

# Machine Learning techniques in V&V of Nuclear Data Bases

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**INDUSTRIALES**  
ETSII | UPM

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## Outlier detection in EXFOR nuclear reactions library by ML techniques

INGENIA Students

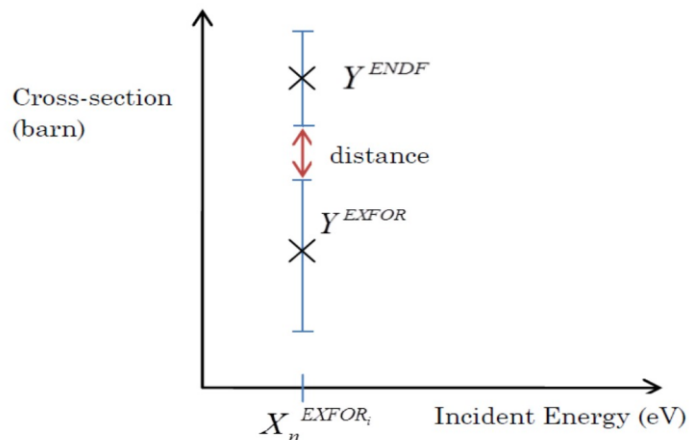
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*Ángela Torrelo*

*Juan Fernández*

*Sergio Moreno*

- ❑ EXFOR library: Compilation of more than 20.000 nuclear reactions experiments.
- ❑ Outliers:
  - Figure of merit ( $\chi$ , *distance*): Weighting the dispersion of the experimental value from the evaluated one.
  - Any kind of data (Cross sections, nu-bar, angular distributions, etc.) can be checked with the same test.
  - Special Case: Reactions with resonances.



$$\chi = \left| \frac{\sigma_{Ex} - \sigma_{Ev}}{\Delta\sigma_{Ex}} \right|$$

Figure. Principle of the method  
 Ref. Verification of the database EXFOR and ENDF.  
 JEFF Meeting 10/2016 (JEFFDOC-1778)

## Methodology

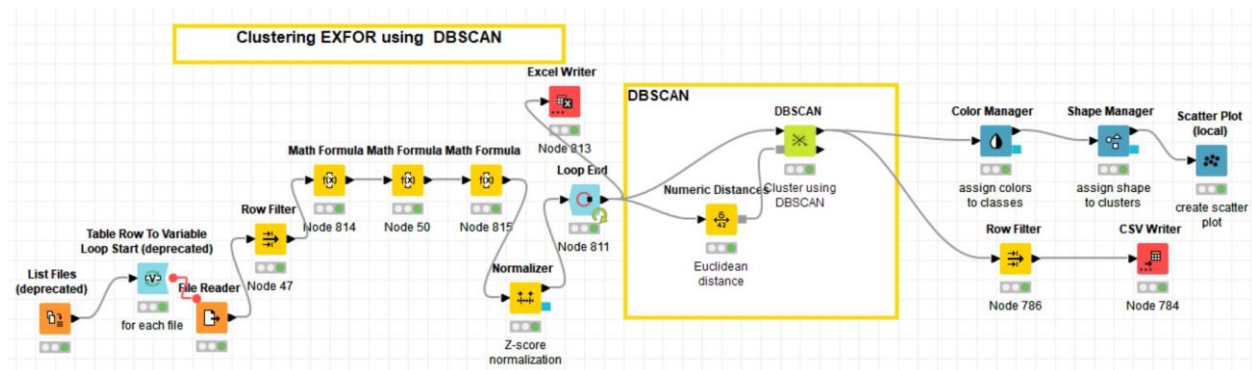
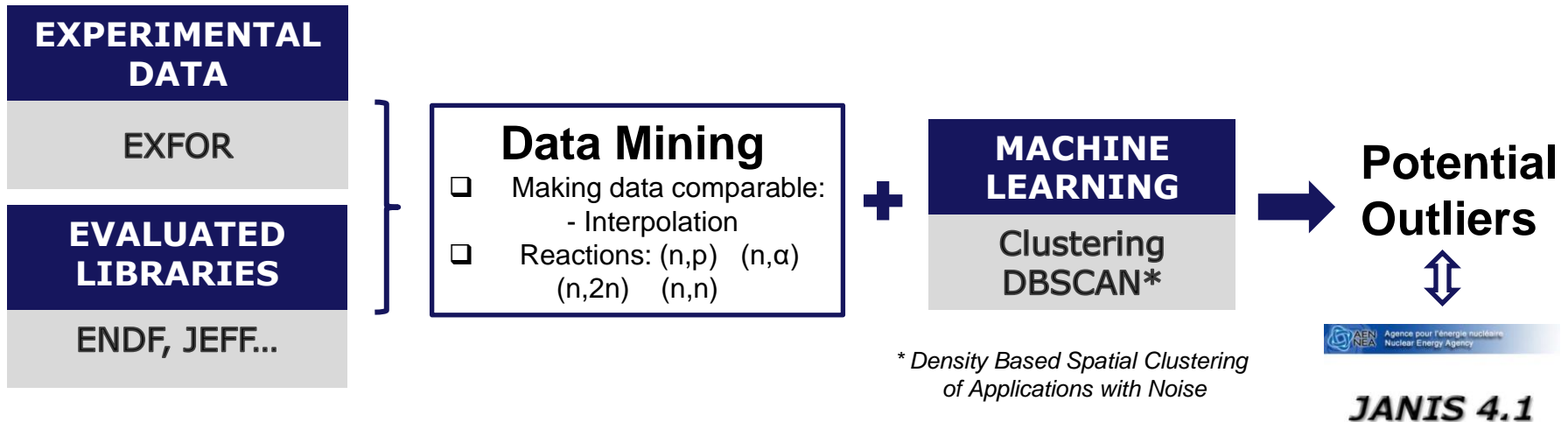


