CRISTAL
FORMULAIRE DE CRITICITÉ

CRISTAL

# CRISTAL V2.0: New Package for Criticality Calculations

J.M. GOMIT *(Project Manager)* - I. DUHAMEL - Y. RICHET IRSN (France)
C. MAGNAUD - A. ENTRINGER - F. MALOUCH - C. CARMOUZE CEA (France)

*Thanks to N. Leclaire for the oral presentation and to F. Fernex for his contribution to LATEC workbench part*

DE LA RECHERCHE À L'INDUSTRIE
cea

AREVA

IRSN
INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ NUCLÉAIRE
Faire avancer la sûreté nucléaire

# CONTENT

# INTRODUCTION

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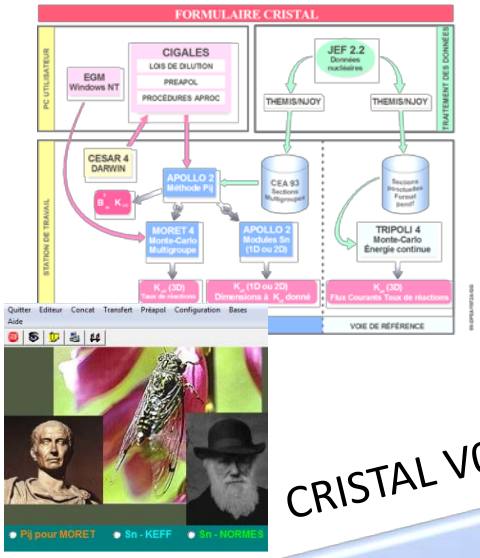
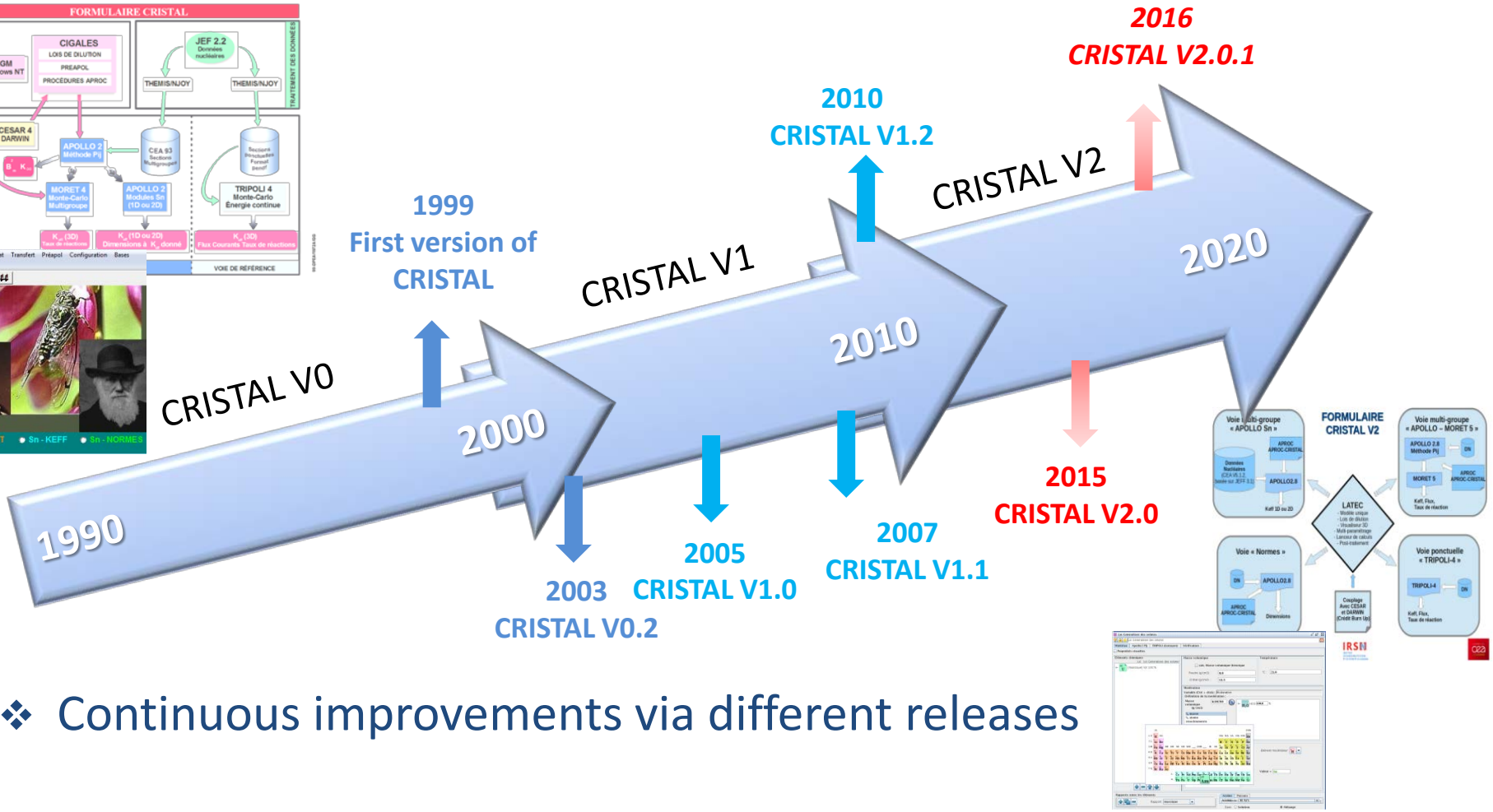
- A long term collaboration between IRSN, CEA and AREVA



