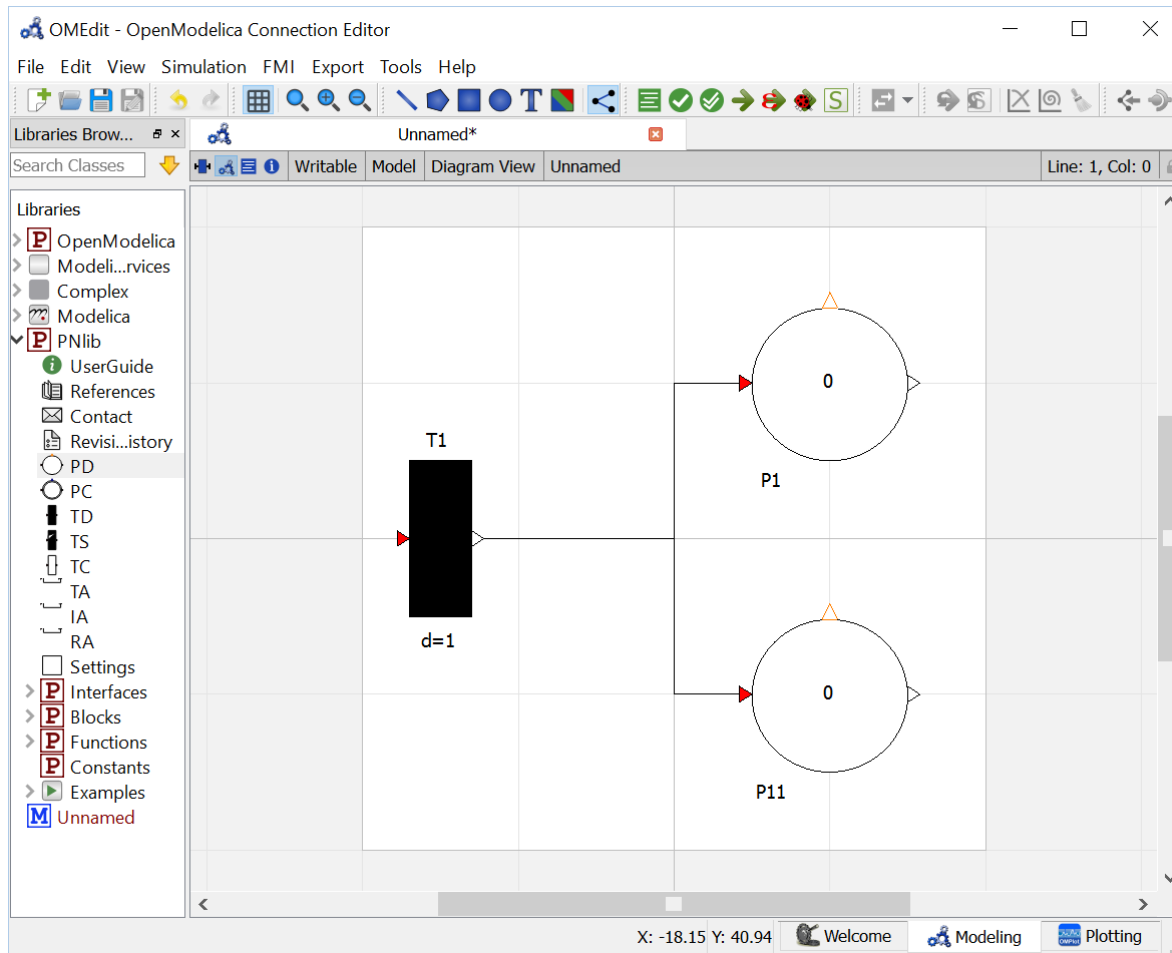
Why not just using OMEdit?

Places/Transitions are using array connectors.



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Places/Transitions are using array connectors.

Unfortunately, **connectorSizing** annotation is not supported yet.

OpenModelica compiler generates useful error messages.

OMEdit - OpenModelica Connection Editor

File Edit View Simulation FMI Export Tools Help

Libraries Browser: Unnamed*

Search Classes: Writable Model Diagram View Unnamed Line: 1, Col: 0

Libraries:

- OpenModelica
- Modeli...rvice
- Complex
- Modelica
- PNlib
 - UserGuide
 - References
 - Contact
 - Revisi...istory
 - PD
 - PC
 - TD
 - TS
 - TC
 - TA
 - IA
 - RA
- Settings
- Interfaces
- Blocks
- Functions
- Constants
- Examples
- Unnamed

Messages Browser:

Continuing flattening by only considering the 'outer' component declaration.

[4] 16:48:32 Translation Error
Subscript '2' for dimension 1 (size = 0) of T1.outPlaces[2] is out of bounds.

[5] 16:48:32 Translation Error
Error occurred while flattening model Unnamed

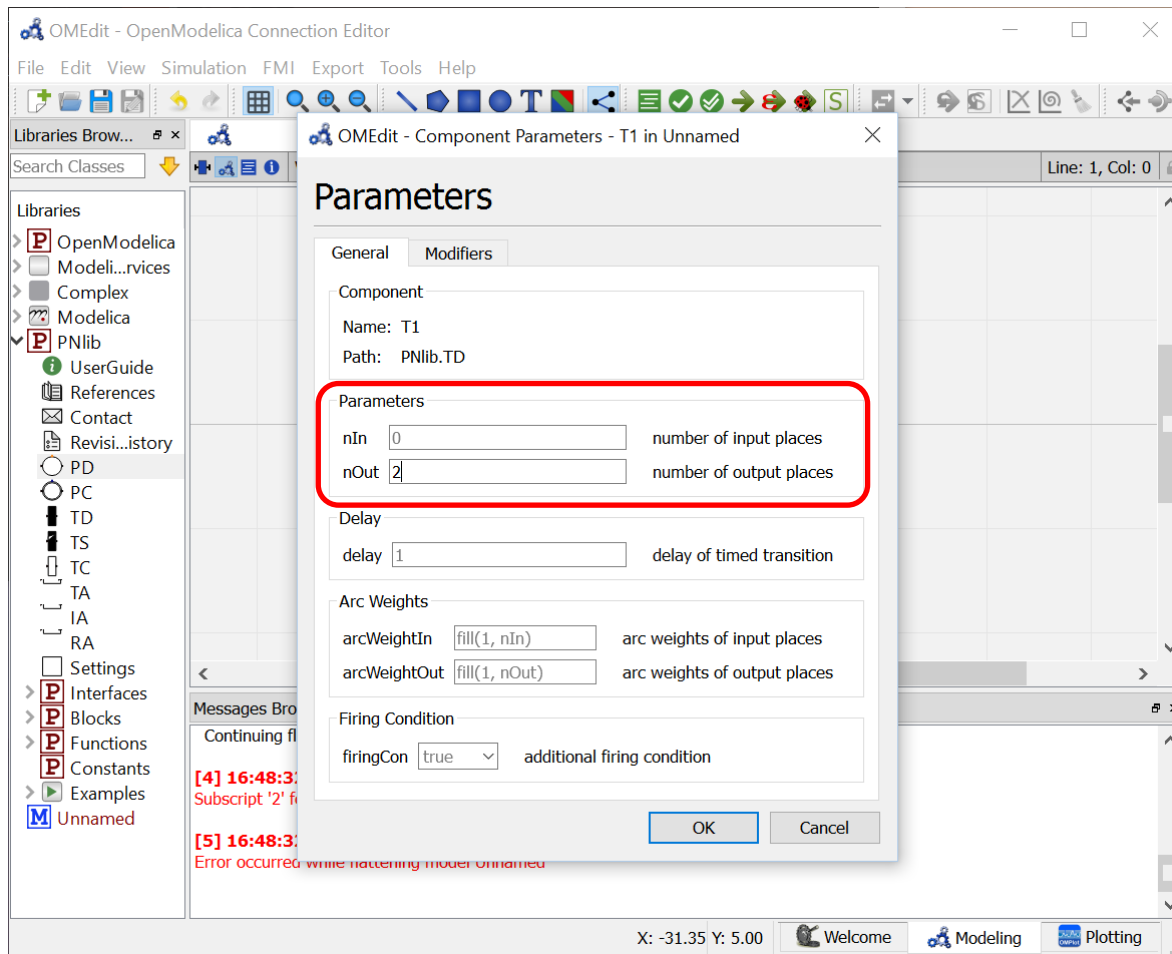
Changes to/from connect mode X: -12.50 Y: 45.00 Welcome Modeling Plotting