Figure. KNIME flowchart using DBSCAN

## Results

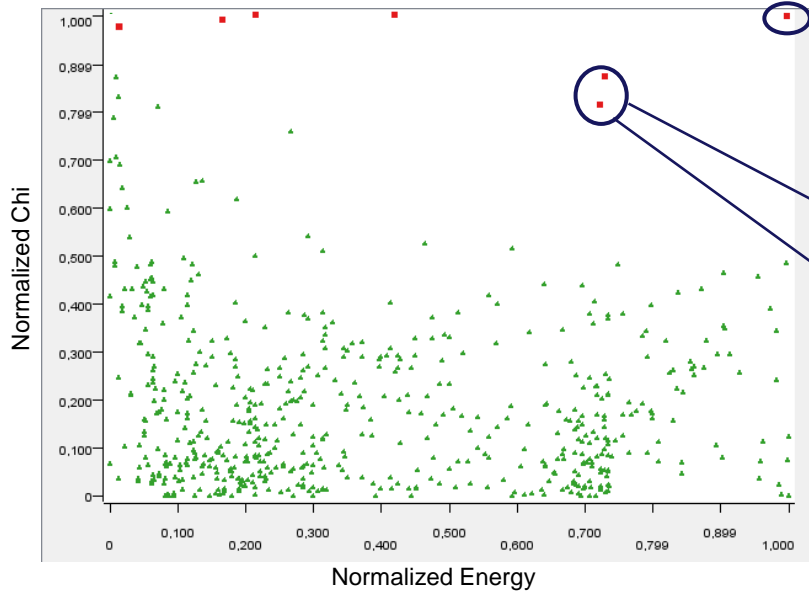
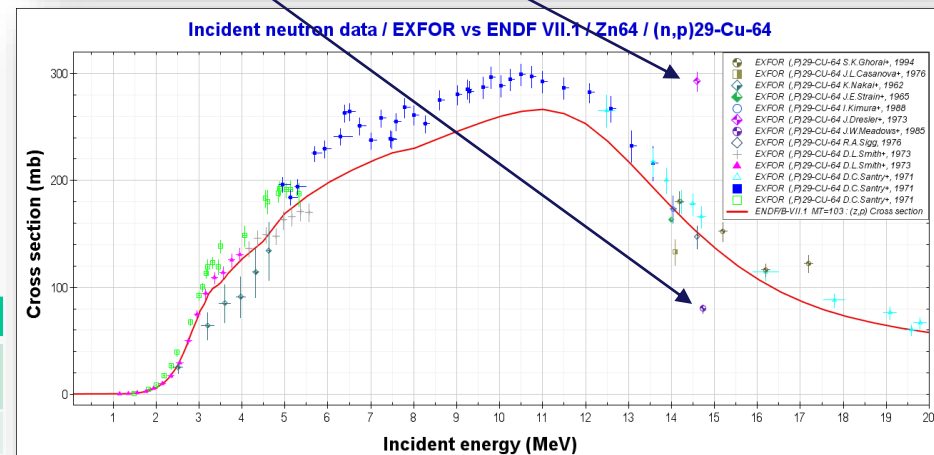
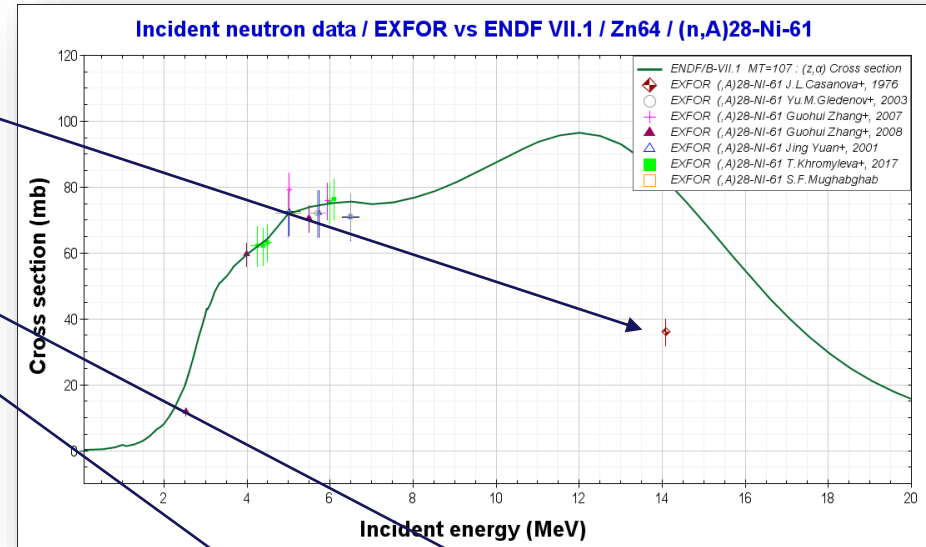


Figure. Clustering Knife  
Neutron incident reactions Zn64

Table. Potential outliers detected in (n,p), (n,α), (n,2n), (n,n) reactions

Material	Zn64	Al27	Pb204	Fe54	Ge76	Se80
Potential Outliers detected	7	7	6	27	1	4
% of total points	1.2%	0.4%	2.1%	2.4%	1.6%	0.9%





