

IRSN

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

IRSN contributions : *from TARs and S/U to V&UQ via DA*

*Key Actions and
New proposals*

MEMBRE DE

ETSON

EUROPEAN
TECHNICAL SAFETY
ORGANISATIONS
NETWORK

Layout

Introduction (motivation)

general statements

Data Assimilation (Bayesian-based inference)

Nuclear Data evaluation

ND libraries V&UQ

problem-oriented basic research

V&UQ using Data Assimilation

basic statements and protocol

required inputs: IEs and CND

TARs: complexities and opportunities

LWRs and safety assessment issues

MSFR concepts and an issue of controllability

Potential deliverables

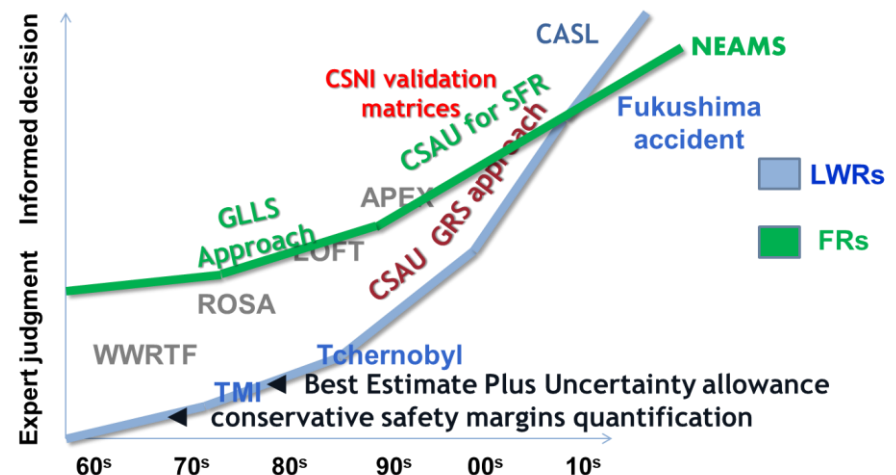
Phenomenological validation: objectives and trends

Commonly shared

- **progressive growth** => computational capacities & enhanced role of simulations
- imperative => all statements **to have a solid basis in reality**
- to be addressed => how far can we rely on modeling and do we have a **guidance for predictive capability maturity (PCM) characterization**
- In our understanding, PCM assessment = Validation => an entity made of => **Application Domain (applicability) characterization + Uncertainty Quantification**
- Validation has become a specific scientific discipline with its own concept system

Good practice and collaborations

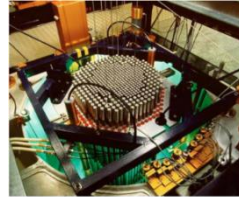
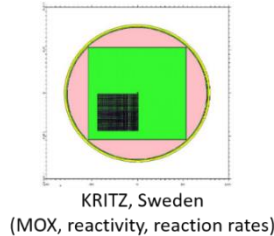
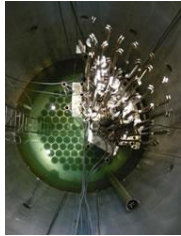
- **comparison with analogues:** Plant Measurements and Observations and experiments data (ex. CASL: *Consortium for Advanced Simulation of Light water reactors* www.casl.gov, 2014)
- **an understanding of sources** of uncertainties: Uncertainty identification and propagation (ex. GRS-like approach: *E. Ivanov, B. Rearden, J. Baccou and K. Velkov, "Role of a phenomenological validation and integral experiments for maturing the predictive simulations", NED, V 362, 2020*)



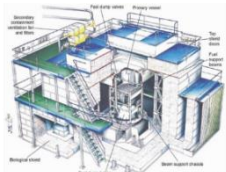
Phenomenological validation: practice and worldwide trends

From comparison

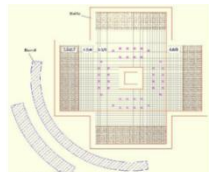
Legacy and newly designed IEs



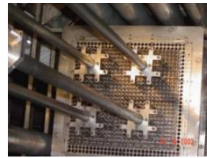
CROCUS, Switzerland
(transient processes)



Dimple, UK
(low power/ burnt fuel ~1% fima)



VENUS, Belgium
(zero power facility)



IPEN, Brazil
(UOX, reactivity, rates, kinetics)

Experiment	K-eff	Power/ Reaction rate	Temp. Effects	Spectral Indices	Kinetics	Borated/ Unborated	UO2/ MOX
CREOLE PWR (CREOLE-PWR-EXP-001)	Yes	Yes	Yes			Yes/ Yes	Yes/ Yes
CROCUS (CROCUS-LWR-RESR-001)	Yes				Yes	Yes/ No	Yes/ No
IPEN MB1 (IPEN(MB01)-LWR-RESR-001)	Yes			Yes	Yes	No/ Yes	Yes/ No
KRITZ1 (KRITZ-LWR-RESR-001, -002, -003)*	Yes	Yes	Yes			Yes/ No	No/ Yes
TCA (TCA-LWR-EXP-001)	Yes		Yes			Yes/ Yes	Yes/ No
DIMPLE (DIMPLE-LWR-EXP-001, -002)*	Yes	Yes		Yes		No/ Yes	No /Yes
VENUS-1 (VENUS-PWR-EXP-001, -003, -005)*	Yes	Yes				No/ Yes	Yes/ No
VVER Reactor (LR0-VVER-EXP-001)**	Yes	Yes	Yes	Yes		Yes/ No	Yes/ No

Origin, basis and remarks

References

- Dinh, Nam. *CASL Validation Data: An Initial Review*. United States: N. p., 2011. Web. doi:10.2172/1017862
- Hongbin Zhang, Review of Experiments for CASL Neutronics Validation (CASL-U-2012-0039-000)
- Joel A. Kulesza, Fausto Franceschini, Thomas M. Evans and Jess C. Gehin, **Overview of the Consortium for the Advanced Simulation of Light Water Reactors (CASL)**, EPJ Web of Conferences, 106 (2016) 03002

Notes:

- An intuitive - an expert-based judgement
- Cases selected to be similar to design, phenomena and processes one plan to deals with (<= in particular, LWRs core behavior)
- No one could be considered as fully representative (<= gaps existence)
- Once gaps being identified to be filled by newly evaluated or designed IEs data

Phenomenological validation: practice and worldwide trends

Basis and remarks

References

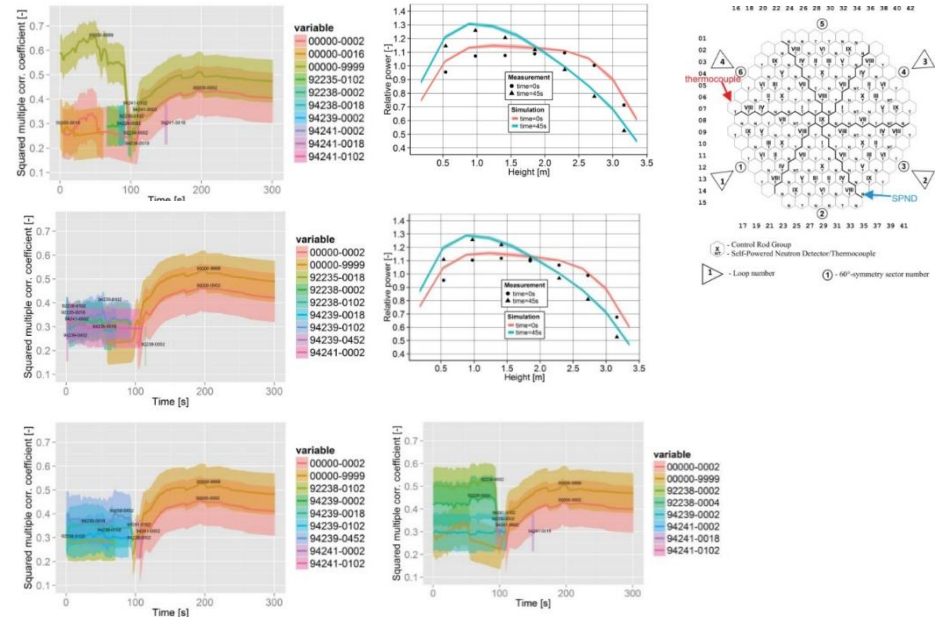
- E. Ivanov, B. Rearden, J. Baccou and K. Velkov, “Role of a phenomenological validation and integral experiments for maturing the predictive simulations”, NED, V 362, 2020
- A. Aures, N. Berner, W. Zwermann, (2020). Closing the Gap Between Sensitivity Analyses Based on Perturbation Theory and Random Sampling.
- W. Zwermann et al, Nuclear data U/S analysis with XSUSA for fuel assembly depletion calculations, Nuclear Engineering And Technology, Volume 46, Issue 3, 2014
- J.S. Martinez, W. Zwermann, O. Cabellos et al, Propagation of Neutron Cross Section, Fission Yield, and Decay Data Uncertainties in Depletion Calculations, Nuclear Data Sheets, Volume 118, 2014

Conditioned

- (IF) fully credible Covariance matrices of Nuclear Data (CND) and other uncertainties
- Continuous dependence on parameters and no methodological errors

From understanding of uncertainties

- GRS safety assessment approach (since 90s) => SUSAS, XSUSA, etc.

