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DATA ASSIMILATION AND BEST-ESTIMATE MODEL VALIDATION ACTIVITIES IN EURATOM-FISSION PROGRAMS

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OUTLINE

- “Sensitivity and Uncertainty Analysis” and “Data Assimilation for Best-Estimate Adjustment (DABE)” Activities within the NURESIM FP6-Project (2005-2008)
- “Model Validation” and “DABE” Activities within the NURESP FP7-Project (2008-2010)
- Model Validation within the Sustainable Nuclear Fission (Energy) Technology Platform (21.09.2007-)

NURESIM: European Platform for Nuclear Reactor Simulations

Coordinator: CEA; Time-Frame: 02.05 – 02.08 (7.6 M€)

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Sub-Projects

- Core Physics (UP Madrid)
- Thermal-Hydraulics (CEA)
- Multi-Physics Coupling (PSI)
- Model Validation, Sensitivity & Uncertainty Quantification (U-KA)
- Integration in SALOME (CEA)

Objectives

- **Industrial Needs**
- **Scientific challenges (physical modeling, numerical methods)**

Results

- **Integration in a multi-scale multi-physics software platform (SALOME)**
- **Towards validated software standards**
- **Improvement of efficiency in simulations**

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Time-Dependent Data Assimilation for Best-Estimate Adjustment (DABE) (1/4)

- Discretized time-span: $\mathbf{J}_t = \{1, \ldots, N_t\}$
- Parameters: $\boldsymbol{\alpha}^{\nu} = \left\{ \boldsymbol{\alpha}_i^{\nu} \mid i \in \mathbf{J}_{\alpha} \right\}, \quad \nu \in \mathbf{J}_t \qquad \mathbf{J}_{\alpha} = \{1, \ldots, N_{\alpha}\}$
- Parameter covariances:

$$\mathbf{C}_{\alpha} = \begin{bmatrix} \mathbf{C}_{\alpha}^{11} & \mathbf{C}_{\alpha}^{12} & \cdots & \cdots \\ \mathbf{C}_{\alpha}^{21} & \mathbf{C}_{\alpha}^{22} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \mathbf{C}_{\alpha}^{N_t N_t} \end{bmatrix} \qquad c_{\alpha,ij}^{\nu\mu} = \left\langle \Delta\boldsymbol{\alpha}_i^{\nu} \Delta\boldsymbol{\alpha}_j^{\mu} \right\rangle$$

Time-Dependent Data Assimilation for Best-Estimate Adjustment (DABE) (2/4)

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- Computed responses: $\mathbf{R}^{\nu} = \left\{ \mathbf{R}_n^{\nu} \mid n \in \mathbf{J}_R \right\}, \quad \nu \in \mathbf{J}_t$

$$\mathbf{J}_R = \{1,\dots, \mathrm{N}_R\}$$

- Covariance of computed responses (using first-order sensitivities only):

$$\mathbf{C}_R^{\nu\mu} = \sum_{\rho} \sum_{\eta} \mathbf{S}^{\nu\rho} \mathbf{C}_{\alpha}^{\rho\eta} \left(\mathbf{S}^T \right)^{\mu\eta} , \qquad \rho, \eta \in \mathbf{J}_{\nu}; \;\; \nu, \mu \in \mathbf{J}_t$$

- Measured responses: $\mathbf{M}^{\nu} = \left\{ \mathbf{M}_n^{\nu} \mid n \in \mathbf{J}_M \right\}, \;\; \nu \in \mathbf{J}_t \qquad \mathbf{J}_M = \{1,\dots, \mathrm{N}_M\}$

- Covariances for measured responses: $\mathbf{C}_M$

- “Response deviations”: $\boldsymbol{d}^{\nu} = \boldsymbol{R}^{\nu} - \boldsymbol{M}^{\nu}$

- Response-Parameter Covariances: $\mathbf{C}_{\alpha R}$

- Note: $\mathbf{C}_M$ and $\mathbf{C}_{\alpha R}$ have the same “time-structure” as $\mathbf{C}_{\alpha}$

Time-Dependent Data Assimilation for Best-Estimate Adjustment (DABE) (3/4)

Bayes' Theorem yields:

Adjusted ("best-estimate") parameters:

$$\left(\boldsymbol{\alpha}^{BE}\right)^{\nu} = \boldsymbol{\alpha}_o^{\nu} + \sum_{\mu} \left\{ \left[\left(\left(\mathbf{C}_{\alpha R}^{\nu\mu}\right)^T - \sum_{\eta} \mathbf{C}_{\alpha}^{\nu\eta} \left(\mathbf{S}^{\mu\eta}\right)^T \right) \times \left[\sum_{\eta} \left(\mathbf{C}_d^{-1}\right)^{\mu\eta} \mathbf{d}^{\eta} \right] \right] \right\} , \quad \mu \in J_t \, , \; \eta \in J_t$$

where $\boldsymbol{C}_d = \boldsymbol{C}_R + \boldsymbol{C}_M - \boldsymbol{S}\boldsymbol{C}_{\alpha R} - \boldsymbol{C}_{\alpha R}^T \boldsymbol{S}^T$