Why not just using OMEdit?

Places/Transitions are using array connectors.

Unfortunately, **connectorSizing** annotation is not supported yet.

Connector sizes need to be set manually.

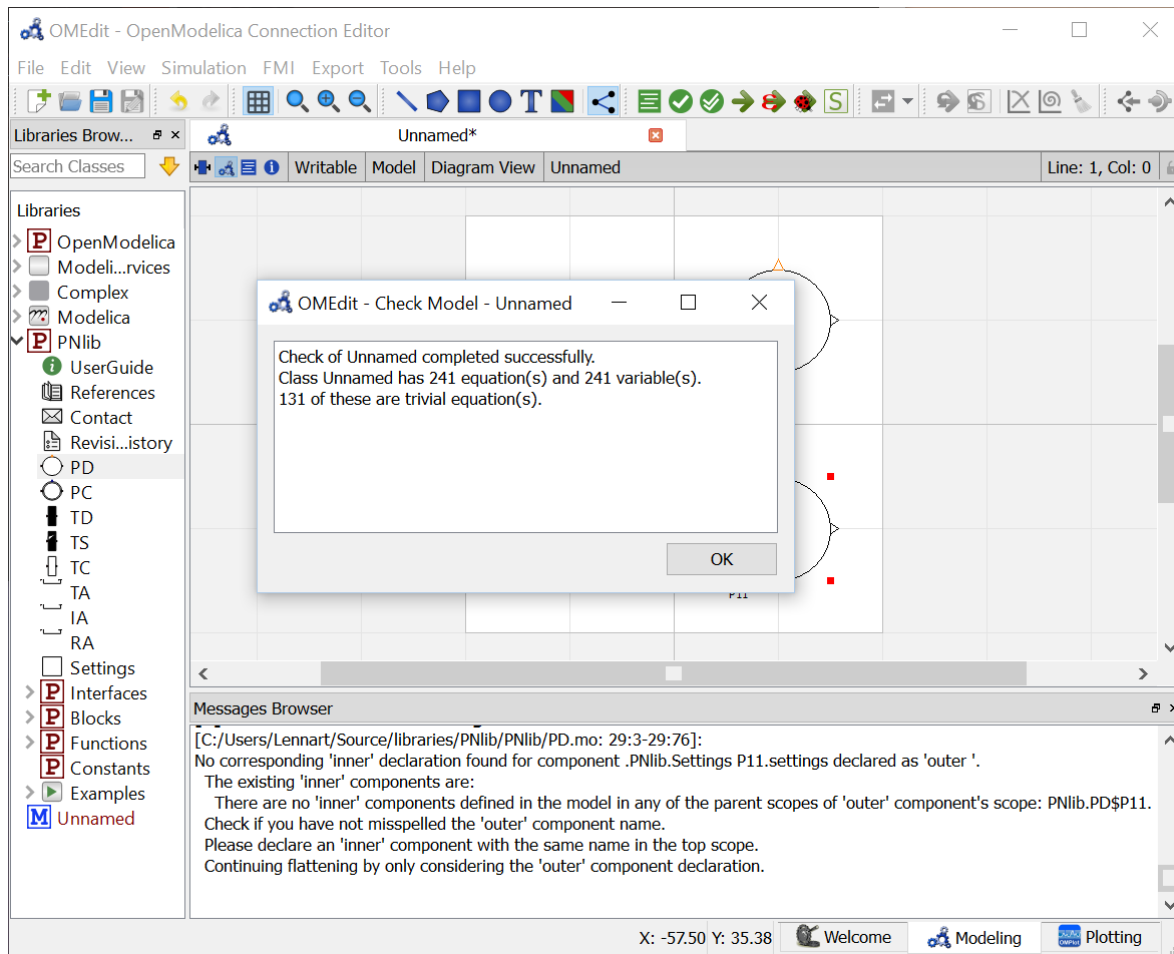


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