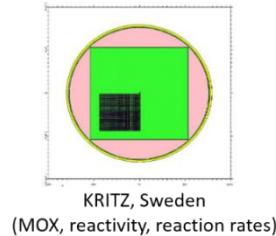
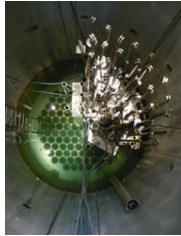


- Advantage => PMOs => known “macroscopic” output
- non-intrusive simple sampling frameworks
- Inferred contributions by XS uncertainties (CND) =>
- No links between available IEs and CNDs

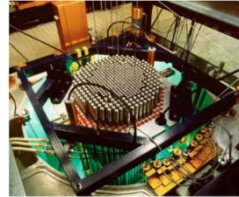
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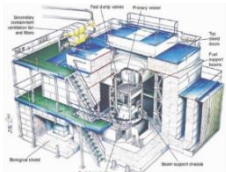
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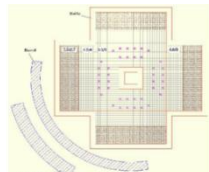
KRITZ, Sweden
(MOX, reactivity, reaction rates)



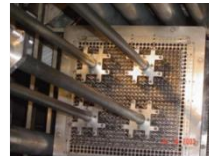
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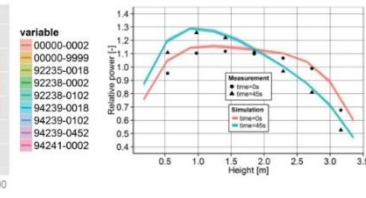
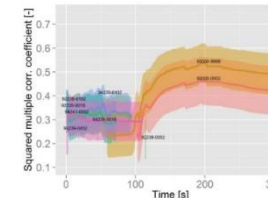
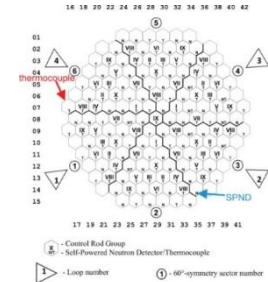
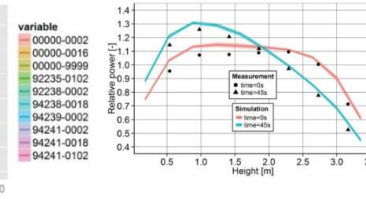
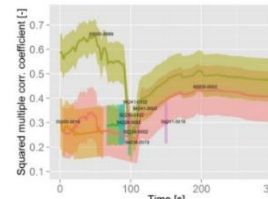
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(UOX, reactivity, rates, kinetics)

Questions to be addressed

- What is beyond an Experimental Domain => could any plausible set of IEs entirely "encompass" demanded Application Domains

From understanding of uncertainties

- GRS safety assessment approach (since 80s) => SUSAS, XSUSAS, etc.



Not academic but practical interest to V&UQ => reliance to a Decision making support
Step toward "science-driven" validation => merging approaches within a Data Assimilation

G. Palmiotti, M. Salvatores, "The Role of Experiments and of Sensitivity Analysis in Simulation Validation Strategies with Emphasis on Reactor Physics," *Ann. Nucl. Energy*, 52, 10-21 (2013)

Data Assimilation ⇔ best fit within uncertainty bounds 1#3

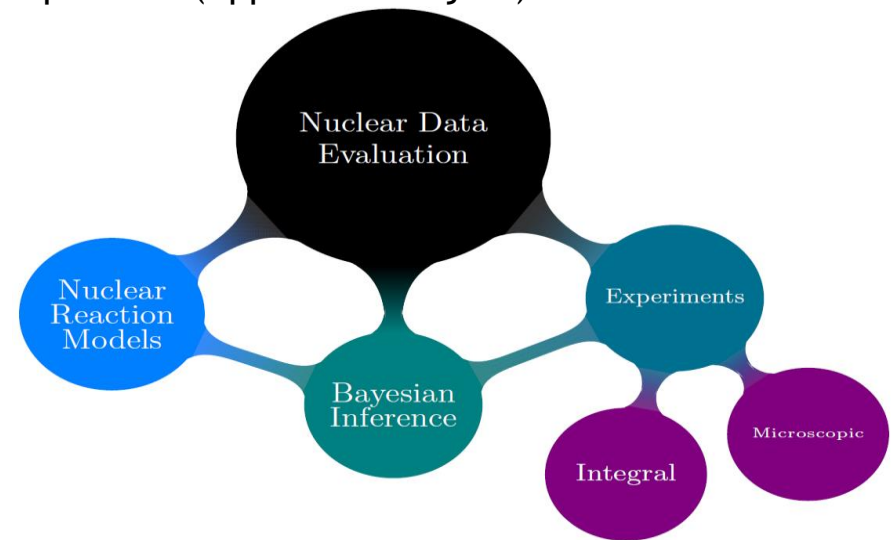
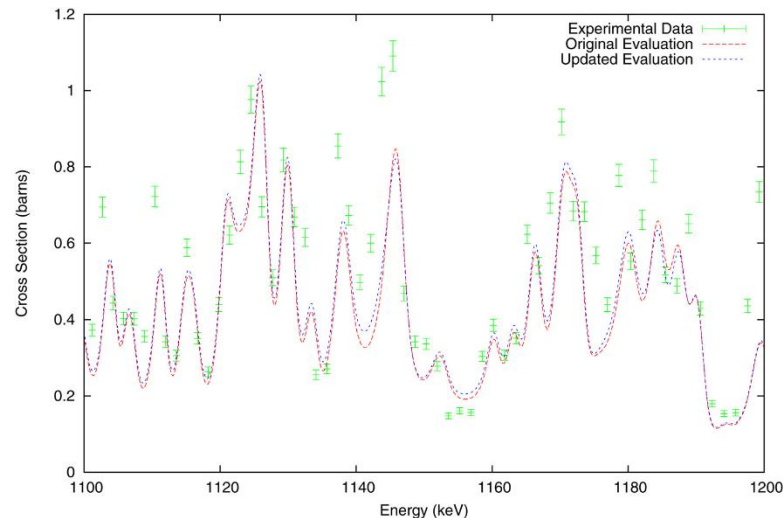
Simple lack of knowledge - *we don't know what we know* - theoretical model ⇔ almost fully consistent

Given => new IEs data => of higher resolution than existing one [selected representative IEs]

Task => to adjust libraries (parameters inherent to nuclear reaction modeling) => data adjustment

=> to generate design-oriented library => ERALIB1, ABBN-78 (SFRs), ENDF/B-V (LWRs), etc.

=> to adapt general-purpose library to a given problem (Application object)



Vladimir Sobes, Luiz Leal, Goran Arbanas, Benoit Forget, Resonance Parameter Adjustment Based on Integral Experiments, Nuclear Science and Engineering | Volume 183 | Number 3 | July 2016 | Pages 347-355 (⁵⁶Fe inelastic XS)

C. De Saint Jean, P. Archier, E. Privas, G. Noguère, B. Habert, P. Tamagno, Evaluation of Neutron-induced Cross Sections and their Related Covariances with Physical Constraints, Nuclear Data Sheets, Volume 148

Given => PMO (boron concentrations, burn-up, reactivity effects, transfer function)

Task => to “tune” a design-oriented (or exploitation support) tool => limited predictive capabilities

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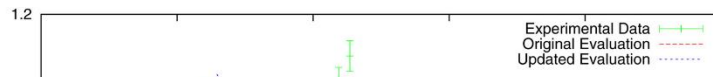
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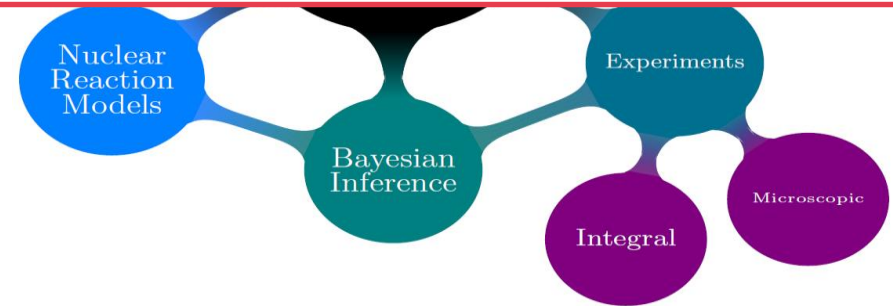
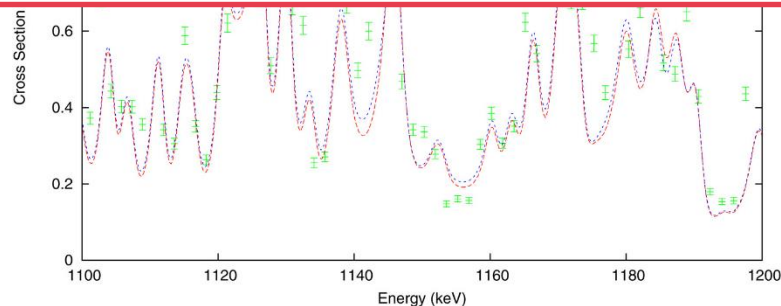
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The 1st application of Data Assimilation involving IEs data in a scientific turnover



