On the interaction of VANESA, PNlib, and OpenModelica

Lennart Ochel[1,2] and Christoph Brinkrolf[2]

[1]Department of Applied Mathematics, University of Applied Sciences Bielefeld
[2]Bioinformatics Department, Faculty of Technology, Bielefeld University

MoRitS is a cooperation between:

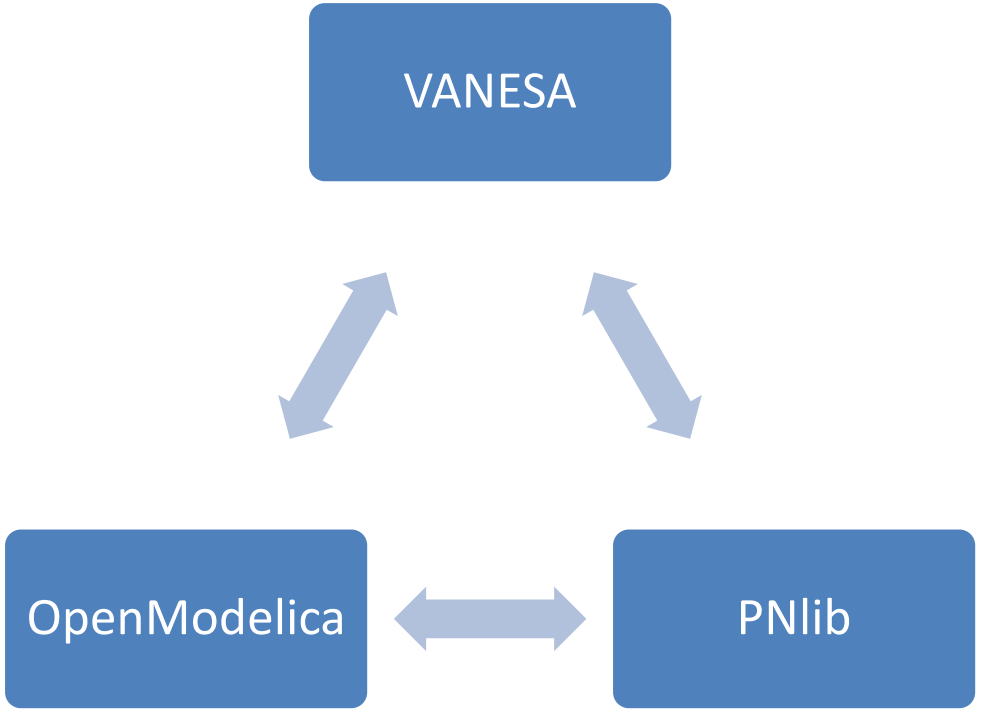
FH Bielefeld
University of
Applied Sciences

With the support of:

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

Outline

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



VANESA in a Nutshell

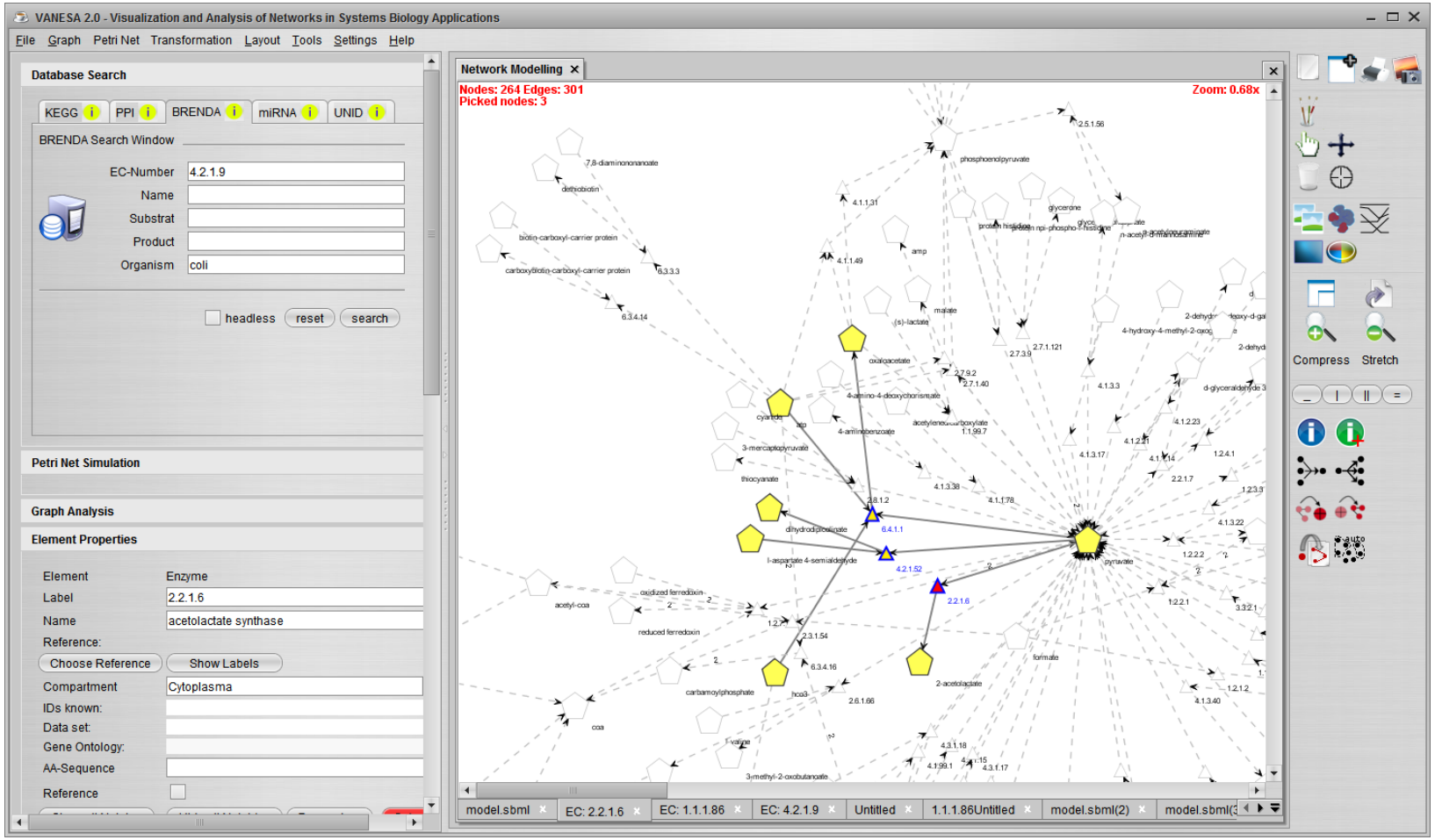
- Department of Bioinformatics (Prof. Hofestädt), Bielefeld University
- Development since 2009
- Graph-based editor for Systems biology applications
  - Modeling of Cell-to-Cell Communication Processes with Petri Nets Using the Example of Quorum Sensing
  - Hydrogen production in *Chlamydomonas reinhardtii*
- 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

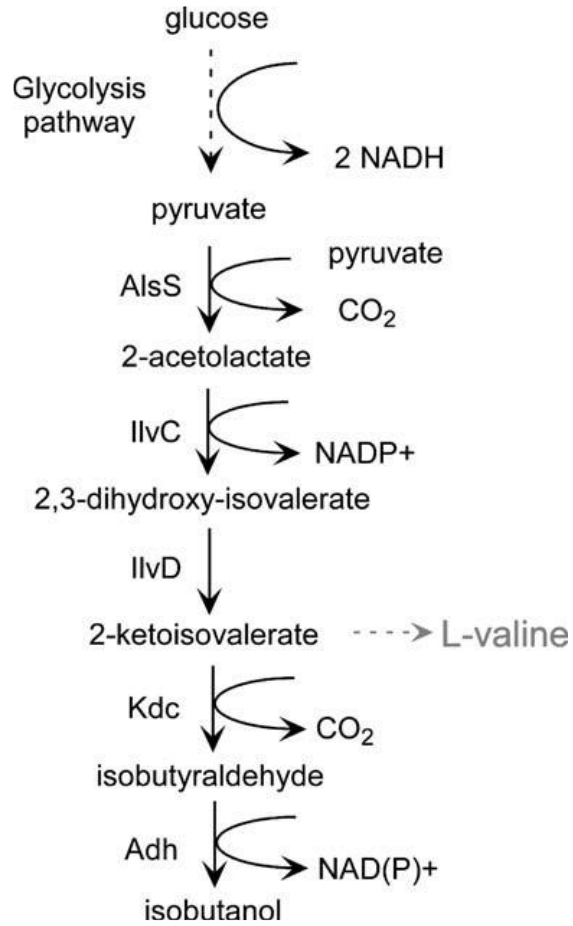
- Simulation of biological systems using Petri nets
  - Biological network → Petri net → Modelica model
- Visualizing of simulation results
  - On-the-fly
  - Tokens, token flow, firing speed mapped on nodes and edges
- Applying algorithms on networks
  - Discrete PN: reachability and coverability
 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

VANESA in a Nutshell



VANESA: Introductory Example

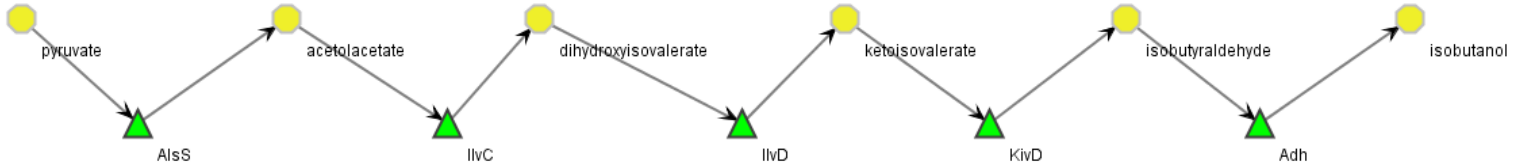
- Production of isobutanol in *Escherichia coli*
  - Isobutanol is renewable bio fuel
- Database connection
  - Exploration of pathways
  - Database-supported modeling of pathways
- Network simulation
  - Automatic transformation to Petri net formalism
  - Modelica-based simulation



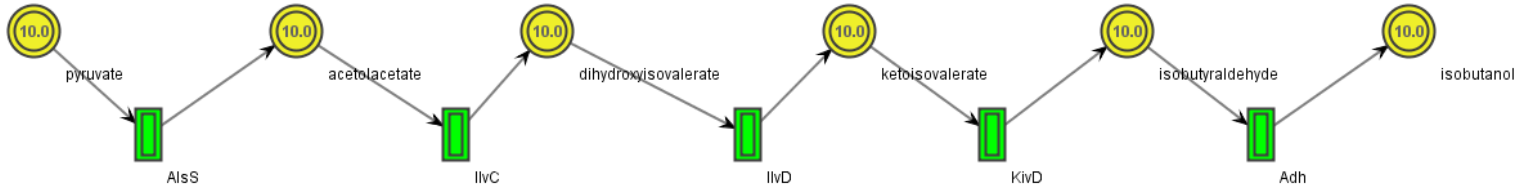
VANESA: Introductory Example

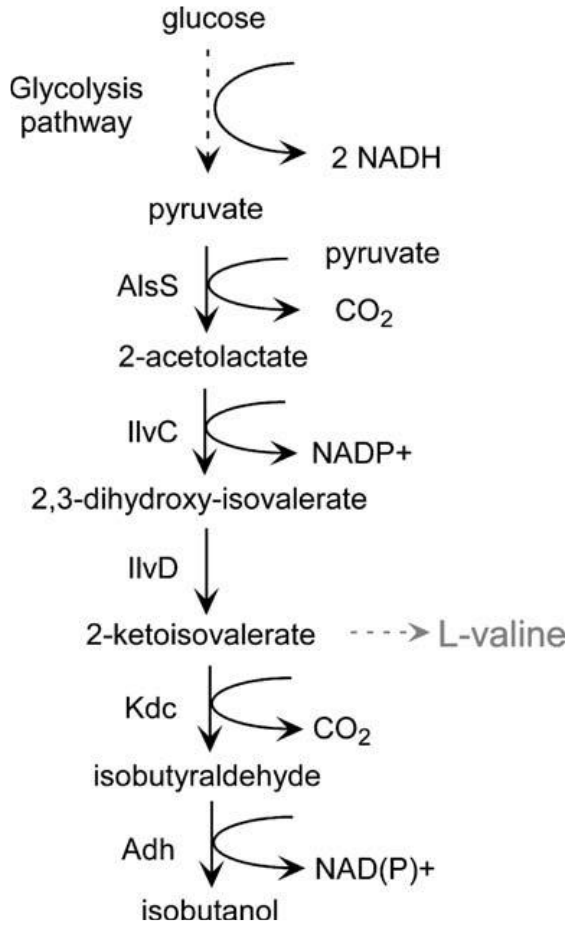
- Production of isobutanol in *Escherichia coli*