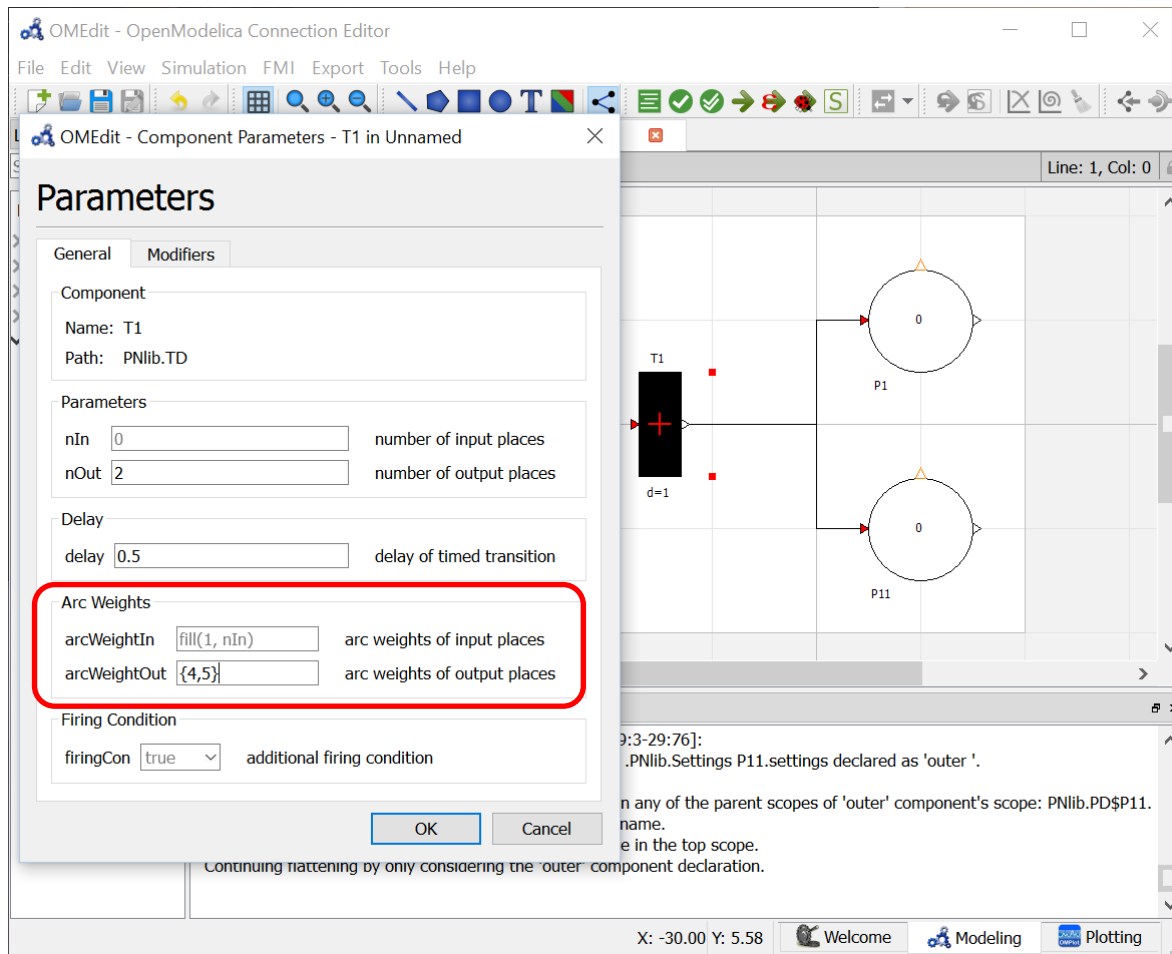
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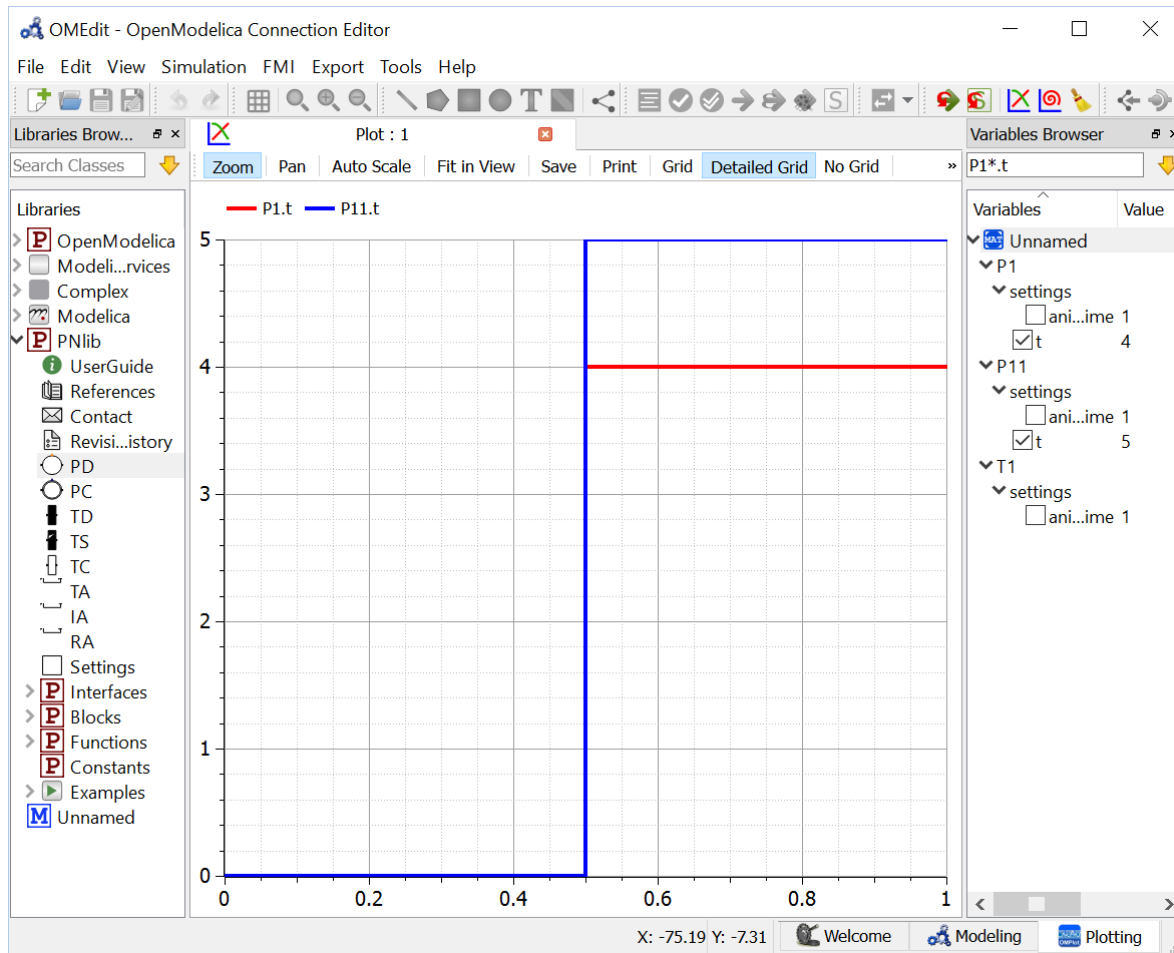
Why not just using OMEdit?

Arc weights are stored within transitions.

Arc weights are mapped on corresponding connector array.