- Adjusted ("best-estimate") responses:

$$\left(\mathbf{R}^{BE}\right)^{\nu} = \mathbf{R}_M^{\nu} + \sum_{\mu} \left\{ \left[\left(\left(\mathbf{C}_{M}^{\nu\mu}\right)^T - \sum_{\eta} \mathbf{C}_{\alpha R}^{\nu\eta} \left(\mathbf{S}^{\mu\eta}\right)^T \right) \times \left[\sum_{\eta} \left(\mathbf{C}_d^{-1}\right)^{\mu\eta} \mathbf{d}^{\eta} \right] \right] \right\} , \quad \mu \in J_t \, , \; \eta \in J_t$$

Time-Dependent Data Assimilation for Best-Estimate Adjustment (DABE) (4/4)

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Bayes’ Theorem yields…

- adjusted (“best-estimate”) parameter covariances:

$$\left(\mathbf{C}_{\alpha}^{BE}\right)^{\nu\mu}=\mathbf{C}_{\alpha}^{\nu\mu}-\sum_{\eta}\left[\sum_{\rho}\left(\left(\mathbf{C}_{\alpha}^{\nu\rho}\right)^{T}-\sum_{\pi}\mathbf{C}_{\alpha R}^{\nu\pi}\left(\mathbf{S}^{\rho\pi}\right)^{T}\right)\left(\mathbf{C}_{d}^{-1}\right)^{\rho\eta}\right]\left(\mathbf{C}_{\alpha}^{\eta\mu}-\sum_{\pi}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha R}^{\pi\mu}\right),$$

$$\nu,\mu,\eta,\rho,\pi\in J_{t}$$

- adjusted (“best-estimate”) response covariances:

$$\left(\mathbf{C}_{R}^{BE}\right)^{\nu\mu}=\mathbf{C}_{R}^{BE}-\sum_{\eta}\left[\sum_{\rho}\left(\mathbf{C}_{R}^{\nu\rho}-\sum_{\pi}\mathbf{C}_{\alpha R}^{\nu\pi}\left(\mathbf{S}^{\rho\pi}\right)^{T}\right)\left(\mathbf{C}_{d}^{-1}\right)^{\rho\eta}\right]\left(\mathbf{C}_{R}^{\eta\mu}-\sum_{\pi}\mathbf{S}^{\eta\pi}\left(\mathbf{C}_{\alpha R}^{\pi\mu}\right)^{T}\right),$$

$$\nu,\mu,\eta,\rho,\pi\in J_{t}$$

- “C & E” Consistency Indicator: $\chi^{2}=\boldsymbol{d}^{T}\boldsymbol{C}_{d}^{-1}\boldsymbol{d}$

Time-Dependent Data Assimilation & Adjustment: Particular Cases

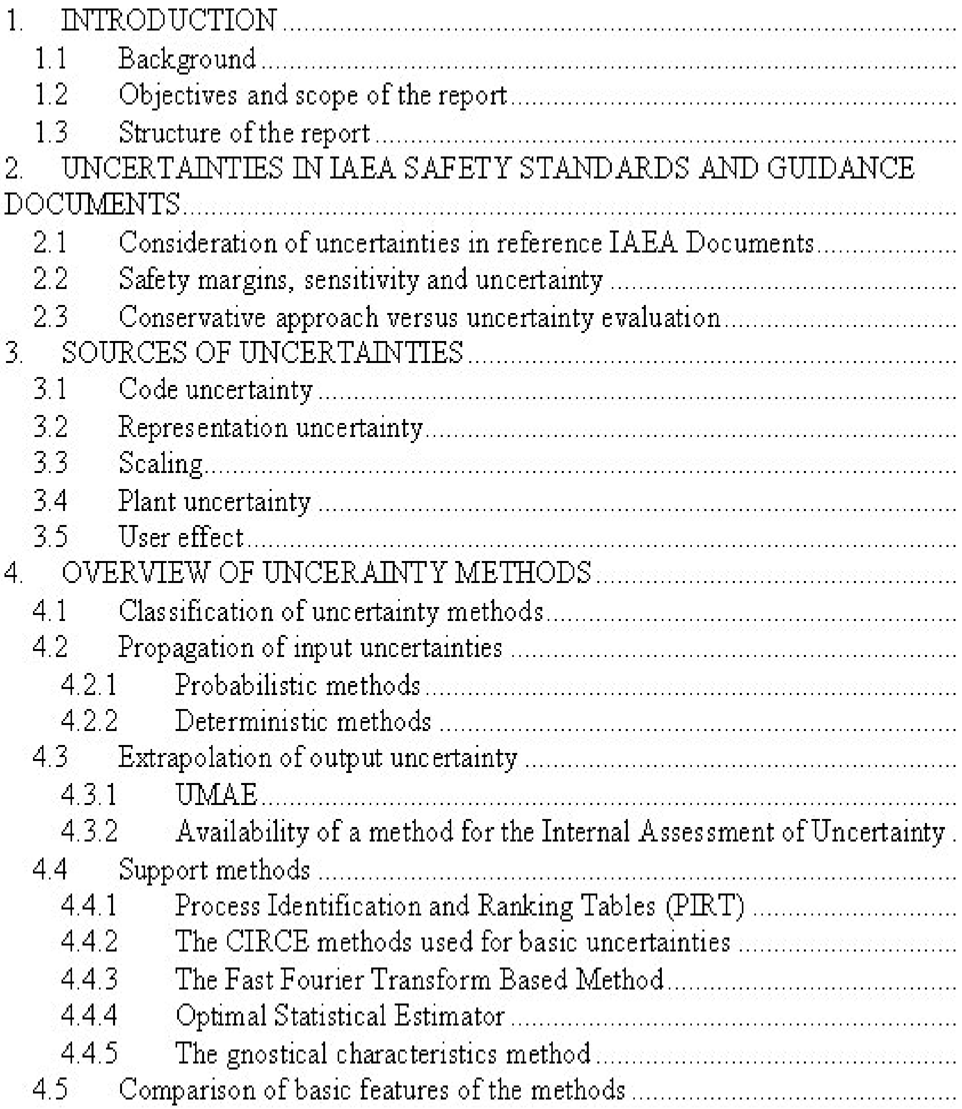
On-Line Data Adjustment/Assimilation:

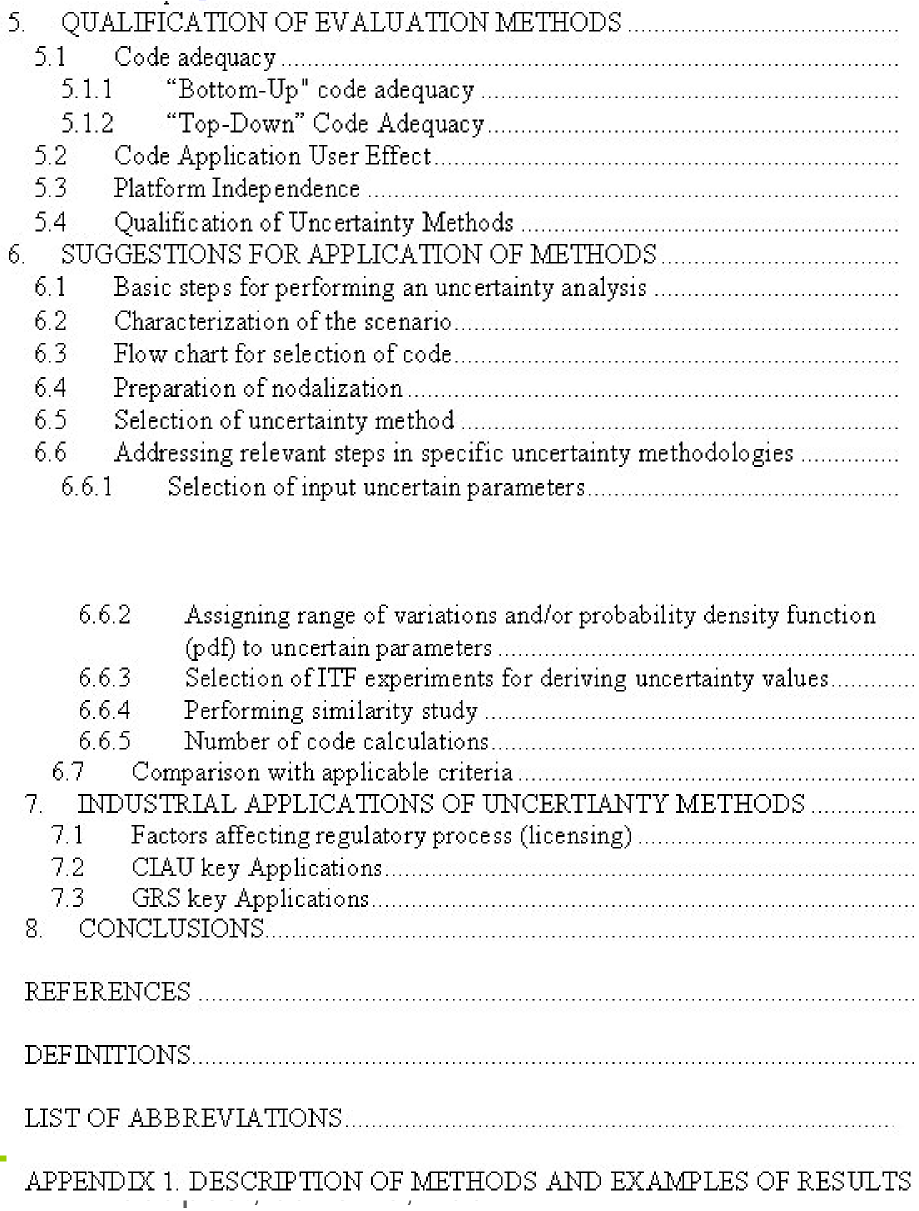
- At a given time node *v*, ***all*** of the "best estimates" $\left(\boldsymbol{\alpha}^{BE}\right)^{\mu}$ at times $\mu < \nu$ are used and ***continually updated*** to obtain $\left(\mathbf{R}^{BE}\right)^{\nu}$ at node *v.*
- This procedure implicitly accounts for all sensitivities and covariances relating to parameters at all nodes $\mu < \nu$ so that only sensitivities and covariances at node *v* will explicitly appear in the expressions of the constraints and of the objective function.
- The uncertainty analysis is performed: (i) sequentially in time; and (ii) interactively with the code that computes the dependent variables and responses, thus updating their values iteratively at every time-node.