Biological network



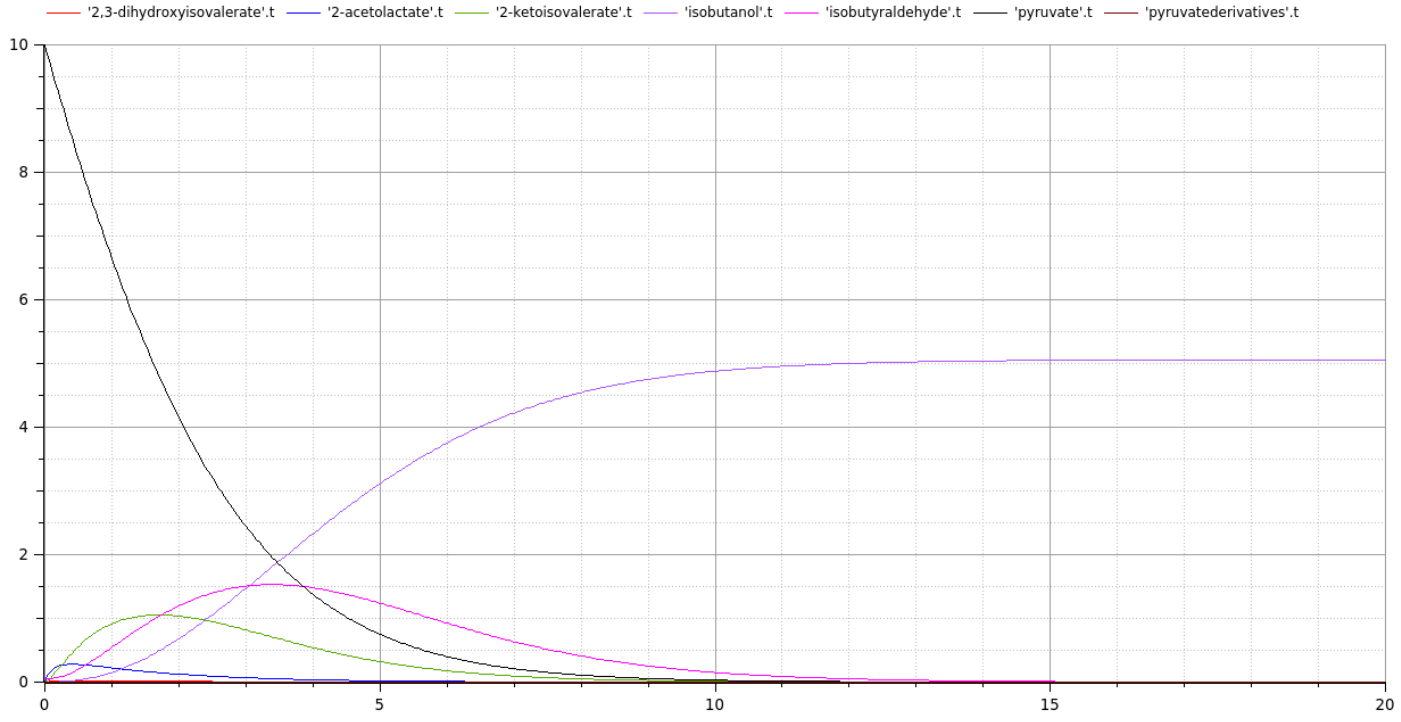
Petri net

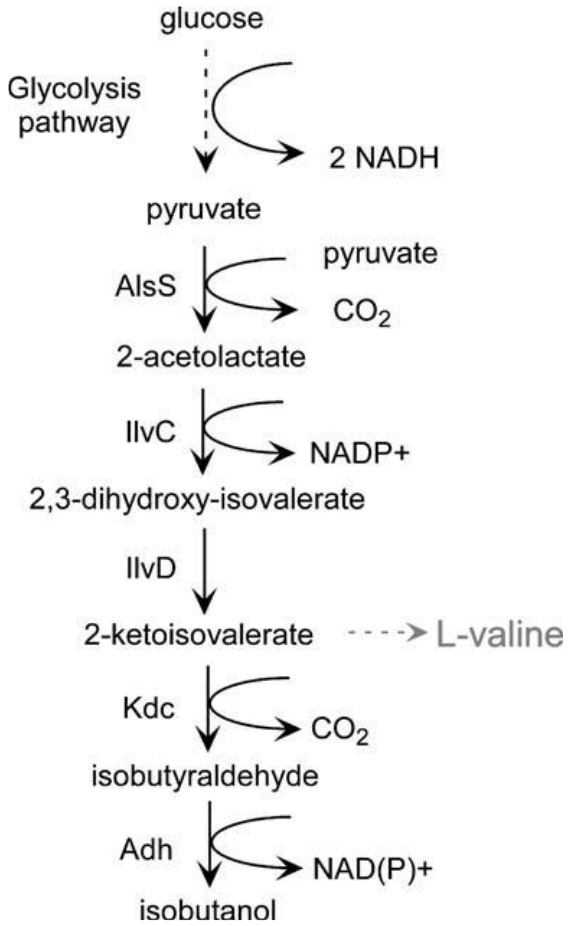




VANESA: Introductory Example

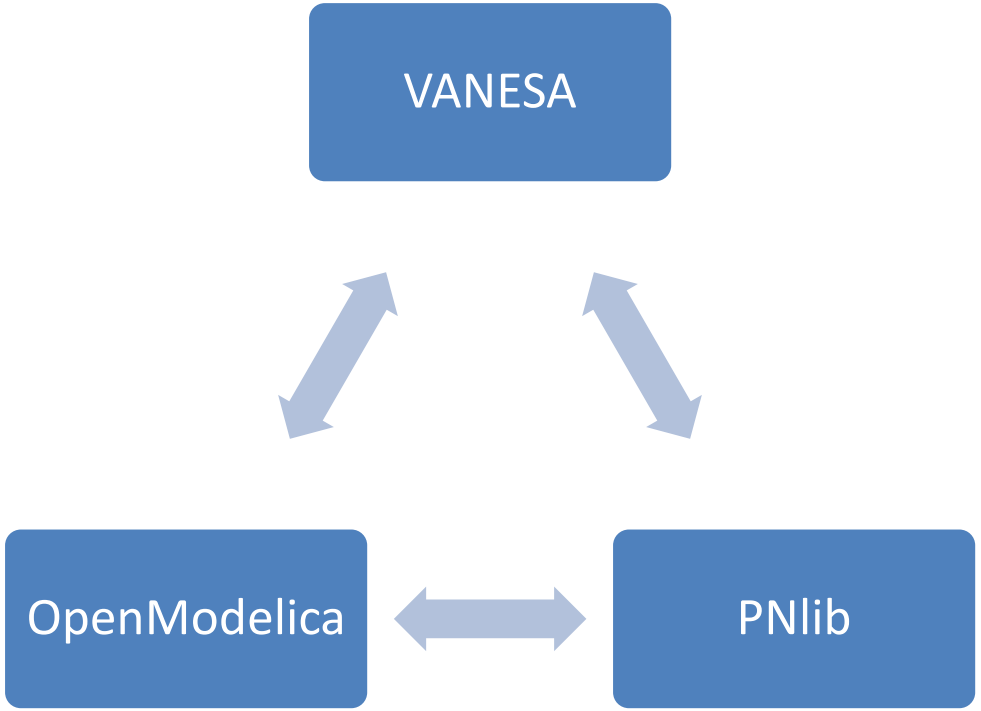
- Production of isobutanol in *Escherichia coli*