# Nuclear Data Validation using Statistical Parameters

INGENIA Students

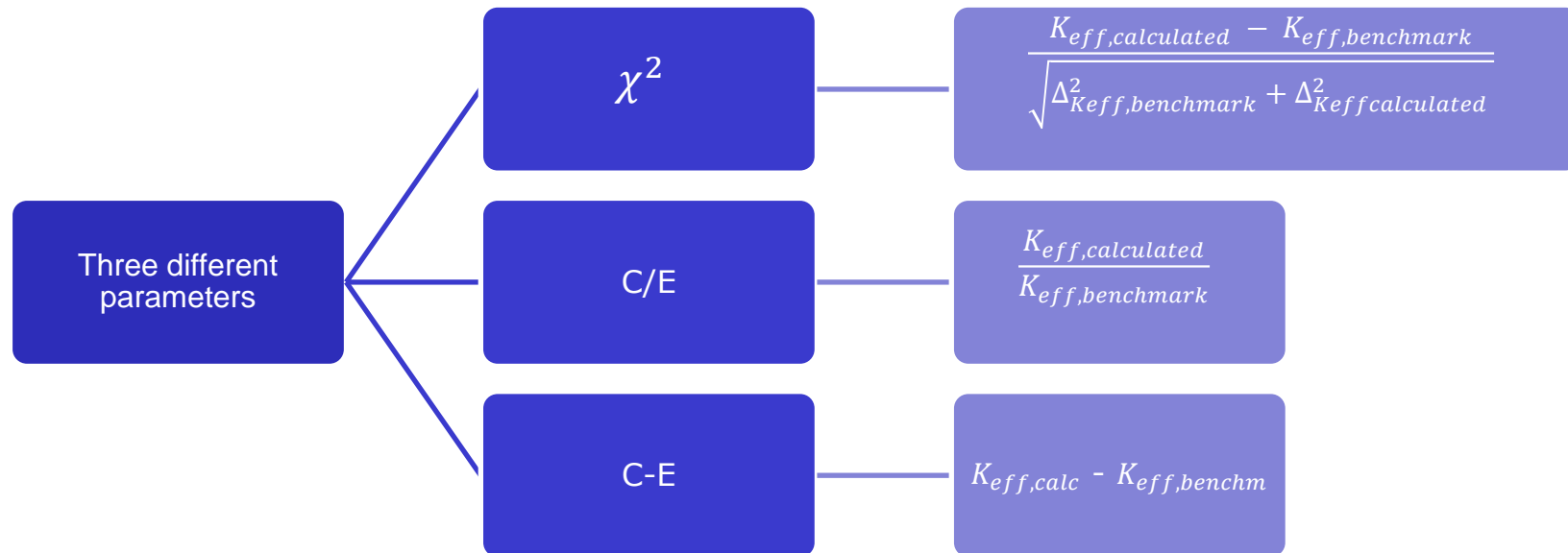
*Rodrigo Herráiz*

*Héctor Gutiérrez*

*Jorge Moreno*

*Beatriz Moreno*

❑ Nuclear Data Validation using Statistical parameters:



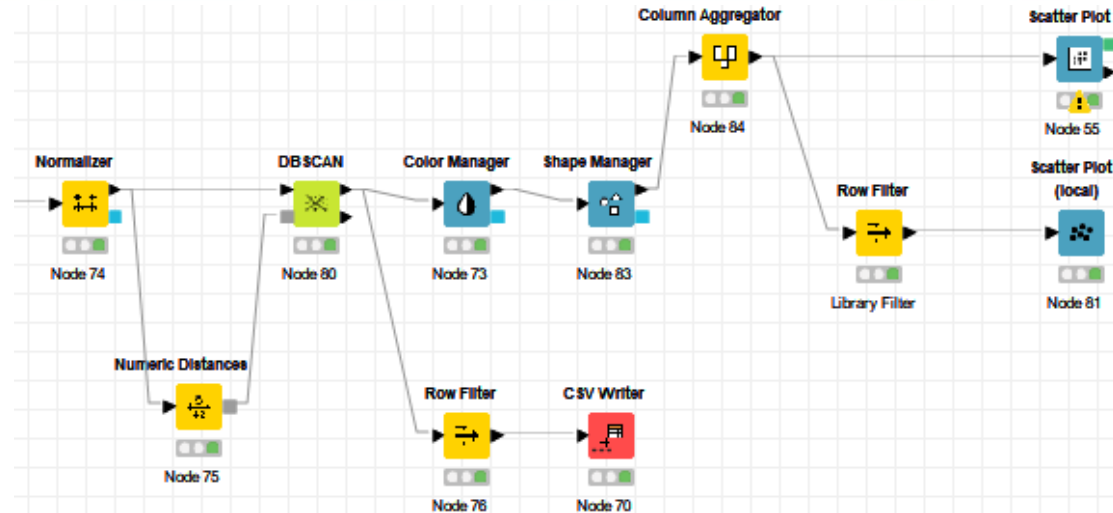
- ❑ Data from ICSBEP database.
- ❑ Detection of Outliers using Machine Learning.
- ❑ Identifying trends with DICE.
- ❑ Establishing comparisons between libraries.

ENDF Libraries
JEFF-3.3
ENDF/B-VIII.0
ENDF/B-VII.1
JEFF-3.1.1

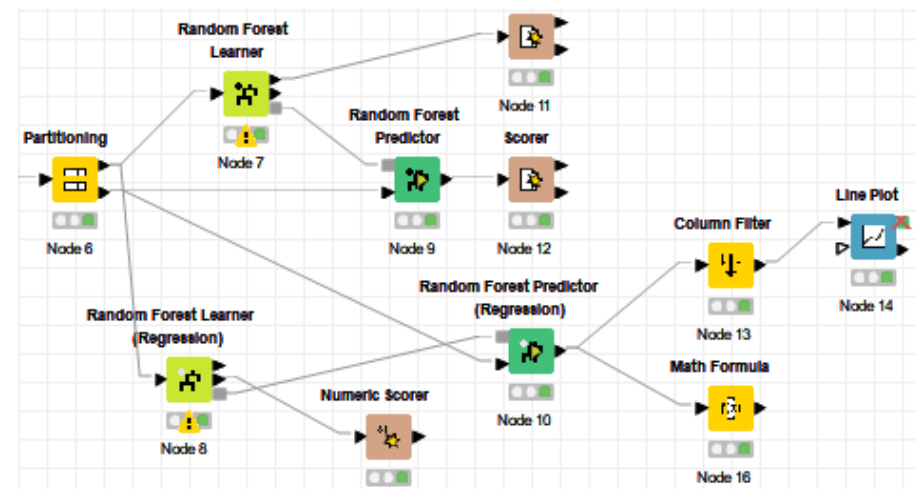
*Keff calculated by courtesy of SVDM. ~2200 benchmarks*



