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# INVAP NEUTRONIC CALCULATION LINE

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**Abstract**. The improvements in the computational systems (increasing the memory and storage capacity and reducing the computational time) allows the development of innovative methods for reactor calculations, including not only more detailed theories and highly accurate numerical methods, but also adding more prediction capabilities and additional engineering information to perform the engineering analysis of the system. As an example, it is possible nowadays to integrate different tools with interdisciplinary or multi engineering information, improving the analysis of the calculated systems. For this reason, INVAP has been on continuous development of the calculation system used for design and optimization of nuclear reactors. The calculation codes have been enhanced with new capabilities for the new challenges. Some of the improvements are developed in the framework of the Upgrade of INVAP´s proprietary calculation line developed with the contribution of the Argentine National Agency of Technological and Scientific Promotion (*Agencia Nacional de Promoción Científica y Tecnológica -ANPCyT*), through the funds of the Argentine Technological Funds (*Fondo Tecnológico Argentino, FONTAR*).
The current state of the code packages enables INVAP to design and follow up nuclear installations with complex geometries using a set of easy-to-use input files. The calculation line is divided, basically, in two main codes: Cell (CONDOR) and Core (CITVAP) codes. The homogenized and condensed macroscopic Cross Section (XS) is one of the main parameters used as interface between both codes; they are calculated by the cell code and used as input by the core code. A set of intuitive graphic pre and post-processors have also been developed providing a fast and complete visualization tool for the parameters obtained in the calculations and several post-processors were developed to ease the interface between the different codes. This work describes the whole INVAP calculation line starting from the nuclear XS data, up to the different interfaces with third party codes.

## 1 INTRODUCTION

The variables needed in reactor physics analysis depend on the interaction of the neutron with the matter. The properties of the matter are basically given by the nuclear XS and engineering data. The engineering data depends on operational conditions (for example temperature, density, cooling conditions, etc) and the nuclear XS depends basically on energy and temperature, and but also in the specific engineering data like crystal and molecular structure of the materials. To obtain the neutron distribution in a reactor core (through the neutron flux) the transport equation need to be solved. For this purpose different methods and tools are usually used. Furthermore the neutronic flux depends on Position, Angle, Energy and Time, thus the solution of the flux in the whole reactor taking into account all the details of system on these variables requires a large amount of computational resources.

Most of current available calculation lines use the fact that a nuclear reactors is normally designed using several fuel assemblies and they are of the same or similar design. This allows dividing the calculation of the reactor at least in two steps: Calculation of the Fuel Assembly, and the calculation of the core:

- The first step (named cell calculation) is carried out in a small system, for example a FA, but with high spatial and energy detail. In this step, to solve the transport equation using a highly precise method is mandatory (such as Collision Probabilities, Discrete Ordinates or MonteCarlo)
- The second one (named core calculation) is carried out in the whole reactor core, but without this level of details. The reduction of the level of detail is done condensing and homogenizing the nuclear XS.
  In this step to solve the transport equation, a less precise method can be used (such as Diffusion approximation).

### 1.1 General Description of the calculation line.

Figure 1 shows INVAP´s calculation line (Mochi, 2011) which has been used by INVAP and several of its customers for the design, optimization and follow-up of several reactors throughout the world obtaining optimal results, like RA-6, NUR, RA-8, ETRR2, OPAL, CAREM, CNA-II, etc. These codes are also used by nuclear engineering students, master's and doctoral thesis students of the Balseiro Institute, performing a large number of calculations for different reactor types such as MTR, PWR, BWR, PHWR, TRIGA, FBR, ADS and Homogeneous reactors.

A few of the characteristics of this calculation line are:

- Well defined calculations steps: Library generation, cell and core calculations.
- Integration between deterministic and stochastic codes.
- Capability to perform calculations with macroscopic or microscopic XS.
- Capability to perform thermal-hydraulic analysis for coupled neutronic/thermal-hydraulic calculations. This feature is very important for power feedback coefficients, thermal-hydraulic margins to critical phenomena and the calculation of the growth of oxide layer, which is a very limiting factor for high performance MTR fuel assemblies.
- Capability to generate specific data for third party codes.