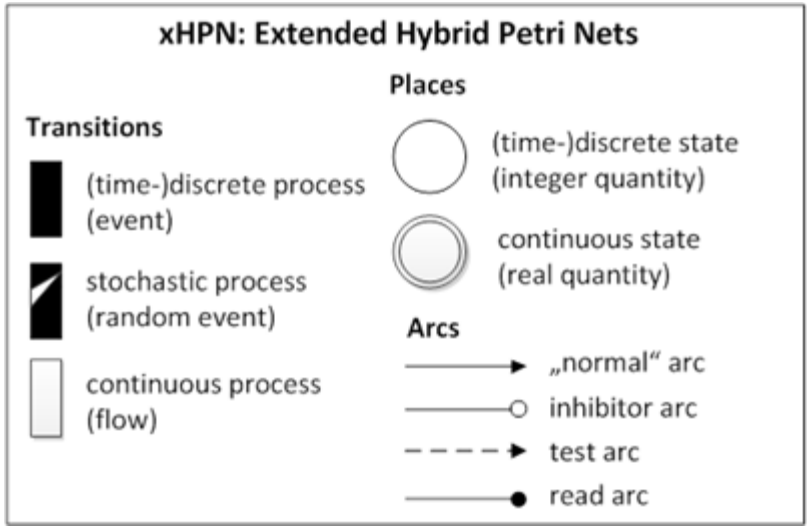
Outline

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



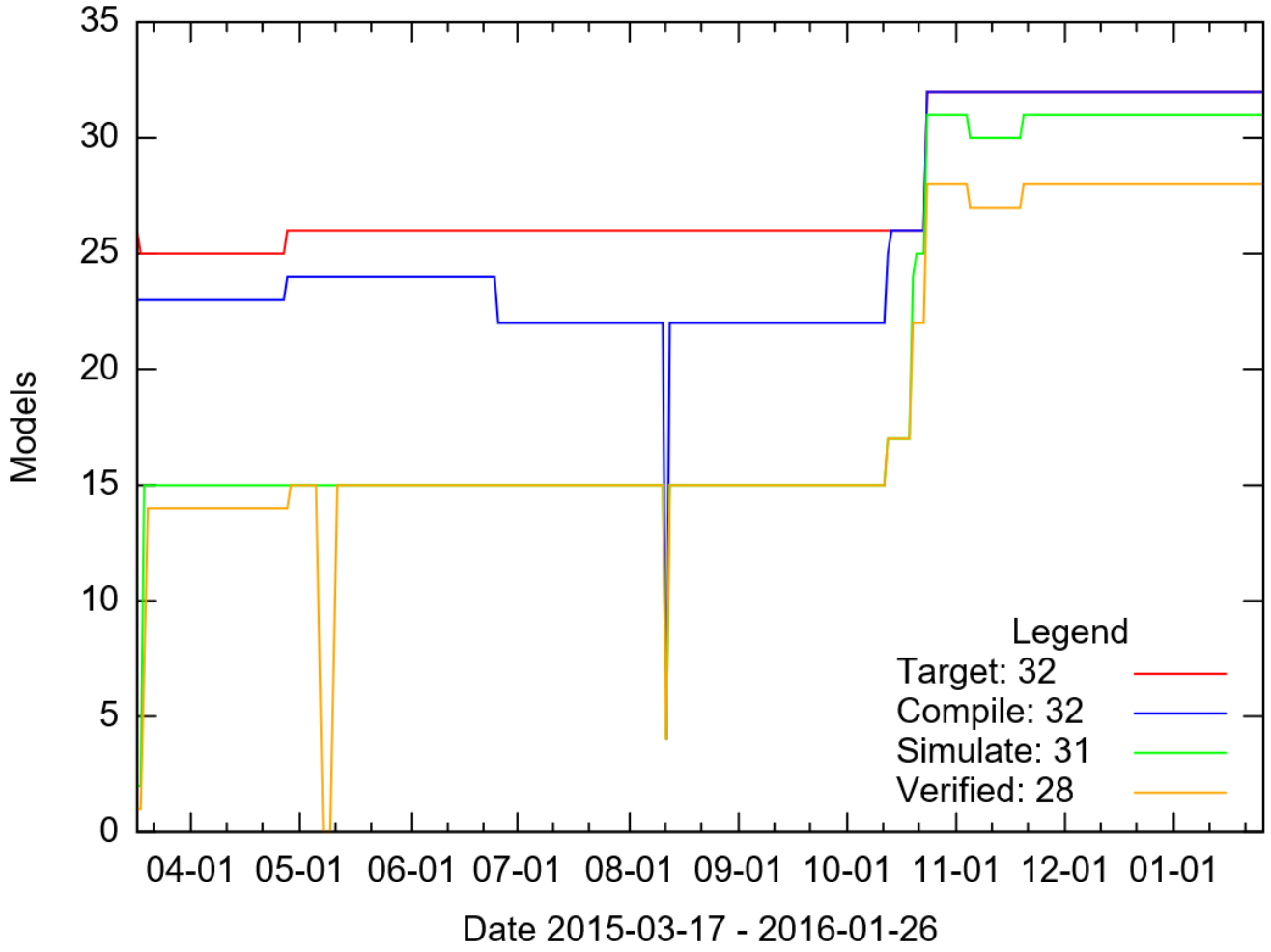
PNlib

- 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



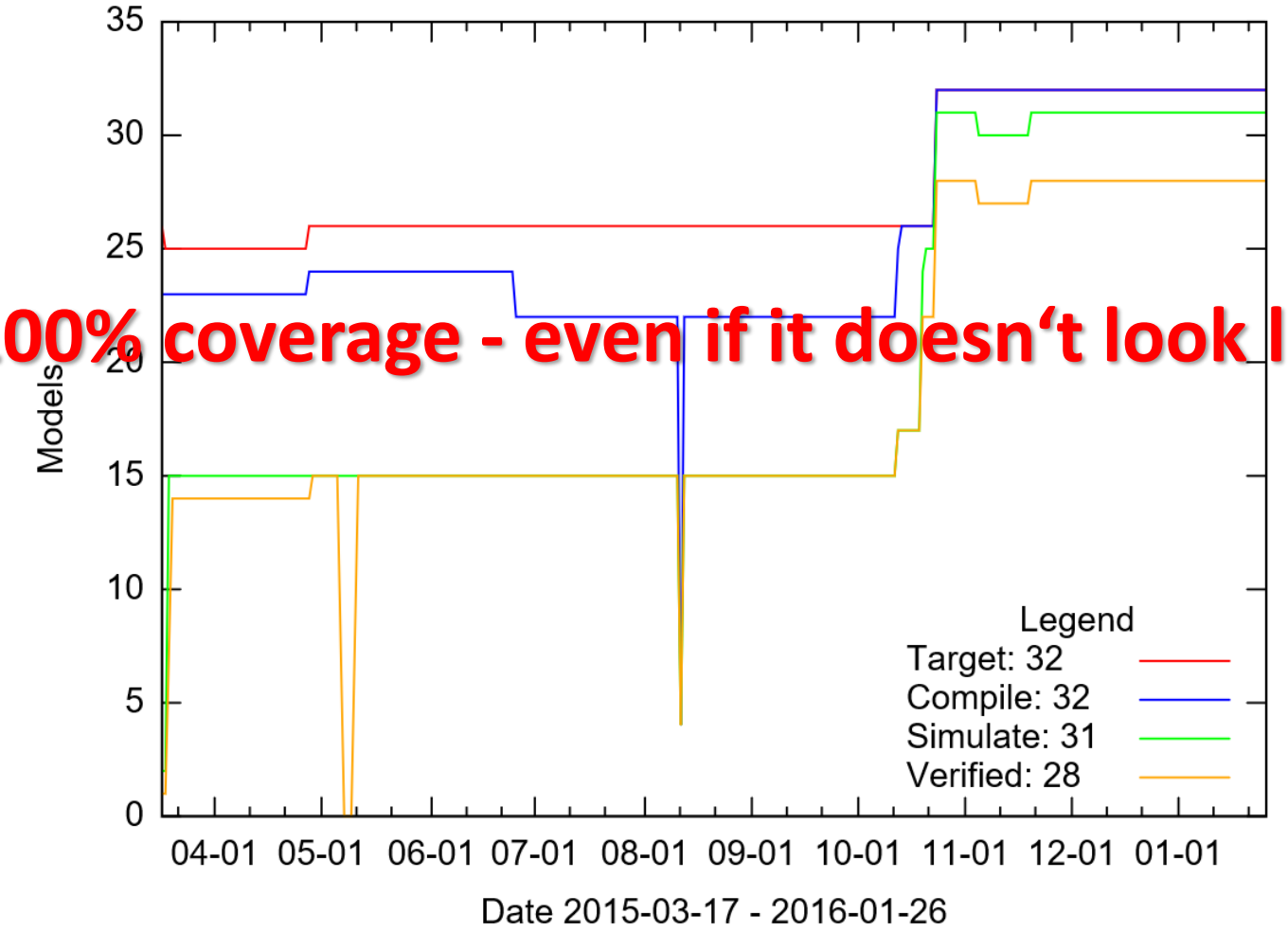
→ https://github.com/modelica-3rdparty/PNlib

OpenModelica - PNlib Coverage Trend



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

OpenModelica - PNlib Coverage Trend

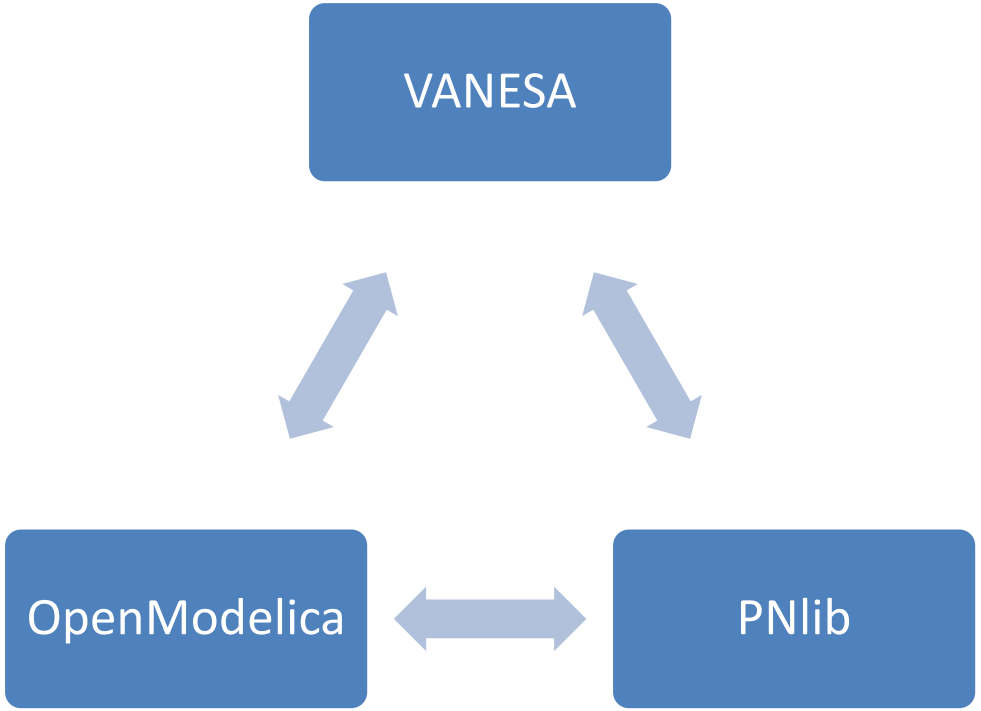


100% coverage - even if it doesn‘t look like

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

Outline

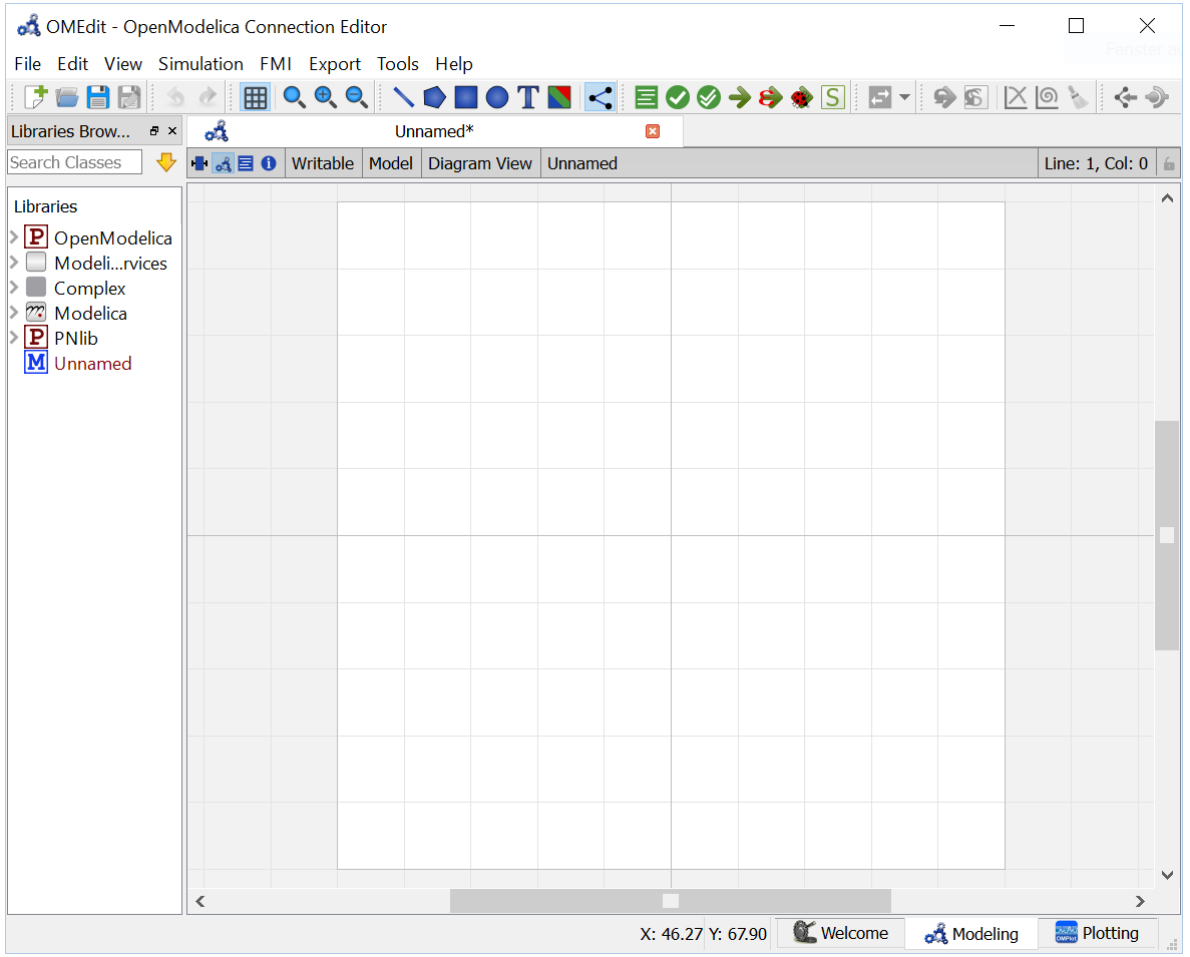
- VANESA
- PNlib
- **OpenModelica**
- Summary



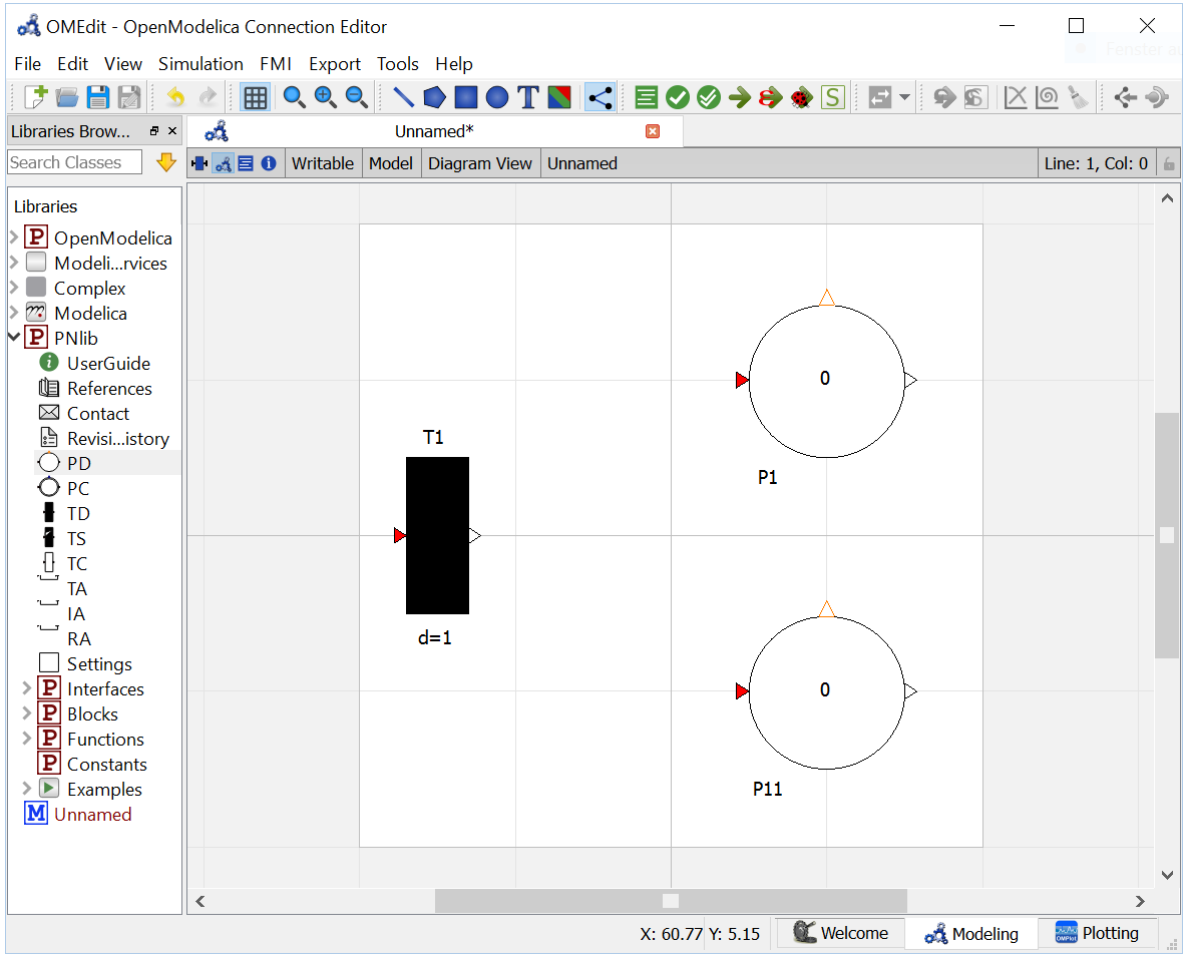
OpenModelica

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

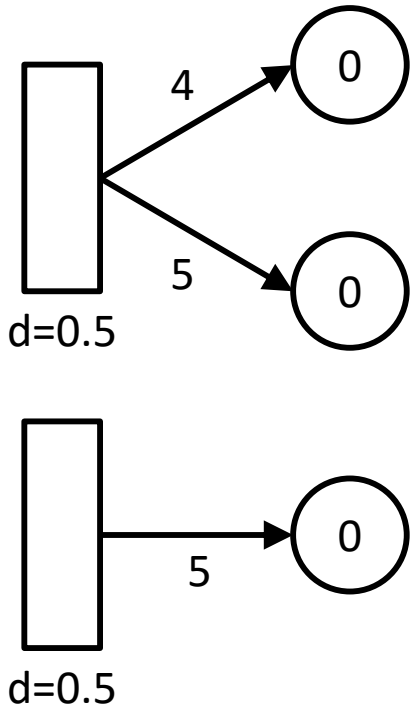
Why not just using OMEdit?