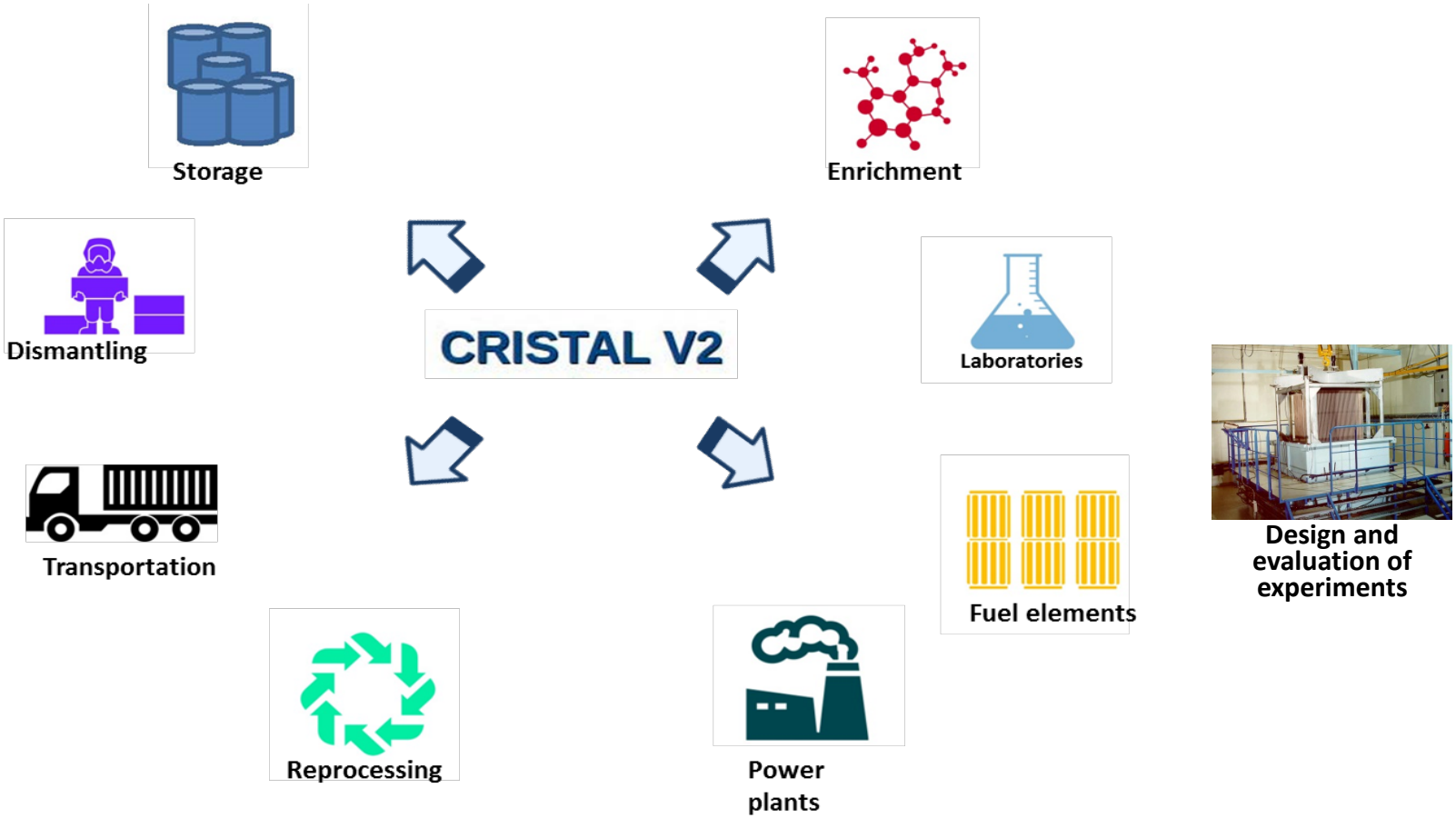




- Continuous improvements via different releases

# APPLICATION AREAS



- CRISTAL V2.0 : a criticality calculation package designed and validated
  - To cover the needs of criticality practitioners in the fields of nuclear fuel cycle facilities and transportation of fissile materials



# CRISTAL V2 PACKAGE

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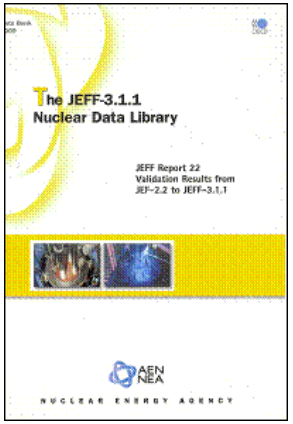
CRISTAL