- ❑ KNIME Workflows
- ❑ Clustering Algorithms
  - DBSCAN algorithm
- ❑ Trends algorithms:
  - Random Forest Learner
  - Random Forest predictor
- ❑ Representing results:
  - CSV Writer
  - Scatter Plot
  - Line Plot

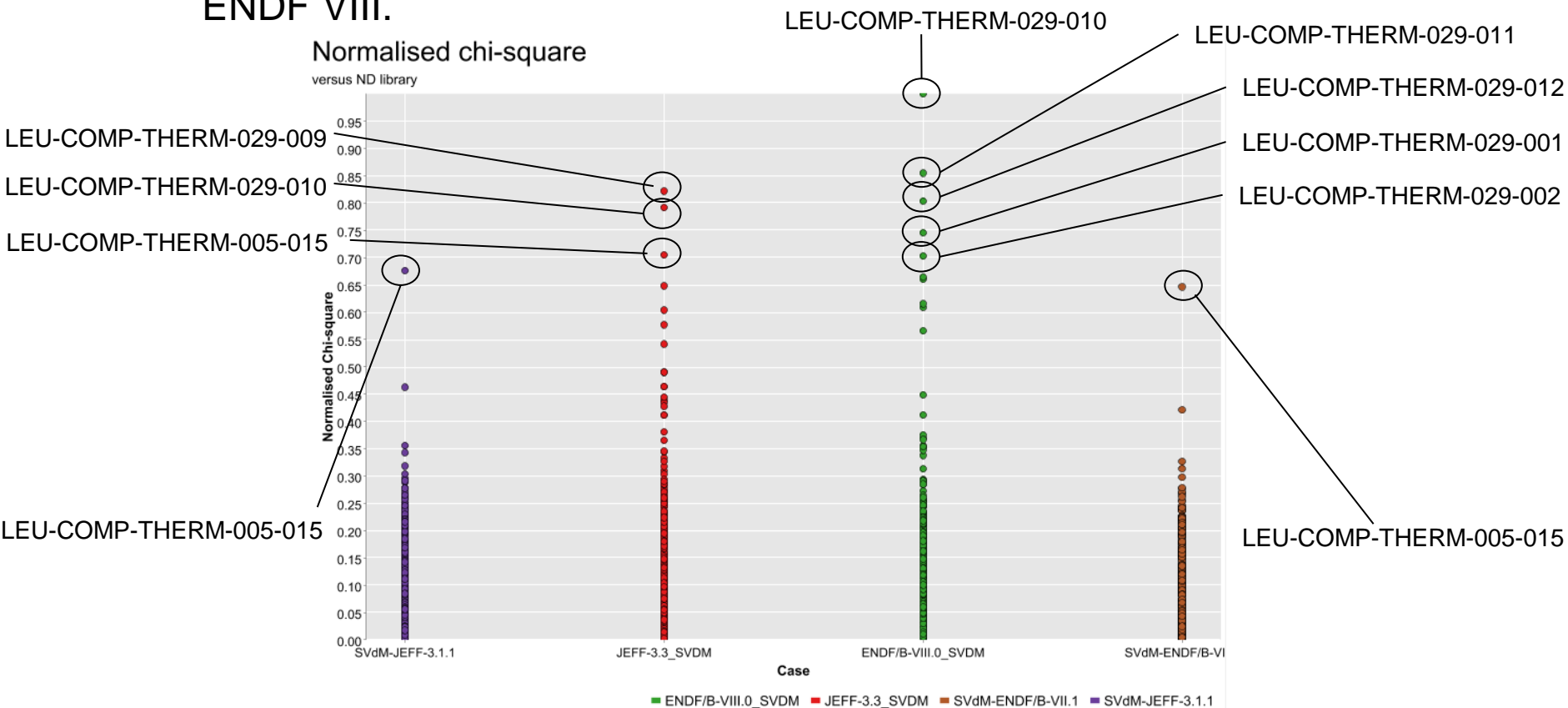


KNIME Workflow - Clustering



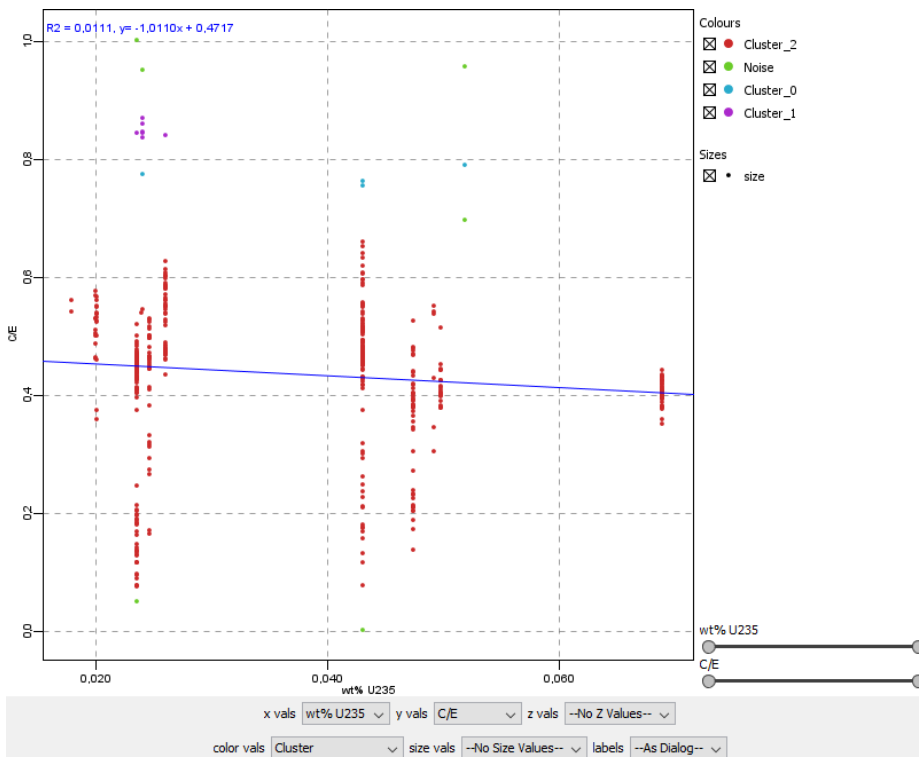
KNIME Workflow - Trends

- ❑ Outlier Detection: comparison between libraries
  - ❑ Evaluation LEU-COMP-THERM: more outliers in libraries JEFF 3.3 and ENDF VIII.