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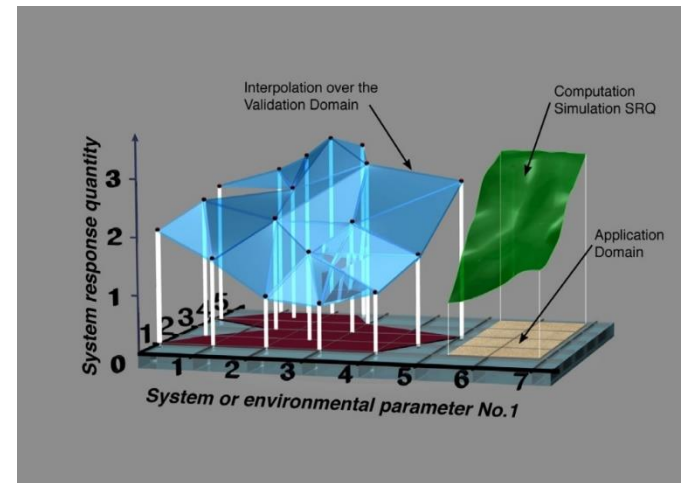
Data Assimilation ⇔ best fit within uncertainty bounds 2#3

Epistemic uncertainties - *we know that we don't know* - gaps in knowledge ⇔ theoretical model of limited consistency

Given => Objective Observations (C/E and relevant CIEs) against new IEs data (experiment-based benchmarks) => [**no one to be ignored** unless explained or of too low-fidelity]

Task => to characterize bias and uncertainty within an Application Domain (ill-posed inverse problem)

Notes => 1) Validation => Application-dependent; 2) Science-driven validation => Validation and Uncertainty Quantification; 3) extrapolation (transposition) => by parametrized model



In our case DA => to confirm a usefulness of general-purpose library within a given Application Domain

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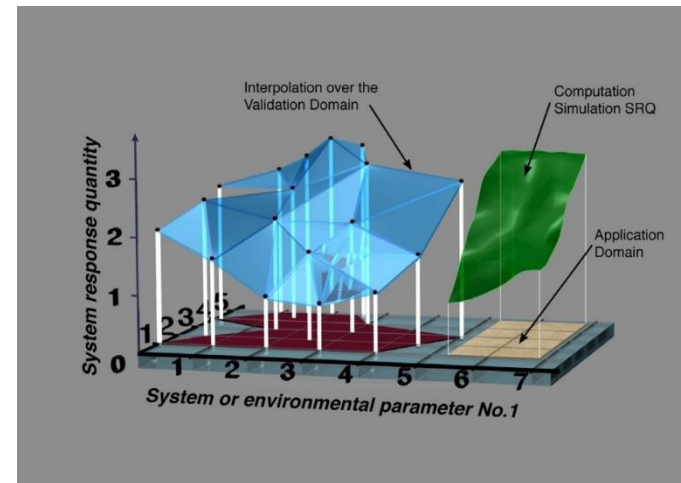
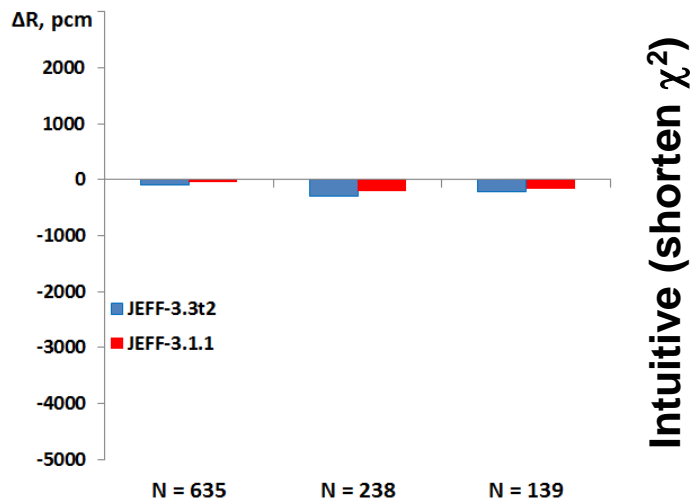
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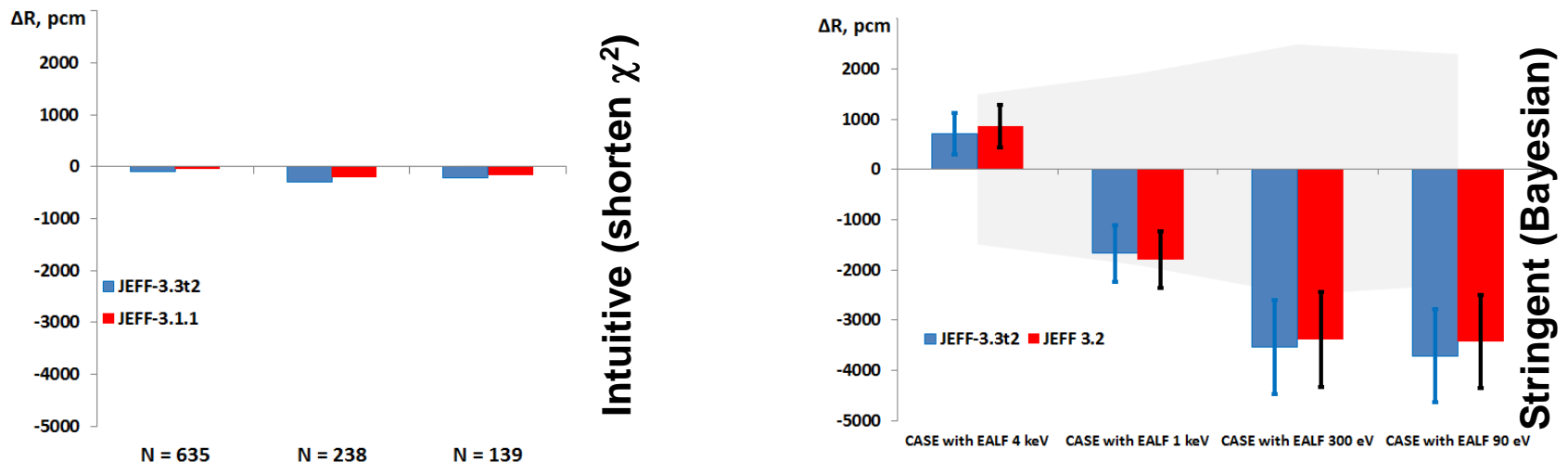
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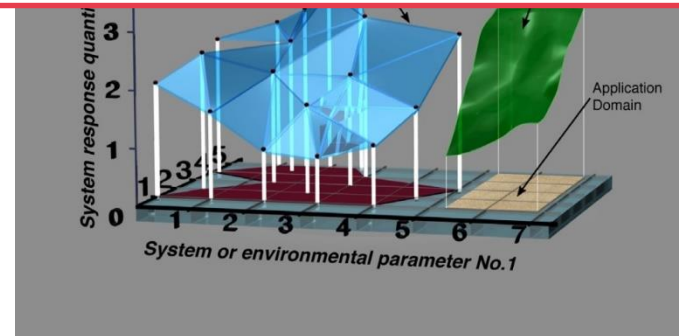
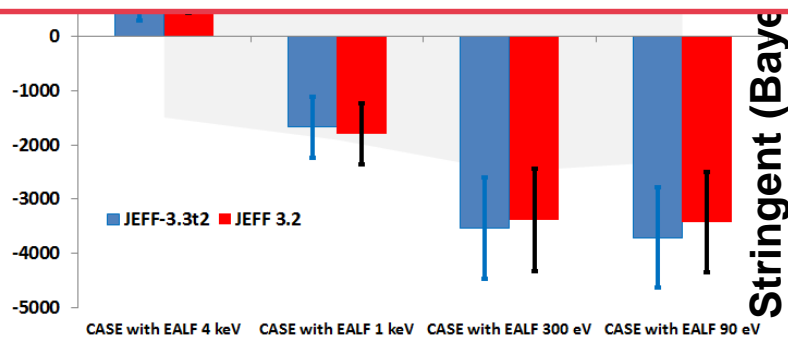
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The 2nd application of Data Assimilation providing an evidence-based background to V&UQP