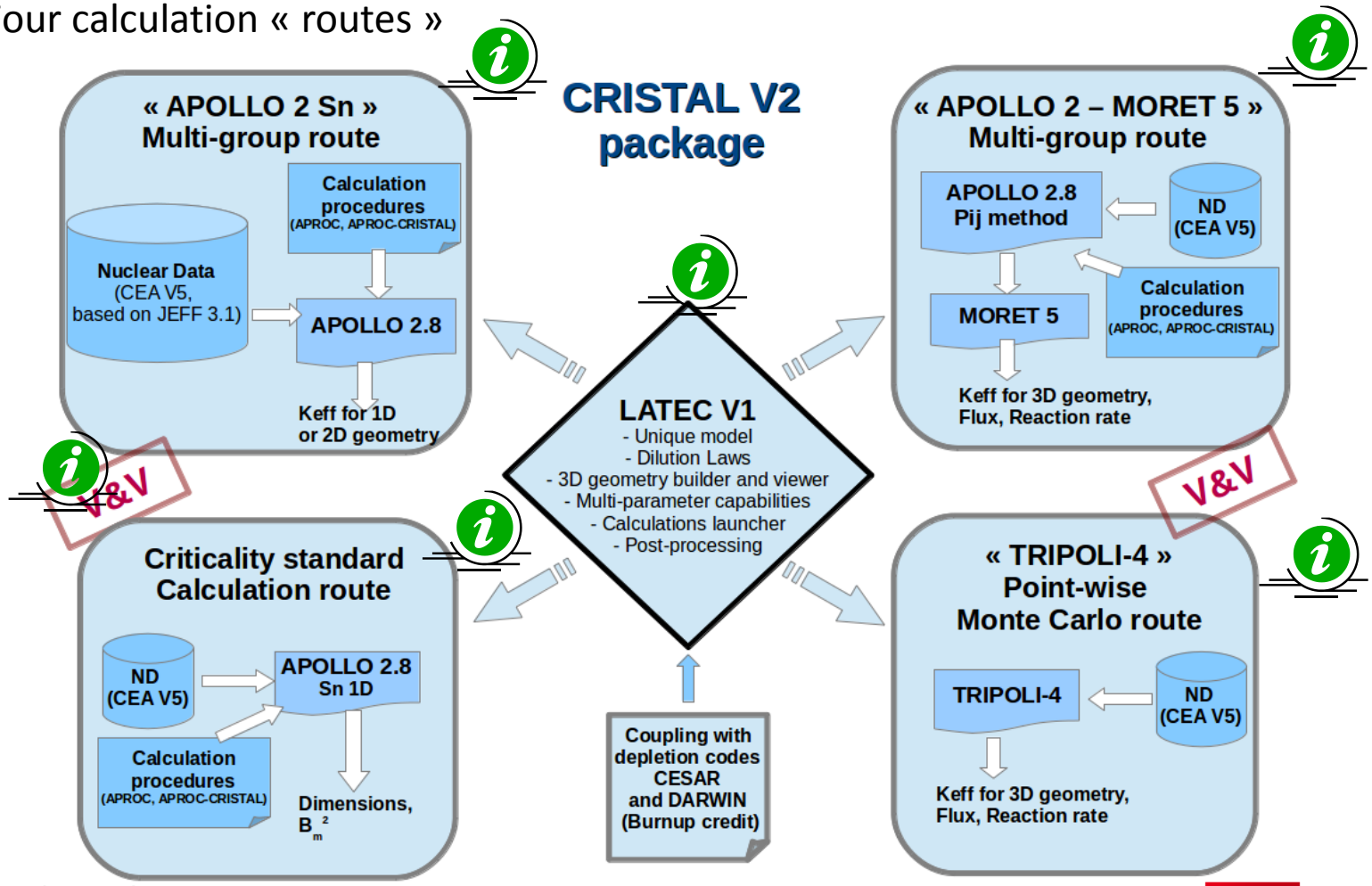
- User-friendly and easy-to-use package including
  - Consistent nuclear data libraries based on JEFF3.1.1 evaluation
  - Procedures libraries *(embedding recommended calculation schemes)*
  - New versions of transport codes *(deterministic and Monte Carlo ones)*
  - User-friendly workbench including parametric capabilities
  - An extended validation database (more than 3000 experiments)




- Four calculation « routes » dedicated to criticality
  - Multigroup and point-wise routes
  - Various density laws implemented
  - Burnup Credit Calculations using directly output files from various French depletion codes