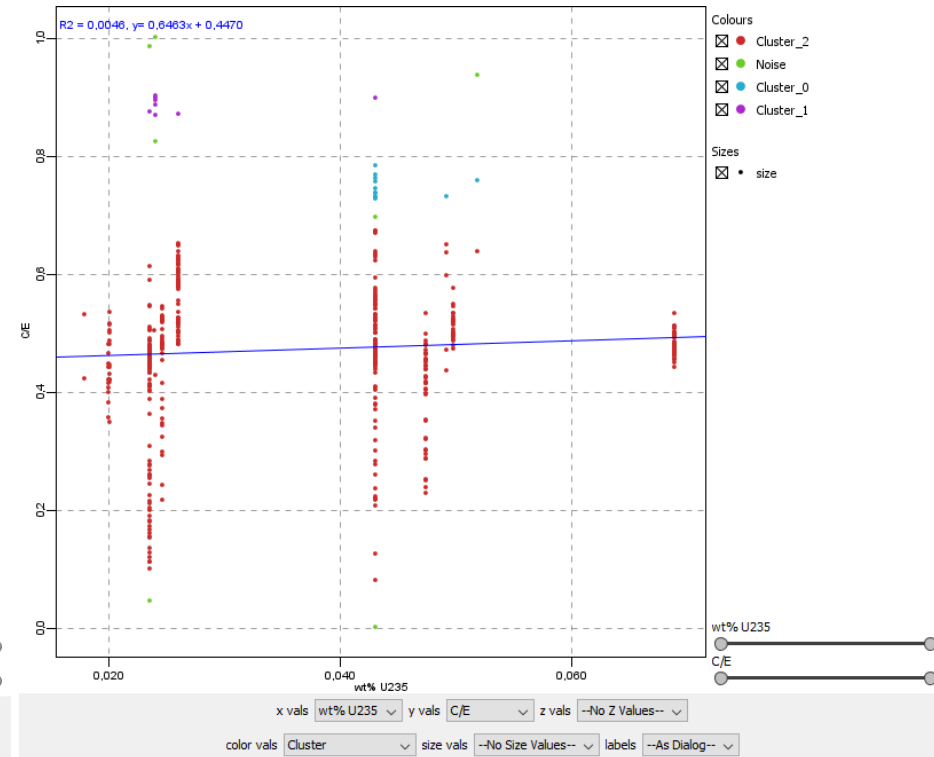


Outlier Detection per library LEU-COMP-THERM cases

## Identifying trends: LCT cases, C/E vs %wt U235

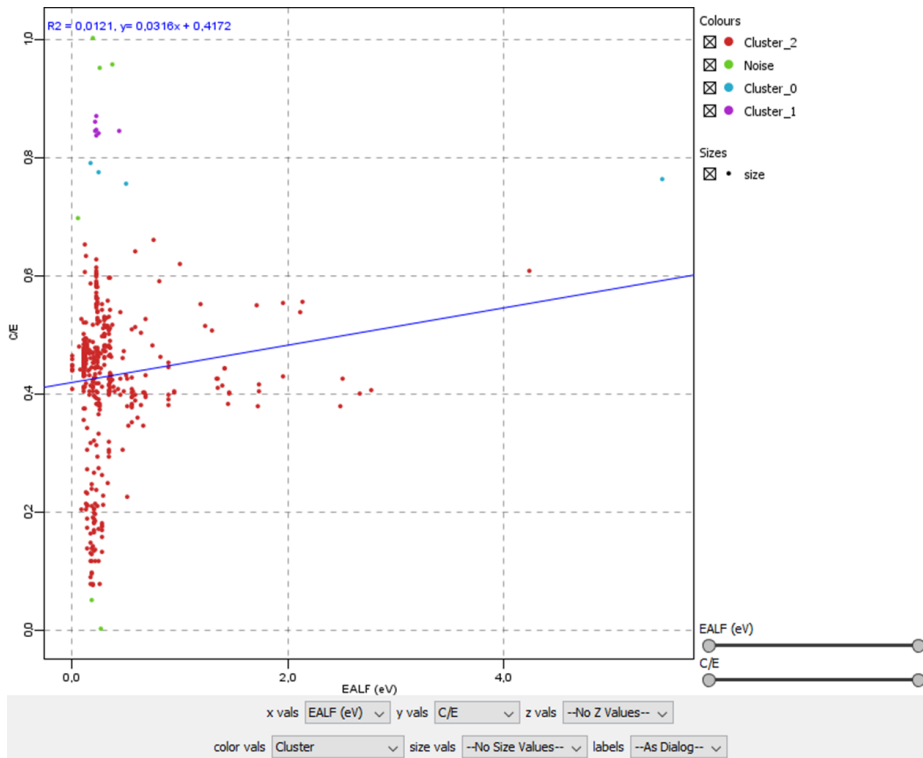


C/E vs.%U235 Trend - ENDF/B-VIII.0

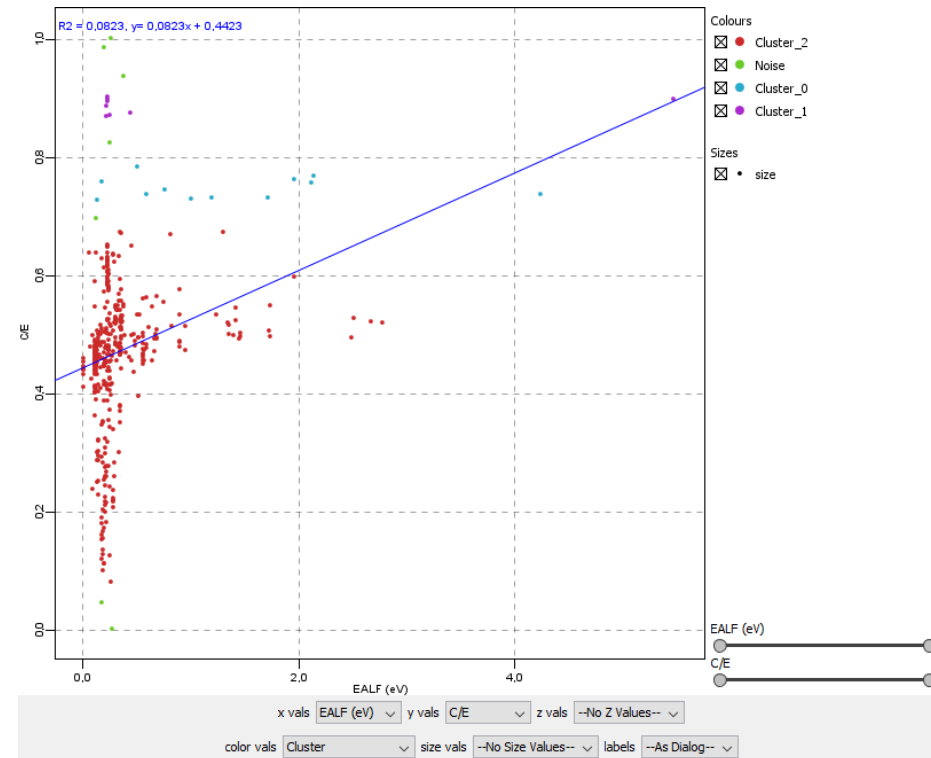


C/E vs.%U235 Trend – JEFF 3.3

## Identifying trends: LCT cases, C/E vs EALF (eV)



C/E vs. EALF - ENDF/B-VIII.0



C/E vs. EALF - JEFF 3.3



# Nuclear Data Verification using Uncertainty Calculations

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- ML using Uncertainty Evaluation
  - Keff Uncertainty ( $\Delta K_{eff}^{ND}$ ) due to Nuclear Data Uncertainties
  - Bias of Keff: C/E, C-E, chi-squared
  - Detecting potential Outliers and trends in the Databases