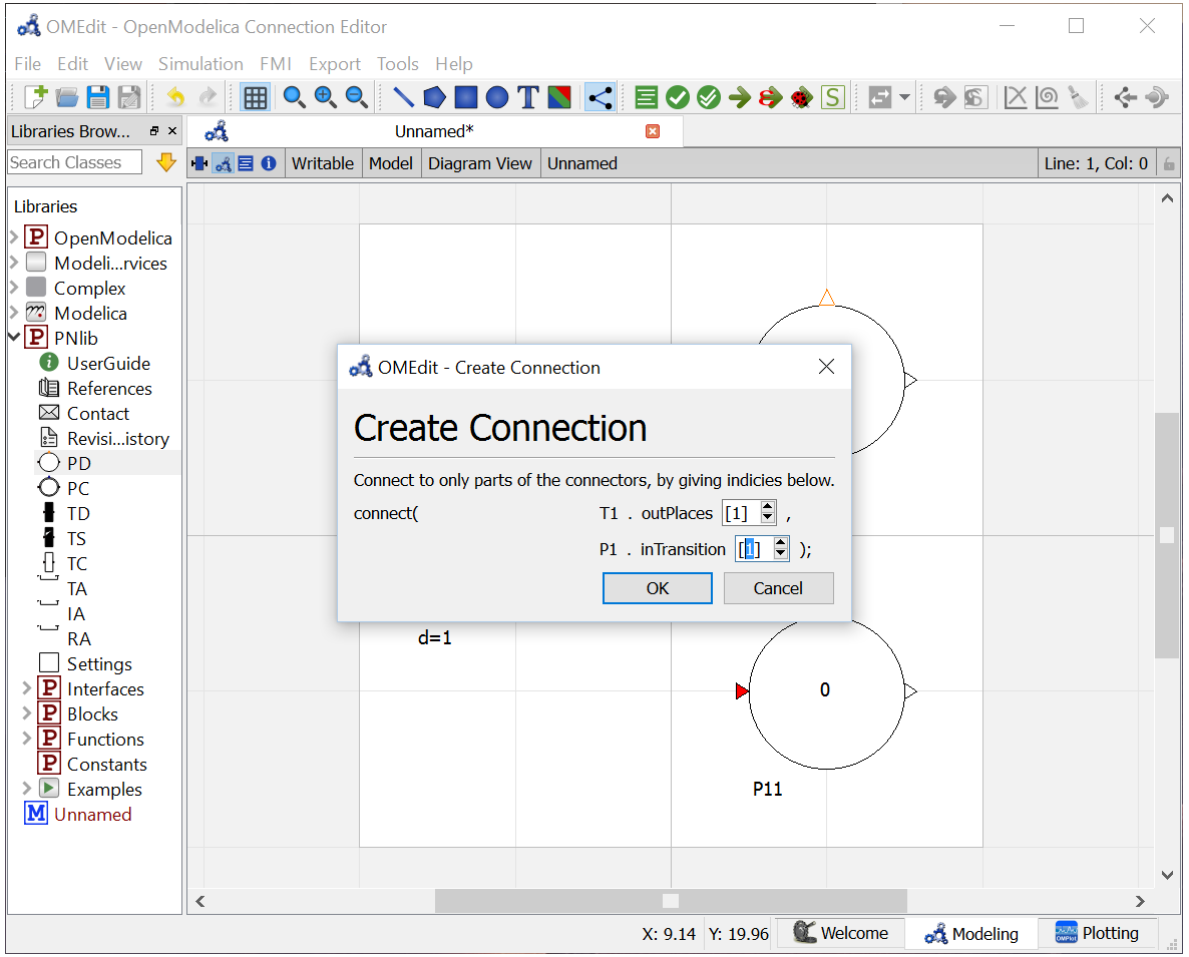
Why not just using OMEdit?



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

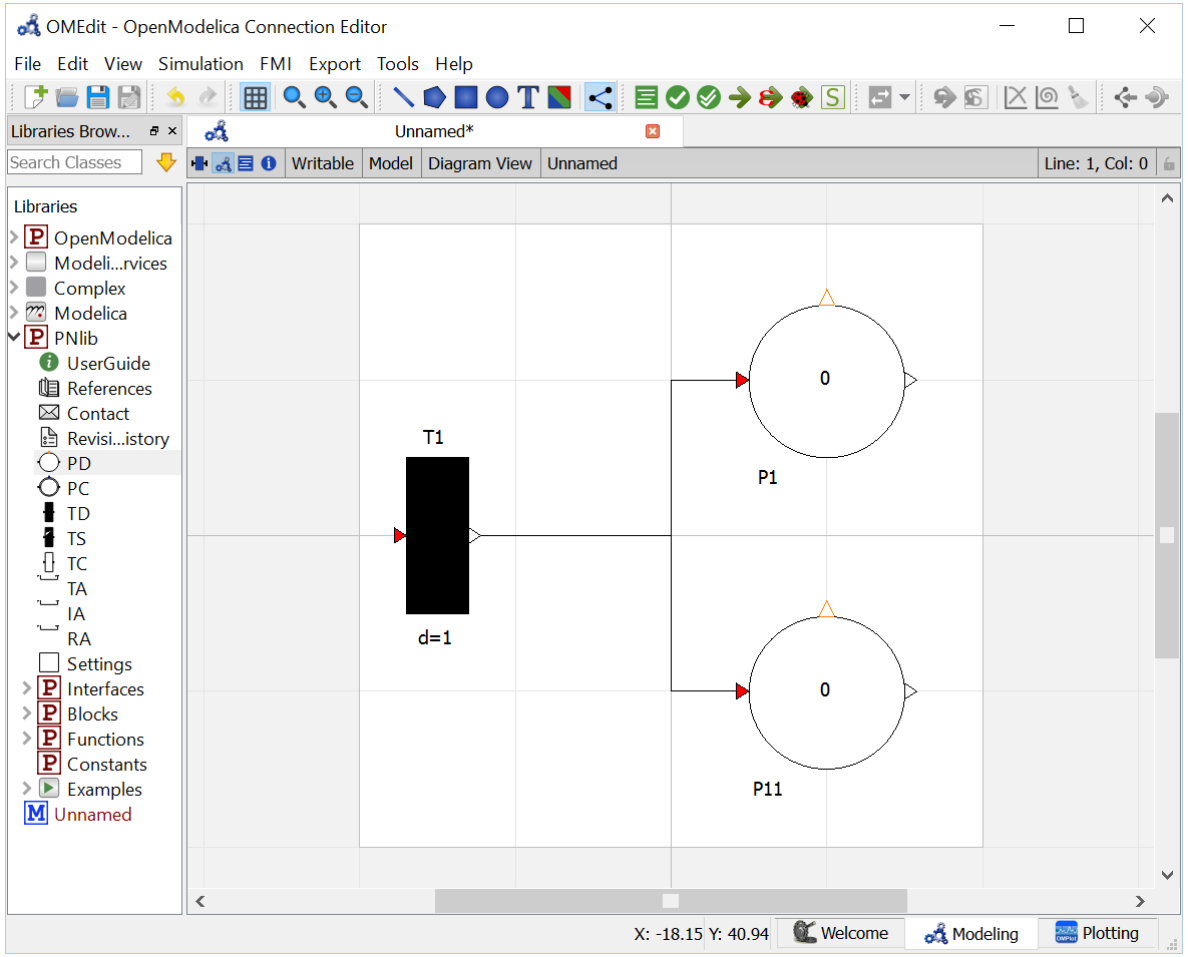


Why not just using OMEdit?



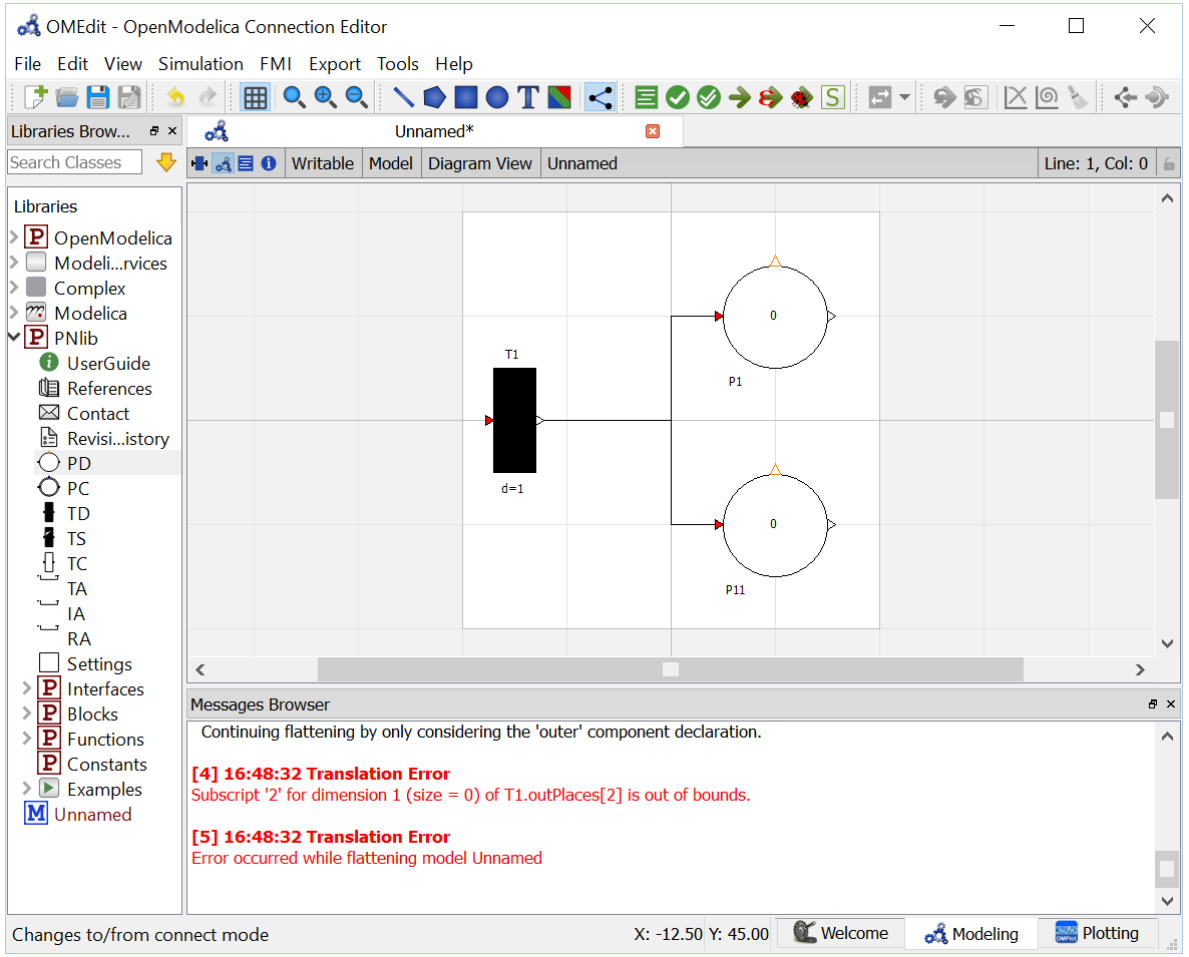
Places/Transitions are using array connectors.

Why not just using OMEdit?



Places/Transitions are using array connectors.

Why not just using OMEdit?