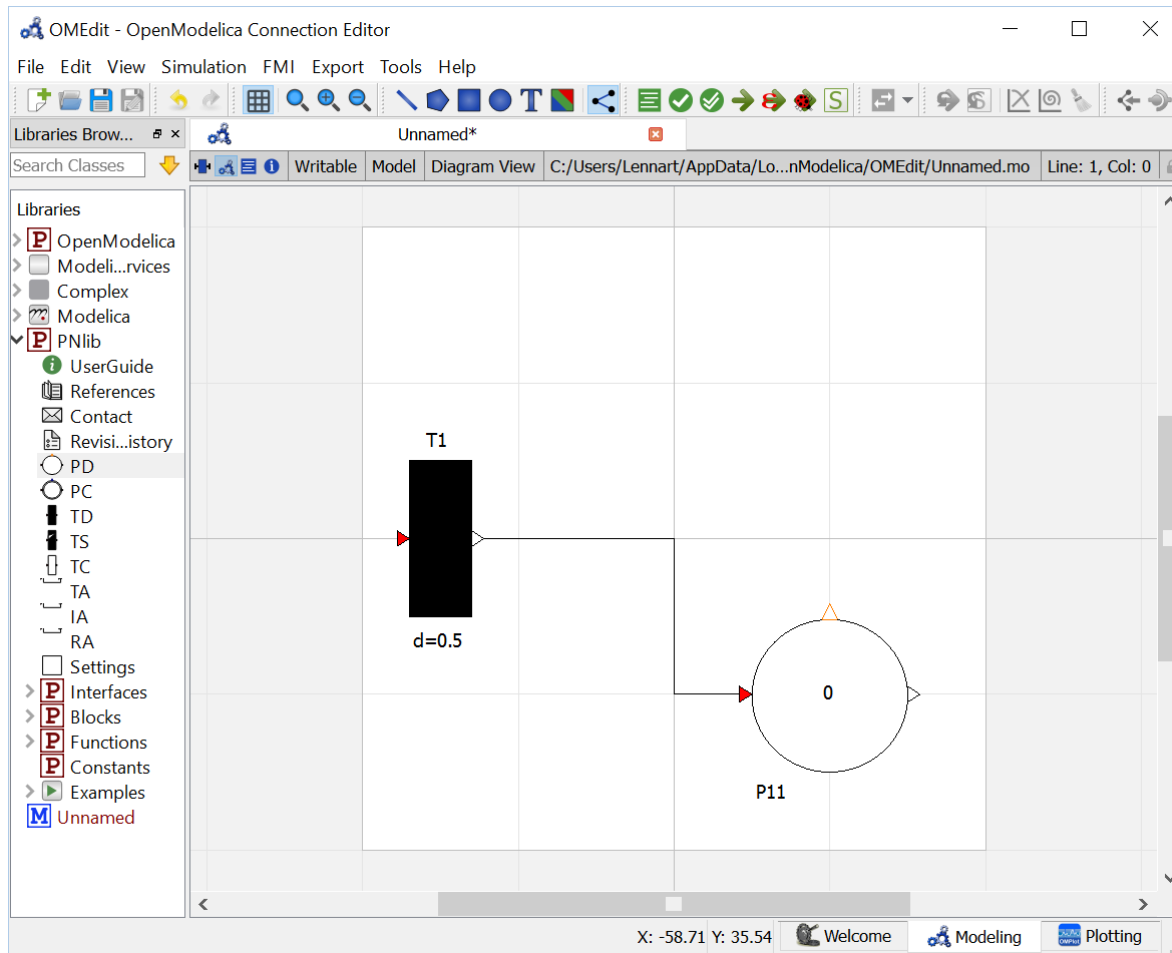


Why not just using OMEdit?



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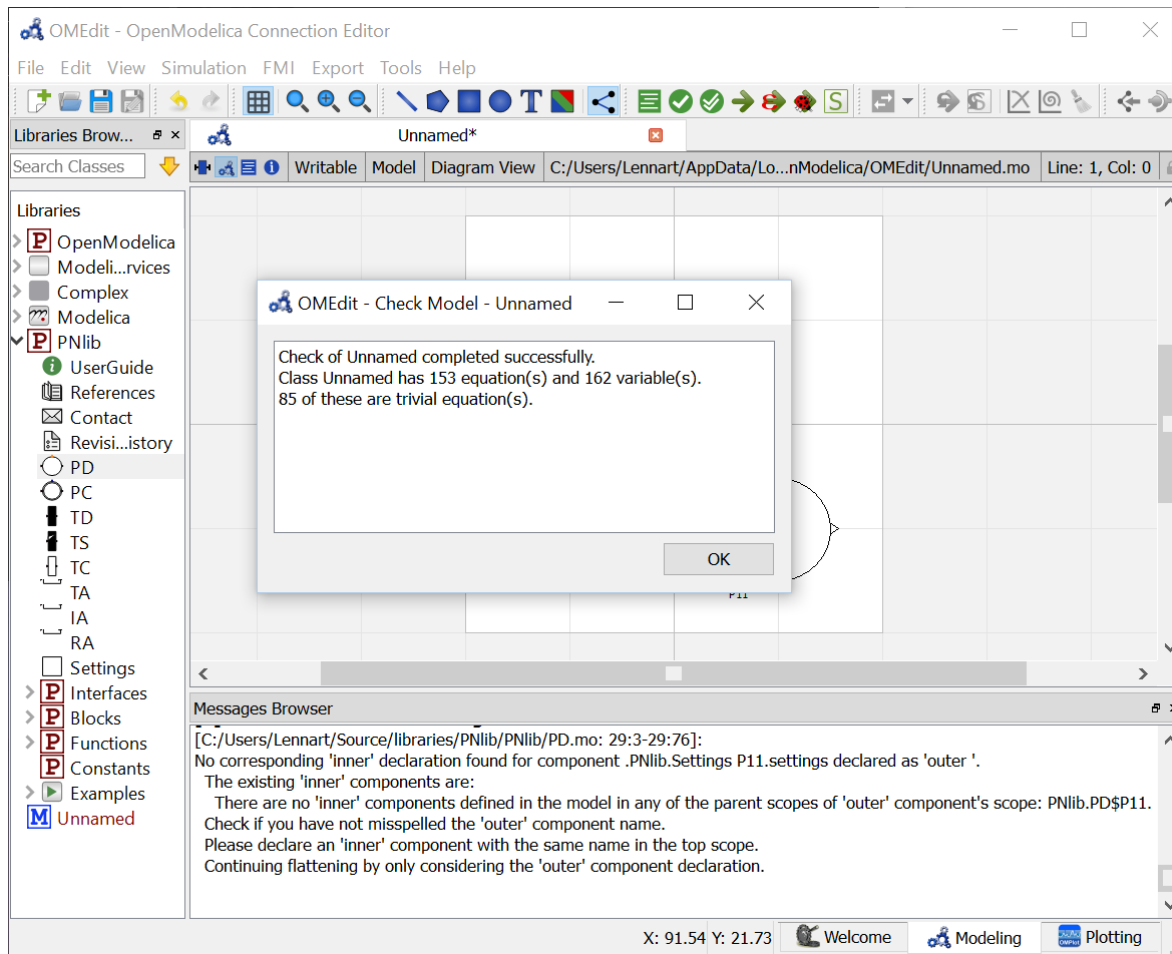
Problems occur once existing connections are changed/removed.