Off-Line Data Adjustment/Assimilation Without Foresight:

- Same procedure as above, but without any iterative updating.

S&U Methods for Safety & Licensing: Preliminary Table of Contents (U-Pisa & Uni-KA)





ASAP-CIAU Benchmark: Blowdown from a Vessel Containing Pressurized Gas (in progress: U-Pisa & Uni-KA)

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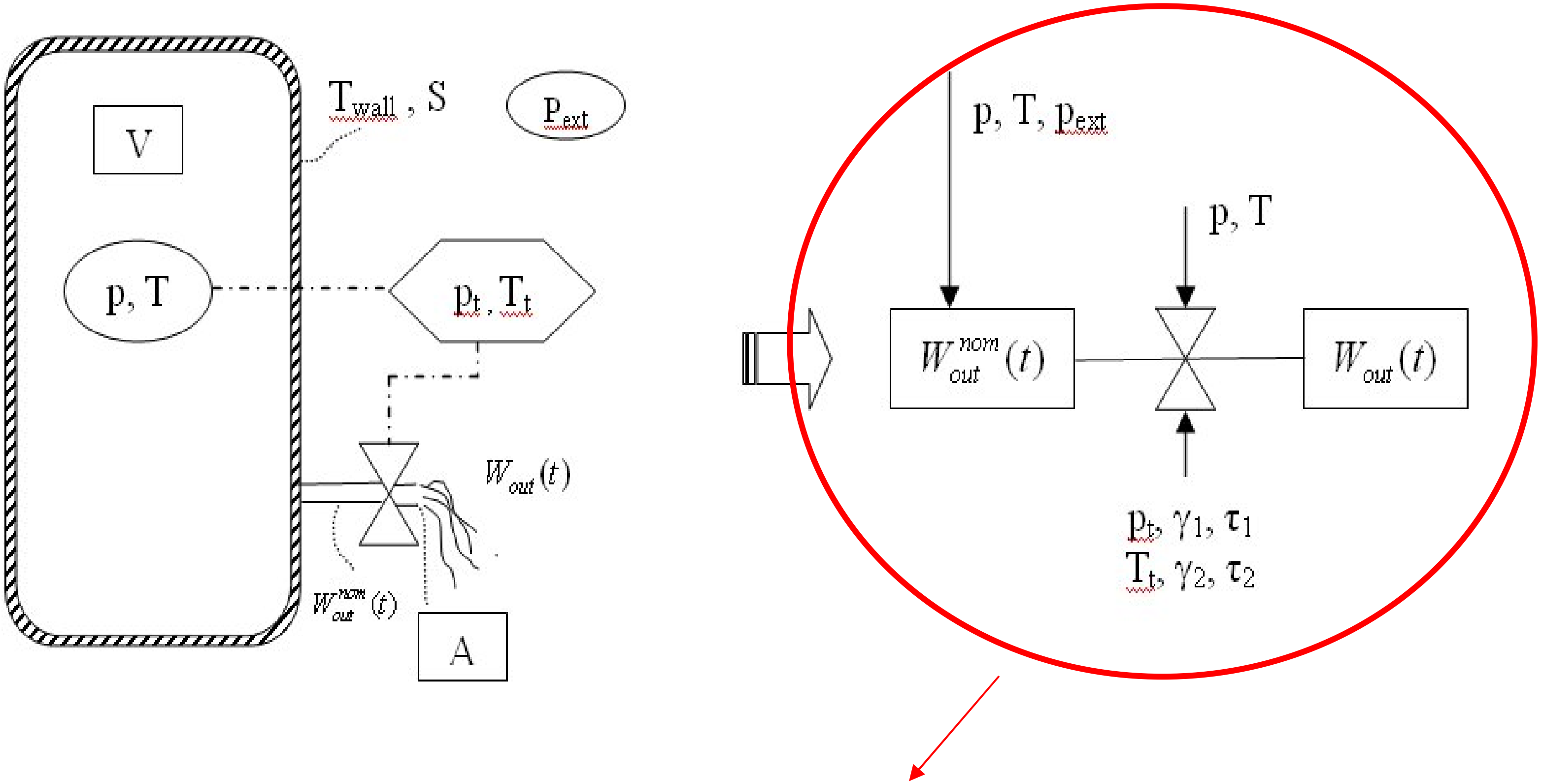