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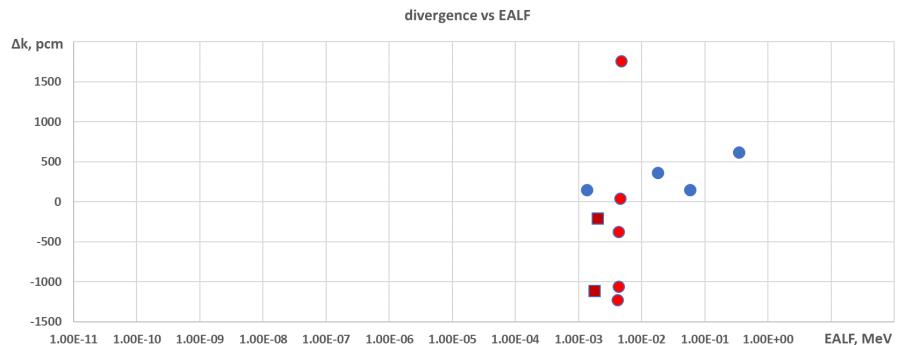
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Data Assimilation ⇔ best fit within uncertainty bounds 3#3

Ontological uncertainties (Ont) - *we don't know that we don't know* - deficiency in theoretical model

Given => Observations to be explained => **[seeking credible IEs data]**

Task => to clarify possibility to arise an ontological issue **[contribution to HPRL]**



C/E for dedicated experimental cases

Unexpectedly large divergences have been found if EALFs were one through tens of keV

T. Ivanova, I. Hill, Methodology and issues of integral experiments selection for nuclear data validation, *EPJ Web Conf.*, **146**, 2017

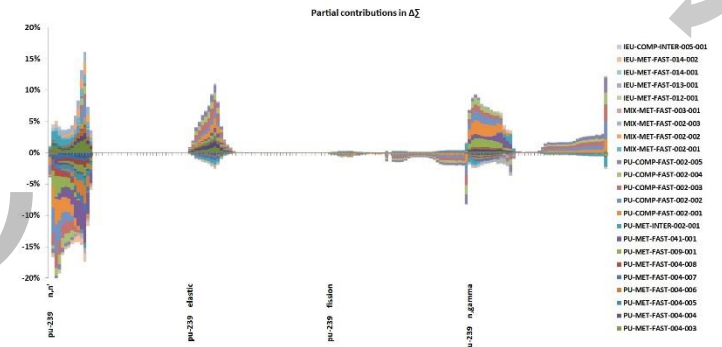
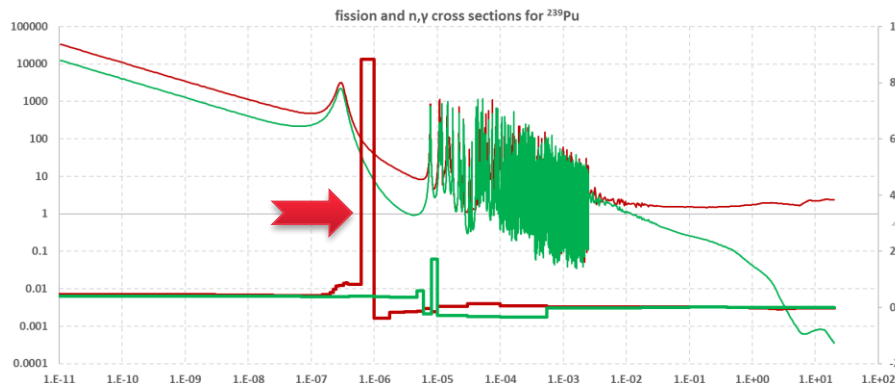
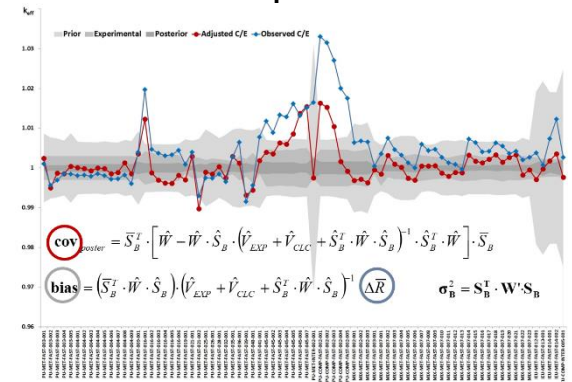
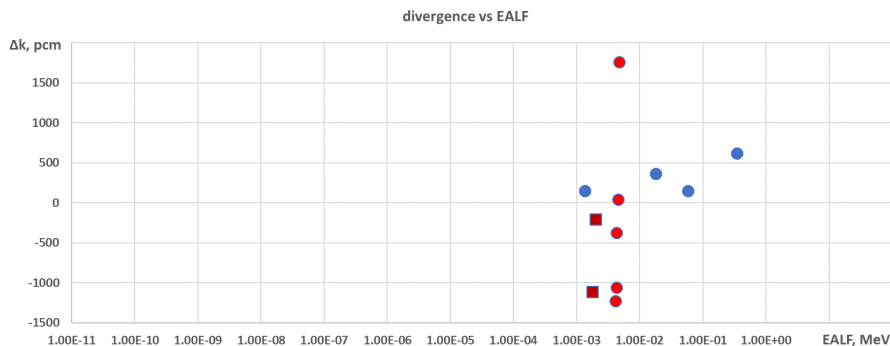
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The peaks on lower-left corner are NOT corrections but ratio between corrections with and w/o new IEs - *no more continuous dependence on a parameter - the only assumption in a Bayesian inference*

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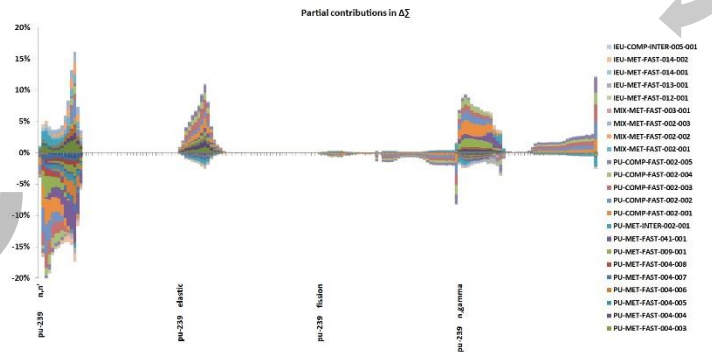
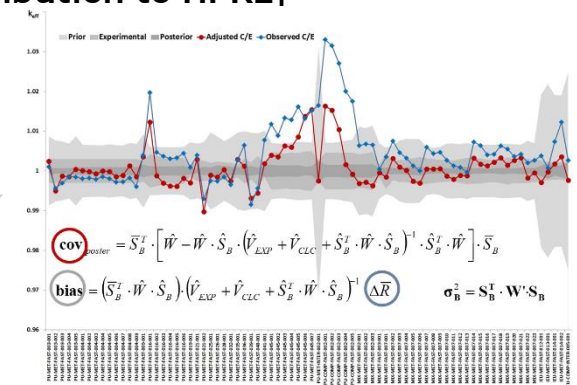
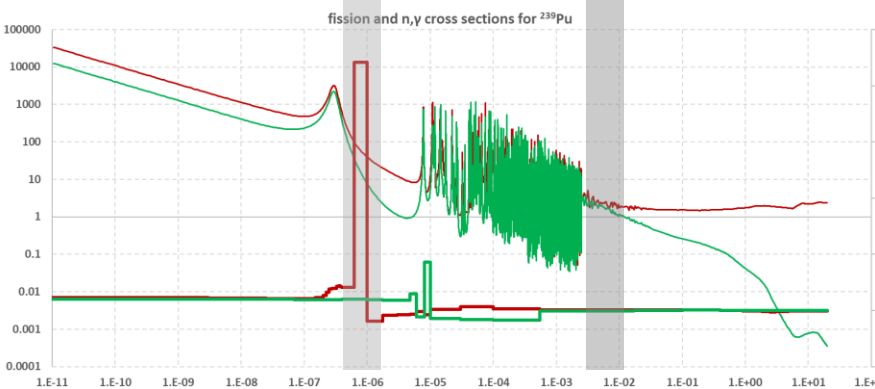
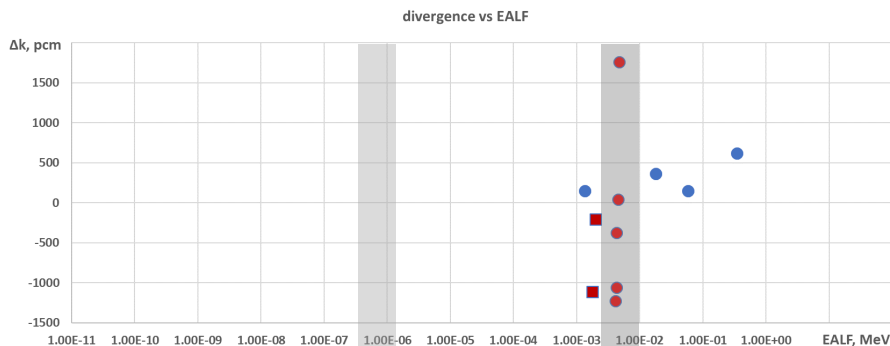
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Note => **Ont** surprisingly contradicts to the first guess: ^{240}Pu , EALF~100 keV => ^{239}Pu fission 0.3-0.8 eV