$$\Delta K_{eff} = \frac{\Delta K_{eff}}{\Delta \sigma} \Delta \sigma = \left[ \frac{\partial k}{\partial \sigma_1} \dots \frac{\partial k}{\partial \sigma_n} \right] * \begin{bmatrix} var(\sigma_1) & \dots & cov(\sigma_n, \sigma_1) \\ \vdots & \ddots & \vdots \\ cov(\sigma_1, \sigma_n) & \dots & var(\sigma_n) \end{bmatrix} * \begin{bmatrix} \frac{\partial k}{\partial \sigma_1} \\ \dots \\ \frac{\partial k}{\partial \sigma_n} \end{bmatrix}$$

*Keff Uncertainty Calculation*

Variable	Tool	Result
Covariance	JANIS/NEA	Errors or lack of covariance in libraries
Sensitivity	ICSBEP	Outlier Detection
Uncertainty	NDAST	Relation between Bias and Keff uncertainty

*Table. Parameters used in ND evaluation*

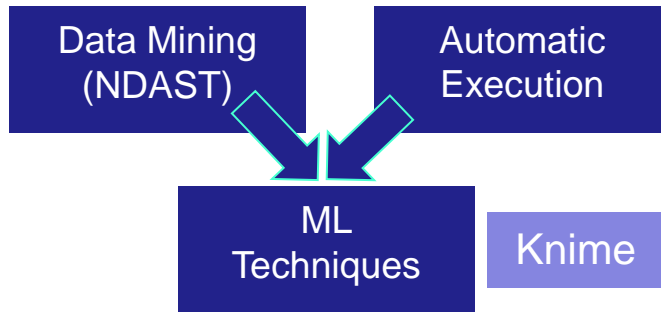
$$\chi^2 = \frac{K_{eff}^C - K_{eff}^{Exp}}{\sqrt{\Delta K_{eff}^{Exp2} + \Delta K_{eff}^{C2} + \Delta K_{eff}^{ND2}}}$$

