FSK-ML
Food Safety Knowledge
Markup Language

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Federal Institute for Risk Assessment

Established	November 2002 (predecessor founded in 1876)
Annual budget	Ca. 65 Mio €
Research budget	Ca. 6 Mio €
Staff	Ca. 750 employees (550 scientists)
Location	Berlin

BfR - Areas of work

- Microbiological and substance-chemical safety and assessment of foods

- Safety and assessment of substances (chemicals, plan protection products, biocides)

- Selected products (commodities, cosmetics, tobacco products, textiles, …)

- Risk communication

- Research

- Alternatives to animal experiments where the safety of substances can be determined

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BfR-Strategy

Available online at www.sciencedirect.com

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International Journal of Food Microbiology

INTERNATIONAL JOURNAL OF
Food Microbiology

www.elsevier.com/locate/ijfoodmicro

A strategy to establish Food Safety Model Repositories

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Software Tools

Model exchange formats

Rules for model annotation

Community Contributions

Food Safety Knowledge Bases
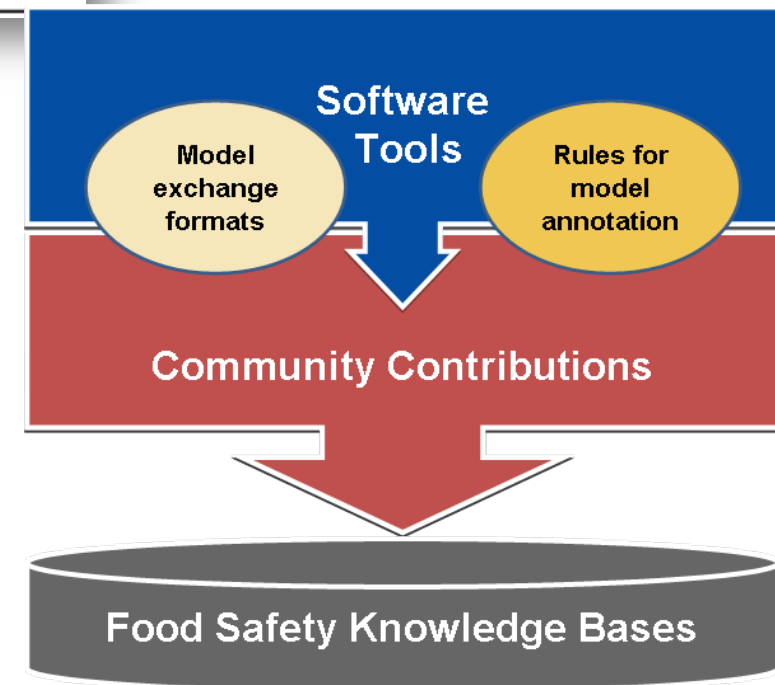
http://www.researchgate.net/publication/273791203_A_strategy_to_establish_Food_Safety_Model_Repositories

Step 1.: Standardized Data format for Models

Predictive Modelling in Food Markup Language (PMF-ML)
Software Developer Guide
Version 1.0

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- ✓ Based on SBML v3

- ✓ Mathematical expressions encoded as MathML

- ✓ Meta data encoded using domain-specific controlled vocabularies

http://sourceforge.net/projects/microbialmodelingexchange/

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Step 2: Standardized Data Format for Script-based Models

KNIME
Open for Innovation

R   MATLAB

Data

manifest

XML
Model meta
Data
(FSK-ML)

XML
Settings for
simulations
(SED–ML)

Simulation
results

FSKX

PDF

Publications

Step 2: Standardized Data Format for Script-based Models

- PMF-ML extended for allowing the exchange of knowledge embedded in script programming languages
- Goal: Harmonization of the exchange of food safety knowledge (like predictive models)
- New COMBINE-based format:
  - Parameterized model + model meta data
  - No more rules: Math no longer in SBML but a script
  - Model meta data in PMF-ML
- Software dependent

- Introduce a COMBINE-based format:
  - Parameterized models + Model metadata
- Parameterized models written in script-based programming languages (R, Matlab or Python)
- Model metadata written in PMF-ML
  - Extended SBML (Predictive Modelling in Food Markup Language)

