



Presentation No: TT07
Stream: Trends & Technology (TT)

PHUSE US Connect 2021

Visual Programming for ADaM Derivation



Robert Adams

Clara Beck

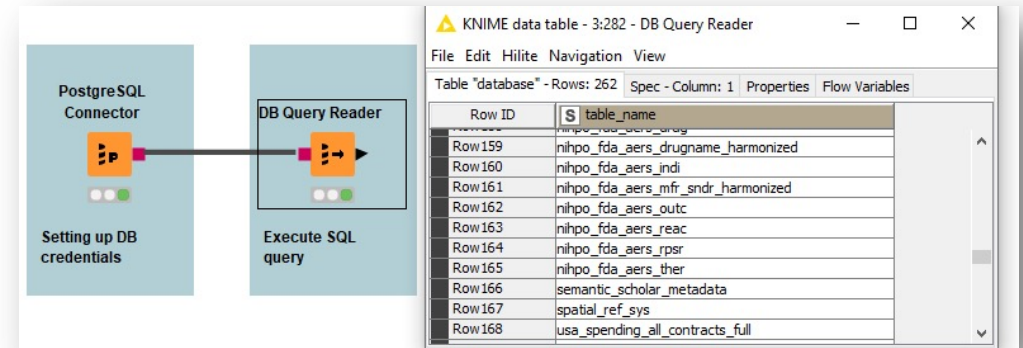




Rationale – Why Visual Programming?

An alternative way of deriving clinical analysis data sets

- Double programming / validation alternative
- Intuitive visualization of data flows within the “program”
 - “The program is the documentation”
- Accessibility to new learners
- Standardization
- “Lowest common denominator”
 - Data science concepts shared across different programming & skills backgrounds

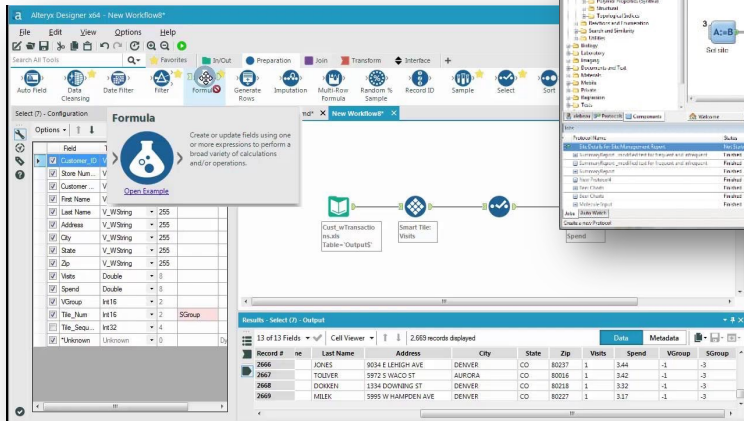


- Immediate clarity of algorithmic approach for anyone with programming / data science backgrounds
- Optimization of workflows straight forward

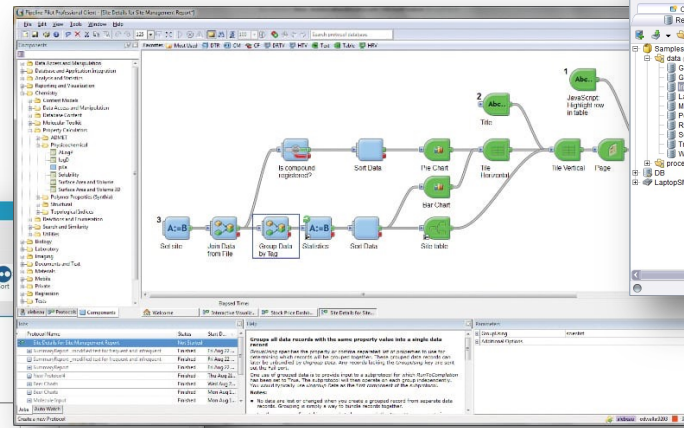


Rationale – Visual Programming Software (low-code tools)