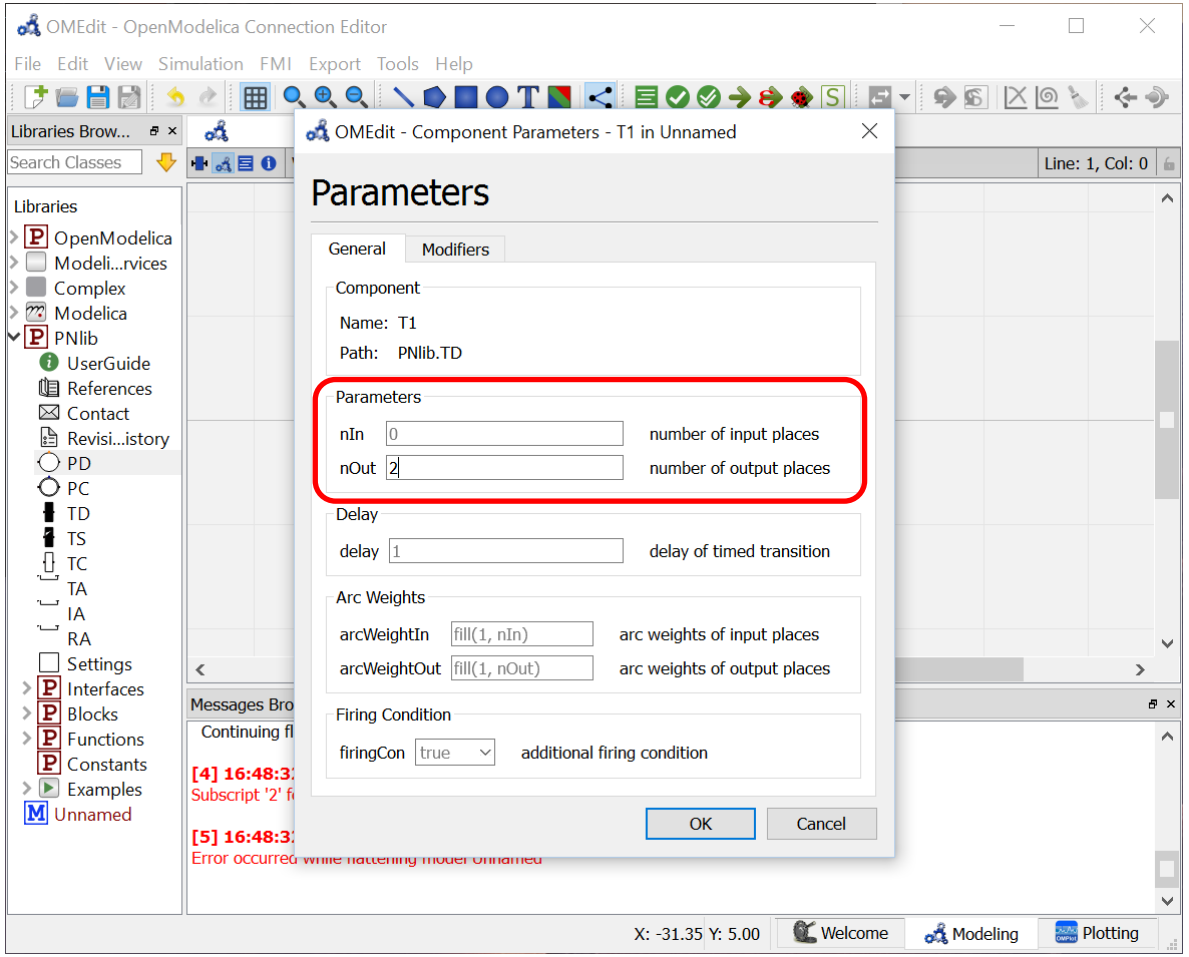


Places/Transitions are using array connectors.

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

OpenModelica compiler generates useful error messages.

Why not just using OMEdit?

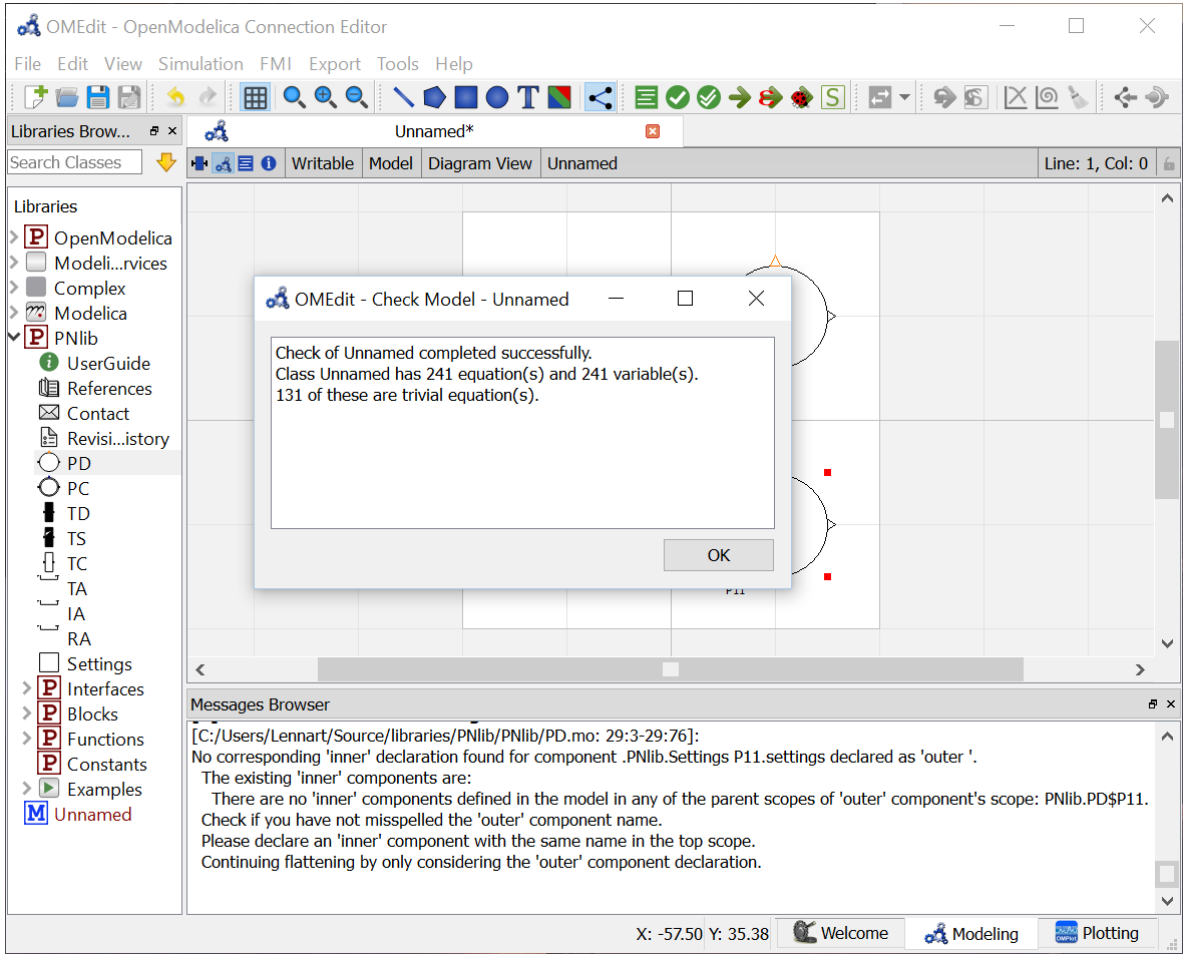


Places/Transitions are using array connectors.

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

Connector sizes need to be set manually.

Why not just using OMEdit?

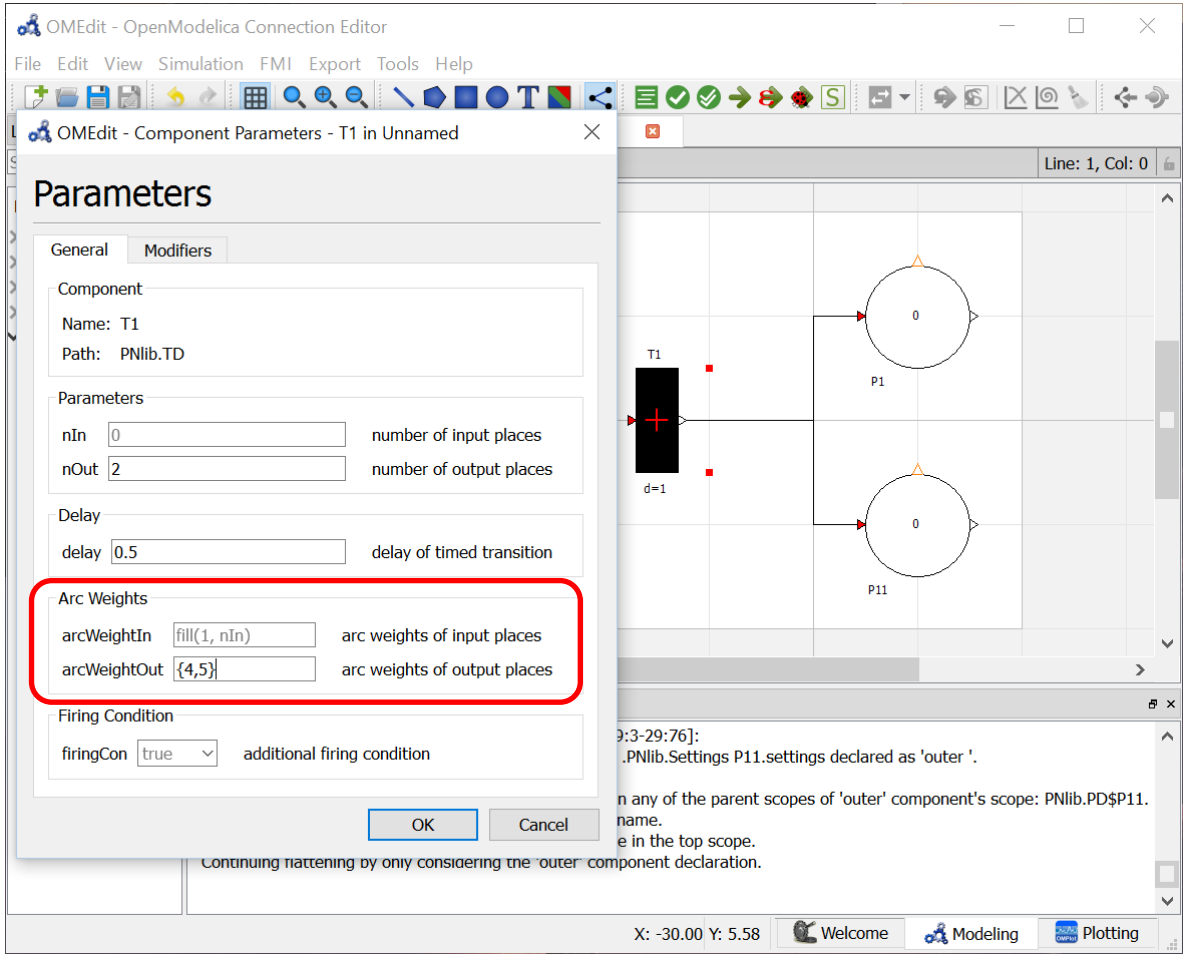


Places/Transitions are using array connectors

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

Connector sizes need to be set manually.