TRIP LOGIC BASED ON PRESSURE AND TEMPERATURE DIFFERENCE SIGNALS

Scope of FP-7 EURATOM-Project NURESP (2008-2011)

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- **Participants (23): CEA, EdF, GRS, FZD, Uni-KA, PSI, ASCOMP, TU-Delft, KTH, U-Pisa, UP-Madrid, UCL, JSI, VTT, LUT, IRNE, NRI, KFKI, FZK, Imp. College, IRSN, NRG, Chalmers**

- **Goal (continuing): “develop the next generation of experimentally validated best-estimate tools for modeling thermal-hydraulics and core physics for present PWRs and BWRs, as well as for future reactors, using a well proven software platform *(SALOME)*.”**

- **Main topics for priority development:**

  (i) coupling of core physics, thermal hydraulics, and fuel models for reactor safety;

  (ii) sensitivity and uncertainty analysis using deterministic and statistical methods;

  (iii) experimental validation and qualification of codes, using benchmarks, industrial plant data and results of (existing or new) experiments;

Basic Types of Uncertainties:

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- ***(a)* *Stochastic uncertainties*:** arise because the system under investigation can behave in many different ways;
- ***(b)* *Subjective or Epistemic uncertainties:*** arise from the inability to specify an exact value for a parameter that is assumed to have a constant value in the respective investigation.

Nuclear Power Plants involve both stochastic and epistemic uncertainties:

- ***Stochastic uncertainties* arise due to the hypothetical accident scenarios which are considered in the respective risk analysis.**
- ***Epistemic uncertainties* arise because of uncertain parameters that underlie the estimation of the probabilities and consequences of the respective hypothetical accident scenarios.**

NOTE: NURESIM (2006-2008) addresses epistemic (subjective) uncertainties only!

Code (Model) Verification, Validation, Verification…

- **“Code Verification”** = “is the code solving the mathematical model correctly?”

- **“Code Validation”** = “does the model represent reality?”

- **“Code Qualification”** = “certifying that a proposed simulation/design methodology/system satisfies all performance and safety specifications”

- ***Although the above “definitions” have been adopted for most modeling activities in USA, this is still not the case in Europe! Adopting uniform definitions for NURESP & Beyond is urgently needed!***

✓Code validation and qualification (V&Q) can be attained only by selected benchmarking, taking into account systematically (i.e., using sensitivities) all sources of uncertainties (computational, experimental, etc.)

Dealing with Uncertainties in Reactor Safety…

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- **“Conservative Codes”…** use deliberately pessimistic and unphysical assumptions; it is then argued that the overall predictions of such codes are “worse than reality”.

- **“Best - Estimate Codes”…** use “best estimate input data” to obtain a “best estimate output / result”; for safety studies, it is necessary to value (or to overvalue) the uncertainty attached to this estimation.

Best - Estimate Codes Are Used for Safety and Economical Reasons

- ➢"Conservatism" of results produced by "conservative" codes is difficult to prove (e.g., cancellation of effects).

- ➢Best-estimate codes can improve accident management procedures by providing a better understanding of accident progression.

- ➢Best-estimate codes are expected to permit relaxing technical specifications and core operating limits set by conservative calculations, thereby improving economics.

- ➢**"Best-estimate uncertainty analysis methods"** must be used in conjunction with best-estimate codes (particularly for reactor safety) in order to evaluate ***safety margins*** around the ***best-estimate values***.

Code Validation Procedure Used by Utilities and TSOs

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✓Four sequential steps; the end-status of each step determines if the procedure can be continued (or not);

➢First step: identification of code applicability analysis, uncertain parameters, and responses of interest for post-processing;

➢Second step: identification of uncertain parameters potentially significant during the physical phenomena observed during the target transient;

➢Third step: derivation of uncertainty bands (interval spans) and subjective probability density functions for all the uncertain parameters, using the code's qualification matrix (vs. experiments), the experimental uncertainties of the initial and boundary conditions, and expert judgment.

➢Fourth step: propagate modeled uncertainties, using a *statistical method*, to obtain a response surface for evaluating the response uncertainties.