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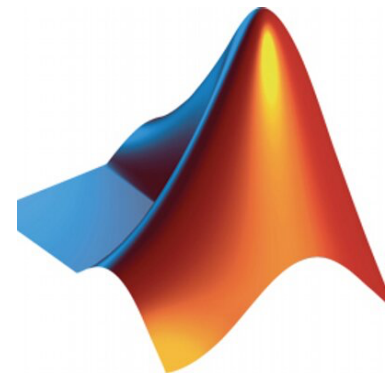
FSK Terminology

Model

- Mathematical description of a system
- May be parameterized → Models may carry predefined values obtained in a parameter fitting process
- **Parameter**. Variables with predefined values
- **Example**. Parameterized model based on experimental data on the growth of a certain pathogen within a temperature range.

Simulation

- Model-based predictions generated from different parameterizations of the same model
- Simulation settings in SEDML (parameters values, simulation type, etc.)
- Simulation results in NuML

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FSK types

Supported types in FSK	
Numeric	Real numbers
Integer	integer
Character	Strings
Vector	1D array
Matrix	2D array

```r
# Examples of scalar data types
pi = 3.14
year = 2016
name = "Miguel, Lord of Westeros"

# Vectors
cookies_per_meeting <- c(10, 5, 20, 15, 10)
cookies_per_meeting <- c(10, "fünf", 20, "fünfzehn", 10)
cookies_per_meeting <- c("zehn", "fünf", "zwanzig", "fünfzehn",
        "zehn")

# Matrices
menus = matrix(
        c("Hänchen", "Reis", "Fishfilet", "Geschnezeltes", "Spinach",
                "Boulette"),
    nrow = 2, ncol = 3, byrow = TRUE,
    dimnames = list(
        c("Menu 1", "Menu 2"), c("Montag", "Dienstag", "Mittwoch")))
```

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FSKX file – model script and libraries

Model script

Script stored within the FSKX archive that calculates the values of the model.

```
#############################################################################
test_model_1 = function(a, b, c){
  res = 100*(rbeta(a, shape1 = b + 1, shape2 = c - b + 1))
  return(res)
}
```
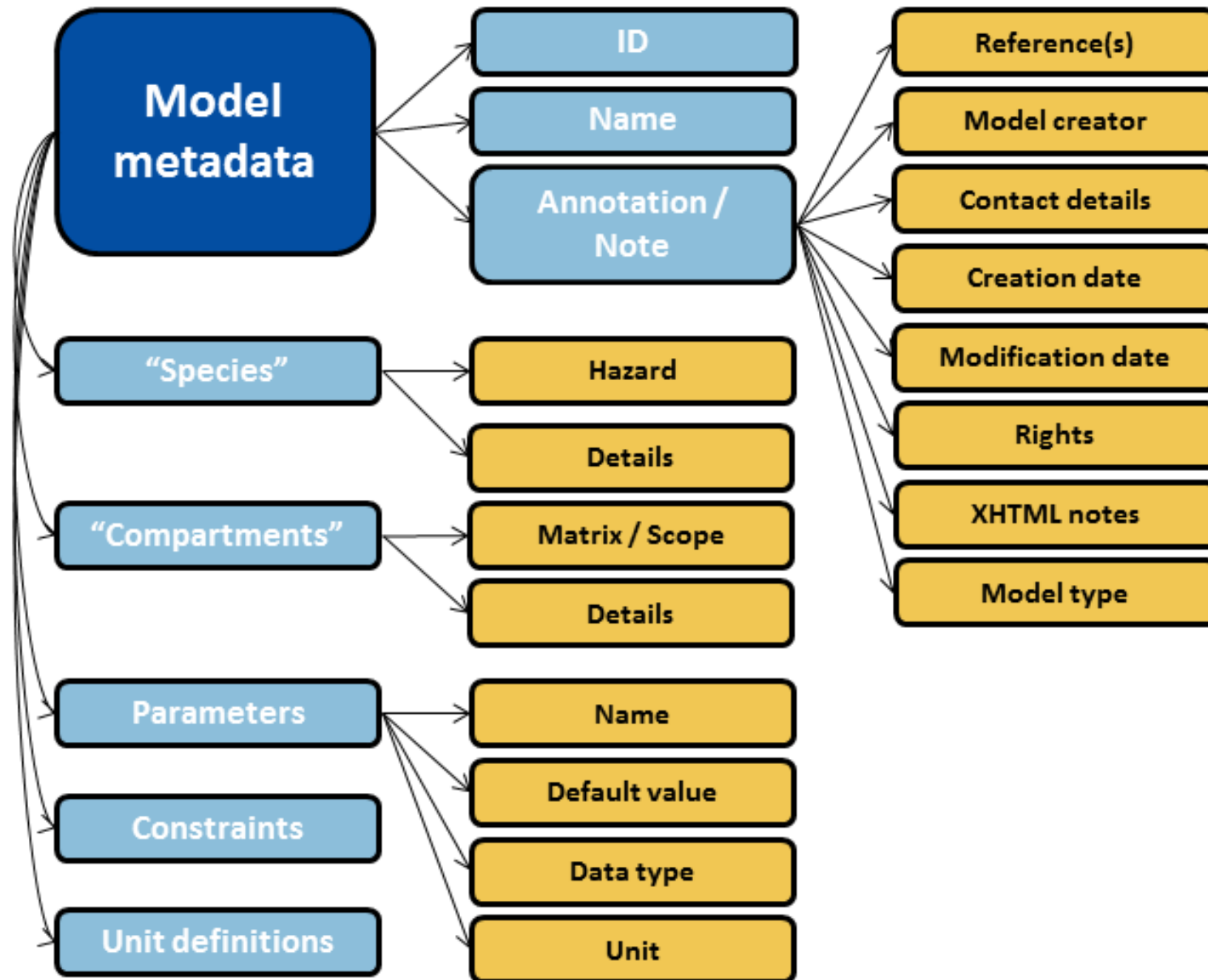
Model script example