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After removing one of the places, the system becomes unbalanced without any helpful message.



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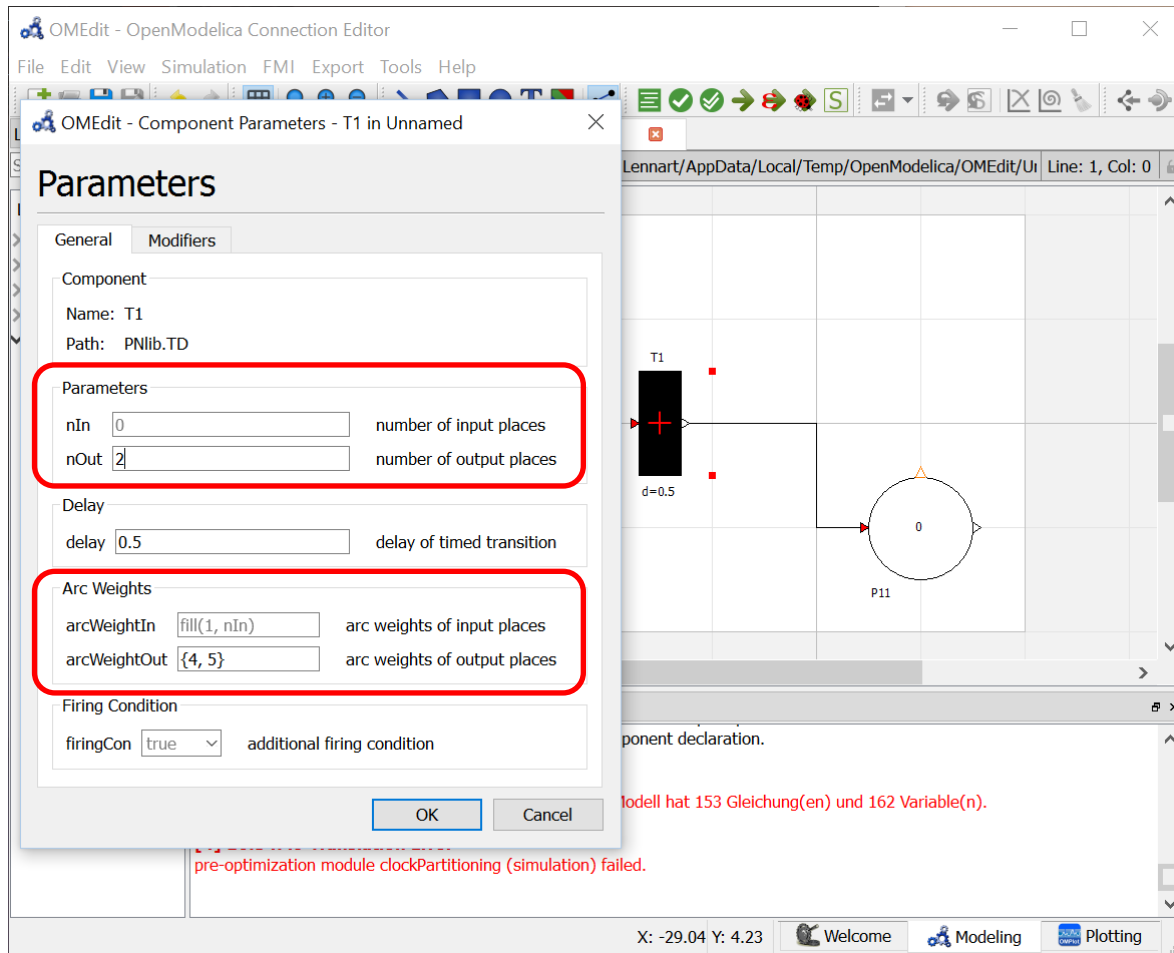
After removing one of the places, the system becomes unbalanced without any helpful message.

The screenshot shows the OMEdit - OpenModelica Connection Editor interface. The main window displays a Petri net diagram with a transition 'T1' (black rectangle) and a place 'P11' (circle). A line connects the output of T1 to the input of P11. The transition is labeled 'd=0.5'. The interface includes a menu bar (File, Edit, View, Simulation, FMI, Export, Tools, Help), a toolbar, a Libraries Browser on the left, and a Messages Browser at the bottom. The Messages Browser displays two error messages:

```
[3] 16:54:49 Symbolic Error
Zu wenige Gleichungen - unterbestimmtes System. Das Modell hat 153 Gleichung(en) und 162 Variable(n).

[4] 16:54:49 Translation Error
pre-optimization module clockPartitioning (simulation) failed.
```

Why not just using OMEdit?