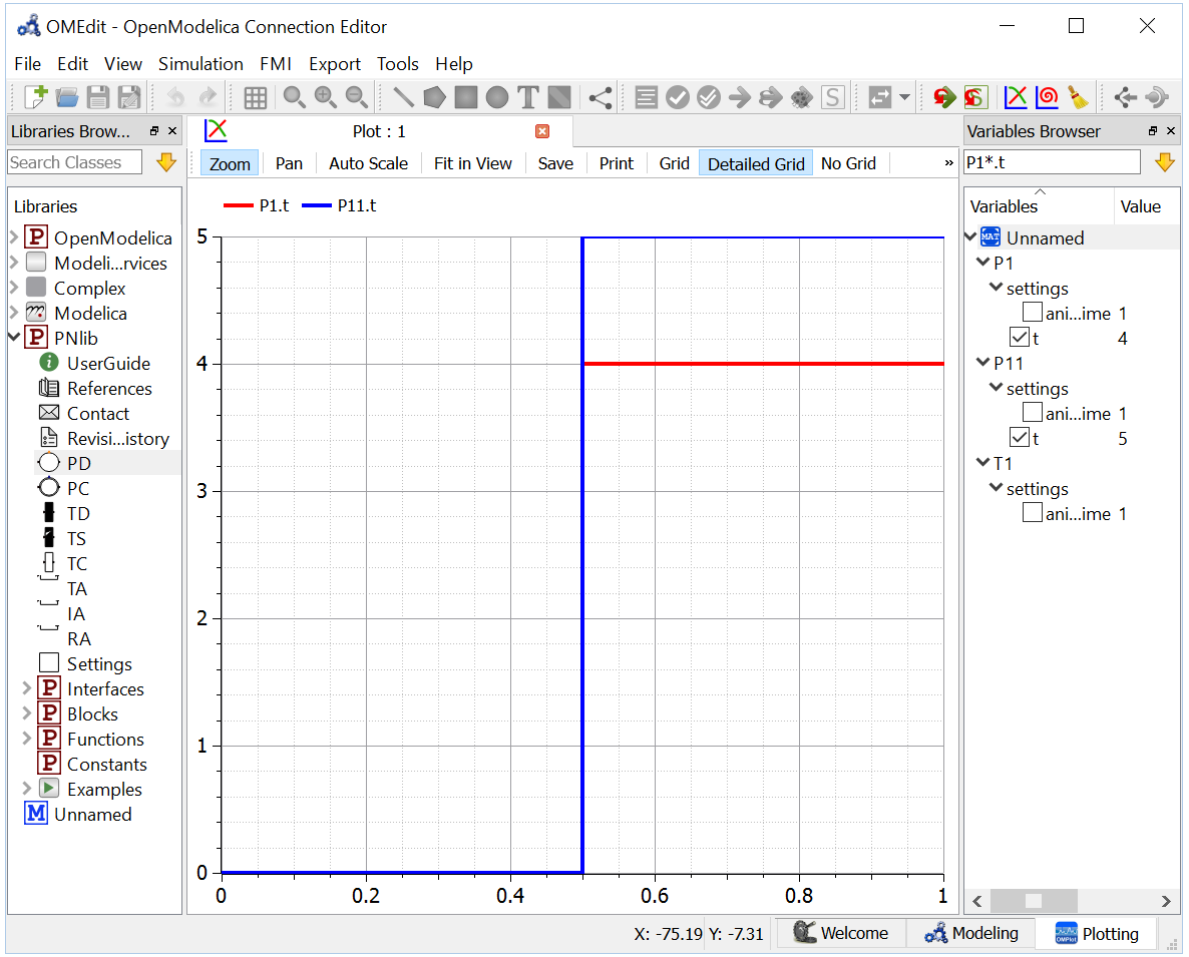
Why not just using OMEdit?



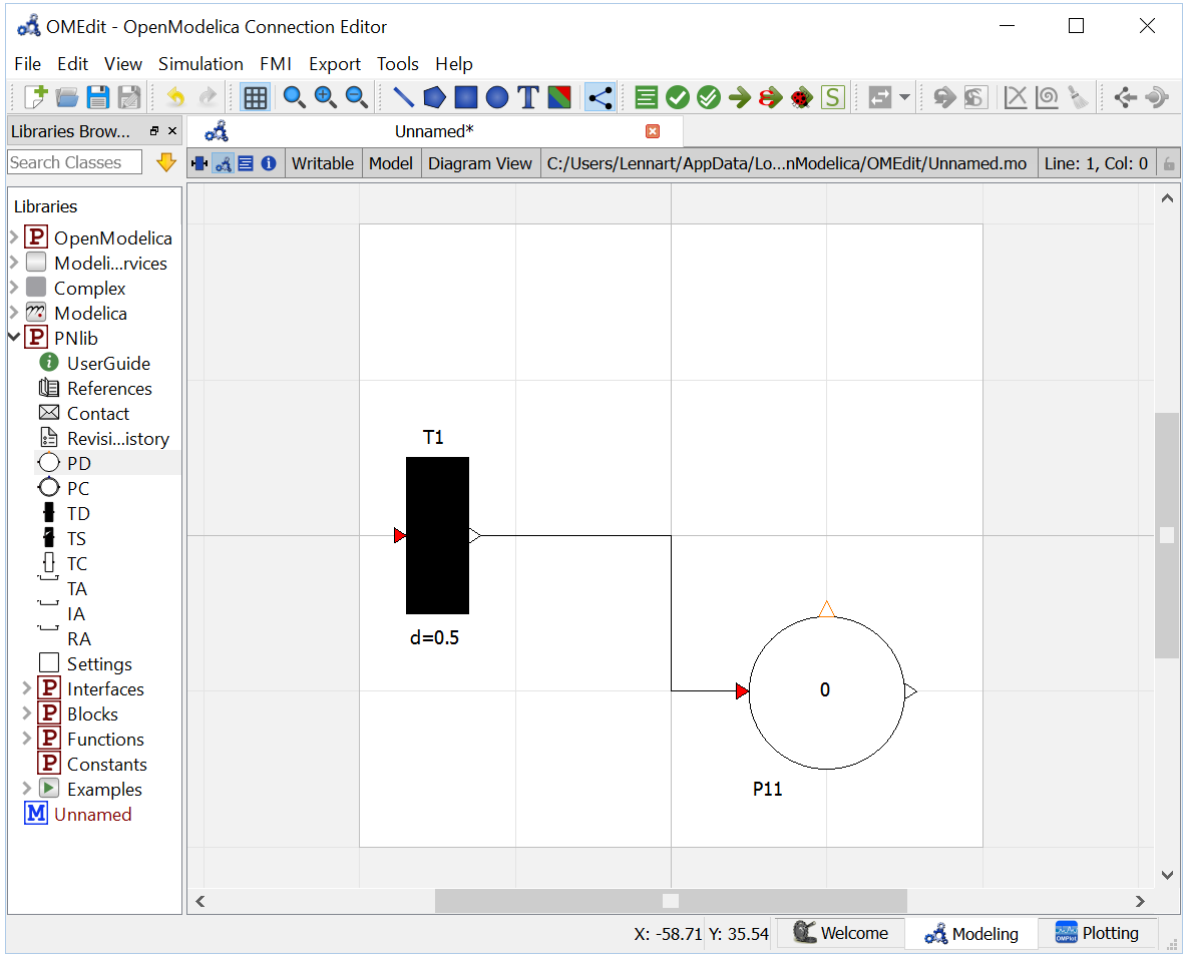
Arc weights are stored within transitions.

Arc weights are mapped on corresponding connector array.

Why not just using OMEdit?

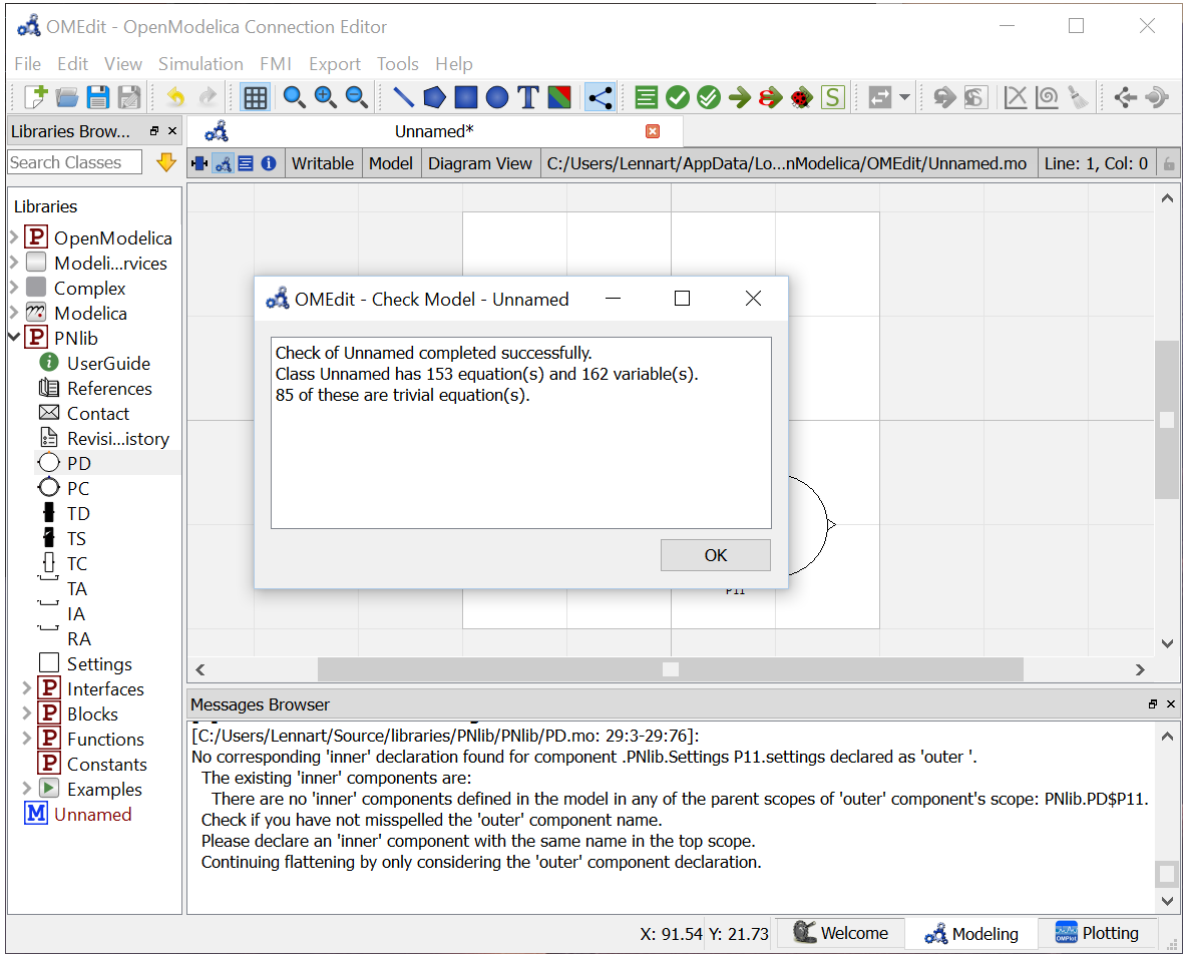


Why not just using OMEdit?



Problems occur once existing connections are changed/removed.

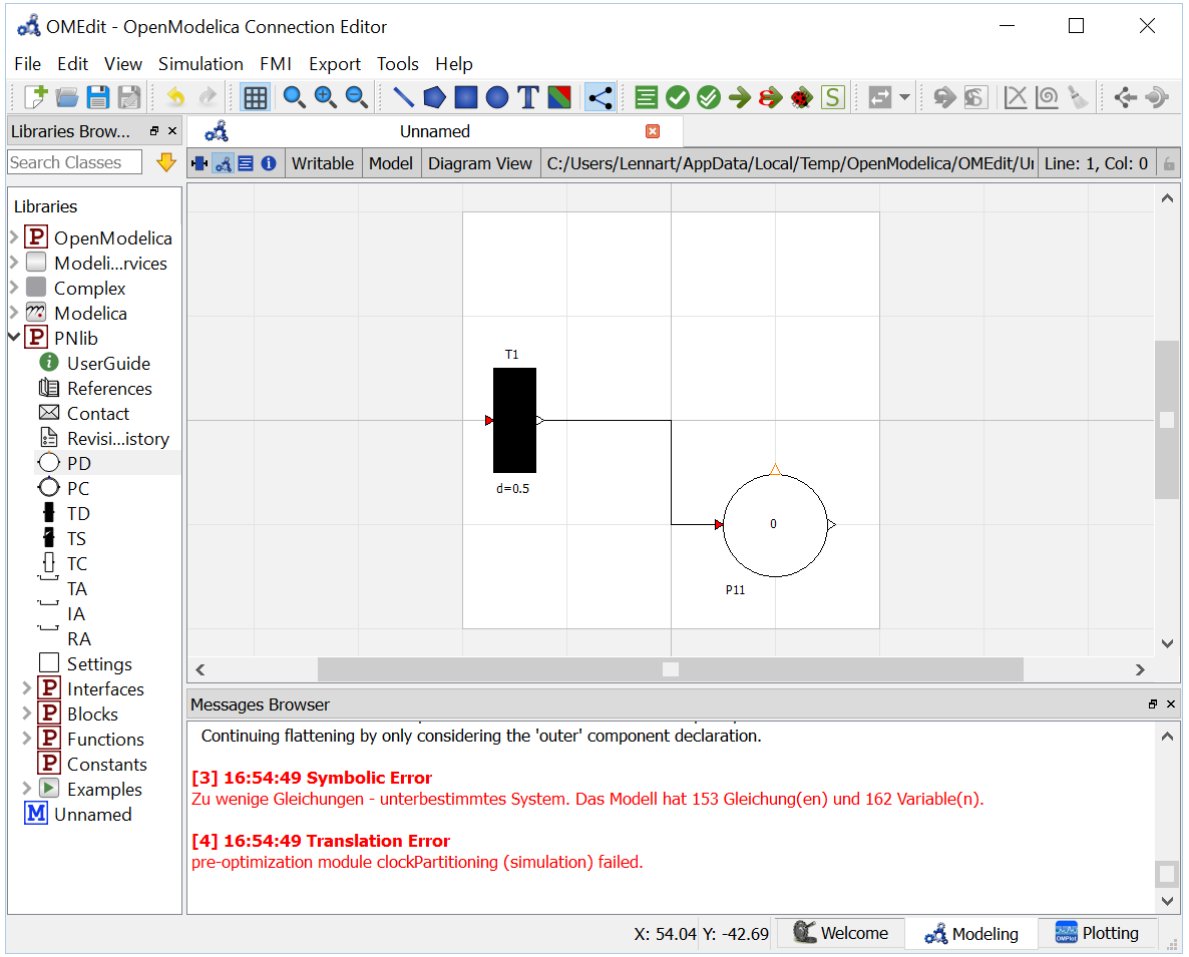
Why not just using OMEdit?