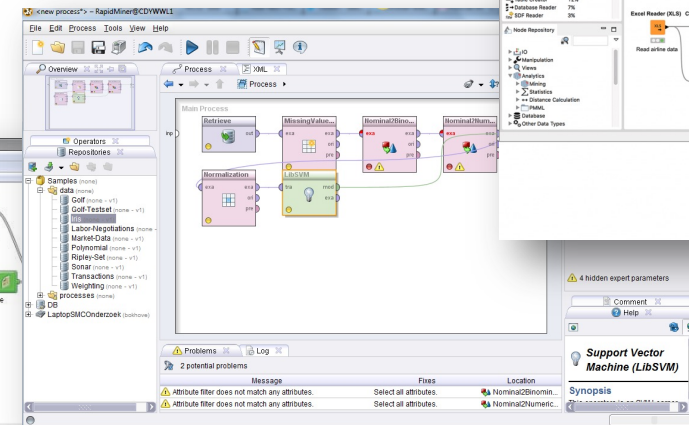
Alteryx



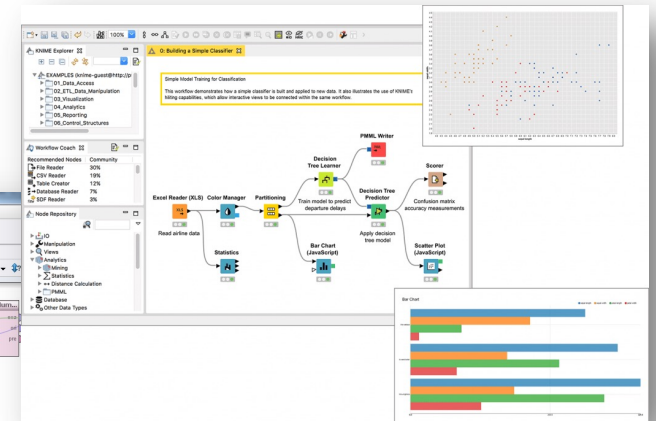
Pipeline Pilot



RapidMiner



KNIME





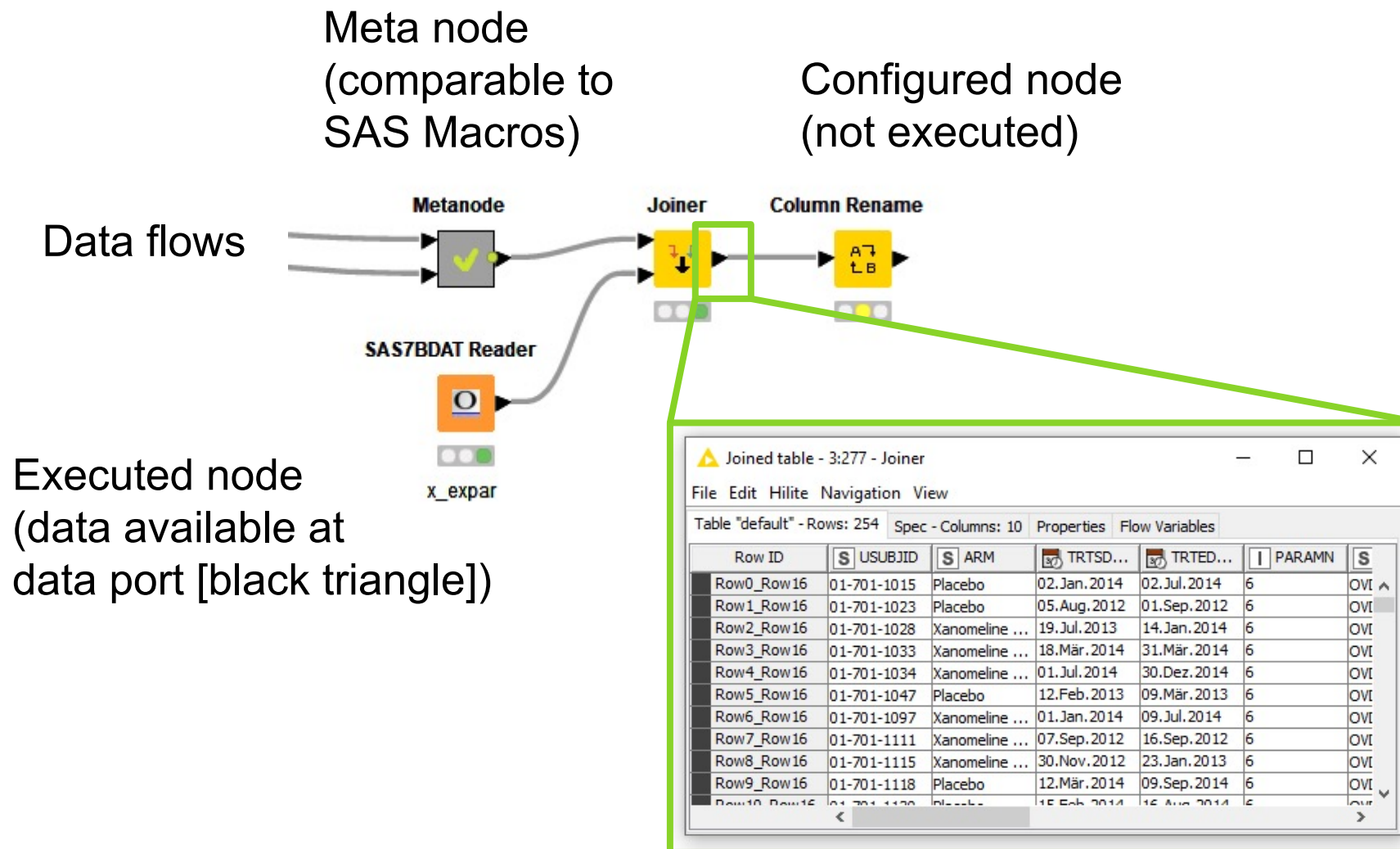
Rationale – KNIME

www.knime.org

- Free software (desktop version) for data analytics
- GPL license
- Java / Eclipse (IDE) based
 - Available on Windows, Linux, Mac OS
- Strong community support
- Open source
 - Code can be inspected / validated
- Java, R, Python integration
- Codeless deep learning (Keras integration)



Main Concepts



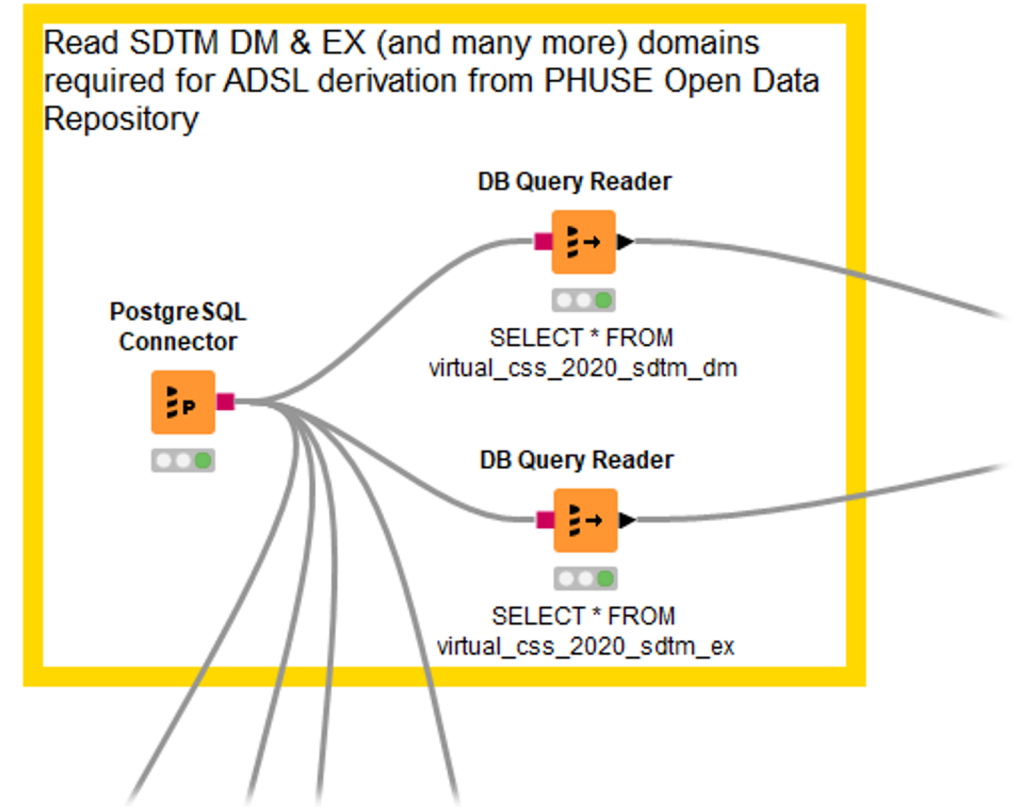


ADSL – Data Retrieval

<https://github.com/phuse-org/PODR>



- “PODR integrates health-related Open Data across agencies”
- Sample data sets
 - SDTM, ADaM ... and more





ADSL – Data Retrieval

<https://github.com/phuse-org/PODR>

Dialog - 0:368 - PostgreSQL Connector

File

Output Type Mapping | Flow Variables | Job Manager Selection

Connection Settings | JDBC Parameters | Advanced | Input Type Mapping

Configuration

Database Dialect: PostgreSQL

Driver Name: PostgreSQL [ID: PostgreSQL]

Location

Hostname: podr.phuse.global Port: 5.432

Database name: nihpo

Authentication

☐ Credentials

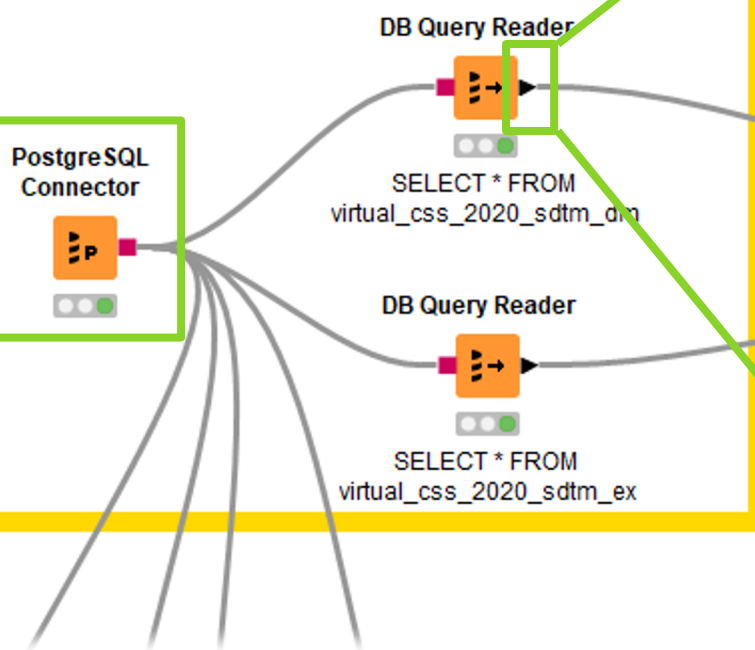
☒ Username & password

Username: phuse_rfl3ghlh8

Password:

OK Apply Cancel ?

Read SDTM DM & EX (and many more) domains required for ADSL derivation from PHUSE Open Data Repository



KNIME data table - 6:373 - DB Query Reader (virtual_css_2020_sdtm_dm)

File Edit Hilite Navigation View

Table "database" - Rows: 306 Spec - Columns: 25 Properties FI

Row ID	S STUDYID	S DOMAIN	S USUBJID
Row0	CDISCPIL01	DM	01-701-1015
Row1	CDISCPIL01	DM	01-701-1023
Row2	CDISCPIL01	DM	01-701-1028
Row3	CDISCPIL01	DM	01-701-1033
Row4	CDISCPIL01	DM	01-701-1034
Row5	CDISCPIL01	DM	01-701-1047
Row6	CDISCPIL01	DM	01-701-1057
Row7	CDISCPIL01	DM	01-701-1097
Row8	CDISCPIL01	DM	01-701-1111
Row9	CDISCPIL01	DM	01-701-1115
Row10	CDISCPIL01	DM	01-701-1118
Row11	CDISCPIL01	DM	01-701-1130
Row12	CDISCPIL01	DM	01-701-1133
Row13	CDISCPIL01	DM	01-701-1145
Row14	CDISCPIL01	DM	01-701-1146
Row15	CDISCPIL01	DM	01-701-1148
Row16	CDISCPIL01	DM	01-701-1153
Row17	CDISCPIL01	DM	01-701-1162
Row18	CDISCPIL01	DM	01-701-1176
Row19	CDISCPIL01	DM	01-701-1180
Row20	CDISCPIL01	DM	01-701-1181
Row21	CDISCPIL01	DM	01-701-1188
Row22	CDISCPIL01	DM	01-701-1192
Row23	CDISCPIL01	DM	01-701-1203