Practical Limitations of Statistical Methods

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- **The results of sampling-based uncertainty and sensitivity analysis depend entirely on the distributions assigned to the sampled parameters; hence, the proper assignment of these distributions is essential to avoid producing spurious results. However, these distributions are not available in practice!**

- **Since the response sensitivities and parameter uncertainties are inherently amalgamated, improvements in parameter uncertainties cannot be directly propagated to improve response uncertainties; rather, the entire set of simulations must be repeated anew.**

- **Since many thousands of simulations are needed, statistical methods are expensive (even for small systems) or impracticable (for exhaustive analysis of large scale time-dependent systems).**

- ***Data Assimilation & Best-Estimate Adjustment (DABE) procedures are the only systematic way for obtaining "best-estimate" codes. However, such procedures have not yet been implemented for nuclear design & safety simulation tools. Hence, bona fide "best-estimate" codes are still not really available!***

Local vs. Global Sensitivity and Uncertainty Analysis

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- ***Global analysis**: to determine all of the system's critical points (bifurcations, turning points, response maxima, minima, and/or saddle points) in the combined phase space formed by the parameters and dependent (state) variables, and subsequently analyze these critical points by local sensitivity and uncertainty analysis.*
  - ***Global Adjoint Sensitivity Analysis Procedure (GASAP)***
  - ***Some statistical methods in theory (in practice: only for small-scale examples)***

- ***Local analysis**: to analyze the behavior of the system response locally around a chosen point (for static systems) or chosen trajectory (for dynamical systems) in the combined phase space of parameters and state variables.*
  - ***Re-computations, Direct Method, Green's Functions, FSAP, ASAP, and***
  - ***All statistical methods in practice, for large-scale problems!***

URANIE: Platform for Model Validation, Sensitivity & Uncertainty Quantification, and Data Assimilation and Best-Estimate Adjustment

(in NURESP)

- **URANIE is based on ROOT, an object-oriented software multi-platform developed at CERN for storing, treatment an analysis of large amounts of data (ca. 20 PetaBytes/year) generated by the LHC.**
- **URANIE is written in C++, comprising dynamic libraries (automatic loading of "root-maps"), tools visualization and GUIs, C++ interpreter, interfaces with Python and R, internal TTree of ROOT, SQL access to databases (MySQL, PostgreSQL, ...), MPI distribution for intensive computations, optimization package (Simplex, OPT++ from Sandia Labs.), numerical experiment design methods (LHS, qMC, MCMC), response surface methods and surrogate models meta-models (polynomials, neural networks, splines), statistical sensitivity analysis (Pearson, Spearmann, Sobol, Morris).**
- **To be implemented in URANIE (NURESP): GASAP, time-dependent data adjustment & assimilation based on adjoint methods, automatic differentiation, hybrid adjoint/statistical solvers, SFEM (Karhunen-Loewe, polynomial chaos), RaFu.**

NURESP / SP4: *Model Validation, DABE, Sensitivity and Uncertainty Quantification (URANIE)*

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Partners: CEA, Uni-KA. U-Pisa, EDF, Imp. College, IRSN, NRG,

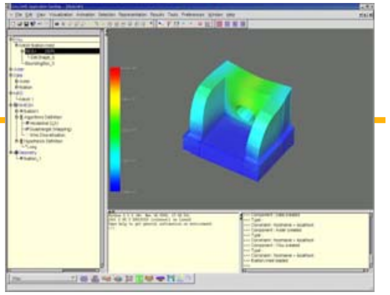
- **WP4.1:** *Implementation of the existing NURESIM-KALIF Modules into the new Platform URANIE*
- **WP4.2:** *Development of New Methods and Software Modules for Local and Global Adjoint Sensitivity and Uncertainty Analysis for URANIE*
- **WP4.3:** *Development of New Methods and Software Modules for Statistical Sensitivity and Uncertainty Analysis for URANIE*
- **WP4.4:** *Development of New Hybrid Methods and Software Modules for Combining Adjoint and Statistical Sensitivity and Uncertainty Analysis Methods for URANIE*
- **WP4.5:** *Development of Global Methods and Software Modules for Data Assimilation and Best-Estimate Adjustment (combining GASAP with DABE) for URANIE*

NURESP / SP4: *Model Validation, DABE, Sensitivity and Uncertainty Quantification (URANIE)*

Partners: Uni-KA, CEA, U-Pisa, EDF, Imp. College, IRSN, NRG,

- **WP4.6:** *Development of Formal Procedures (for Industry-Wide Standards) for Model Validation & Sensitivity & Uncertainty Qualification (VSUQ) Procedures and Tools within URANIE, Including Adaptation of URANIE to Selected High Performance Computing (HPC) Architectures*
- **WP4.7:** *Development of a Formal Procedure to Account for Scaling Effects on Sensitivity and Uncertainty Analysis of Thermal-Hydraulics System Codes within URANIE*
- **WP4.8:** *Coordination with the User's Group, NURESP Sub-Projects, and Outside-NURESP Projects for Multi-Scale and/or Multi-Physics Model Validation*