$$\frac{C}{E} = \frac{K_{eff}^C}{K_{eff}^{Exp}}$$

$$C - E = K_{eff}^C - K_{eff}^{Exp}$$

*Keff Bias used in evaluation*

## Methodology



Retrieving covariance data in JANIS Database

Executing JANIS and NDAST in Command Line

Clustering Algorithms

- DBSCAN algorithm
- K-means workflow

Regression models

- $R^2$  and squared error minimization

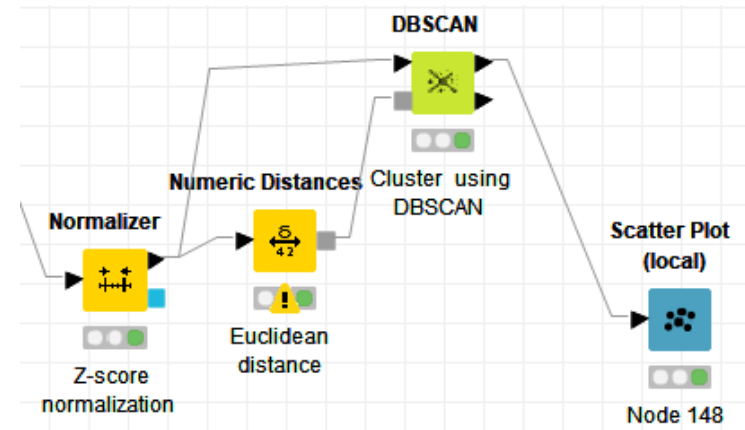


Figure. DBSCAN Algorithm with Knime

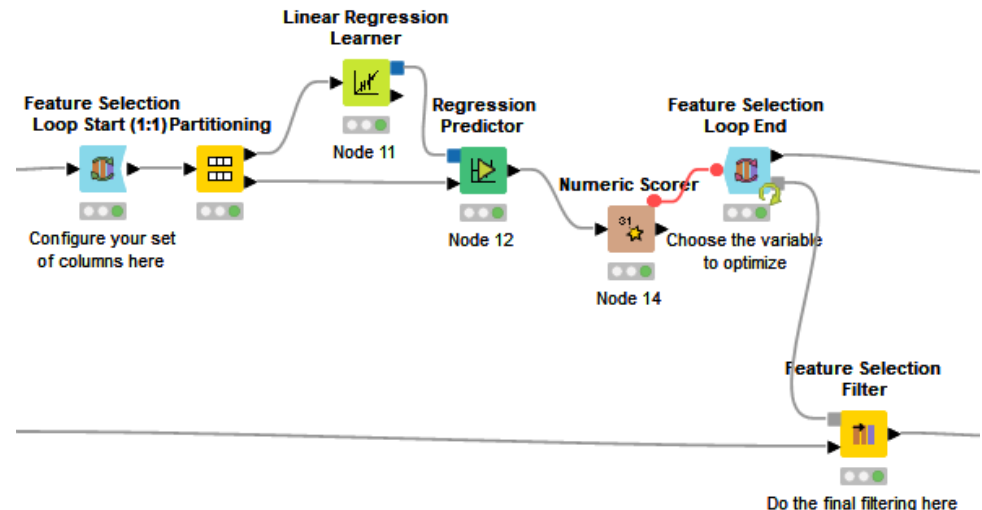


Figure. Regression Model with Knime

## ❑ ND Covariances of JANIS Databases

- JEFF-3.3 evaluation (by courtesy of SVDM ~2200 benchmarks)
- Missing values of covariance in JANIS Database ( $Pu^{242}$  and  $U^{236}$  for instance)
- Error processing covariances: 873 cases with relative error > 100%

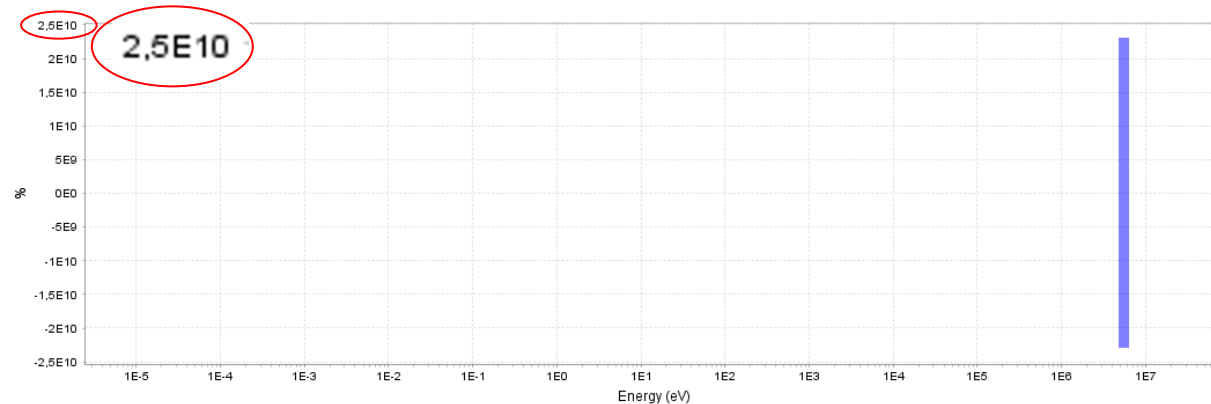


Figure. Relative standard deviation of inelastic reaction of  $^{16}O$

## ❑ Sensitivities of ICSBEP

- Problem running NDAST with “KENO ABBN-93” sensitivities, cause to have high uncertainty deviations in the benchmarks cases.
- Sensitivities are evaluated by elements instead of isotopes

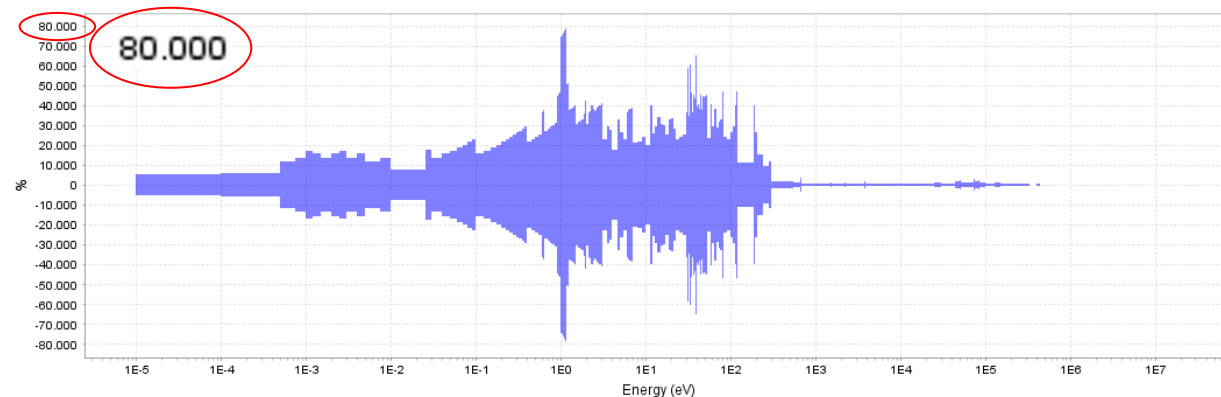


Figure. Relative standard deviation of n-alpha reaction of  $Fe^{57}$

□ Pattern recognition. For thermal systems:  $^1H$  (n,elastic),  $^1H$  (n,gamma),  $^{16}O$  (n,elastic), ...