ADSL – Derivation

Joining (merging) data sets

Joiner Settings | Column Selection | Flow Variables | Job Manager Selection | Memory Policy

Join Mode
Join mode: Left Outer Join

Joining Columns
☒ Match all of the following ☐ Match any of the following

Top Input ('left' table): S RACE
Bottom Input ('right' table): S Label

S RACE	S ETHNIC	S ARMCD
WHITE	NOT HISPANIC OR L...	Pbo
WHITE	NOT HISPANIC OR L...	Xan_Lo
BLACK OR AFRICAN AMERICAN	NOT HISPANIC OR L...	Xan_Lo
WHITE	NOT HISPANIC OR L...	Pbo
WHITE	NOT HISPANIC OR L...	Xan_Hi
WHITE	NOT HISPANIC OR L...	Xan_Lo
WHITE	NOT HISPANIC OR L...	Xan_Hi
WHITE	NOT HISPANIC OR L...	Pbo
BLACK OR AFRICAN AMERICAN	NOT HISPANIC OR L...	Xan_Hi

Table Creator



Codelist Race



Joiner



Merge Codelist

S RACE	I Value	S ETH
WHITE	1	NOT HIS
BLACK OR AFRICAN AMERICAN	2	NOT HIS
WHITE	1	NOT HIS
WHITE	1	NOT HIS
WHITE	1	NOT HIS
WHITE	1	NOT HIS
WHITE	1	NOT HIS
WHITE	1	NOT HIS
BLACK OR AFRICAN AMERICAN	2	NOT HIS
WHITE	1	HISPANI
WHITE	1	NOT HIS

S Label	I Value
WHITE	1
BLACK OR AFRICAN AMERICAN	2



ADSL – Derivation

Column Expressions: Categories

Output table - 3:341 - Date&Time Diffe... — □ ×

File Edit Hilite Navigation View

Spec - Columns: 50 Properties Flow Variables

Table "default" - Rows: 253

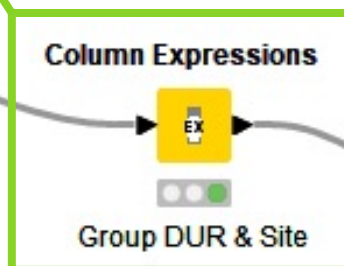
Row ID	MP1...	S COMP2...	31 DISON...	L DURDIS
Row0_Row2_...		Y	2010-04-30	44
Row1_Row2_...		N	2006-03-11	76
Row2_Row1_...		Y	2009-12-16	43
Row3_Row0_...		N	2009-08-02	55
Row4_Row1_...		Y	2011-09-29	33
Row5_Row2_...		N	2009-07-26	42
Row7_Row0_...		Y	2005-09-22	99
Row8_Row0_...		N	2009-04-04	41
Row9_Row0_...		N	2004-05-28	102

Expression	Type	Collection	Replace Column	Output Column
if (column("DURDIS") >= ...	String	☐	☐	DURDSGR1
column("SITEID")	Number (integer)	☐	☐	SITEGR1

Expression Editor

+ column + variable + function

```
1 if (column("DURDIS") >= 12){
2   DURDSGR1 = ">=12"
3 } else {
4   DURDSGR1 = "<12"
5 }
```

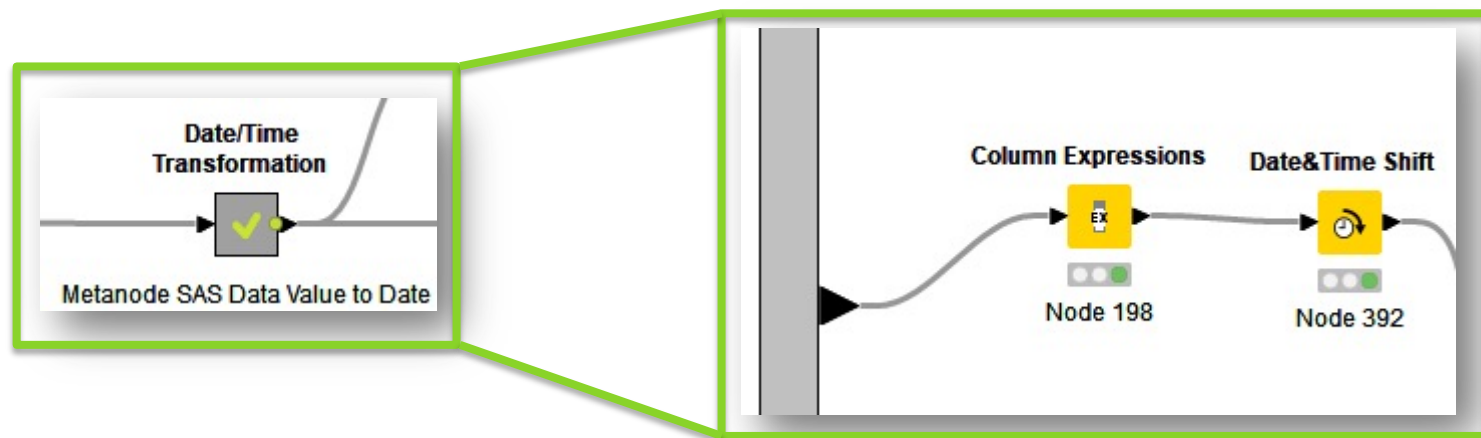


L DURDIS	S DURDS...
77	>=12
33	>=12
19	>=12
11	<12
73	>=12
48	>=12
24	>=12

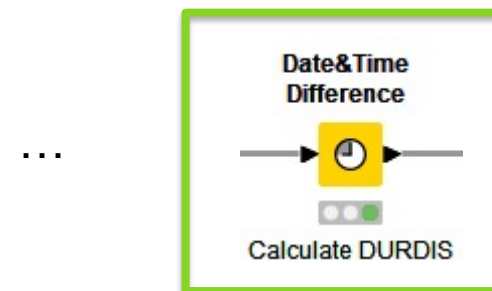


ADSL – Derivation

Coping with date formats



Allow date calculations



SAS date representation

19800
19905
19401
19724

Define SAS origin

1960-01-01
1960-01-01
1960-01-01
1960-01-01

Shift to KNIME dates

2014-01-02
2012-08-05
2013-07-19
2014-03-18

Duration from TRTSTD (e.g. in days)

...

44
76
43
55

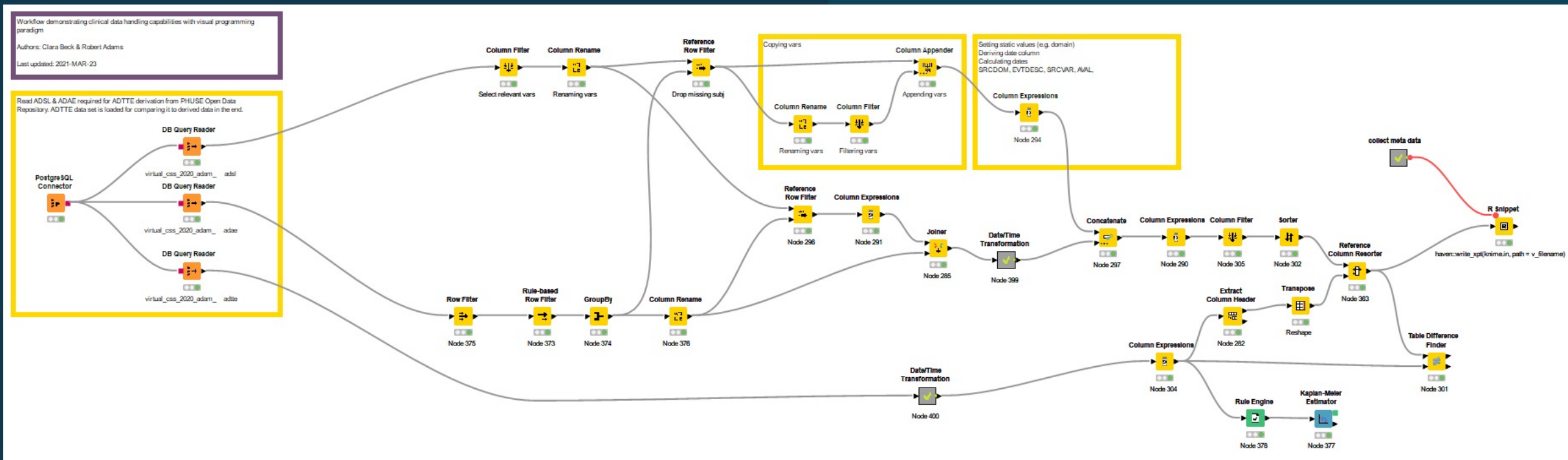


ADaM Derivation - ADTTTE

Data retrieval

Derivation

Visualization
& Testing
& XPT output

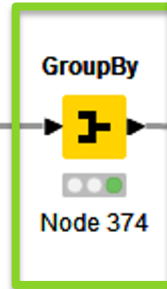




ADTTE – Grouping

Aggregation

[S] USUBJID	[D] TRTSDT	[D] TRTEDT
01-701-1015	19,725	19,906
01-701-1015	19,725	19,906
01-701-1023	19,210	19,237
01-701-1023	19,210	19,237
01-701-1023	19,210	19,237
01-701-1028	19,558	19,737
01-701-1028	19,558	19,737
01-701-1034	19,905	20,087
01-701-1097	19,724	19,913
01-701-1097	19,724	19,913