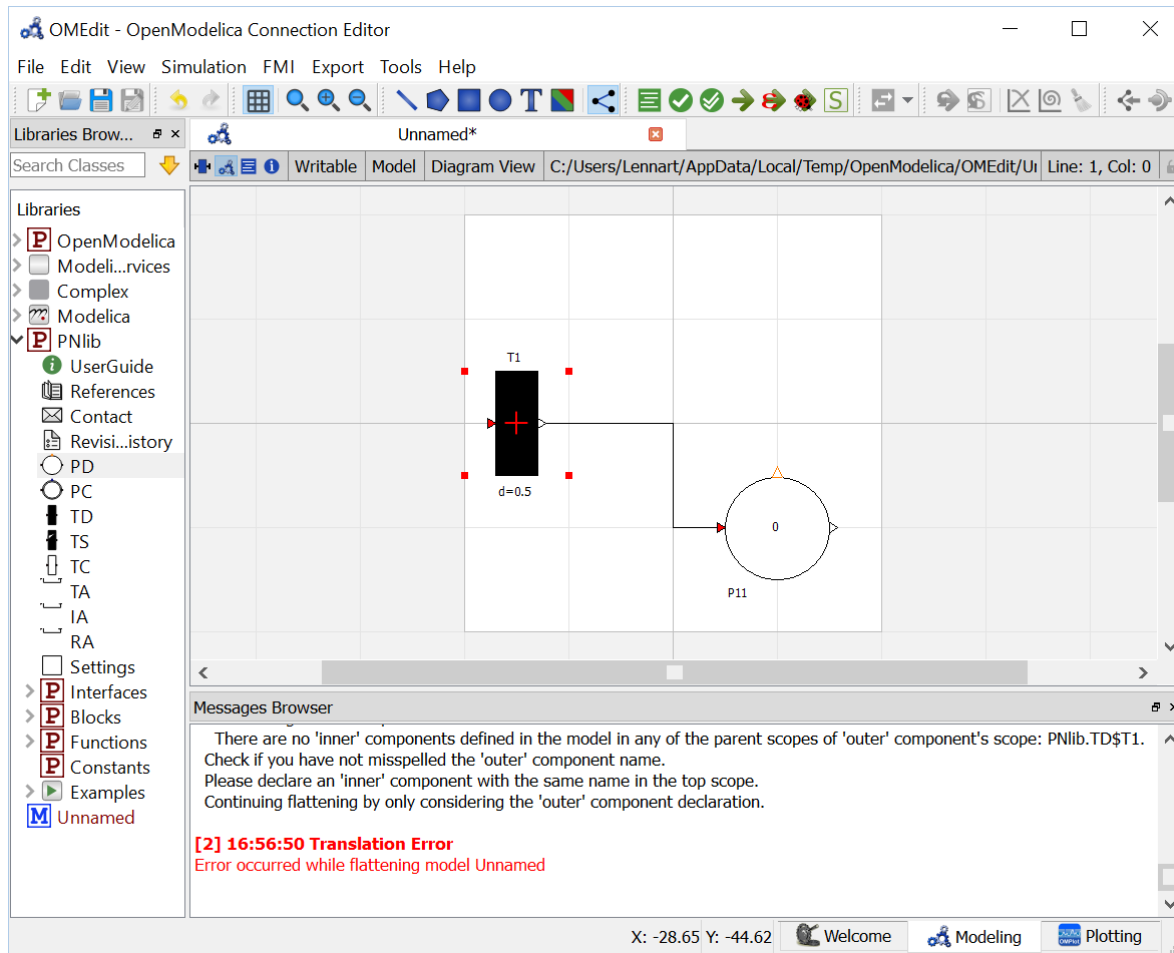


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After removing one of the places, the system becomes unbalanced without any helpful message.

Connector sizes and arc weights need to be adjusted manually.

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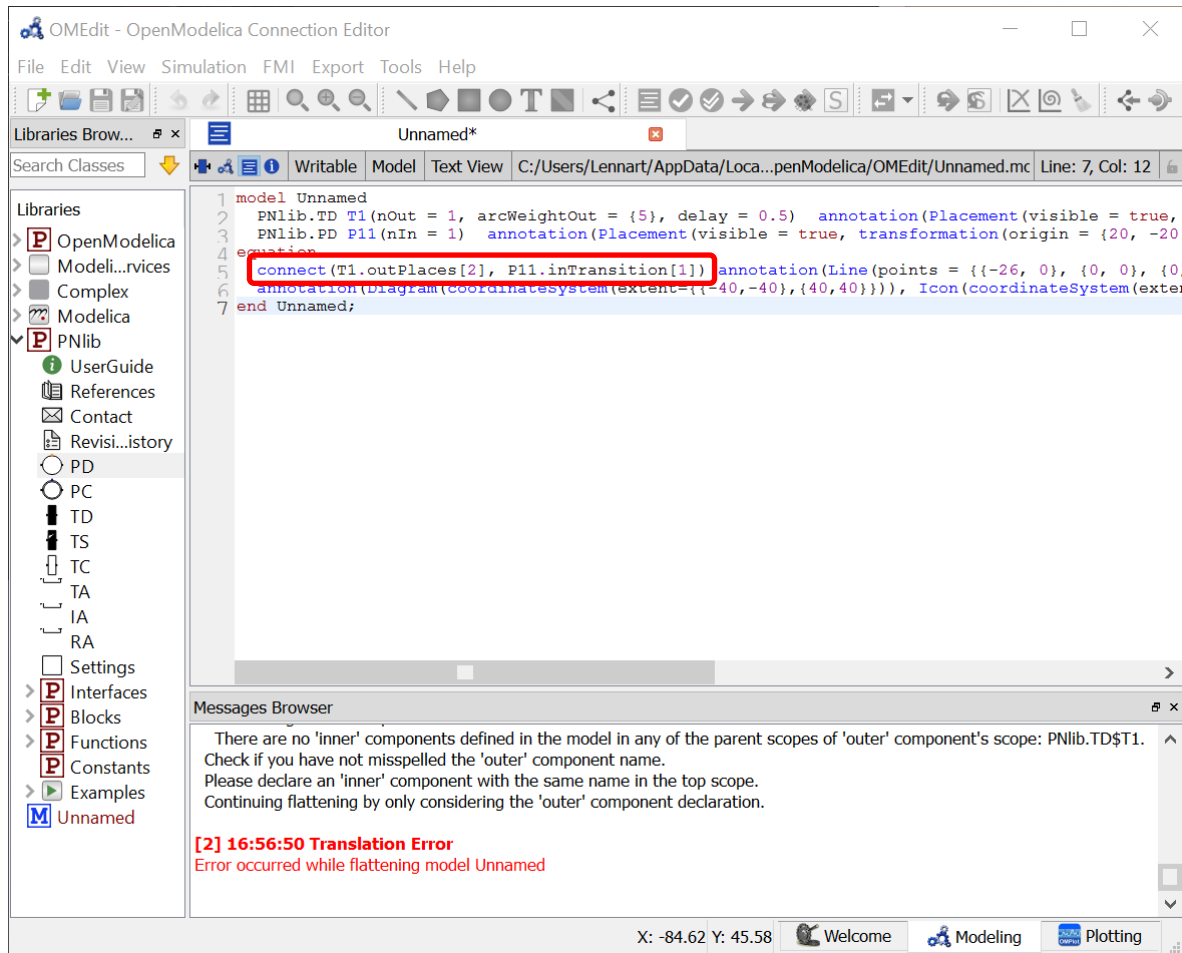
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The model still fails without any helpful notification.