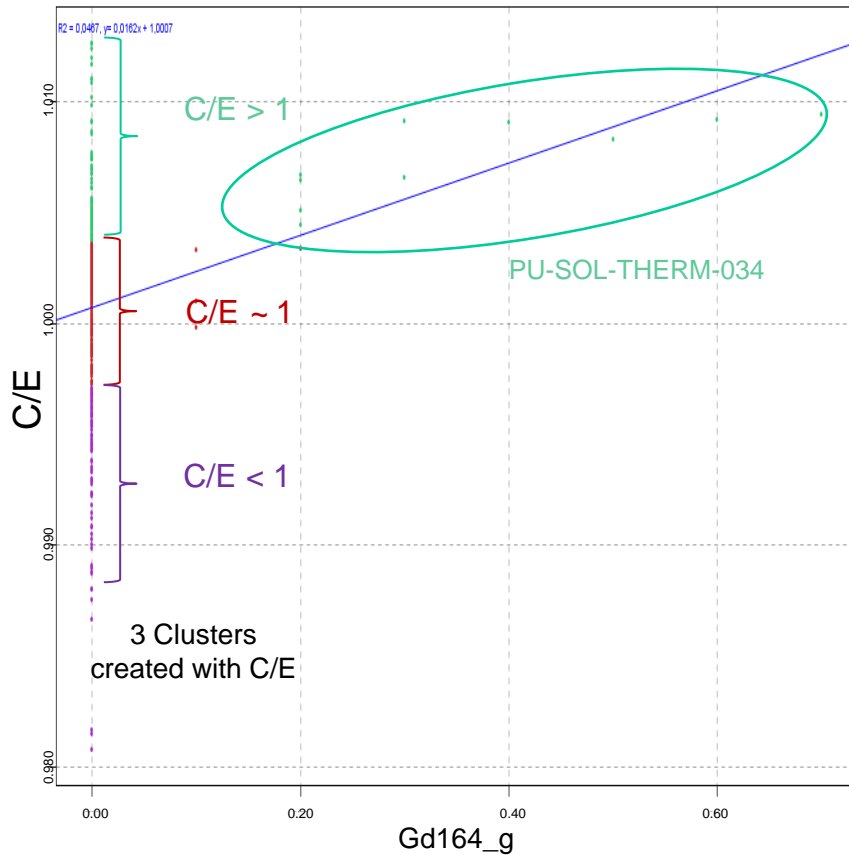


Figure. C/E vs  $K_{eff}$  Uncertainty due to  $^{164}\text{Gd}(n,\gamma)$  reaction for Plutonium experiments

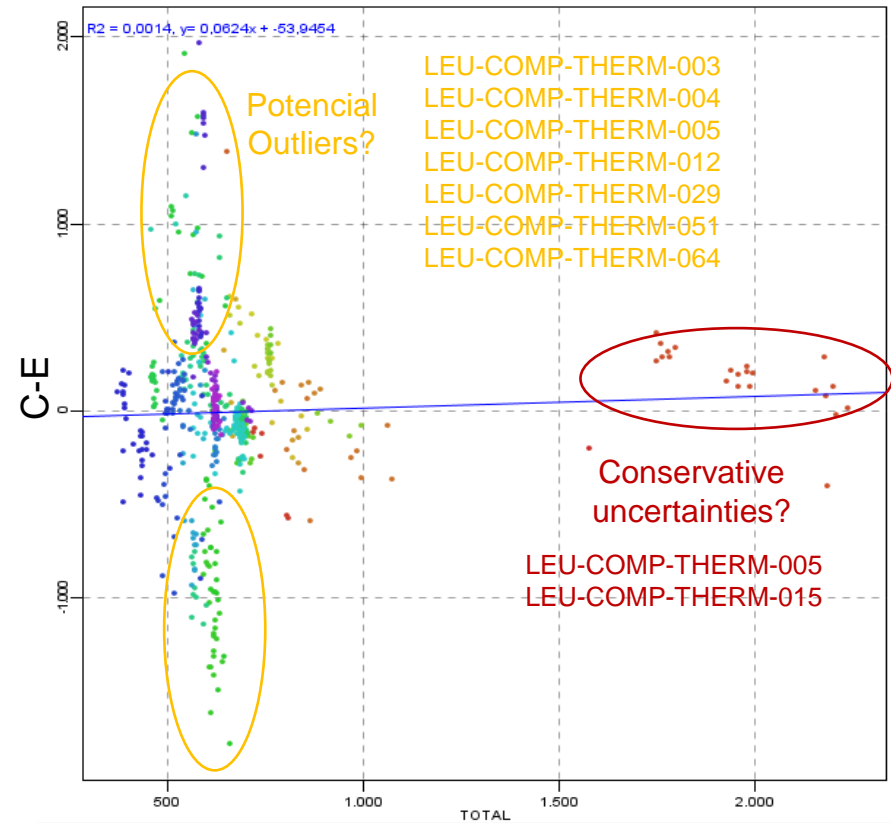


Figure. Bias vs **Total ND Uncertainty** in  $K_{eff}$  for LEU experiments



Thank you for your attention