Settings Description Flow Variables Job Manager Selection Memory Policy

Groups Manual Aggregation Pattern Based Aggregation Type Based Aggregation

Group settings

Available column(s)

Filter

[S] STUDYID
[L] SITEID
[S] TRTA
[D] TRTAN
[D] AGE
[S] AGEGR 1
[D] AGEGR 1N
[S] RACE

Settings Description Flow Variables Job Manager Selection Memory Policy

Groups Manual Aggregation Pattern Based Aggregation Type Based Aggregation

Aggregation settings

Available columns

Filter

[S] STUDYID
[L] SITEID
[S] TRTA
[D] TRTAN
[D] AGE
[S] AGEGR 1
[D] AGEGR 1N
[S] RACE
[D] RACEN
[S] SEX
[S] SAFFL

add >>

add all >>

<< remove

To change multiple columns use right mouse button

Column	Aggregation
[D] TRTSDT	First
[D] TRTEDT	First
[D] ASTDT	First
[S] ASTDTF	First
[D] ASTDY	First
[D] AENDT	First
[D] AENDY	First
[D] ADURN	First
[D] AESEQ	First

[S] USUBJID	[D] First*(T...	[D] First*(T...
01-701-1015	19,725	19,906
01-701-1023	19,210	19,237
01-701-1028	19,558	19,737
01-701-1034	19,905	20,087
01-701-1097	19,724	19,913



ADTTE – Grouping

Available aggregation functions

- Concatenate
- Correlation
- Count
- Covariance
- First
- Geometric mean
- Geometric standard deviation
- Kurtosis

- List
- List (sorted)
- Maximum
- Mean
- Mean absolute deviation
- Median
- Median absolute deviation
- Minimum

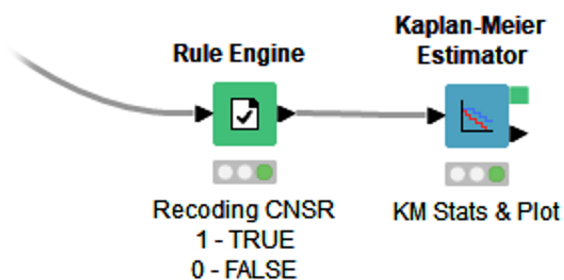
- Missing value count
- Mode
- P² Percentile
- Percent
- Product
- Quantile
- Range
- Second moment

- Standard deviation
- Sum
- Sum of logs
- Sum of squares
- Unique concatenate
- Unique concatenate with count
- Unique count
- Variance



ADTTE – Derivation

Kaplan-Meier Statistics / Plotting

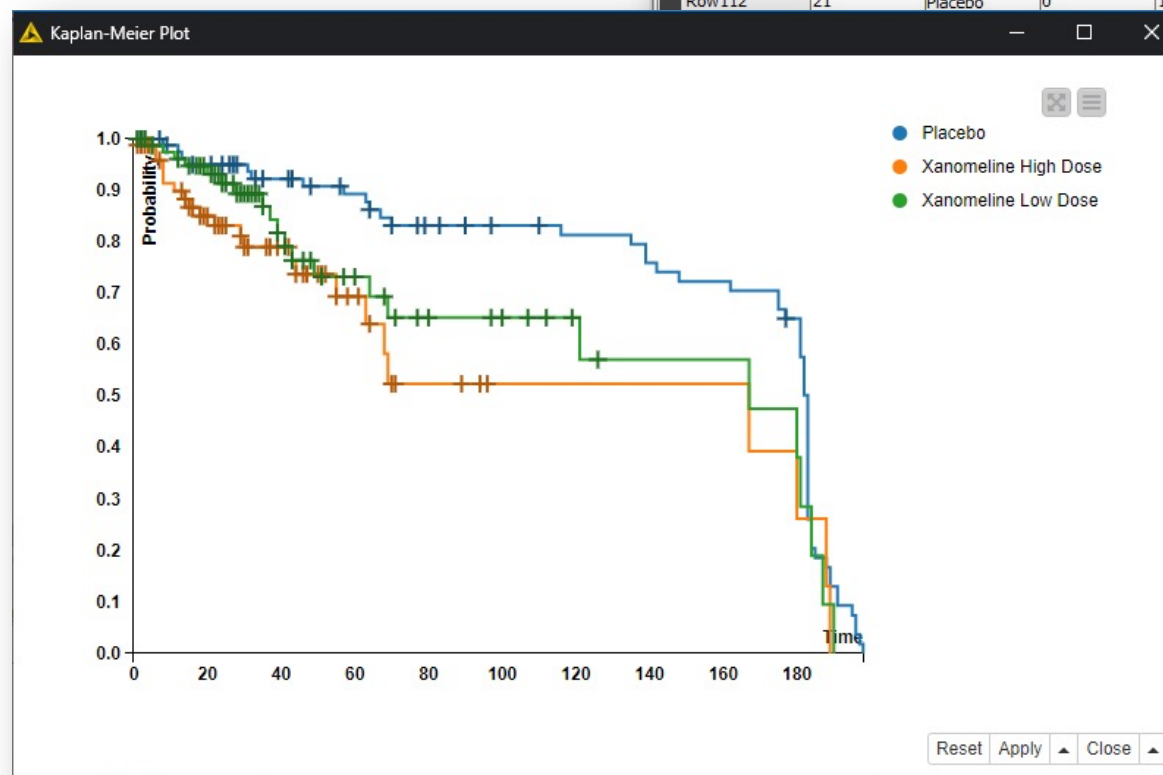


Statistics - 0:379 - Kaplan-Meier Estimator

File Edit Hilite Navigation View

Table "default" - Rows: 161 Spec - Columns: 5 Properties Flow Variables

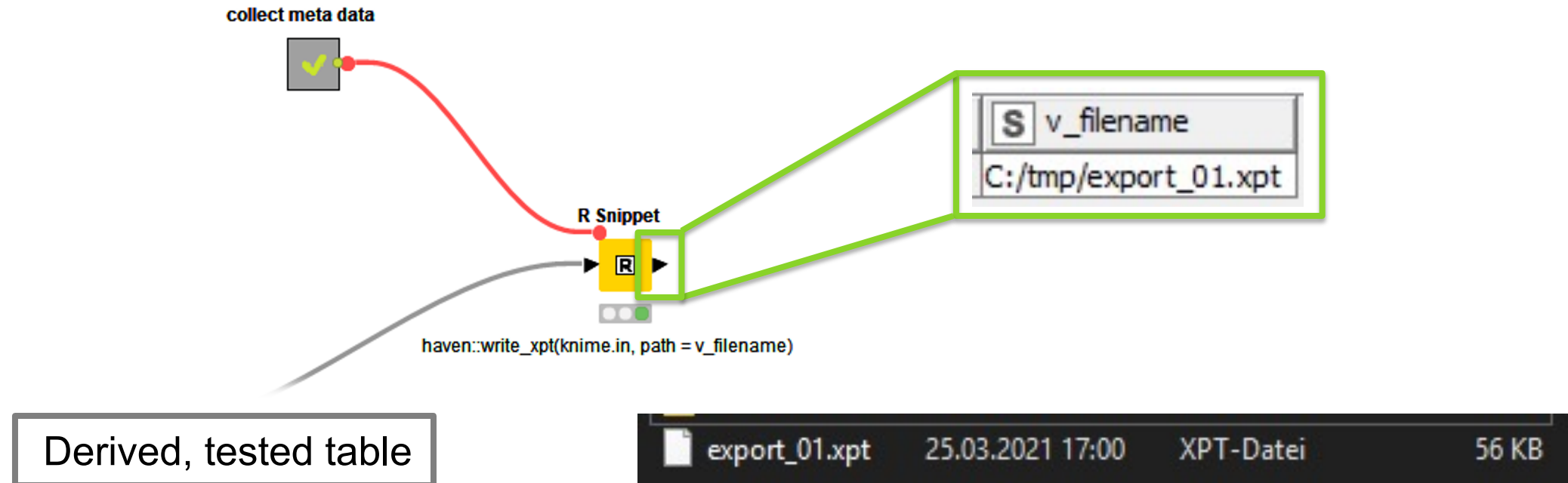
Row ID	D AVAL	S TRTA	I #True(...	I #False(...	D km-esti...
Row152	1	Placebo	0	1	1
Row0	2	Placebo	0	1	1
Row1	3	Placebo	0	2	1
Row134	7	Placebo	0	1	1
Row68	8	Placebo	1	0	0.988
Row159	9	Placebo	0	1	0.988
Row39	12	Placebo	1	0	0.975
Row116	13	Placebo	1	0	0.963
Row29	14	Placebo	1	0	0.95
Row144	16	Placebo	0	1	0.95
Row112	21	Placebo	0	1	0.95