(Binary) libraries

• All the required libraries for the model execution must be provided

• The location in the archive is free

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FSKX file – Model meta data (PMFML)

Model meta data

Simulation files

FSK-SED-ML files

- Extended SED-ML describing the simulation of a model
  - Parameter values
  - Type of simulation: deterministic, statistic or probabilistic
  - Output with the simulation results

Visualization scripts

•Scripts with commands to generate a visualization with the simulation results

•May be referenced or embedded in FSK-SED-ML files

```
hist(test_model_1(200, 20, 100), breaks=50, main="Headline", xlab="Text", col="32")
```
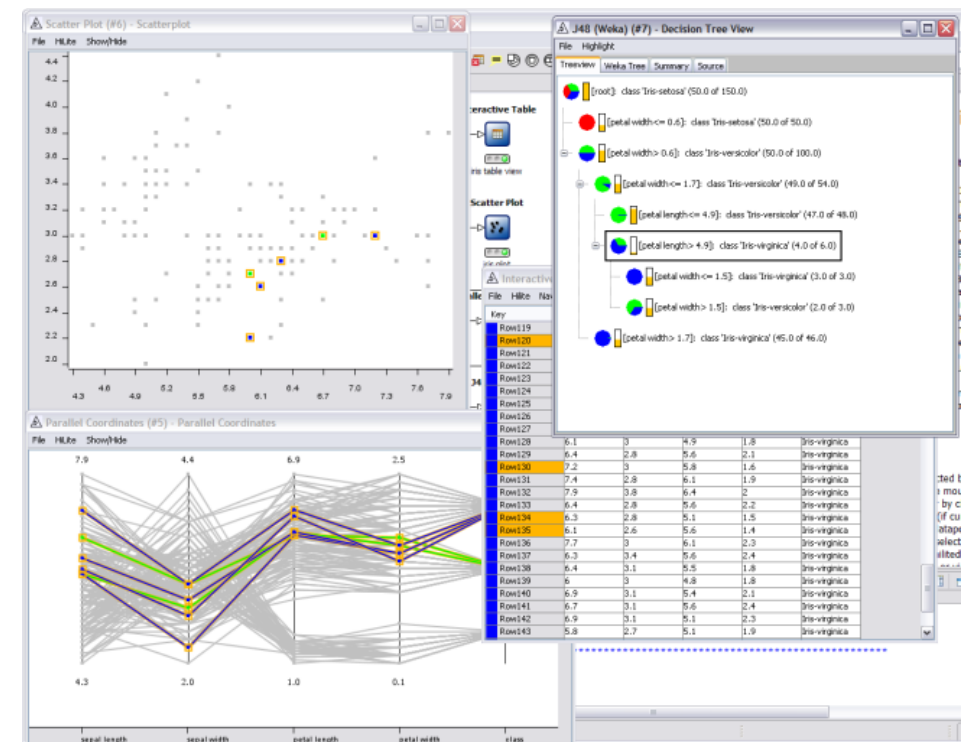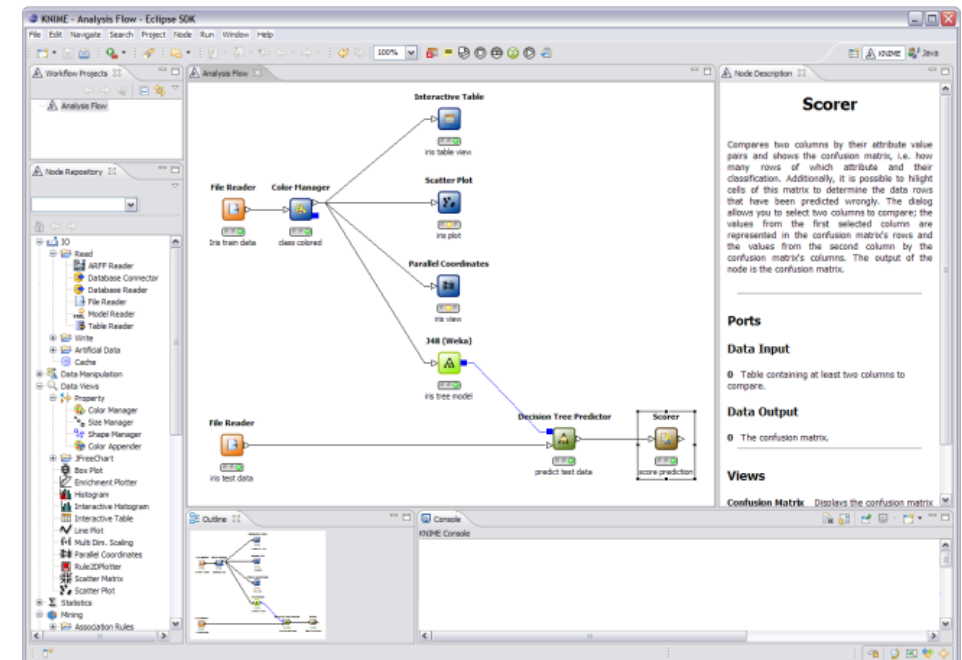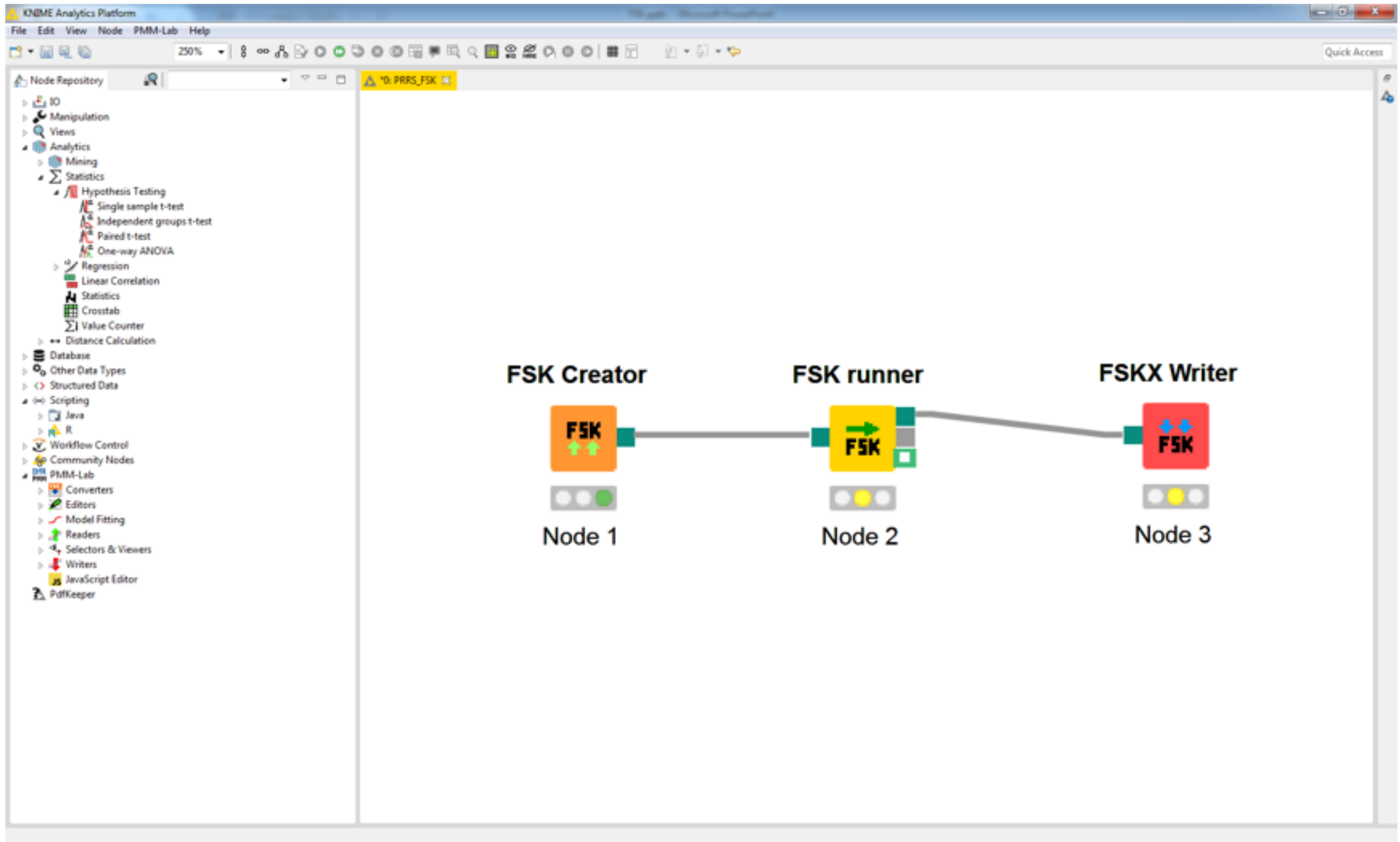**Example visualization script**