Problems occur once existing connections are changed/removed.

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

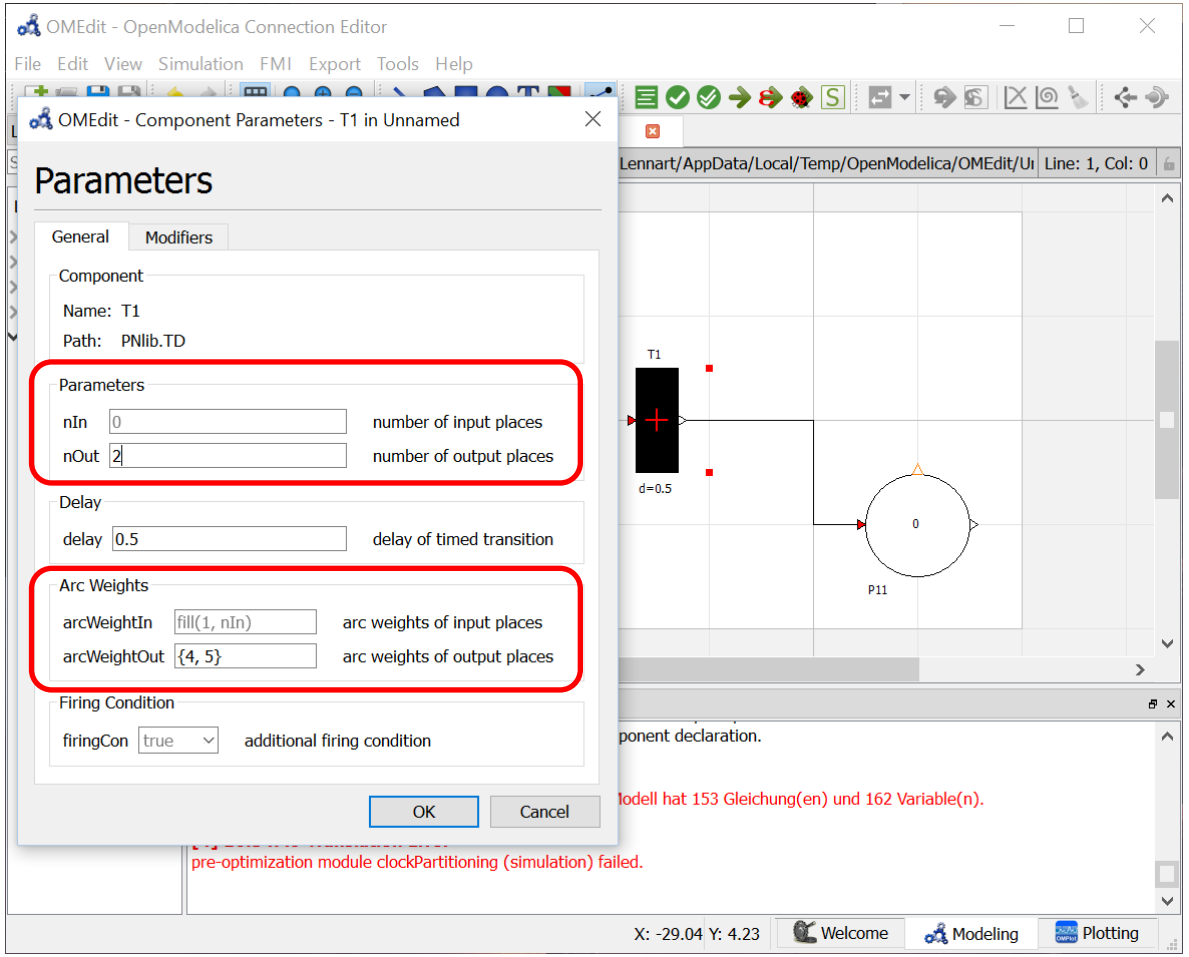
Why not just using OMEdit?



Problems occur once existing connections are changed/removed.

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

Why not just using OMEdit?

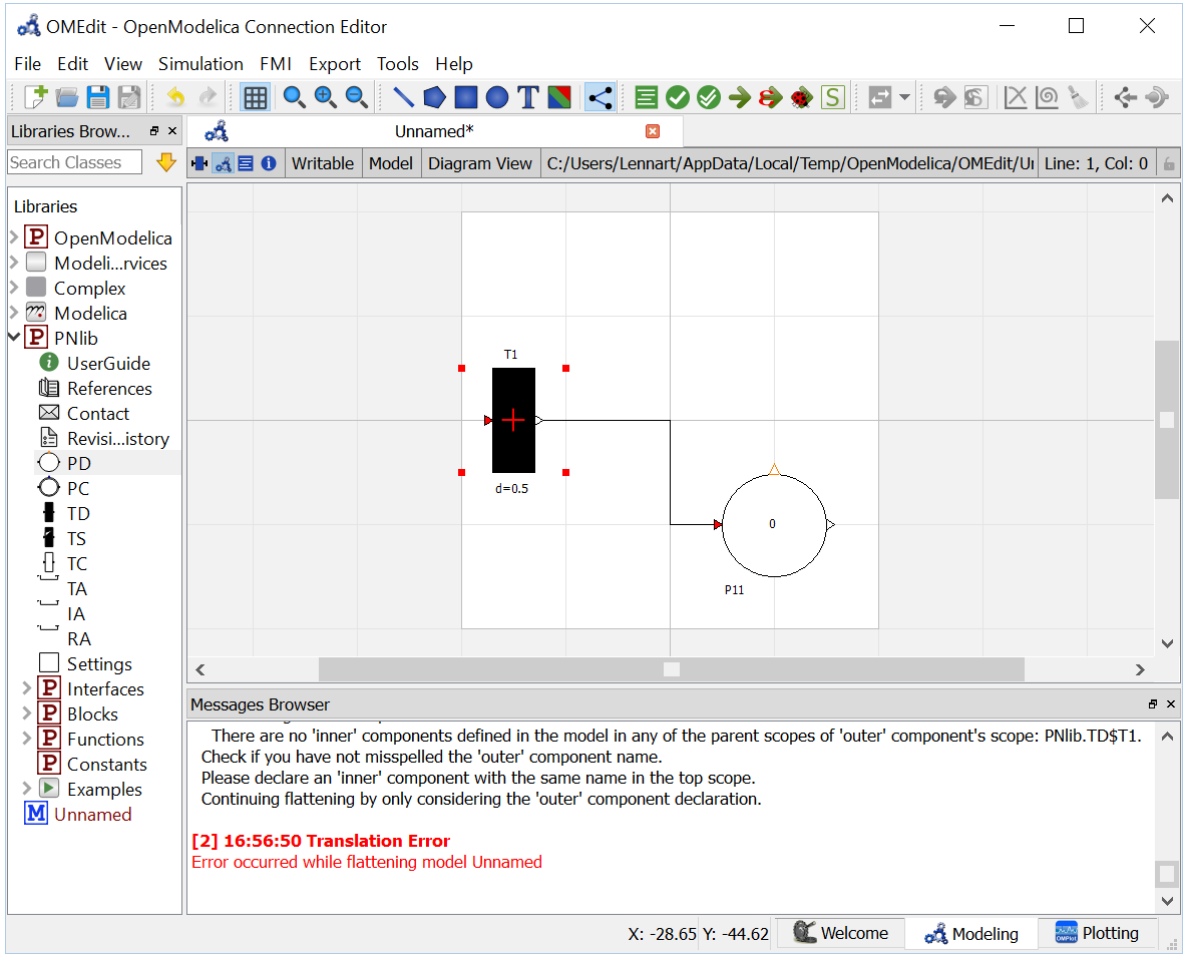


Problems occur once existing connections are changed/removed.

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

Connector sizes and arc weights need to be adjusted manually.

Why not just using OMEdit?



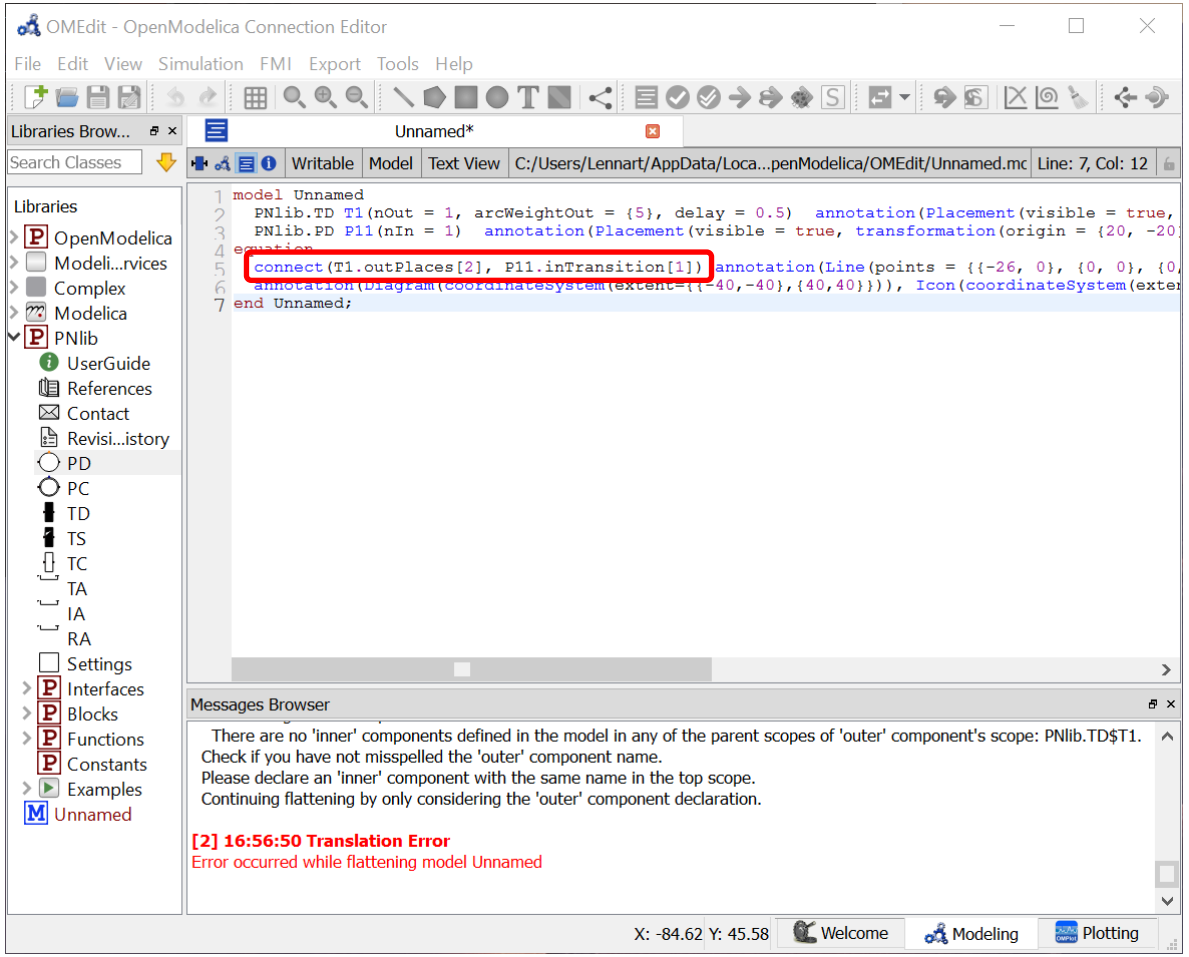
Problems occur once existing connections are changed/removed.

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

Connector sizes and arc weights need to be adjusted manually.

The model still fails without any helpful notification.

Why not just using OMEdit?



Problems occur once existing connections are changed/removed.