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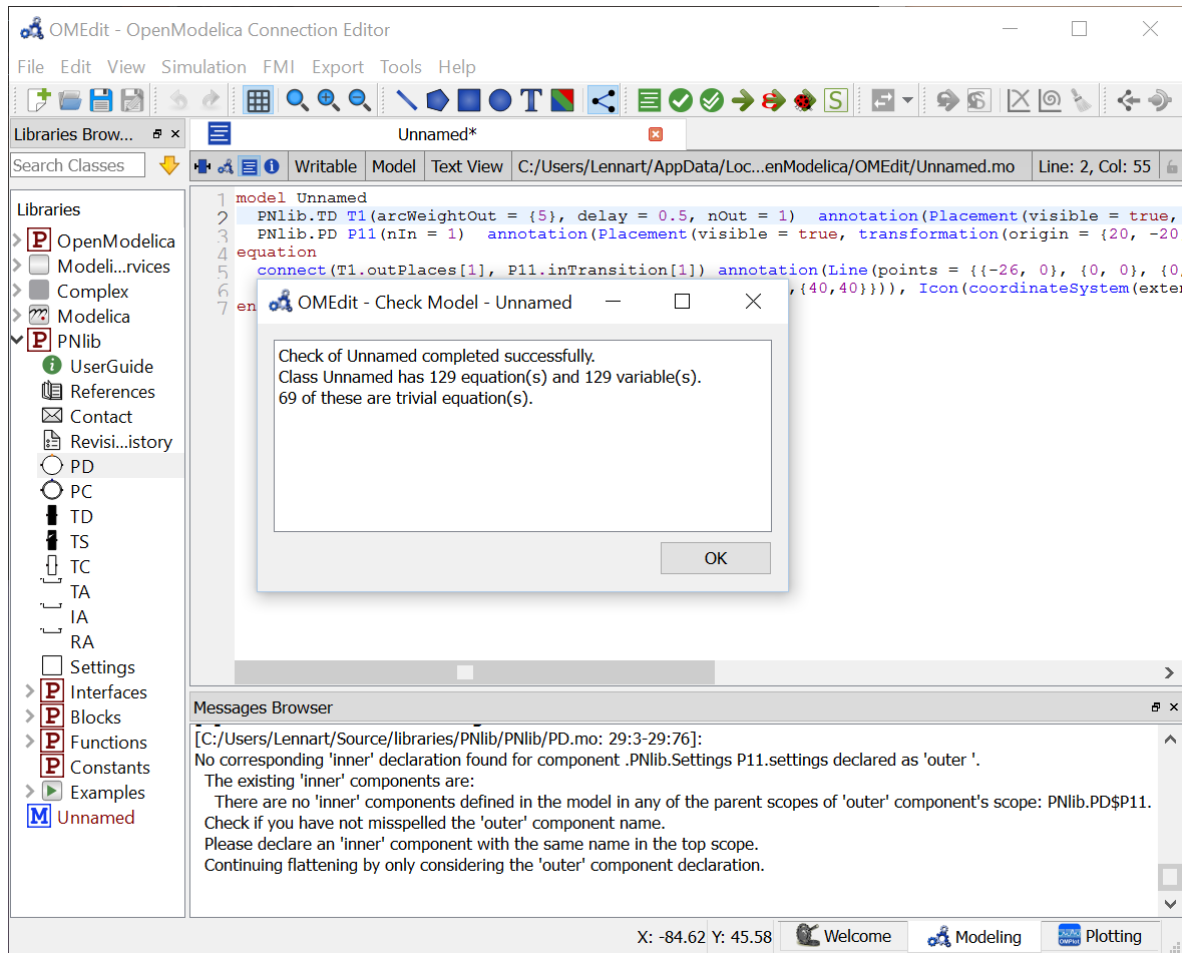
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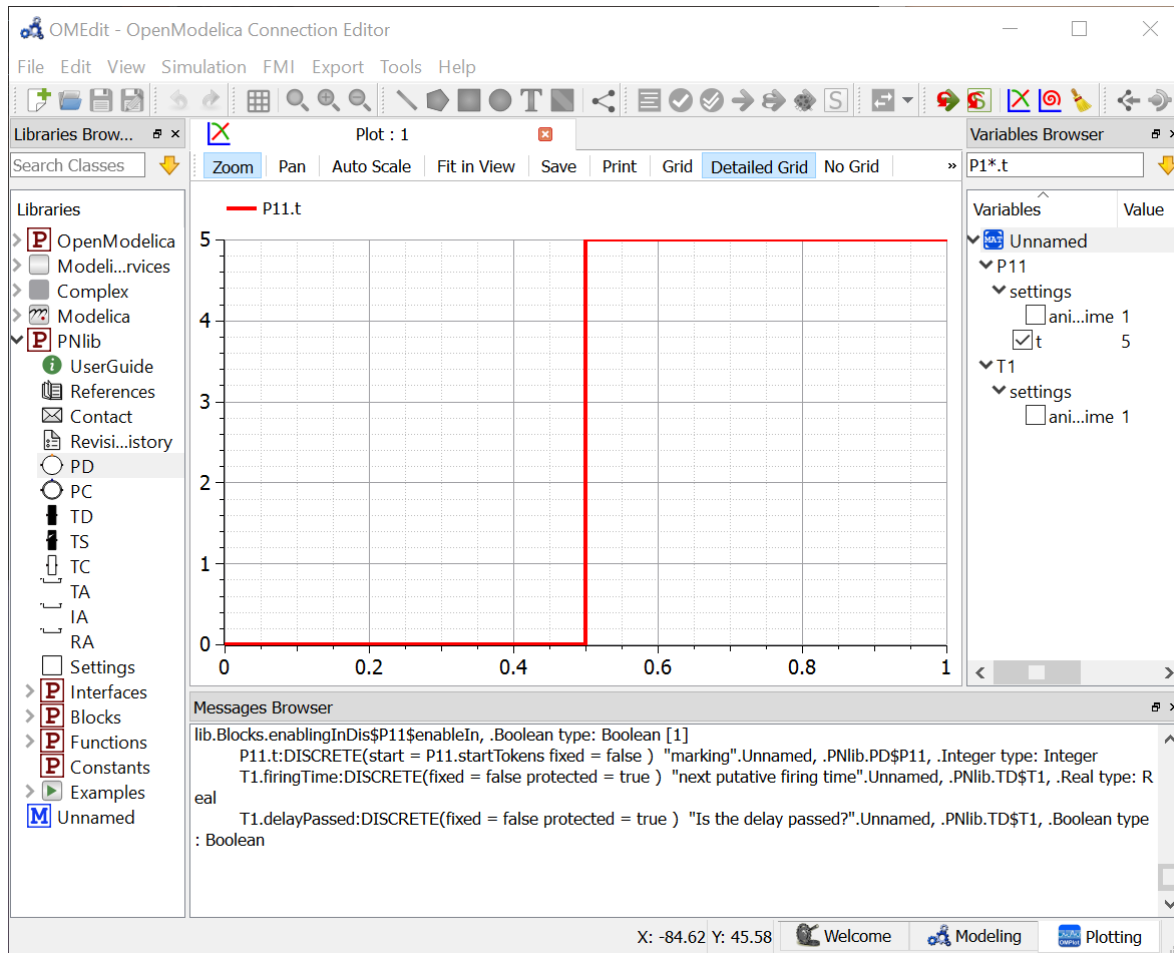
The model still fails without any helpful notification.