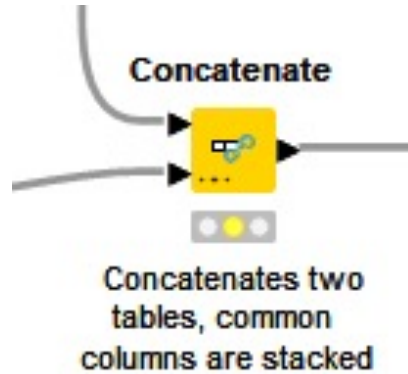
ADTTE – Derivation

Utilizing R to write XPT output

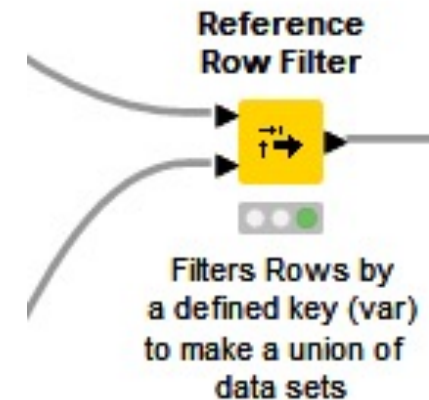
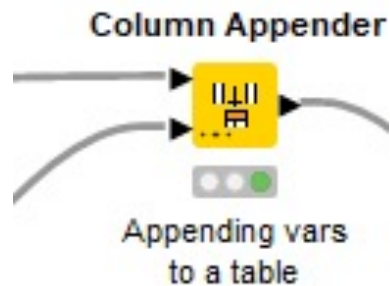
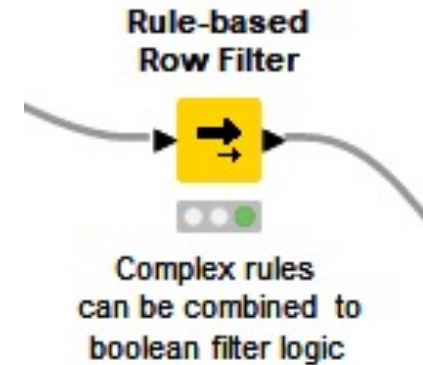




5 Nodes You Need To Know To Be A Clinical KNIME h4xX0r

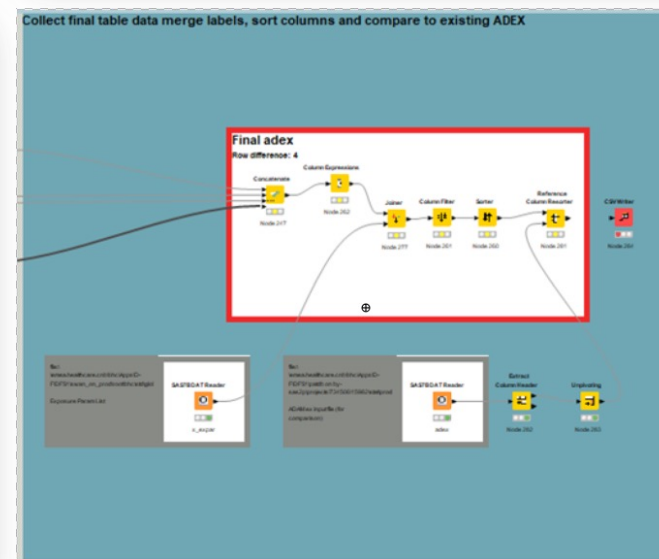
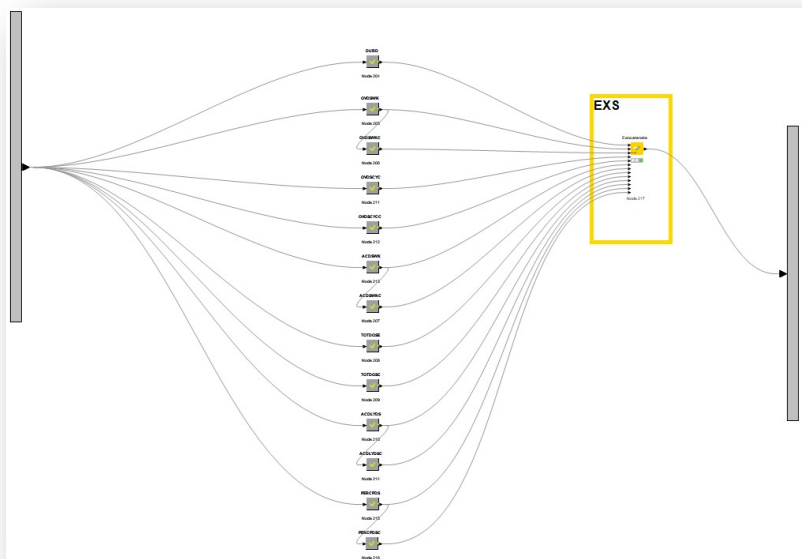
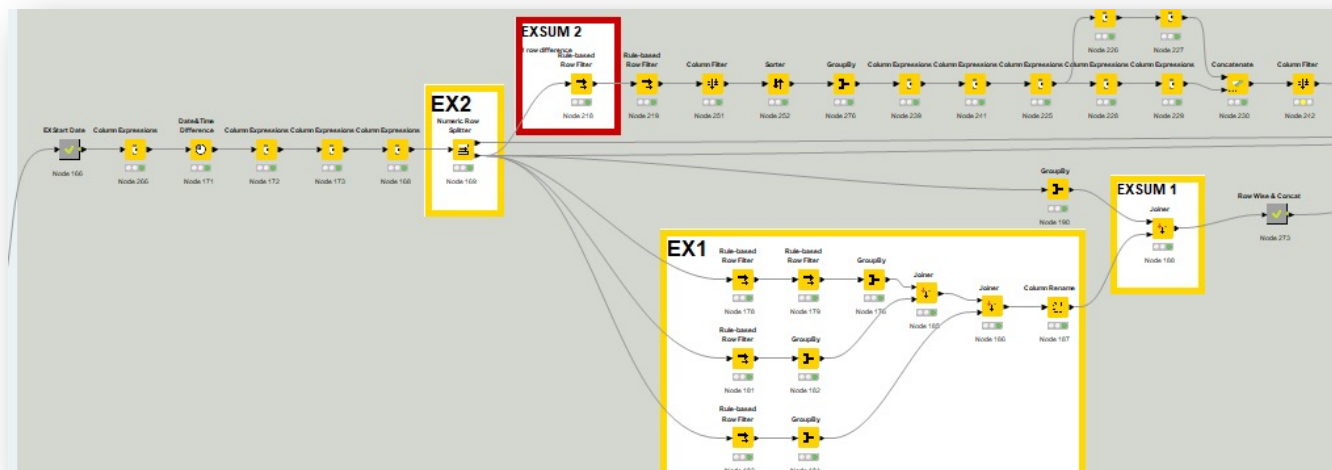
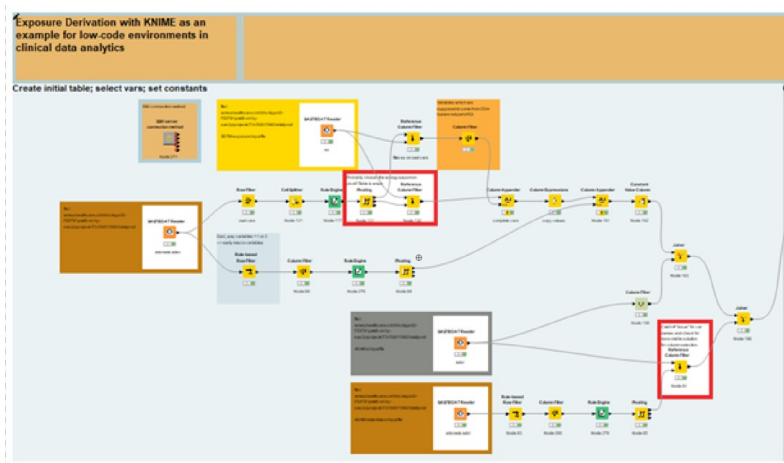