The Salome Platform



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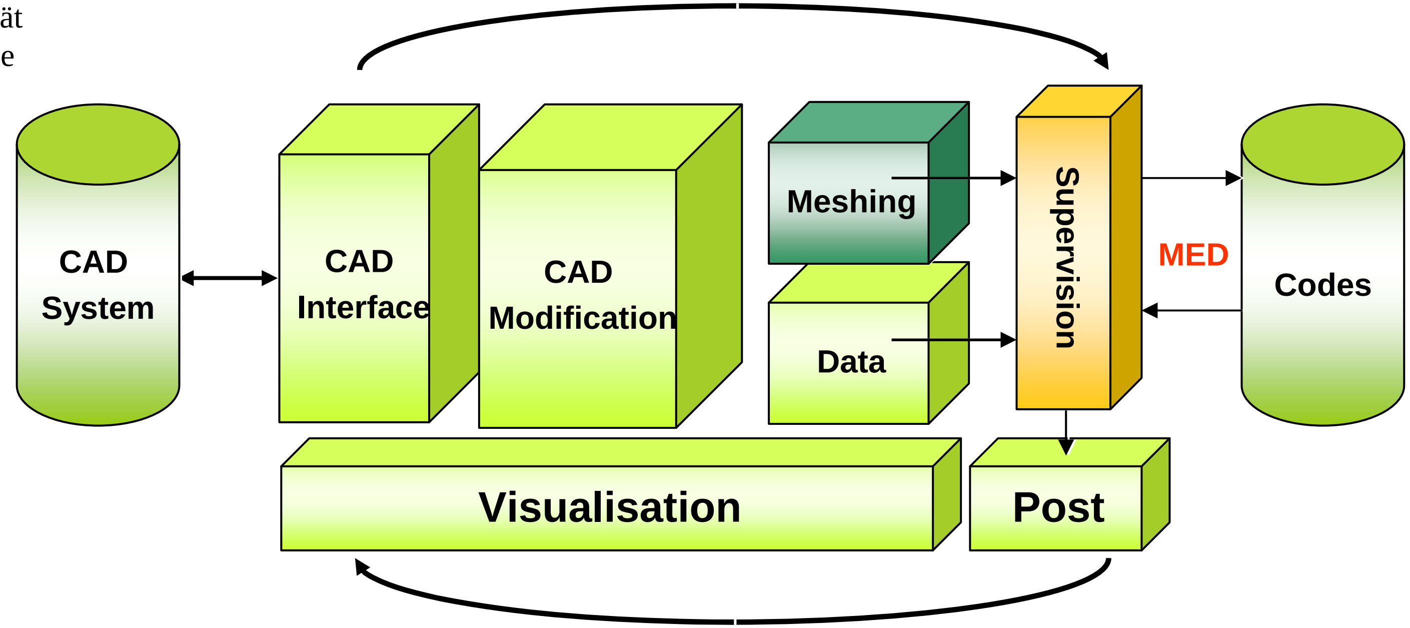
An Open Source Platform *(LGPL license)*
to build multi-physics and multi-scale industrial simulation tools
from CAD to post-processing



CAD System

CAD Interface

CAD Modification

Meshing

Data

Supervision

MED

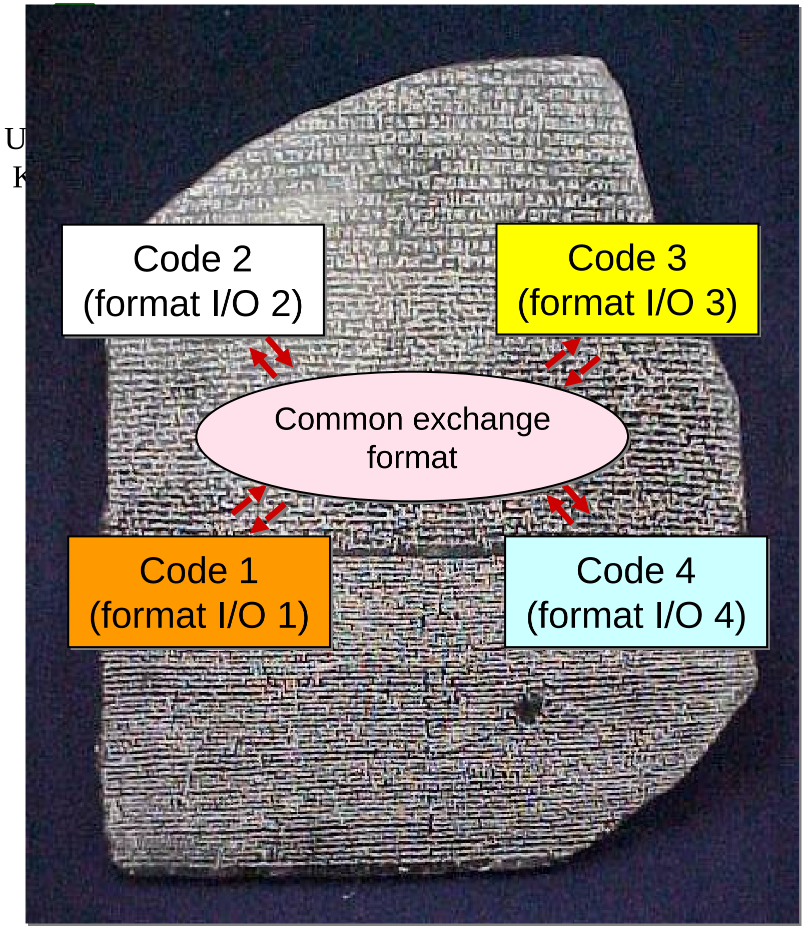
Codes

Visualisation

Post

Download → http://www.salome-platform.org

MED (Data Exchange Model) : the Rosetta Stone of SALOME



Code 2
(format I/O 2)