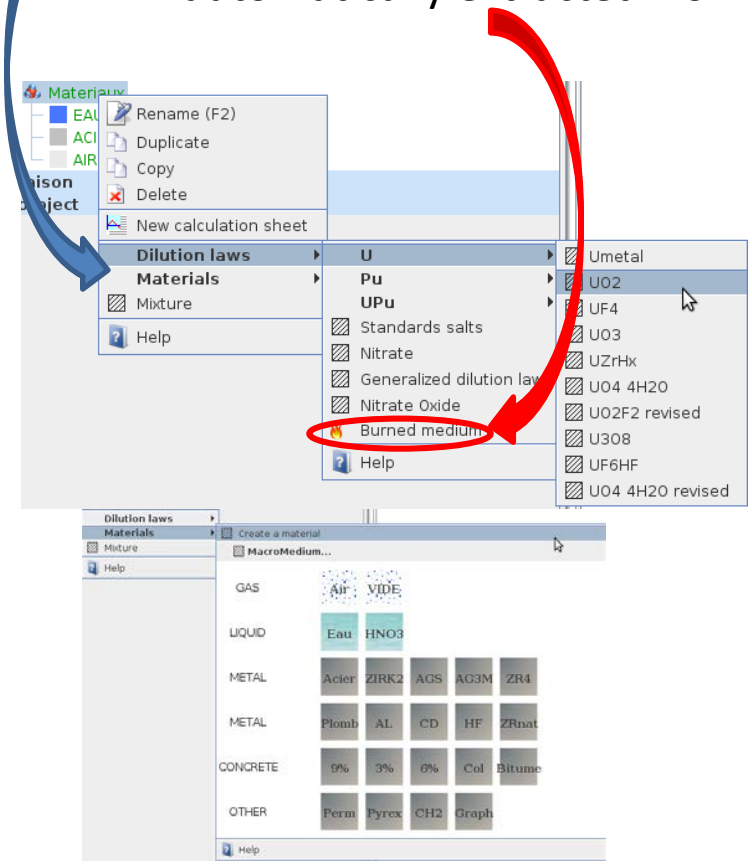
# FUNCTIONAL ARCHITECTURE

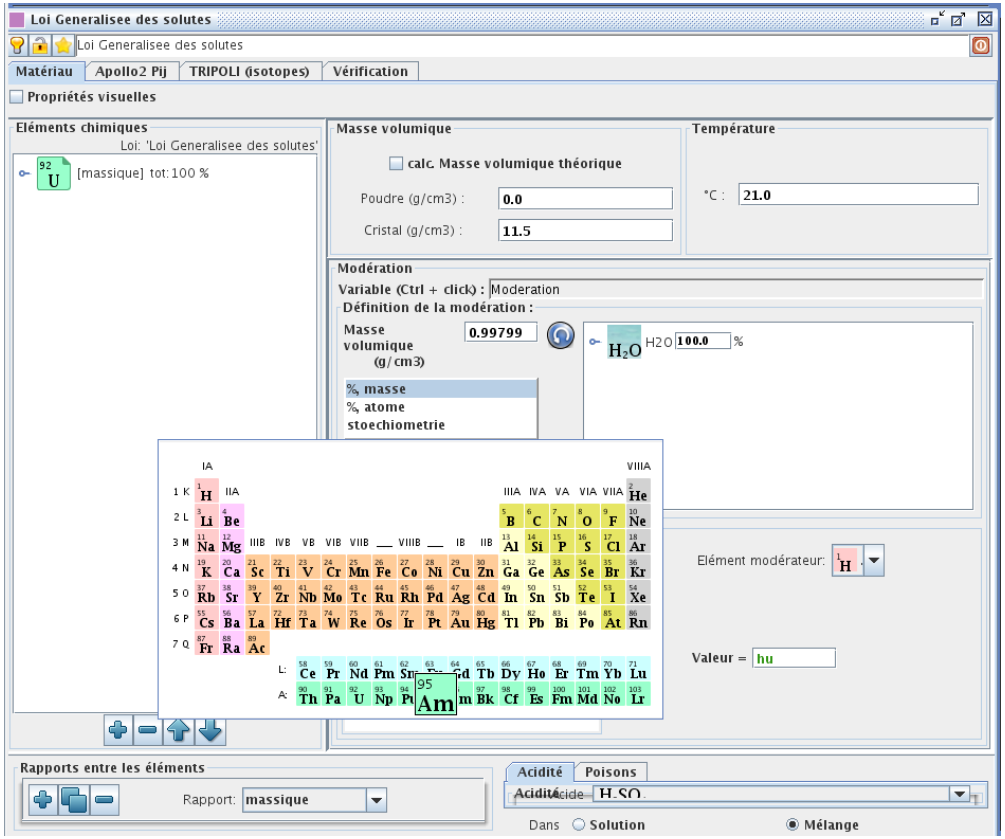
Four calculation « routes »



## ❖ Creation of materials (fissiles and non fissiles)

- Material atomic composition calculations using various density laws
- Burnup credit calculation: creation of irradiated media using isotopic data automatically extracted from CESAR or DARWIN depletion codes