SAS7BDAT Reader



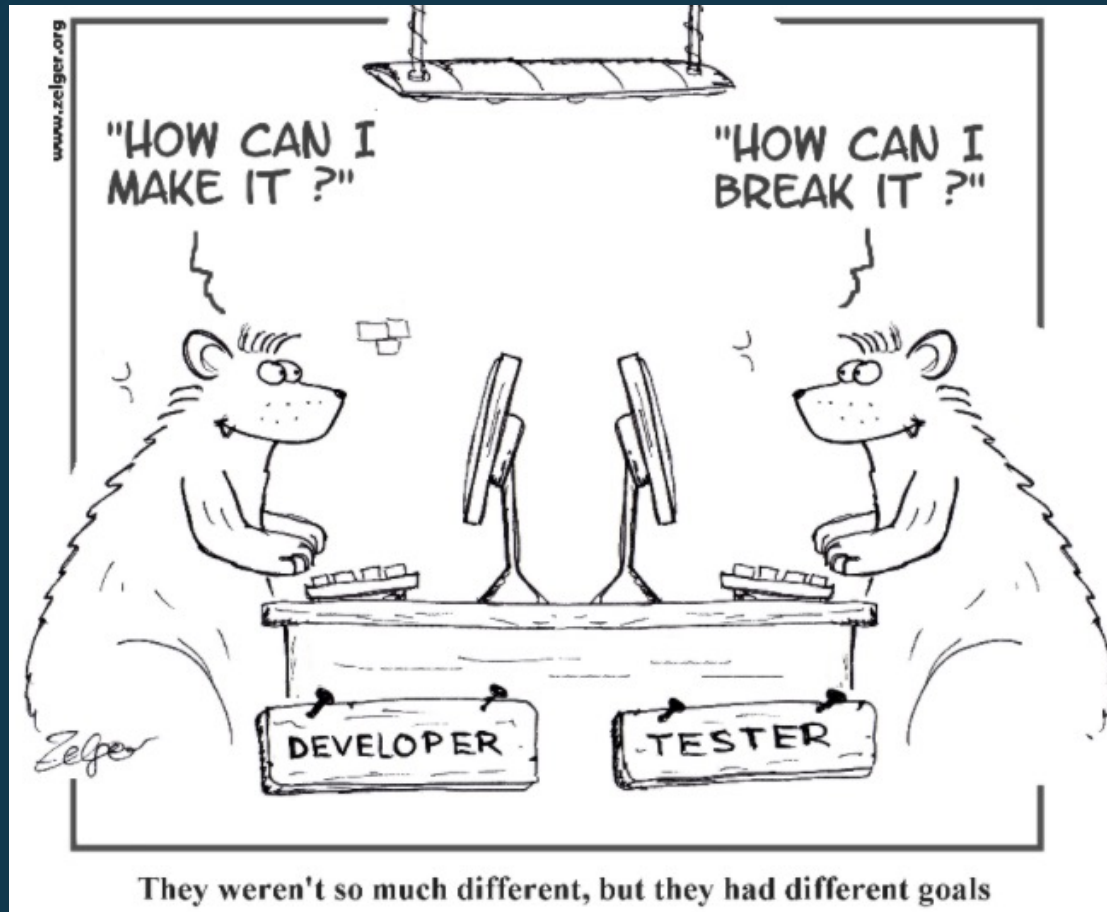


CDISC Guided Exposure Derivation With Real Clinical Data



- Complex derivation of ADEX with internal clinical data
- Annotations enable structuring and documentation

Validation, Testing, Logging, Reporting





Double Programming Validation

Dear PODR – no offense ☺ you have a typo!

Value differences

[S] RowId ...	[S] RowId ...	[S] Column...	[?] Value Compared Table	[?] Value Reference Table
Row0_Row0	Row0	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row1_Row1	Row1	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row2_Row2	Row2	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row4_Row3	Row4	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row6_Row4	Row6	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row8_Row5	Row8	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row10_Row6	Row10	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...
Row11_Row7	Row11	EVNTDESC	Dermatologic Event Occu...	Dematologic Event Occu...

Derived data table

Table Difference
Finder



Compare to Reference

Gold standard data set;
PODR ADTTE
(or SAS derived data)

Domain differences

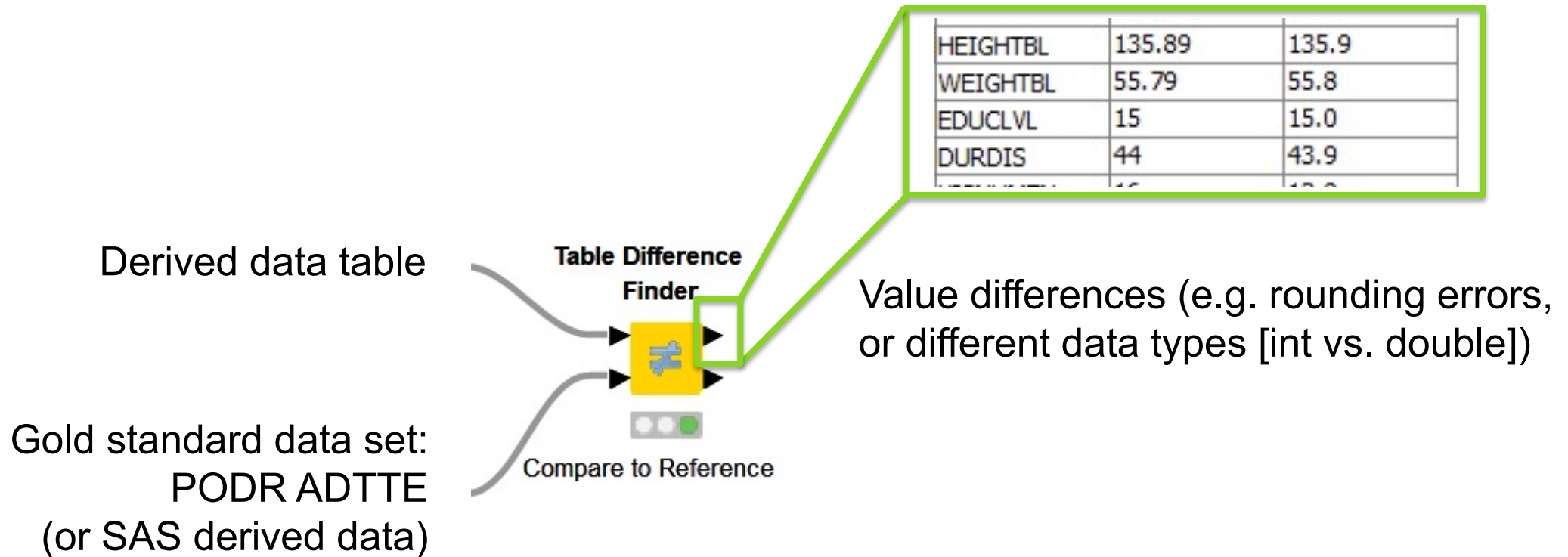
PARAMCD	PARAMCD	true	true	true
AVAL	AVAL	true	false	true
STARTDT	STARTDT	true	true	true
CNSR	CNSR	true	true	true
EVNTDESC	EVNTDESC	true	false	true