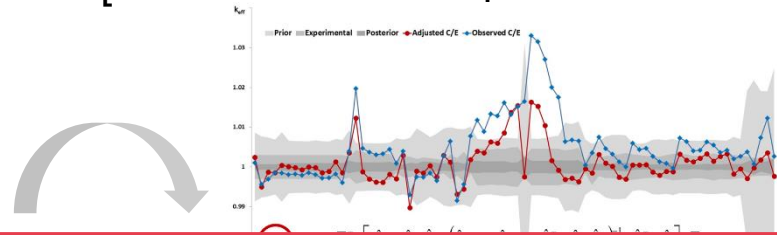
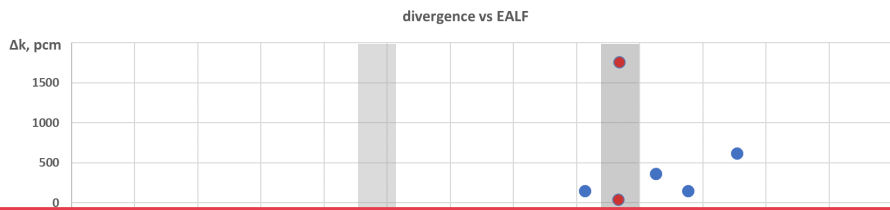
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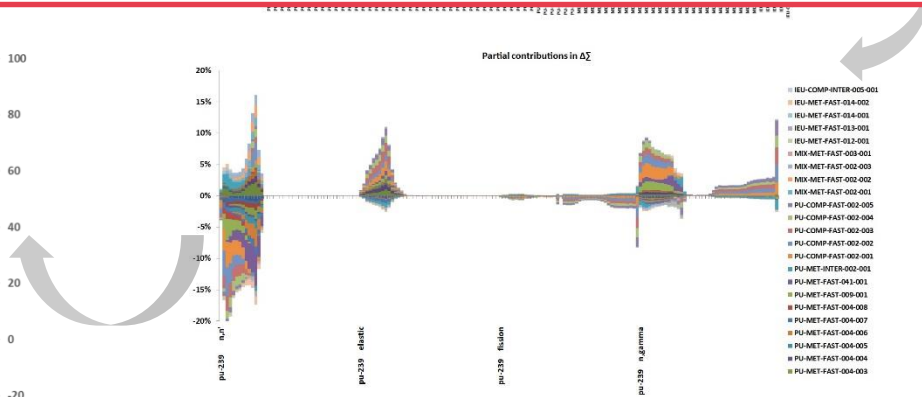
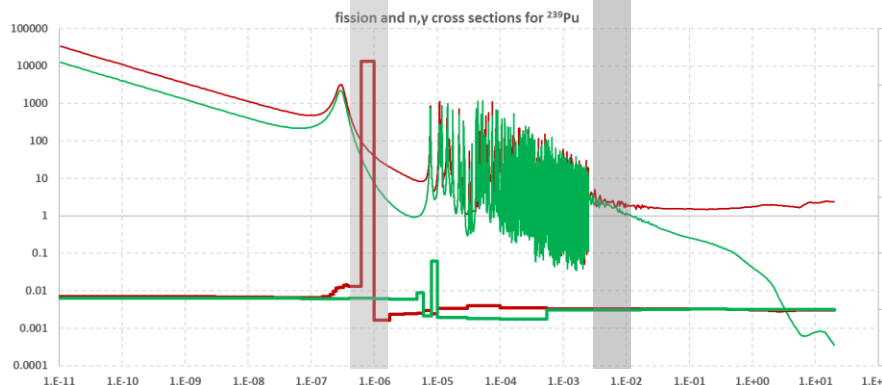
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The 3rd application of Data Assimilation
prioritizing problem-oriented fundamental research programs



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DA ingredients in terms of science-driven Validation process

V&UQ protocol => major phases

- To collect all needed data
- To characterize IEs data and prior uncertainties (CND)

■ To withdraw used IEs from V&UQ **1st application**

- To parametrize model and AO
- To quantify C/E + uncertainties
- To apply/establish Bayesian framework quantifying bias and uncertainties => given parameters

■ To ensure an absence of Ontological issues **3rd application**

- To transpose knowledge (bias + uncertainty) comparing with TARs

DA contributions and other actions

- Testing IEs consistency (reversing Bayesian inferences)

Given: “tuned” libraries =>

■ Identifying used IEs data **Reference to simple adjustment**

- Perturbation Theory or other ROMs
- Examining CND, Establishing CovEX
- Optimizing deterministic (GLLSM-like), stochastic (BMC, HMC, etc.) and hybrid algorithms

■ Prioritizing problem-oriented basic research programs **an ontological uncertainty treatment**

- Performing additional statistical testing, and using given parametrization

Topics to be discussed within the sub-group

Subject

Content

■ TARs related to conceptual design, exploitation and safety assessment

- Reasoned discussion on very basic matters of an establishment of TARs
- Meaningful analysis ↔ linking nuclear technologies and TARs

■ Requirements to IEs and Handbooks

- an elimination of double use of
 - IEs (inherent to a ND evaluation), and
 - libraries (inherent to a benchmarks' evaluation)
- current status of IEs covariances (CovEX)

■ Requirements and status of ND covariances (CND)

- compatibilities and linear-algebra issues
- cross-covariances => analysis and assessment (IEs impacts, eliminations)

Preparatory actions (2#2) prior uncertainties

$$\frac{\Delta\bar{\sigma}}{\bar{\sigma}} = \hat{W} \cdot \bar{S}_{IE} \cdot (\hat{V}_{IE} + \hat{V}_{CLC} + \bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE})^{-1} \cdot \frac{\Delta\bar{R}_{IE}}{\bar{R}_{IE}}$$

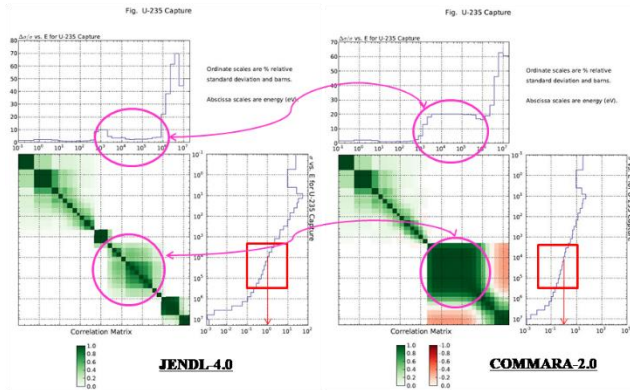
\hat{V}_{IE} as CovEX for all involved IEs data (see above)

$$\frac{\Delta\bar{\sigma}}{\bar{\sigma}} = \hat{W} \cdot \bar{S}_{IE} \cdot (\hat{V}_{IE} + \hat{V}_{CLC} + \bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE})^{-1} \cdot \frac{\Delta\bar{R}_{IE}}{\bar{R}_{IE}}$$

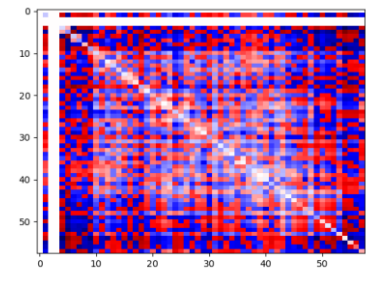
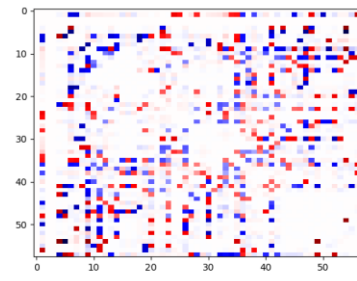
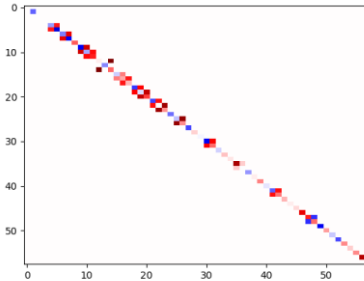
\hat{V}_{CLC} a numerical tool error => minimizing => precise solvers (Monte-Carlo)

$$\frac{\Delta\bar{\sigma}}{\bar{\sigma}} = \hat{W} \cdot \bar{S}_{IE} \cdot (\hat{V}_{IE} + \hat{V}_{CLC} + \bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE})^{-1} \cdot \frac{\Delta\bar{R}_{IE}}{\bar{R}_{IE}}$$

\hat{W} prior Covariance matrix of Nuclear Data (CND) => independent on ND



$$\hat{W}' = \hat{W} - (\bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE}) \cdot (\hat{V}_{IE} + \hat{V}_{CLC} + \bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE})^{-1} \cdot (\bar{S}_{IE}^T \cdot \hat{W} \cdot \bar{S}_{IE})$$



Prior CND => inconsistent but useful

Posterior CND => consistent yet in a local domain (covered by IEs)