Code 3
(format I/O 3)

Common exchange
format

Code 1
(format I/O 1)

Code 4
(format I/O 4)

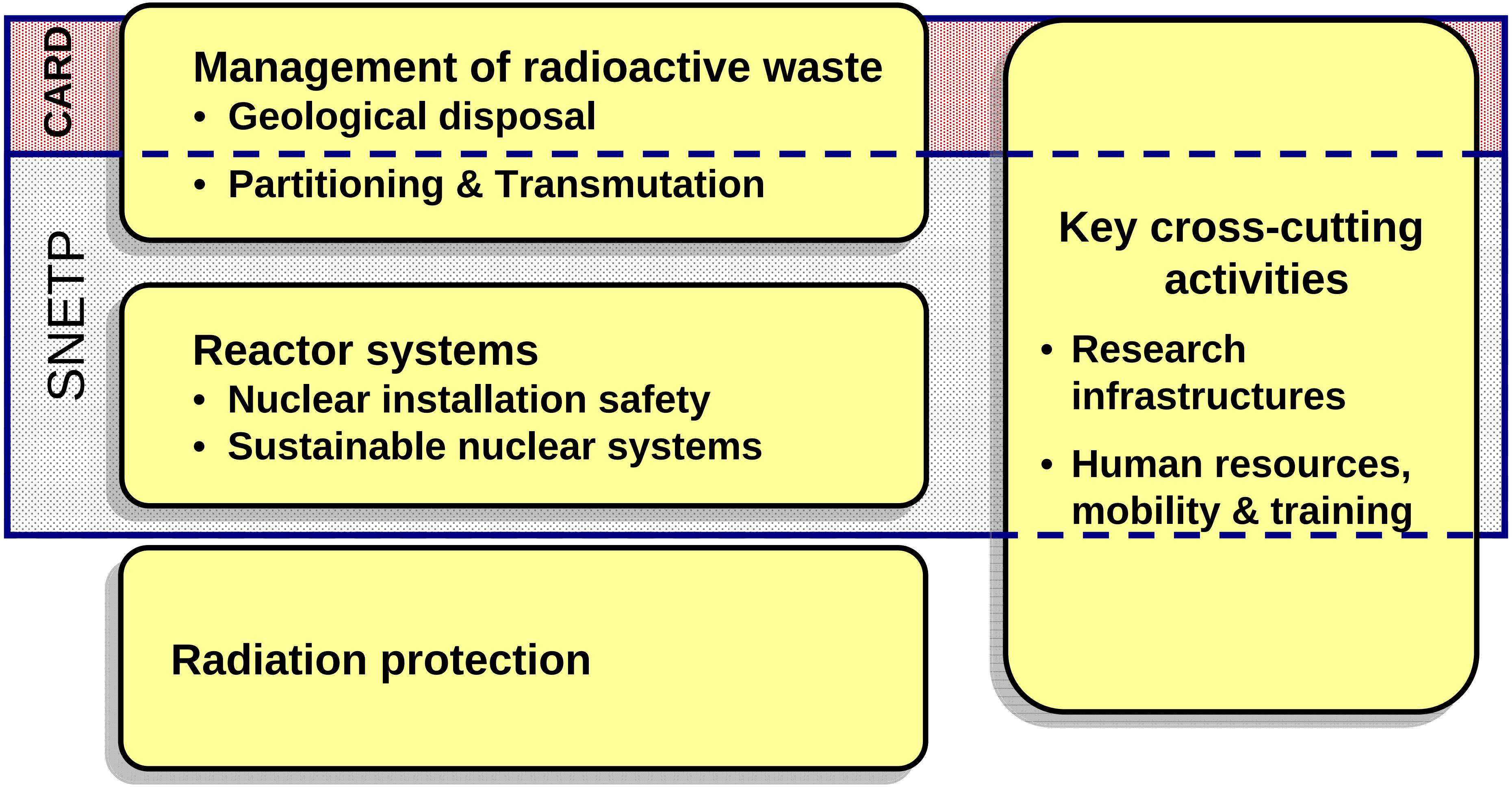
- A common format for facilitating exchanges between solvers

- Integrated solvers can import/export data in a common format

- Sharing high-level services on meshes and fields (interpolation, non-conform meshes,…)

- Ongoing developments for massively parallel architecture

Sustainable Nuclear Energy TP in 7th FP



Management of radioactive waste
- **Geological disposal**
- **Partitioning & Transmutation**

Reactor systems
- **Nuclear installation safety**
- **Sustainable nuclear systems**

Radiation protection

Key cross-cutting activities
- **Research infrastructures**
- **Human resources, mobility & training**

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Thank you for your attention!