Domain differences are an additional
validation layer

For numeric: min / max (range) differs
For nominal: different unique values



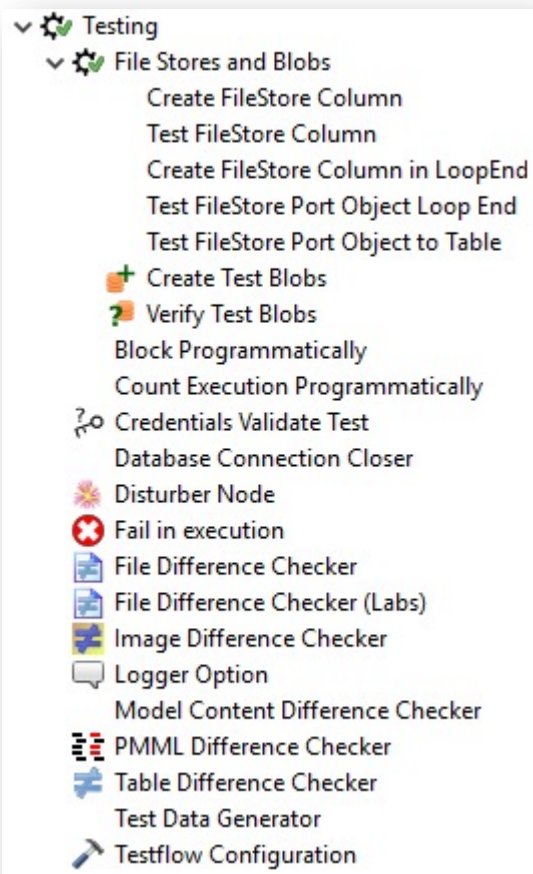
Double Programming Validation





Testing

<https://www.knime.com/blog/enter-the-era-of-automated-workflow-testing-and-validation>

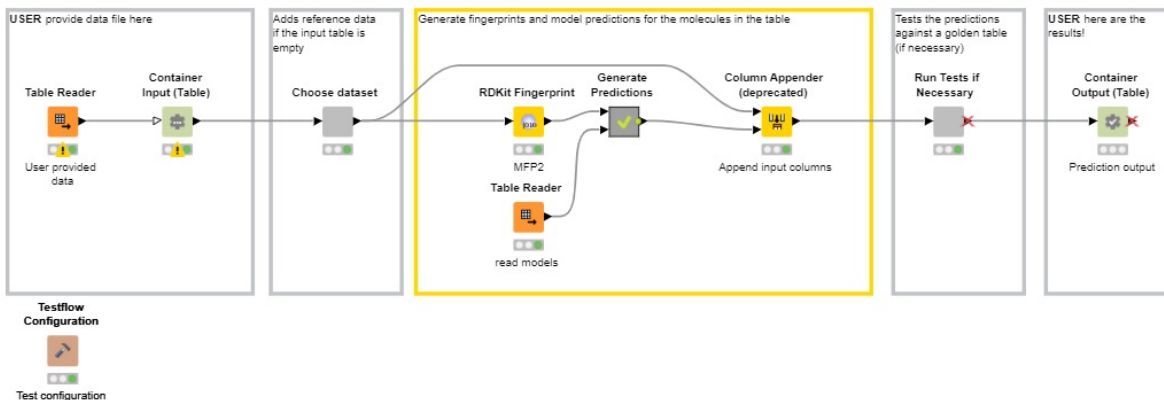


Validating KNIME Workflows

reproducibility validation testing XGBoost RDKit

Last edited: 26 Feb 2021

This workflow demonstrates a technique to deploy a model prediction workflow as a web service and to validate that it is doing what it's supposed to do.



All relevant testing scenarios can be covered



Logging

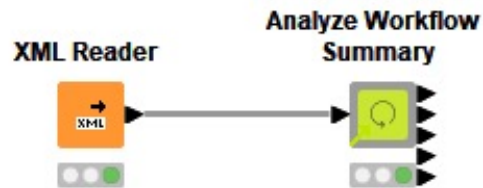
Export executed workflow summary

Verbose XML document traces all data points / transformations throughout a workflow



```
rs > gbeck > Downloads > adslsummary.xml > WorkflowSummary > environment > installation > plugins > plugin
<WorkflowSummary version="1.0.0" summaryCreationDateTime="2021-03-22 14:45:37 +0100"><environment knimeVersion="4.3.2.v202103051236" os="Windows 10"><installation><plugins><plugin
name="org.eclipse.osgi" version="3.15.200.v20200214-1600"/><plugin name="org.eclipse.osgi.compatibility.state" version="1.1.700.v20200207-2156"/><plugin name="javax.transaction"
version="1.1.1.v201105210645"/><plugin name="org.eclipse.equinox.simpleconfigurator" version="1.3.500.v20200211-1505"/><plugin name="cc.mallet" version="2.0.8.v20180913-knime"/
><plugin name="com.amazonaws.aws-java-sdk-core" version="1.11.602"/><plugin name="com.amazonaws.aws-java-sdk-s3" version="1.11.602"/><plugin name="com.amazonaws.aws-java-sdk-sts"
version="1.11.602"/><plugin name="com.epam.parso" version="2.0.2"/><plugin name="com.fasterxml.jackson.core.jackson-annotations" version="2.11.0"/><plugin name="com.fasterxml.
jackson.core.jackson-core" version="2.11.0"/><plugin name="com.fasterxml.jackson.core.jackson-databind" version="2.11.0"/><plugin name="com.fasterxml.jackson.dataformat.
jackson-dataformat-cbor" version="2.11.0"/><plugin name="com.fasterxml.jackson.dataformat.jackson-dataformat-xml" version="2.11.0"/><plugin name="com.fasterxml.jackson.datatype.
jackson-dataformat-yaml" version="2.11.0"/></plugins></installation></environment></WorkflowSummary>
```

Use third party tools or read back into KNIME and use the provided Analyzer component



org.knime.workbench.workflow...	4.3.0.v202011191609
org.knime.workflow.migration	4.3.0.v202011191336
org.knime.xml	4.3.0.v202011212018
org.mortbay.jetty.server	6.1.26
org.mortbay.jetty.util	6.1.26
org.mozilla.javascript	1.7.5.v201504281450
org.objectweb.asm	5.0.4
org.openqa.selenium	3.12.0.v202010300...
org.reactivestreams.reactive...	1.0.3
org.sat4j.core	2.3.5.v201308161310

Installed plugins

Column Expressions	Manipulator	13
Column Filter	Manipulator	2
Column Rename	Manipulator	10
DB Query Reader	Source	9
Date&Time Differ...	Manipulator	2
Date/Time Shift (l...	Manipulator	4
Extract Column H...	Manipulator	1
Extract Context P...	Source	1
Extract System Pr...	Source	1
GroupBy	Manipulator	4
Java Snippet (sim...	Manipulator	1

Used nodes

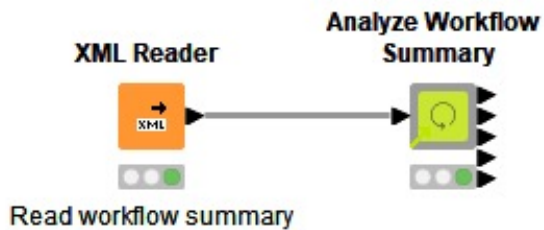
S Knime Version	S OS	S WF Author	S Creatio...	S Last Edi...	S Last Up...	S WF Description	S summaryCreationDate...	S WF Title	[...] WF An...
4.3.2.v202103051236	Windows 10	Robert Adams & Clara Beck	2021-03-02	?	?	PHUSE_Workflow_ADSL_PODR Demonstrates ADSL derivation from PODR data sets for PHUSE US Connect 2021	2021-03-23 11:44:46 +0100	PHUSE_Workflow_ADSL_PODR	[]

Environment & Metadata



Logging

Export executed workflow summary



Node details:

- For each node input, state, configuration, settings, variables
- Data at input port, data at output port
- More verbose than usual SAS logs

Node details - 5:0 - Analyze Workflow Summary

File Edit Hilite Navigation View

Table "default" - Rows: 81692 Spec - Columns: 27 Properties Flow Variables

Row ID	B isComp...	B Deprec...	S parent...	B isMetan...	S OutputPort	S succee...	[...] precedingPort	[...] inputPort	S key	S value	S out_po...	S out_po...	S col_index	S col_name	S col_type	XML column...	XML column...
Row48	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table	7	VSORRES	Number (do...	<?xml v...	<?xml v...
Row49	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table	8	VSORRESU	String (do...	<?xml v...	<?xml v...
Row50	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table	9	VSSTRESC	Number (do...	<?xml v...	<?xml v...
Row51	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table	10	VSSTRESN	Number (do...	<?xml v...	<?xml v...
Row52	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row53	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row54	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row55	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row56	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row57	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row58	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row59	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row60	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row61	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row62	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row63	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					
Row64	false	false	Top Level	false	output port 1 (table)	?	[PostgreSQL Connector:368: output port 1]	[input port 1 (PortTy...	sql_statement	SELECT * F...	1	table					