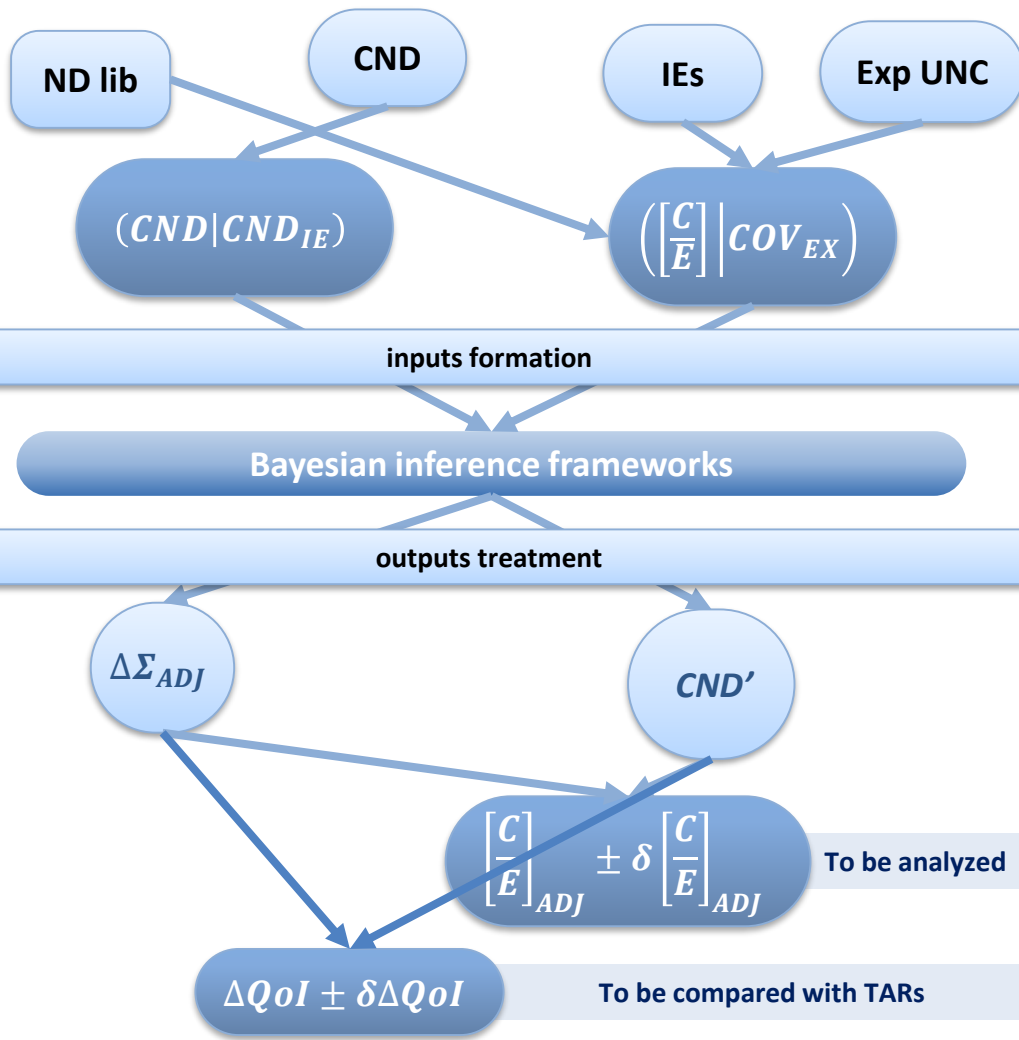
Metrics of information => ratio between functionals given by Prior and Posterior CND

Posterior CND meaning as a pocket of knowledge (information extracted from IEs)

Suggestions: to validate a library => to provide prior CND and

to withdraw IEs have been yet used in data "tuning"

Step towards shared protocol of science-driven V&UQ



Data Assimilation contributions

- Suite of *IEs* collection with *CovEX* (*withdrawing cases used in lib_s tuning*)
- Observations (*C/E*) calculations
- *CND* in a suitable format

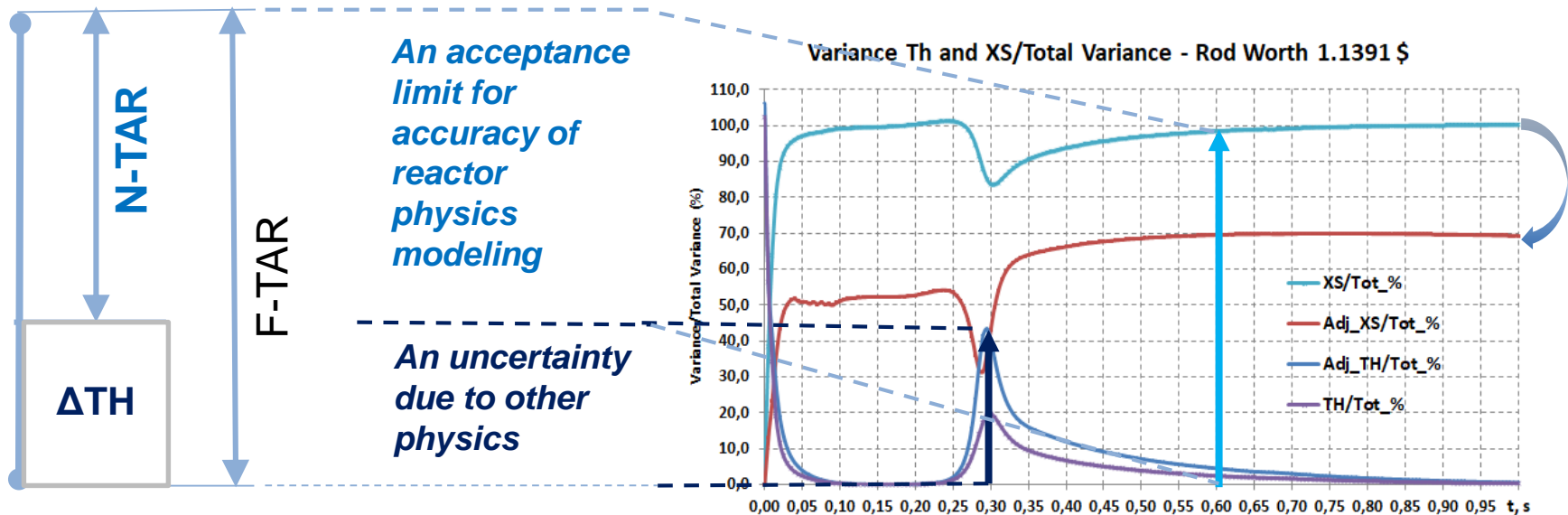
any => *deterministic* or *stochastic*

Data Assimilation outputs

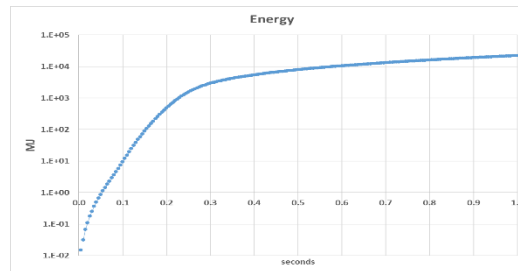
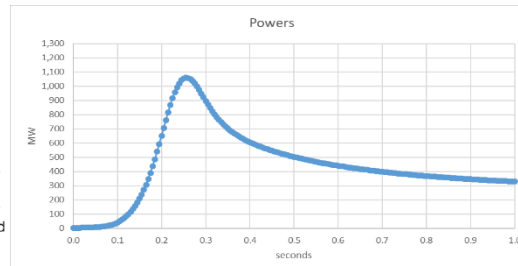
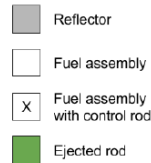
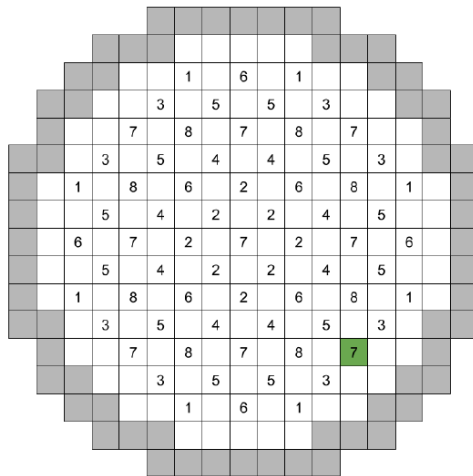
- Ontological issues testing
- Informed Decision Making support

Target accuracy establishment for multi-physics processes

- Target Accuracy Requirements (TARs) represent wishes and acceptance limits established by designers and/or assessors
- Sg46 task => to establish TARs for Nuclear Data libraries
- One should separate (approximately) impacts due to reactor physics and due to other physics => combining sampling and linearized response (sensitivity) studies
- Sampling-based back-propagation with reduced (adjusted) ND uncertainties
- Note: practically used simulations (no exemptions) based on a hierarchic structure; we are following a kind of a gradient descent approach to quantify uncertainties of different nature



UQP for LWR RIA => links to WPRS/EGMUP 1#2



Given:

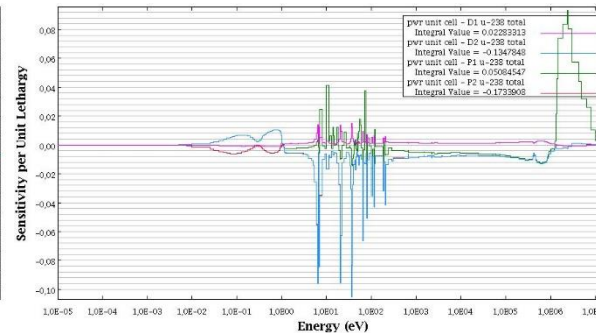
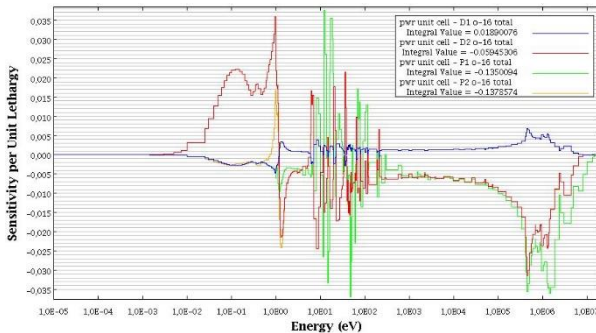
- the case to be assessed => Reactivity Insertion Accident on PWR
- tools available => fully validated TH tools and robust coupled calculational chain

Task:

- to estimate uncertainties of power peak and deposit energy
- to perform UQ basing on an evidence-based background

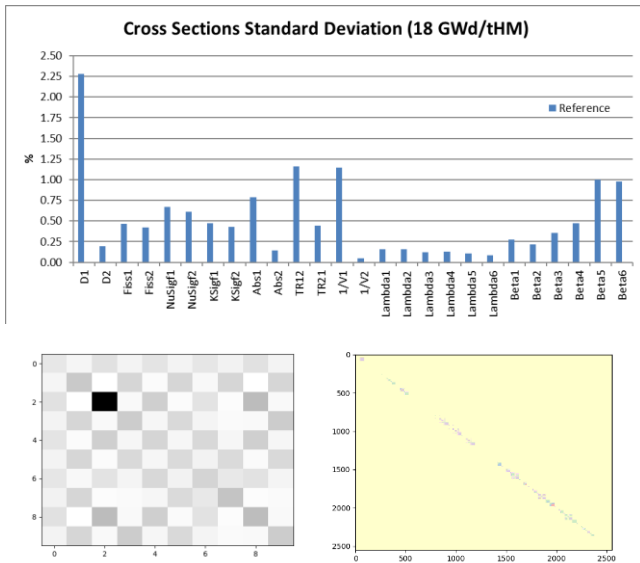
Methodology =>

separated different physics uncertainties, XS and CND calibration, and sampling to an Errors' Propagation



Hierarchic algorithm => cell => lattice => few groups core / coupled modeling
 Uncertainties' calibration => ND + CND => GPT => Posterior few-groups CND

UQP for LWR RIA => links to WPRS/EGMUP 2#2



Homogenization of ND into few groups XS

Uncertainties Quantification and Propagation (UQP) using Generalized Perturbation Theory (GPT)

Prior Uncertainties Propagation

ND contributors in D₁ uncertainties

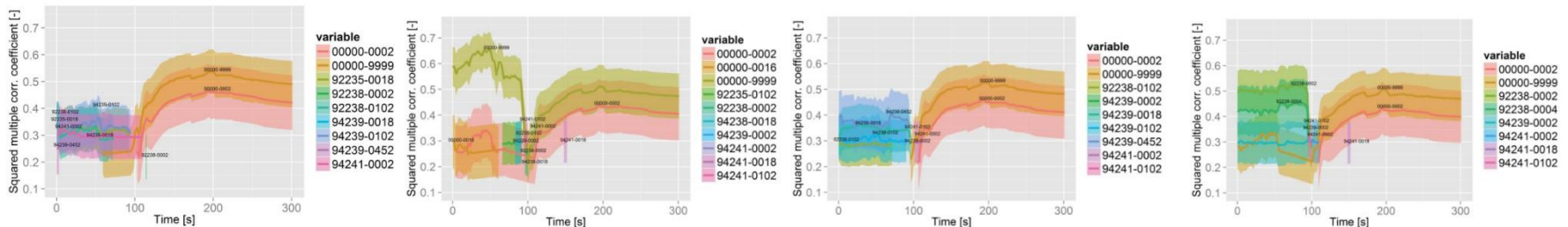
V&UQ differs for different physics (Propagation-based in TH and full DA-based in PhR)

Available => principle contributors in F-TARs and N-TARs <= to commensurate with conservatisms

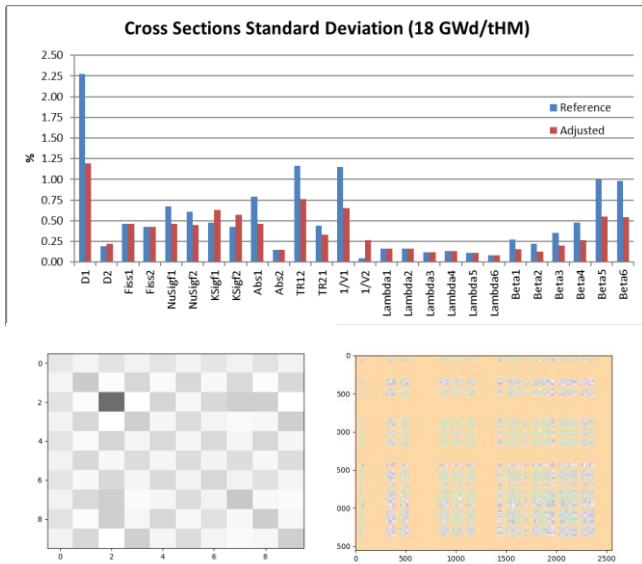
[A.Sargeni, G.Bruna et al, "Evidence-based background for constrained uncertainty quantification in a core transient analysis", ANE, 2021 (to be published)]

ND TARs might be fundamentally different for static and transient AOs [GRS example]

[E. Ivanov et al, "Role of a phenomenological validation and integral experiments for maturing the predictive simulations", NED, V 362, 2020]



UQP for LWR RIA => links to WPRS/EGMUP 2#2



Homogenization of ND into few groups XS
 Uncertainties Quantification and Propagation (UQP) using Generalized Perturbation Theory (GPT)
 Posterior Uncertainties Quantification & Propagation

ND contributors in D₁ uncertainties

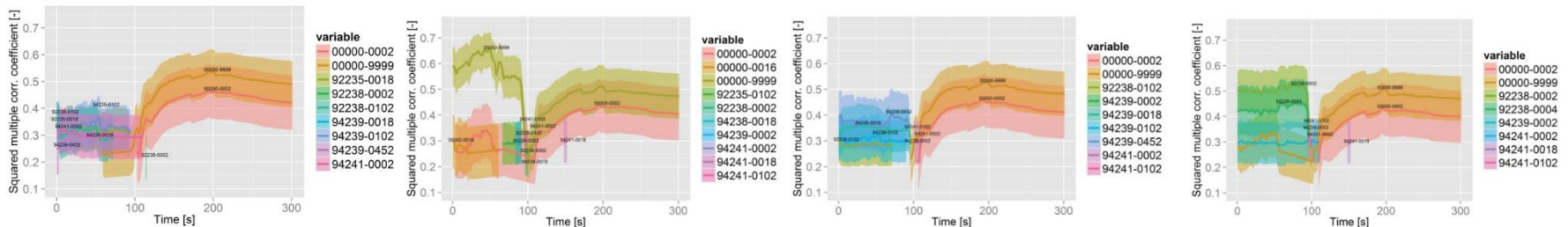
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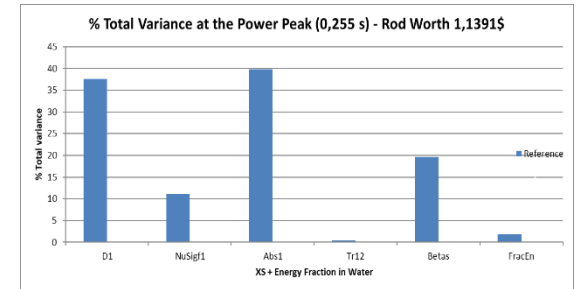
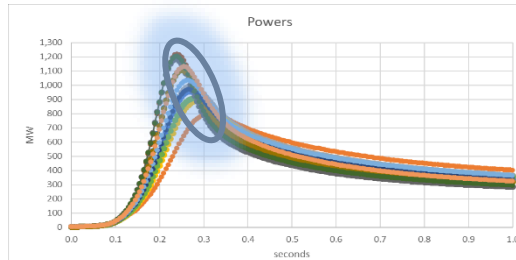
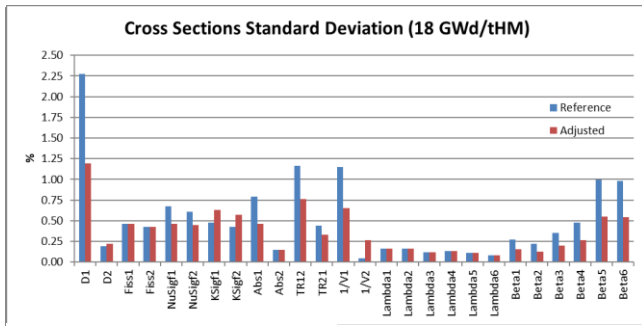
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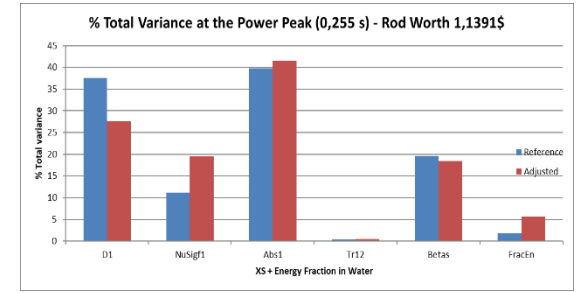
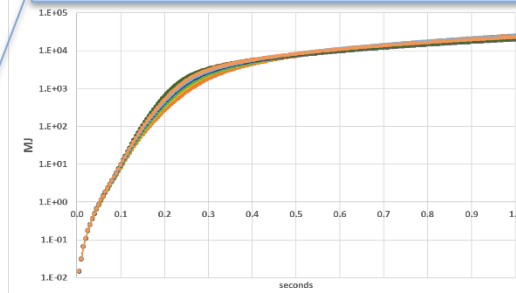
[E. Ivanov et al, "Role of a phenomenological validation and integral experiments for maturing the predictive simulations", NED, V 362, 2020]