Results NuML

•Results of the model encoded in NuML

•Supported data types: numeric, integer, character, vector and matrix

- Konstanz Information Miner
- Created and hosted by KNIME.com
- 1st version released in '06
- Free of charge, OpenSource
- Uses:
  - Data extraction
  - Transformation
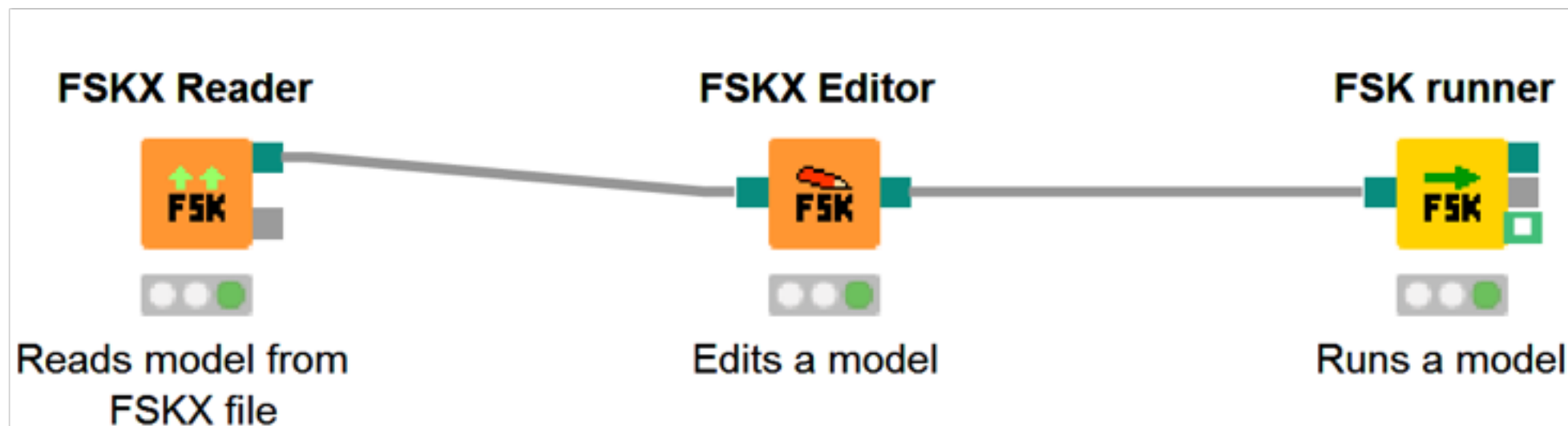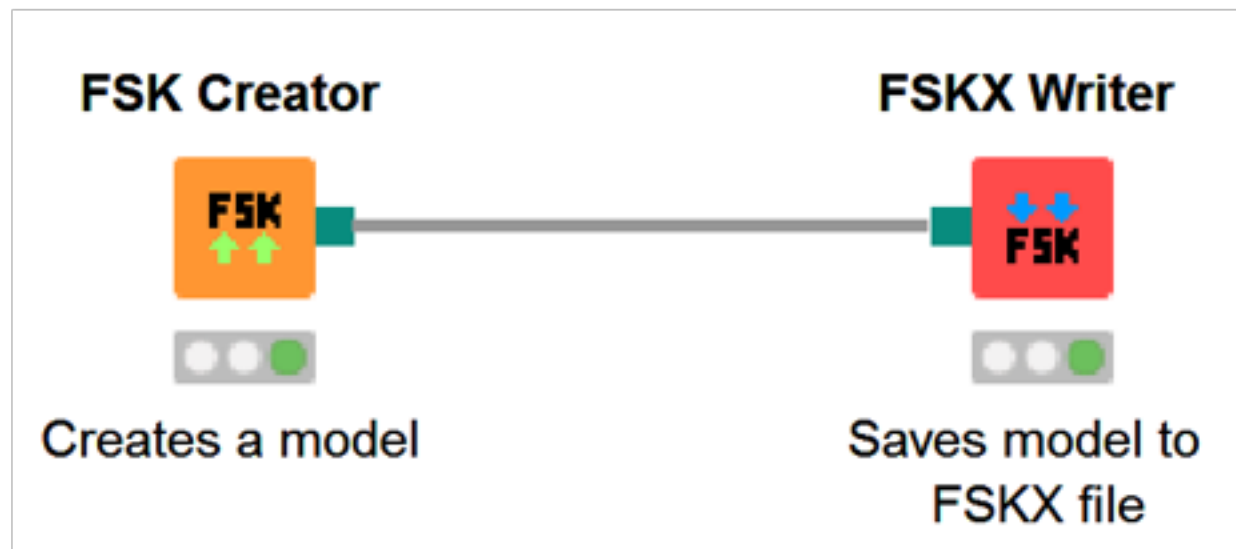