KNIME Console

```
WARN Math Formula 5:2 No configuration available
WARN PostgreSQL Connector 7:368 DB Connection no longer available. Go to advanced settings to
WARN Column Expressions 7:8 An error occurred in script 1:
The provided date must not be null (at line 0, function: 'date')
ERROR Date/Time Shift (legacy) 0:306:199 Execute failed: org.knime.core.data.def.DoubleCell cannot
ERROR Date/Time Shift (legacy) 0:307:199 Execute failed: org.knime.core.data.def.DoubleCell cannot
WARN PostgreSQL Connector 8:368 DB Connection no longer available. Go to advanced settings to
WARN Column Expressions 8:8 An error occurred in script 1:
The provided date must not be null (at line 0, function: 'date')
WARN Column Expressions 8:8 An error occurred in script 1:
```



BIRT extension can be configured to write costumized reports (e.g. log information)

[illegible]



Conclusion & Take-aways



- Powerful (feature complete) alternative for working with (clinical) data
- Clinical data derivation possible
 - Alternative approach for double programming / validation of SAS derivations
 - Verbose logging & validation capabilities
- Visual programming especially for pipeline optimization, automation & educational purposes with great potential



- Academic development
 - Low speed in bug fixing & feature development
- Collaboration not straight forward with the desktop version alone (e.g. versioning of workflows, sharing of workflow files)



Want to learn more?

<https://sway.office.com/iVcxHWRpqzX6kEHK>



An open source Analytics platform for creating data science applications and services

by Clara Beck, Robert Adams & Srinivas Veeragoni

What is KNIME?

The KNIME (pronounced /nalml/, Konstanz Information Miner) Analytics Platform developed in 2006 at the University of Konstanz. It is a free and open source data workflow platform suitable for data integration, analytics, reporting, and system integration. Its graphical user interface is based on an intuitive modular pipeline components that allows the user to assemble different types of nodes into a processing workflow. The extensive library of nodes include functionality to access a diverse set of data sources and databases, perform text processing, apply analytics and machine learning techniques, and many other applications. See Figure 1.

KNIME Analytics Platform



Working principles and paradigms

A visual programming workflow represents small steps of functionality as nodes which are the smallest function blocks. A node can be understood as a function as part of a larger library in other programming languages. A node can be configured (you would normally pass parameters into a function), e.g. by specifying a file path, a query or output formats, or other node specific options. Nodes are connected by edges. The edges represent data flows and connect nodes, i.e. data gets consumed by an incoming edge at the input port, gets transformed / processed and is to be inspected at the output port. Each step of a workflow can be easily inspected in tabular format.

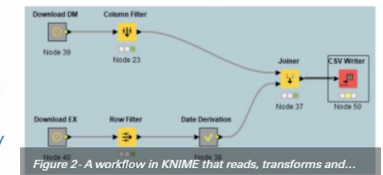


Figure 2 - A workflow in KNIME that reads, transforms and...



Acknowledgements



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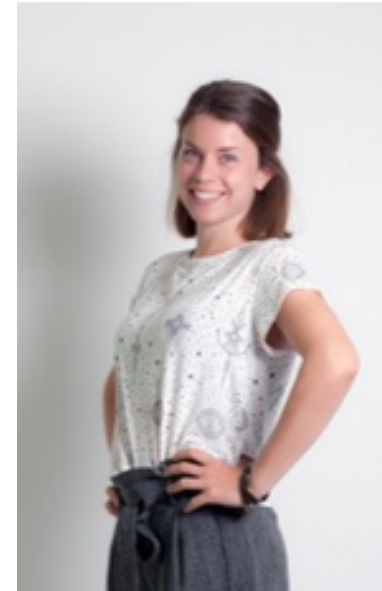
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PHUSE US Connect 2021

Presentation No: TT07

Title: Visual Programming for ADaM Derivation

Stream: Trends & Technology (TT)

Main Author: Robert Adams

Co-Author: Clara Beck



Thank you for the attention





Open the door

**Don't limit yourself to clinical
dataset derivation!**



Features & Extensions

Connectivity

Big data connectors (e.g. Hive, Kafka, Spark, Hadoop)

DBs

Files

APIs

Remote (SSH, Web)

Data wrangling

Text Mining

Cheminformatics

Bioinformatics

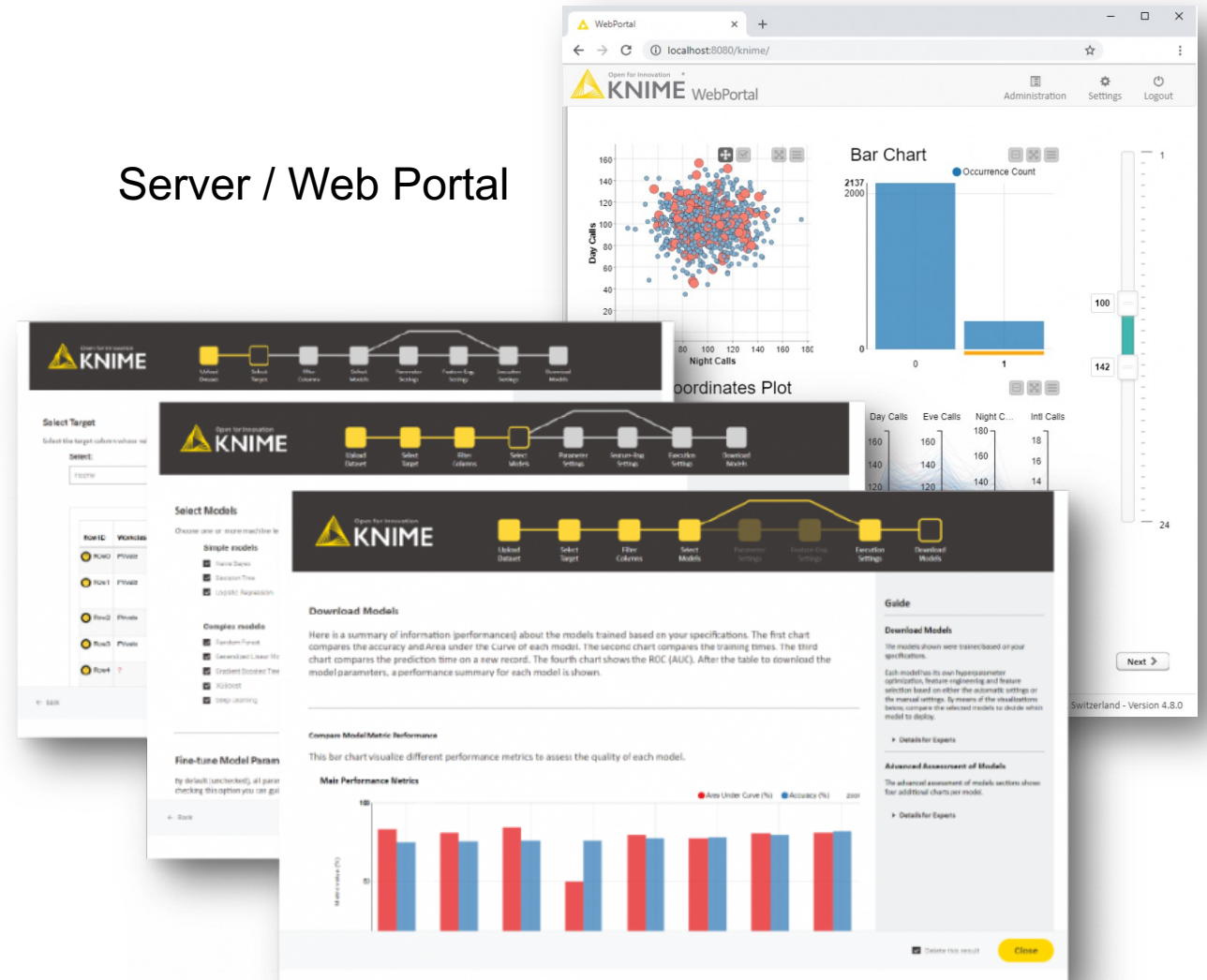
NGS

Image Analysis

Machine Learning / Deep Learning (codeless)

Create REST API endpoints from workflows

Server / Web Portal



Guided Analytics



Replication Instructions

- Download KNIME desktop:
<https://www.knime.com/downloads/download-knime>

KNIME Analytics Platform for Windows (zip archive)

- Extract (unzip)
- Start knime.exe
- Import *.knwf
- Set PODR credentials
- Execute workflow