UQP for LWR RIA => links to WPRS/EGMUP 2#2



ND contributors in D₁ uncertainties



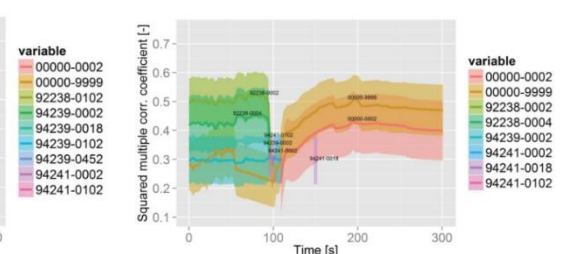
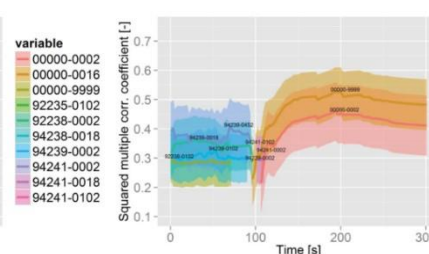
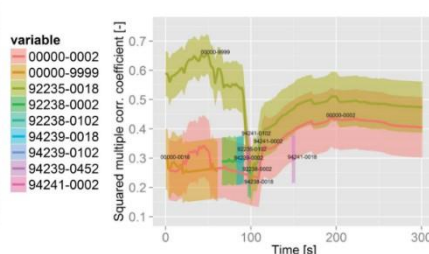
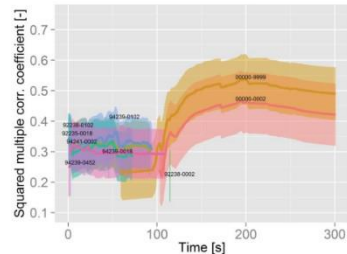
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Molten Salt Fast Reactor functional TARs

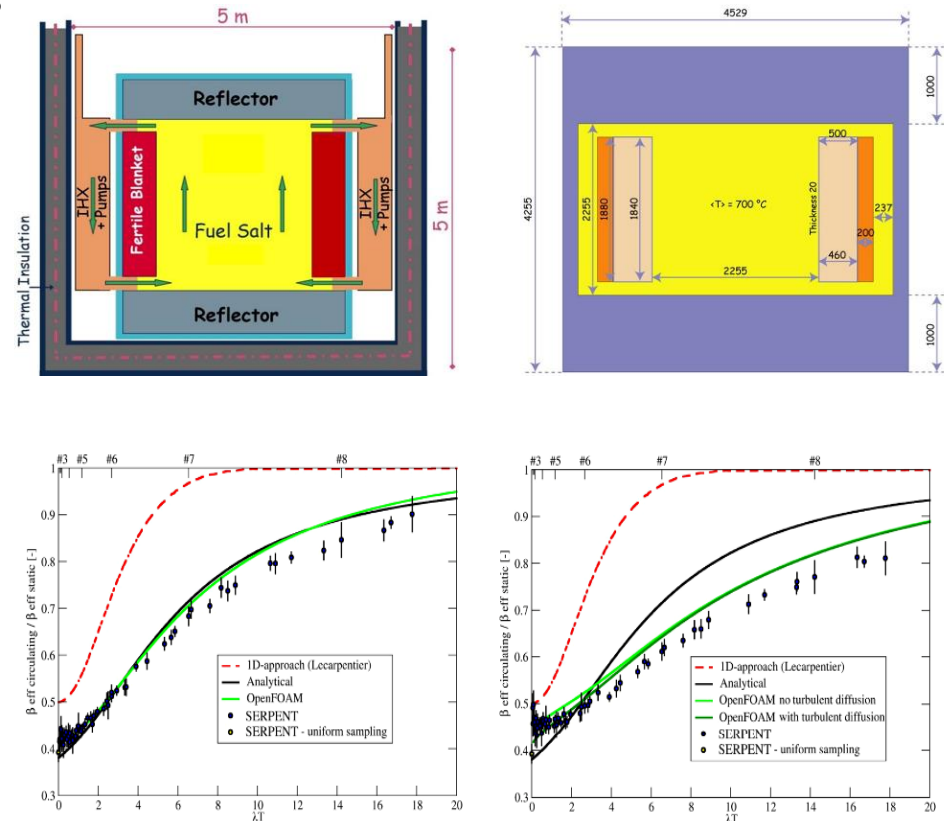
TARs: controllability

TARs have been established basing on the physics behind principles of the entire system control

Peculiarity of MSR => no dedicated power output

- $\Delta k_{eff} \sim 1.0 \%$ if $\omega = 0.0 \text{ m/sec}$ with f.p.
- $\Delta k_{eff} \sim 0.2 \%$ if ω : $\beta_{eff} \cong 0$ & circulating f.p.
- $\frac{c_{232} \Delta k_{eff}}{k_{eff} \Delta c_{232}} \sim 2 \%$ for static case
- $\frac{c_{233} \Delta k_{eff}}{k_{eff} \Delta c_{233}} \sim 3 \%$ for static case
- $\frac{c_{238} \Delta k_{eff}}{k_{eff} \Delta c_{238}} \sim 2 \%$ for static case
- $\frac{c_{239} \Delta k_{eff}}{k_{eff} \Delta c_{239}} \sim 7 \%$ for static case
- $\frac{c_{Zr.Mo.Ce} \Delta k_{eff}}{k_{eff} \Delta c_{Zr.Mo.Ce}} \sim 12 \%$ for static case

Calculational model



MODEL FOR SENSITIVITY STUDIES

Mariya Brovchenko, Jan-Leen Kloosterman, Lelio Luzzi, Elsa Merle, Daniel Heuer, Axel Laureau, Olga Feynberg, Victor Ignatiev, Manuele Aufiero, Antonio Cammi, Carlo Fiorina, Fabio Alcaro, Sandra Dulla, Piero Ravetto, Lodewijk Frima, Danny Lathouwers, Bruno Merk, Neutronic benchmark of the molten salt fast reactor in the frame of the EVOL and MARS collaborative projects, EPJ Nuclear Sci. Technol. 5 2 (2019)

Potential IRSN participation: collaboration and delivery

■ MSFR [IRSN & CNRS] =>

- Quantified TARs for major functionals
- Commented article and inputs for sensitivity coefficients calculations

■ LWRs RIA [IRSN] =>

- Quantified TARs to power and energy yields in a power excursion accident
- Commented articles explaining unconventional options in TARs establishment

■ V&UQP protocol [IRSN and all ?] =>

- Synopsis on major “ingredients” of science-driven (DA-based) V&UQ process
- An example on IEs uncertainties quantification and CovEX establishment
- Draft and consolidated comments to a science-driven V&UQ protocol

Suggestion: to see a meaningful discussion on validation criteria in a reliance (separately) to conceptual design, basic research and safety assessment

Note: [differences in objectives...]

in simple adjustment => uncertainties give a range for variations;

in V&UQ => DA forms [localized] models for evolving uncertainties [related to AO]

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■ Crucial items [all ?]=>

- List of IEs have been used in ND evaluation
- Current Status of CND for XSs, secondary particles yield and cross-correlations

■ One contribution to HPRL [IRSN and all ?]

Thank you for your time

Questions?