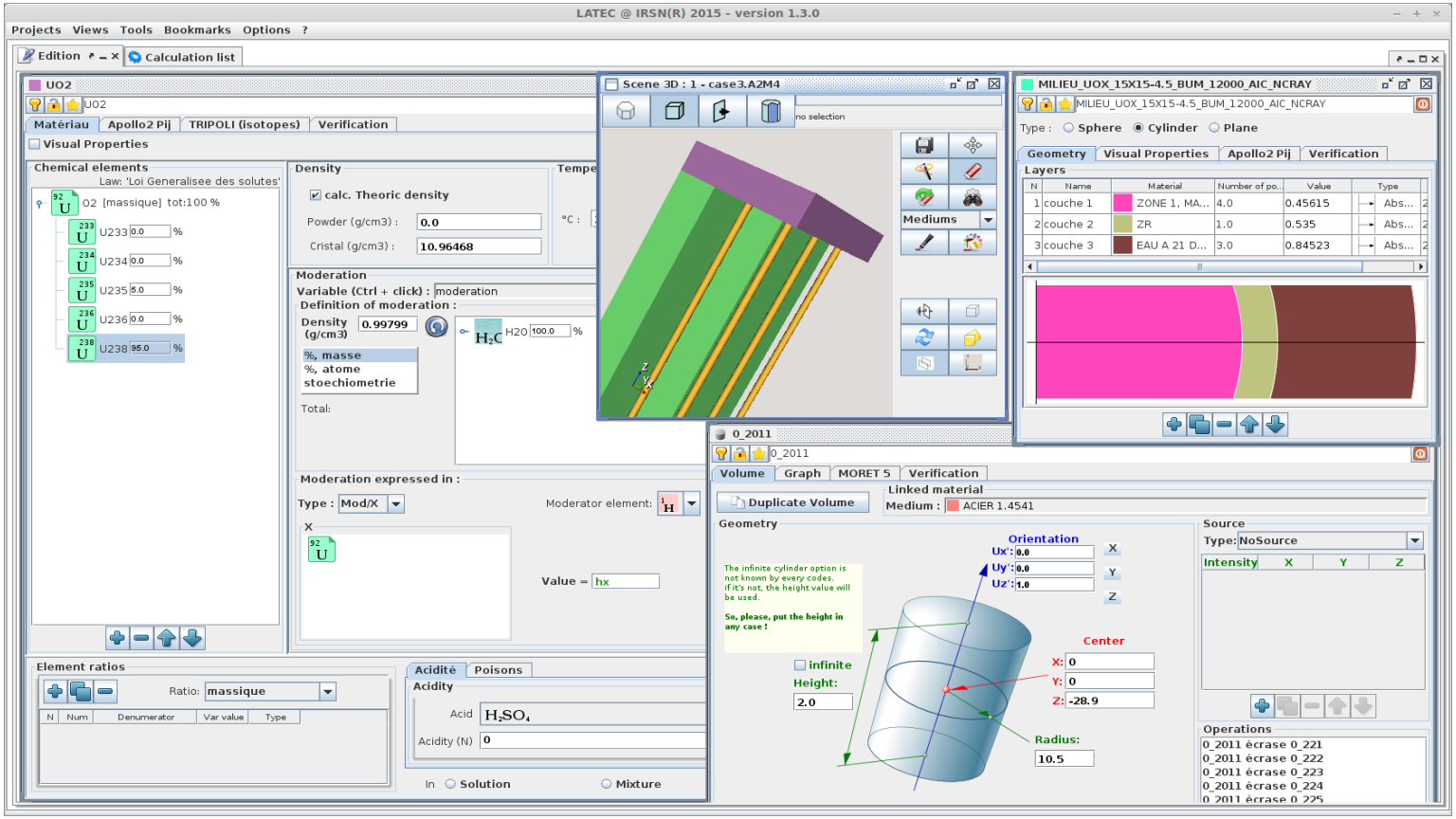


# LATEC V1 WORKBENCH

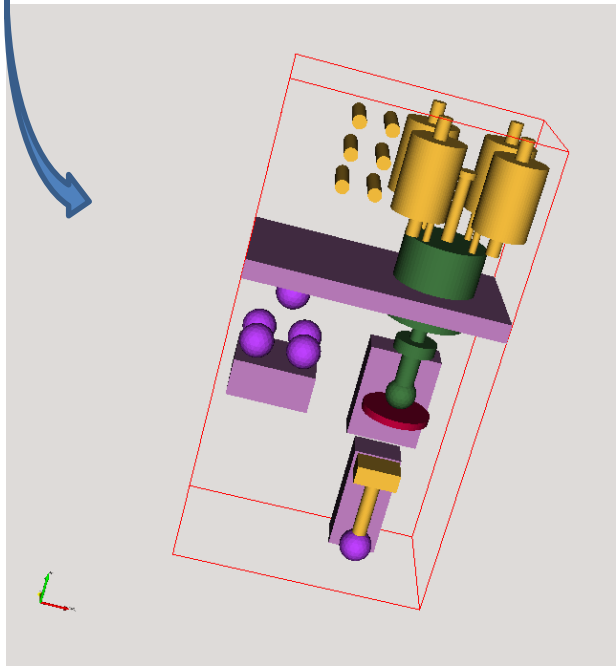


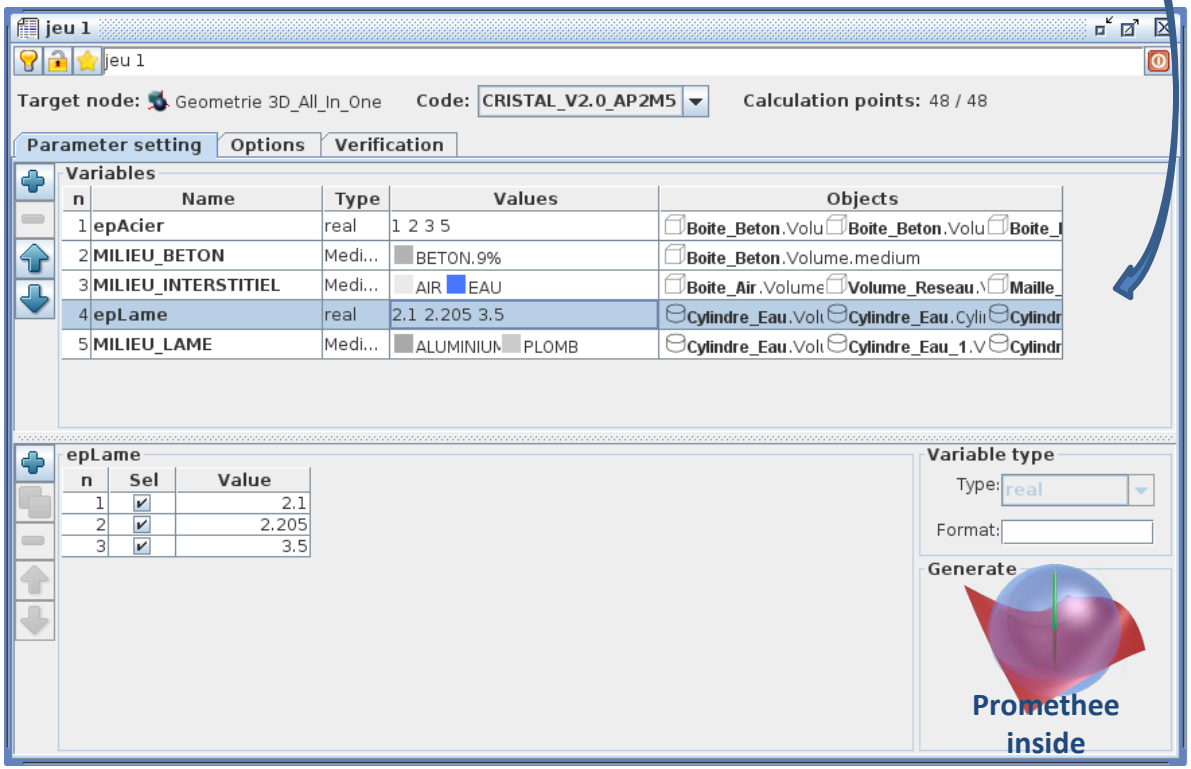
- Creation of geometry and association with the created materials
  - Description of cell pattern and description of an assembly for multi-cell calculation
  - Description of the overall geometry of the model (1D, 2D or 3D) → unique model



# LATEC V1 WORKBENCH

- 3D model visualization with the VTK library
- Example of parametric studies over chemistry and geometry model variables