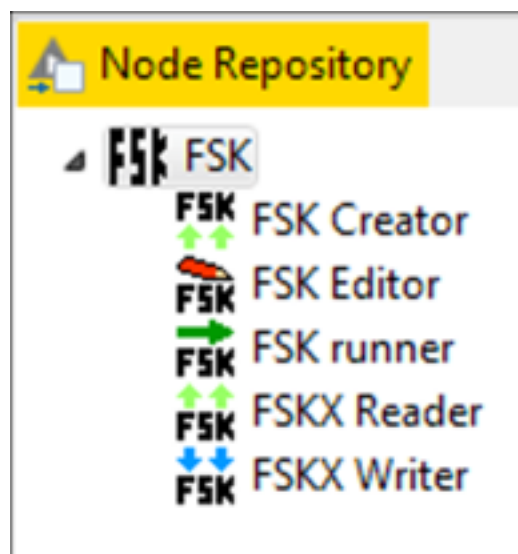 - Modelling
  - Data analysis

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Implementation in detail

Basic workflow to create an FSK model, run it and store it into a local file
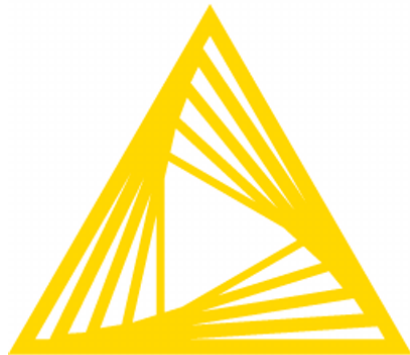
Implementation in KNIME

Implemented FSK KNIME nodes

Want to play?