One need to modify the source code manually.

Why not just using OMEdit?

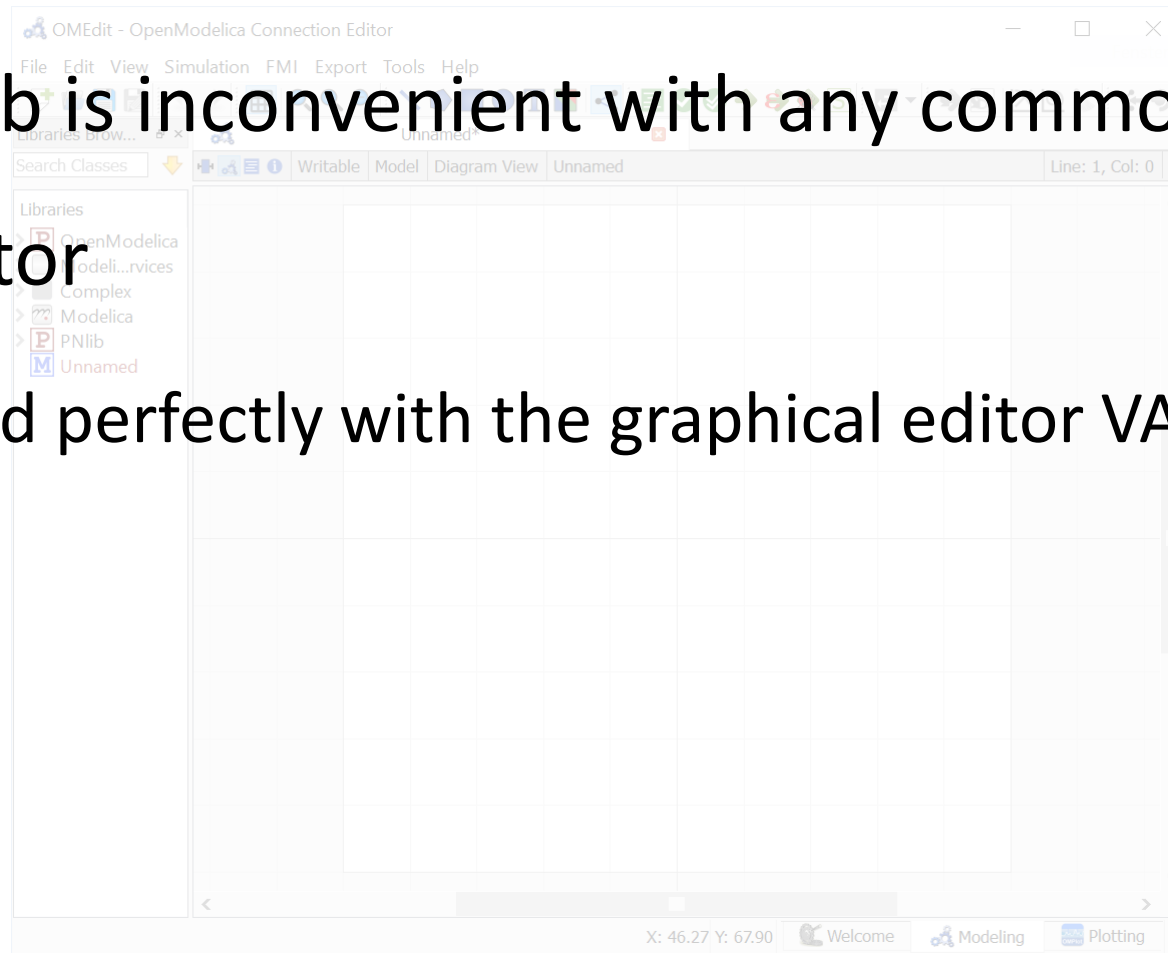


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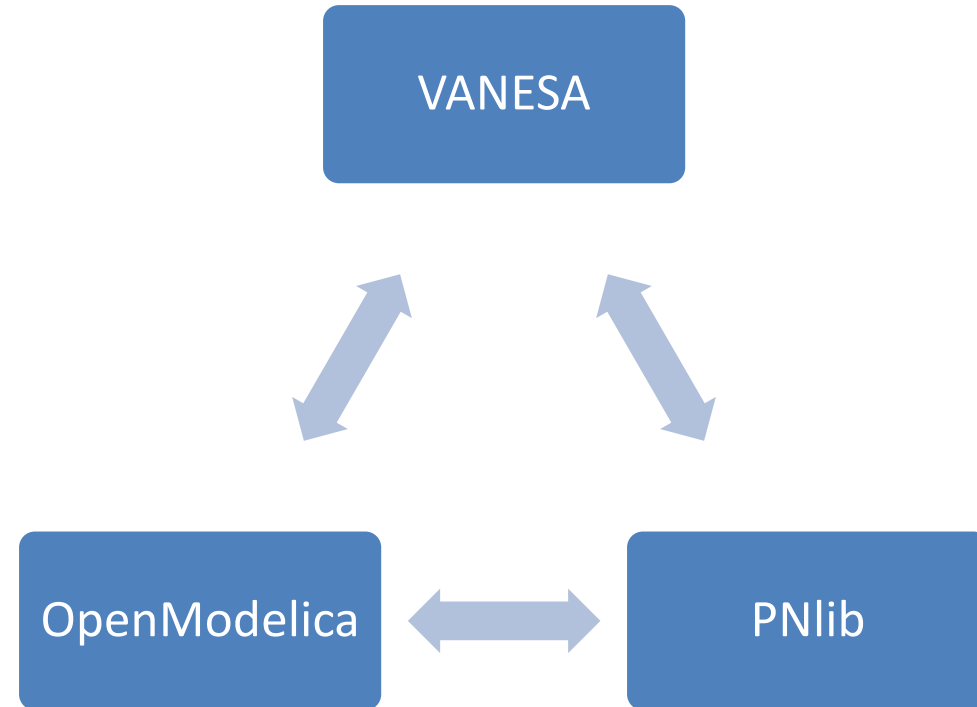
Why not just using OMEdit?

- Usage of PNlib is inconvenient with any common graphical Modelica editor
 - This is solved perfectly with the graphical editor VANESA!



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Summary

- VANESA is network editor for biological use cases
- VANESA can be used as graphical Petri net editor
- PNlib is updated to latest Modelica version
- OpenModelica fully supports PNlib

Wish list/Next steps

- Export Modelica models with graphical annotation
- Extract pure Petri net editor from VANESA
- More comprehensive PNlib coverage testing (e.g. hybrid Petri nets)
- Improve OpenModelica performance – as always