# LATEC V1 WORKBENCH



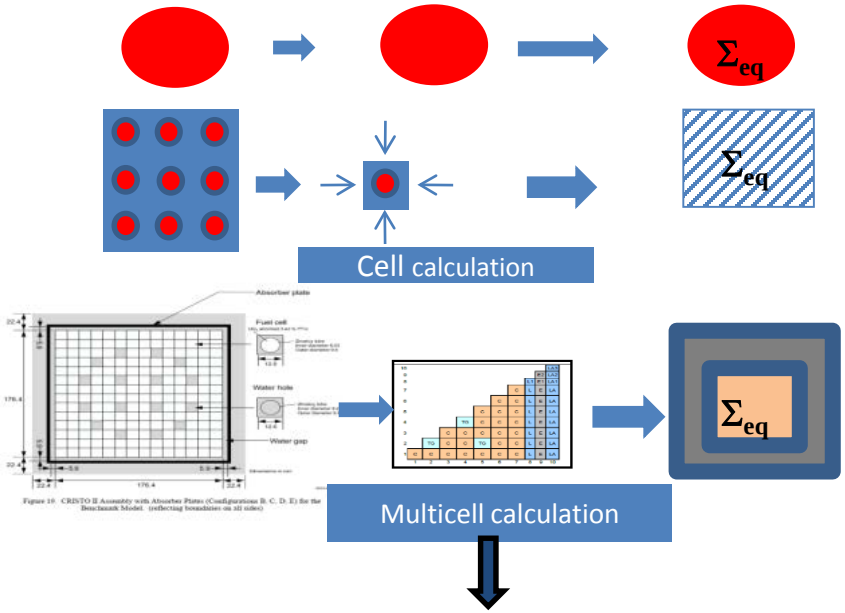
## ❖ Other LATEC functionalities

- Choice of calculation codes, methods ($P_{ij}$, Sn, Monte Carlo...) and calculation options (energy mesh, spatial mesh, ...) through tabs for each code
- Generation of the four CRISTAL calculation routes input decks
- Parallel remote launch and follow up of calculations
- Display of the calculated main results
- Import existing input decks from the previous CRISTAL 1.2 package
- Project verification through a dedicated mode

## ❖ 2 main steps of the Monte Carlo "APOLLO2 MORET 5" route

1 Cell or Multicell calculation using the Probability Collision Method ($P_{ij}$)

- Flux and multigroup self-shielded cross sections
- Spatial Homogenization (281G self-shielded and homogenized cross-sections)




2 Calculation of the $k_{eff}$ using the Monte Carlo MORET code

- Transport calculation in the 3D geometry with the MORET Monte Carlo code
- Anisotropy treatment with a Pn-like model

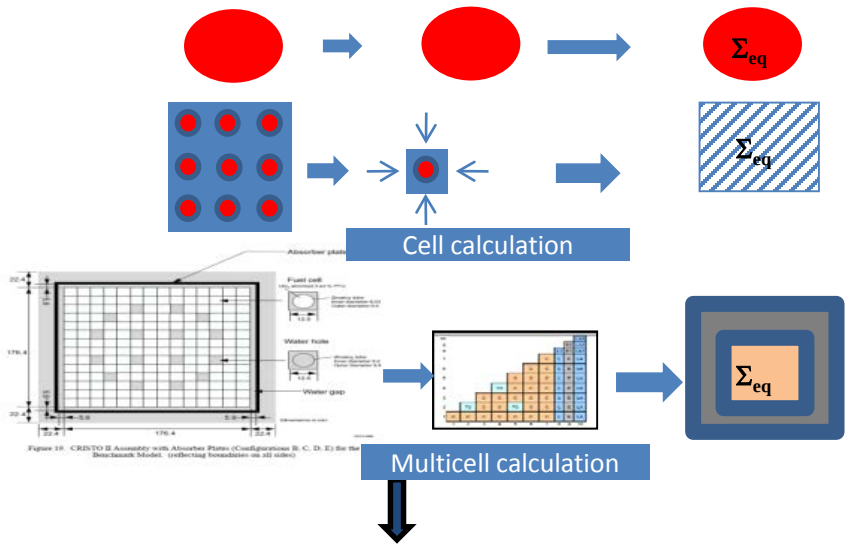
# APOLLO2 SN MULTIGROUP ROUTE



## ❖ 2 main steps of the deterministic "APOLLO2 Sn" route

1 *Cell* or Multicell calculation using the Probability Collision Method ($P_{IJ}$)

- Flux and multigroup self-shielded cross sections
- Spatial Homogeneization and 20-groups collapsing of the cross sections




2 Calculation of the $k_{eff}$ using the discrete Ordinate Method (APOLLO2 Sn)

- Transport calculation in 2D geometry or simplified 1D geometry
- Calculation of the keff of the studied configuration

# POINT-WISE MONTE CARLO ROUTE

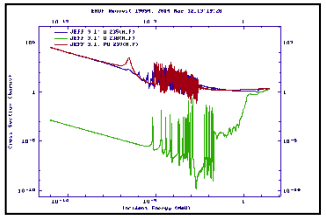
**Point-Wise Nuclear Data**
(continuous energy cross sections library)

↓

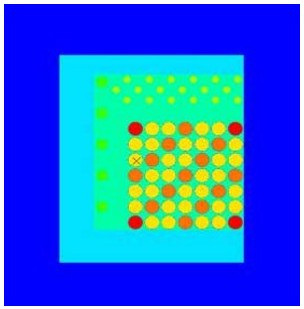
**TRIPOLI-4® Monte-Carlo Code** (version 8.1)