Binary builds available in SourceForge

https://sourceforge.net/projects/pmmlab/
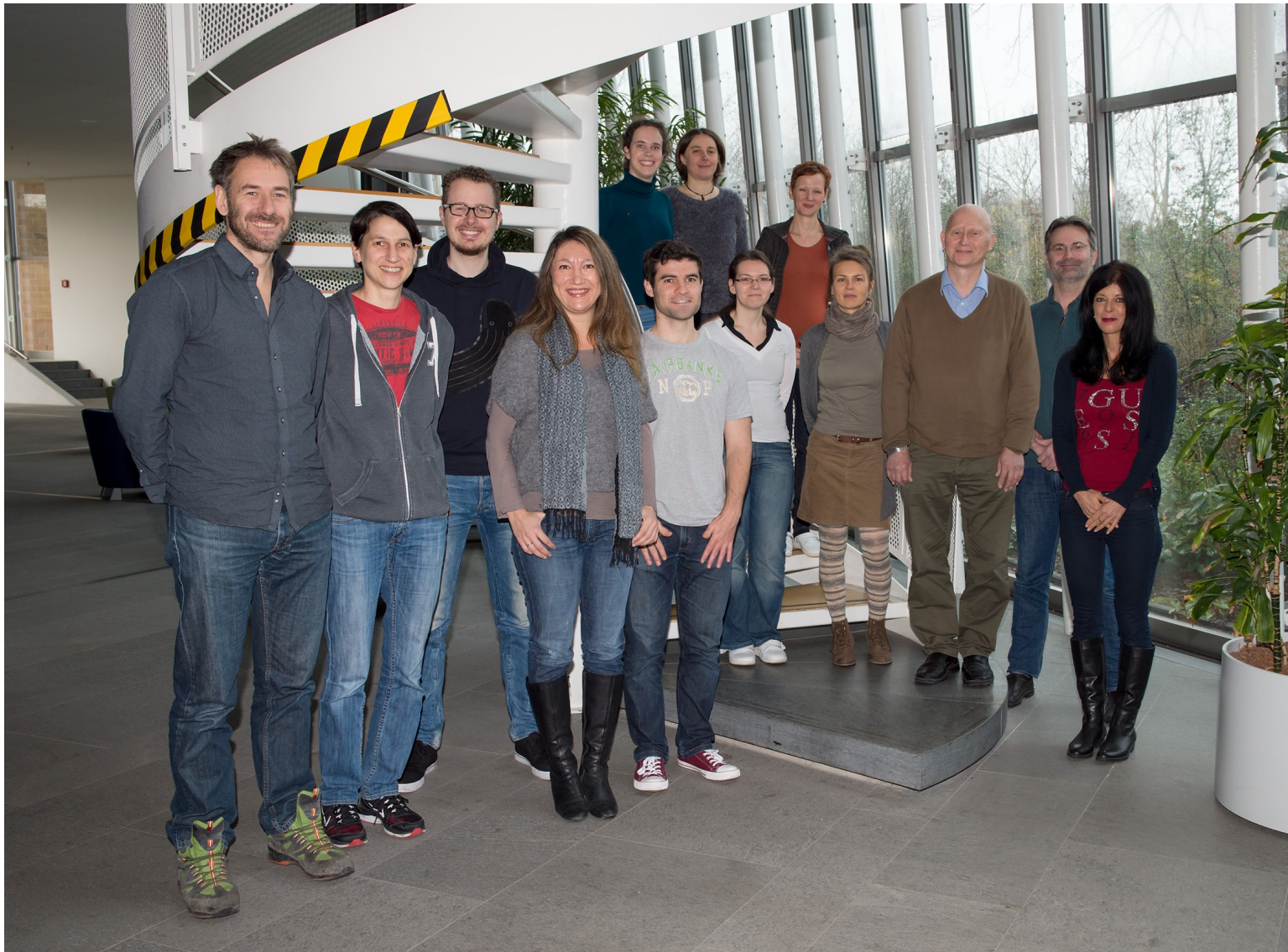
•KNIME build with PmmLab plugins

Vanilla KNIME

•PmmLab is installable with the update site

•http://dl.bintray.com/silebat/test/

Acknowledgments

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