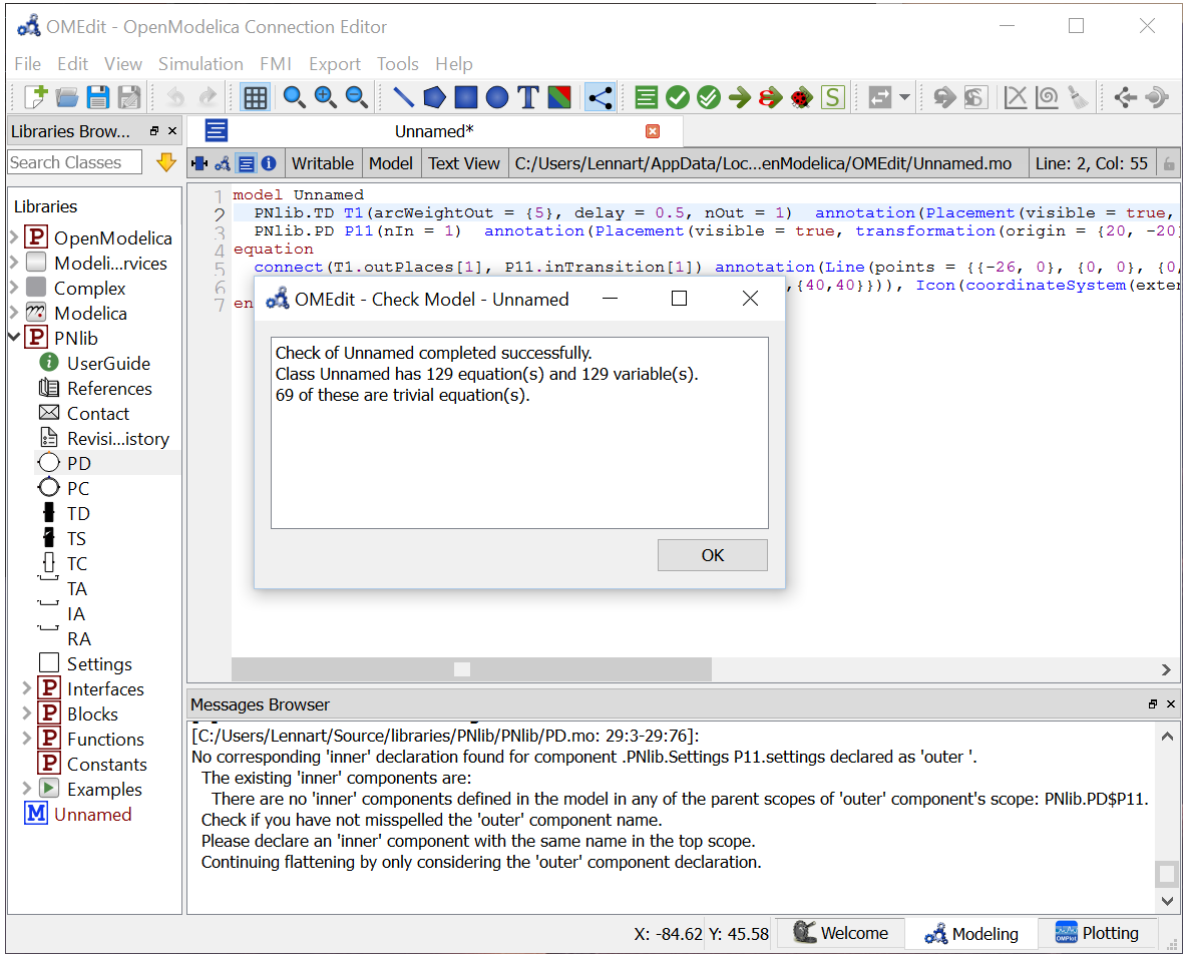
After removing one of the places, the system becomes unbalanced without any helpful message.

Connector sizes and arc weights need to be adjusted manually.

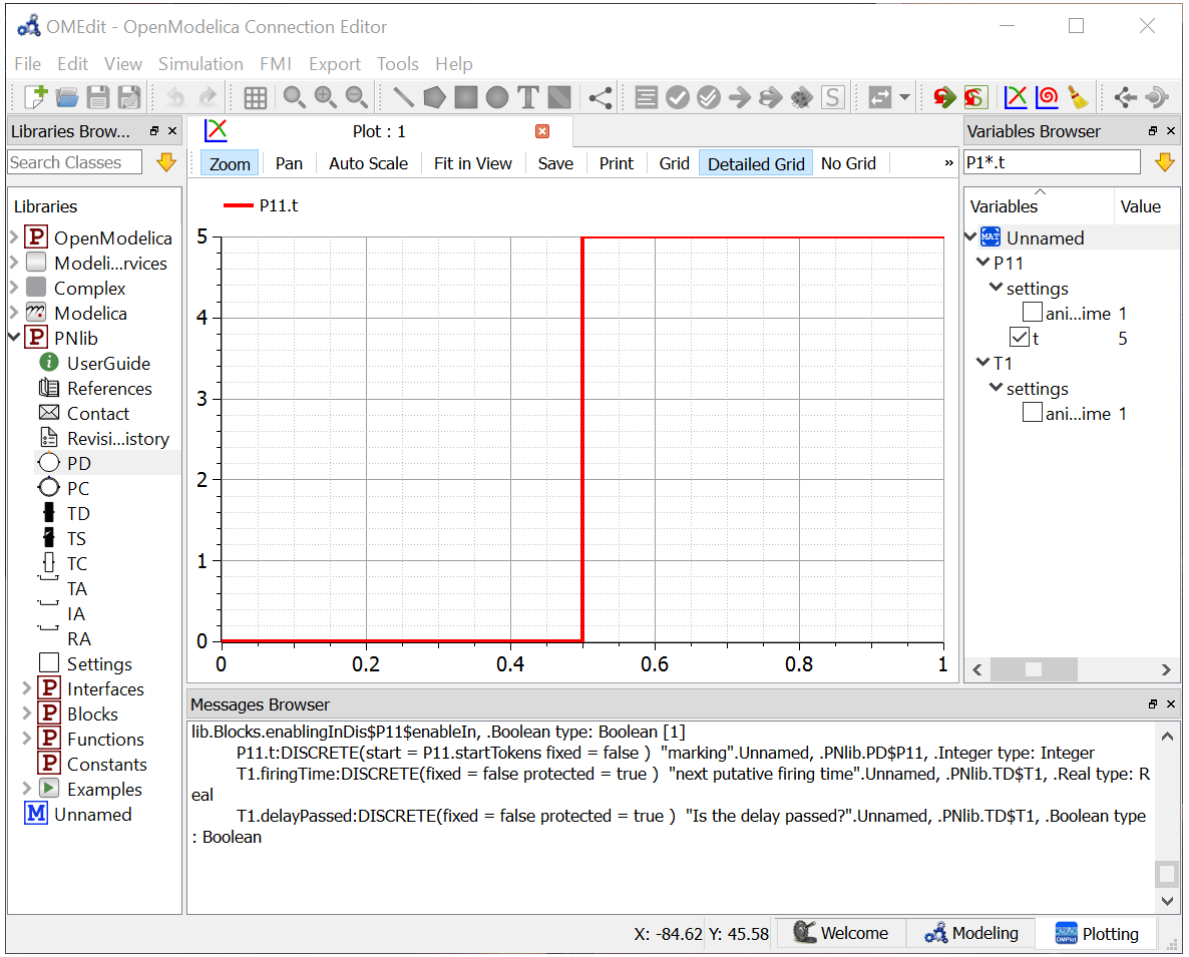
The model still fails without any helpful notification.

One need to modify the source code manually.

Why not just using OMEdit?

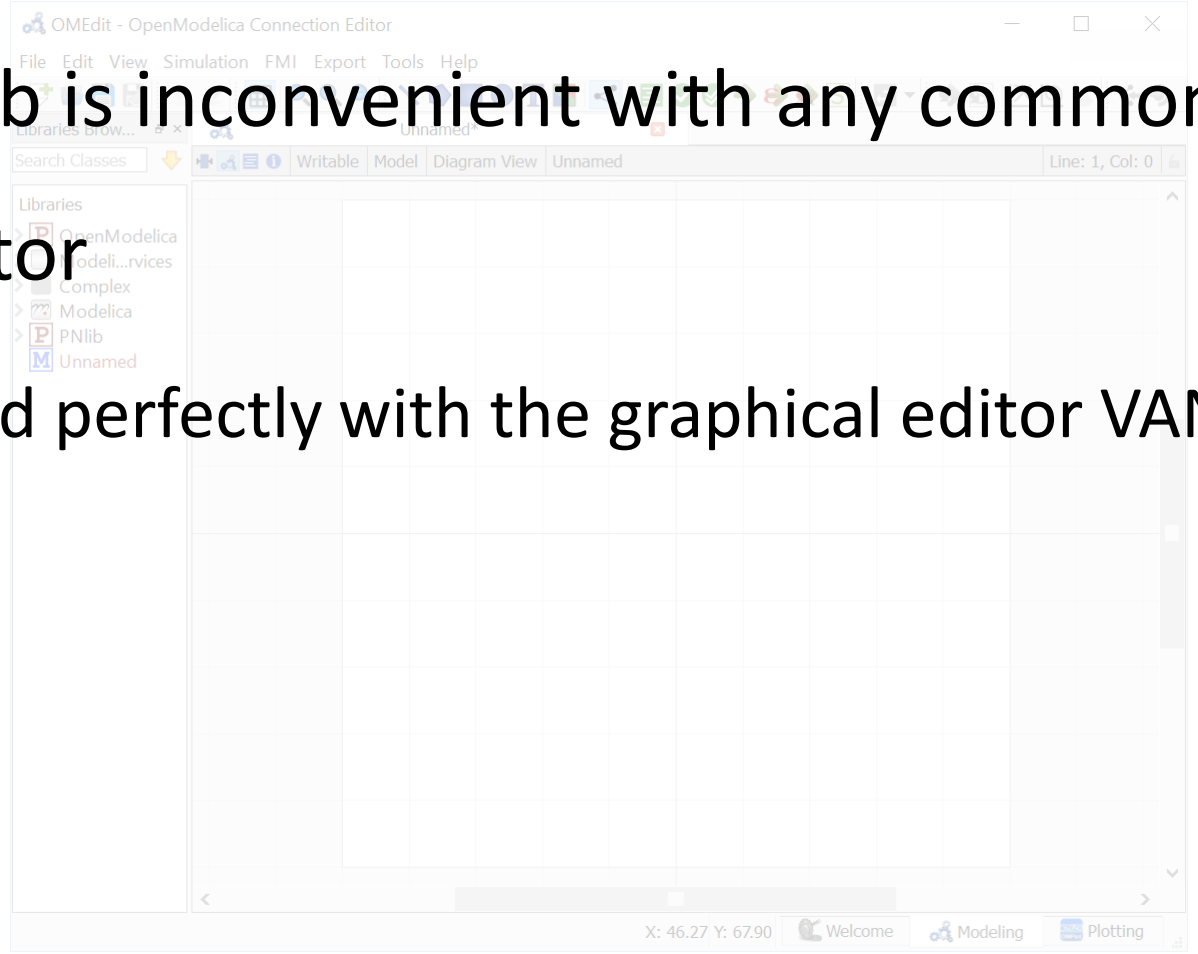


Why not just using OMEdit?



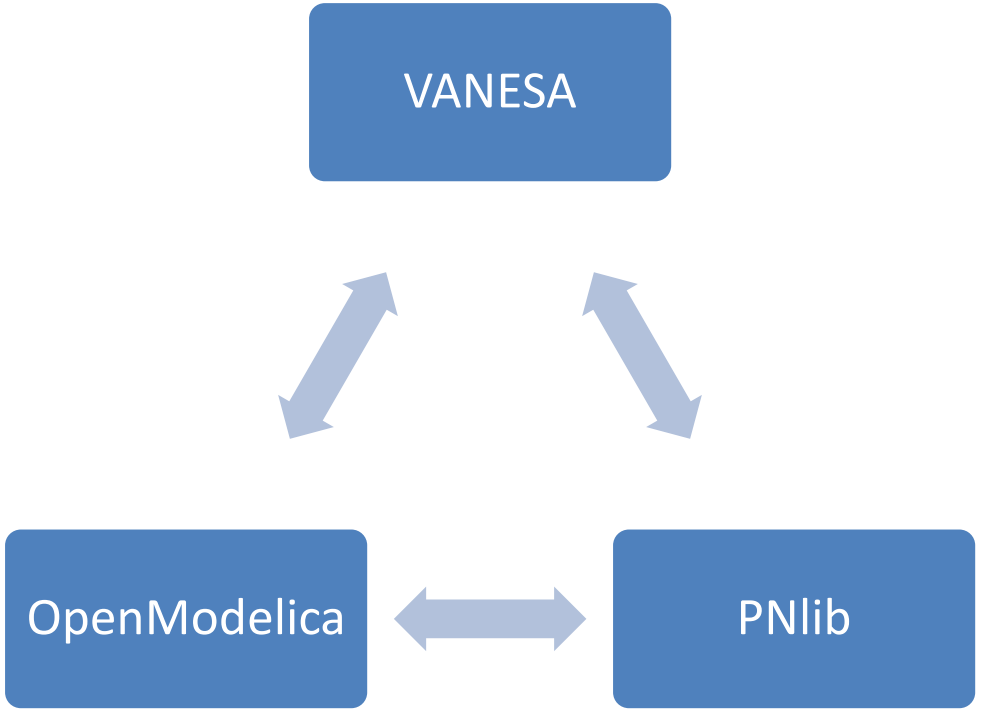
Why not just using OMEdit?

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



Outline

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



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