↓

**$k_{eff}$, flux, Reaction Rates**



Point-wise fission cross-section for $U^{235}$, $U^{238}$ and $Pu^{239}$ issued from JEFF3.1.1 Nuclear Data (CEAV5.1.2 cross-sections library)



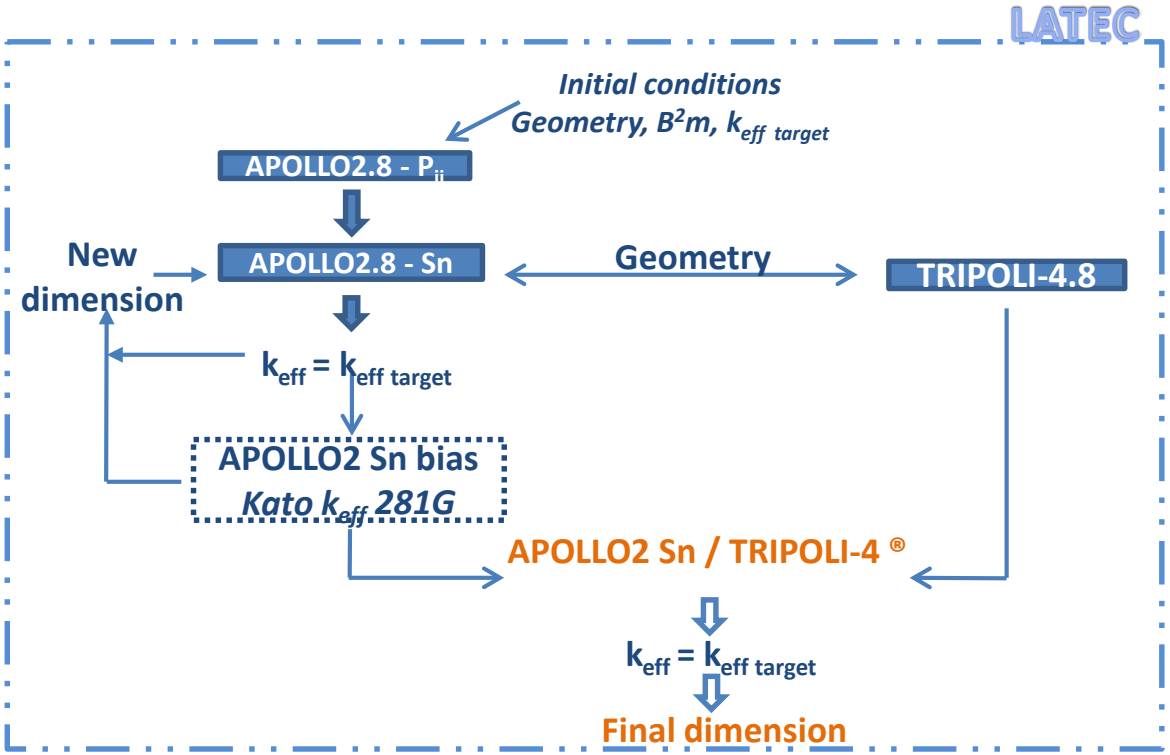
Example of a 3D geometry modeling : fuel disposal configuration


Variation of the configuration $k_{effective}$ versus the thickness of the water gap

- **TRIPOLI-4®: 3D continuous energy Monte-Carlo code**
  - Point-wise cross-sections library (continuous energy)
    - Nuclear data is consistent with the multigroup route of CRISTAL V2.0 (CEA V5.1.2 cross sections library based on JEFF3.1.1 nuclear data evaluation)
  - Probability tables for the unresolved resonance range (URR)
  - TRIPOLI-4® solves the linear Boltzmann equation for neutrons, with the Monte Carlo method, in any 3D geometry and without any approximation

# CRITICALITY STANDARD CALCULATION ROUTE

- **« Standard » route using APOLLO2 $P_{ij}$-APOLLO2 Sn (1D)**
  - Iterative process to determine dimensions (sphere, slab, cylinder) corresponding to a target $k_{eff}$
  - Quantification of bias due to the approximations in $S_n$ Method (spatial and energetic meshes, anisotropy)
- **Possibility to automatically compare with TRIPOLI 4® point-wise route (via LATEC)**



# VERIFICATION AND VALIDATION (V&V)



## ❖ Verification according with a strong QA system

- Separate verification of each code, workbench, procedure, library, …
- Verification of multigroup routes by comparison with point-wise one
- Verification of the complete calculation routes on industrial cases

## ❖ Validation process

- STEP 1 : (C – E) calculation and combined one standard deviation

$$\sigma = \sqrt{\sigma^2_{\text{calculation}} + \sigma^2_{\text{benchmark}}}$$

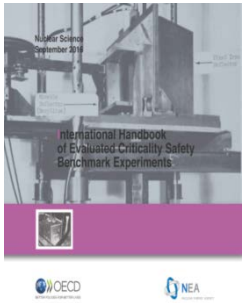
  - Using recommended calculation schemes and procedures
  - Discrepancies within the uncertainties margins
    - Calculation results in good agreement with the benchmarks
  - Comparisons with other available experimental programs in the same field (similar media, materials and/or configurations)
- STEP 2 : (C-E) discrepancies analysis in order to have a feedback to the nuclear data and/or to the calculation schemes by using inter-code comparisons:
  - Between the different CRISTAL V2 routes
  - Using other available calculation results from international codes (MCNP, SCALE, MONK, etc…) using various libraries

# VERIFICATION AND VALIDATION (V&V)



## ❖ An extended validation database

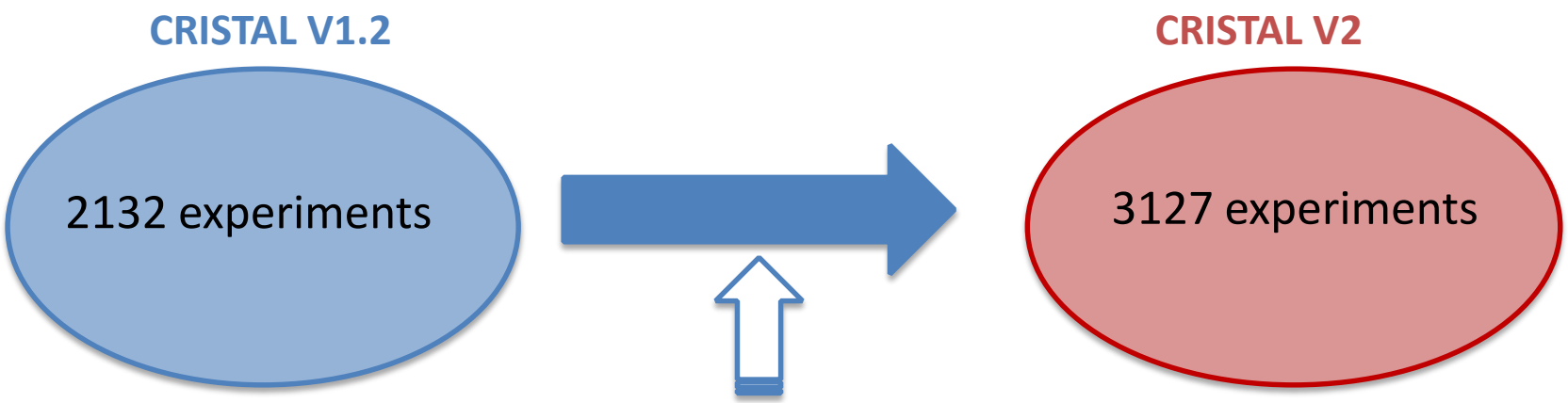
- ≈ 80 % of benchmarks from ICSBEP Handbook
- Additional experiments from French proprietary programs
- Validation performed by the codes development teams
- Benefits from and contributes to JEFF-3.1.1 validation




| FISSILE MEDIUM | NUMBER OF CASES | | | |
|---|---|---|---|---|
| | **Target** | Multigroup route (APOLLO2 – MORET 5) | Multigroup route (APOLLO2 Sn) | Point-wise route (TRIPOLI-4®) |
| **Pu** | **519** | 412 | 145 | 295 |
| **HEU** | **872** | 762 | 264 | 434 |
| **IEU** | **91** | 78 | 24 | 2 |
| **LEU** | **983** | 887 | 174 | 410 |
| **U233** | **59** | 52 | 14 | 42 |
| **MIX** | **597** | 517 | 172 | 167 |
| **SPEC** | **6** | 6 | 0 | 0 |
| **Total** | **3127** | 2714 | 793 | 1350 |

## ❖ Evolution between CRISTAL V1.2 and CRISTAL V2

- 3127 experiments for the three routes
  - 2714 (AP2M5), 793 (AP2Sn), 1350 (TRIPOLI-4)




- Handbook ICSBEP since 2005
- Users needs
  - BUC, Lowly moderated MOX, slabs, structural materials
  - Nuclear future cycles ($^{232}$Th)

# VERIFICATION AND VALIDATION (V&V)



## ❖ Main results

- Use of JEFF-3.1.1 evaluation
  - A significant improvement of calculated $k_{eff}$ compared to the use of JEF2.2 in the previous version of the CRISTAL package
- Use of the 281-group energy mesh and the new treatment of scattering cross-sections of intermediate mass isotopes
  - Bias reduction from 1% to 2.5 % for multi-group calculations for thick reflector compared to 172-group energy mesh library
- New 281-group treatment of $^{238}U$ combined with the JEFF-3.1.1 cross-sections
  - A strong bias reduction of 1.4 % on average for the multi-group Sn deterministic route compared to the previous version of the CRISTAL package
- Calculation results generally in good agreement with the benchmark $k_{eff}$
- Significant over-estimations still observed with the multi-group calculations routes for reflected configurations with thick structural materials (aluminum, steel, nickel), mainly in fast spectra
- Lacks in the validation database coverage : lowly moderated MOX, slab….

# FEEDBACK AND CUSTOMERS SERVICES



## Feedback

- First version of the CRISTAL V2.0 delivered in June 2015
- One year of user's feedback
  - Released version V2.0.1 distributed in June 2016
- A new one, called V2.0.2, under development and validation

## Customers services

- Covering a range of areas of activity like
  - Documentation
  - Hotline
  - Maintenance
  - Training courses

# CONCLUSIONS



## ❖ CRISTAL V2.0 package

- 10 years of development, verification and validation in the frame of a strong collaboration between CEA, AREVA and IRSN
- Represents a coherent system combining the best properties of the APOLLO2, MORET 5 and TRIPOLI-4 codes
- Offers a high level of user friendliness and flexibility with the LATEC workbench
- Proposes an accurate, comprehensive and extended validation database
- Has been designed, verified and validated according with a strong QA system

**Provision of the CRISTAL V2.0 package to the OECD/NEA Data Bank**

NEA Nuclear Energy Agency

# DEPLETION CODES « COUPLING »



- Implementation of Burnup Credit (BUC) methodology in criticality studies of PWR applications
  - Calculations using CESAR5 or DARWIN2.3 depletion codes (CEA) to provide BUC isotopic concentrations
    - Burnup profile 1
    - Isotopic Correction Factors on BUC isotopes retained in the criticality study 2
    - Specific CRISTAL output files created by CESAR or DARWIN providing spent fuel conservative isotopic concentrations after irradiation or cooling time 3