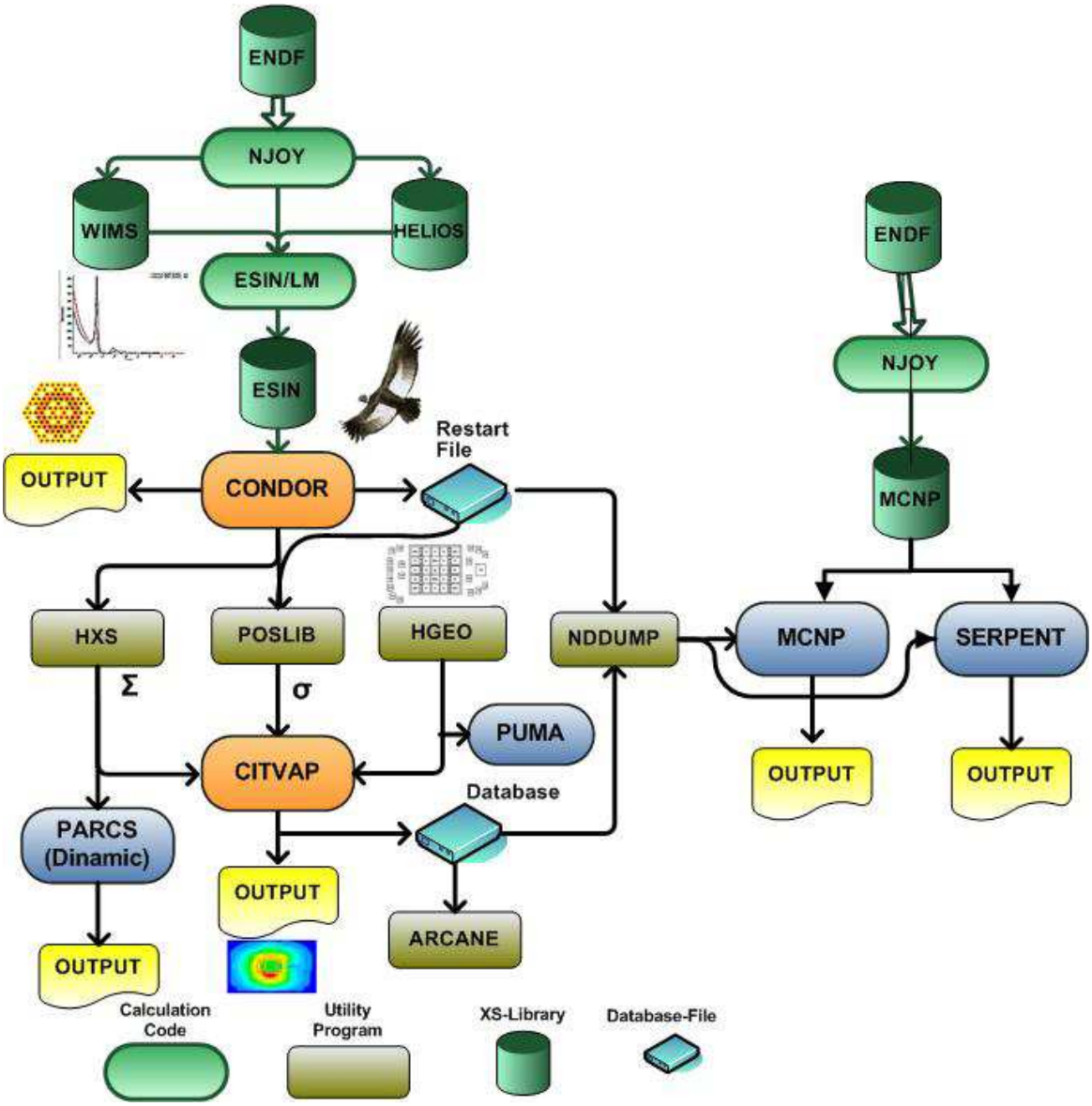


Figure 1: INVAP Calculation Line

## 1.2 Summary Description of the codes

This calculation line includes:

- **ESINLM**: (**ES**cuela **I**ngeniería **N**uclear **L**ibrary **M**anager). This program is used for the maintenance of the nuclear microscopic multigroup XS library. It has for example, the capability to add isotopes from ENDF/B files after NJOY processing.
- **ESINPLOT**: This is a graphical post processor to plot XS available in the nuclear library.
- **CONDOR** (Villarino, 2002): This is the cell code performing the neutronic calculation of the fuel assembly (FA) or any component of the reactor core. CONDOR calculates homogenized and condensed macroscopic XS to be used by the core code. It can be also used for the analysis of the FA, or to generate additional data to be used by other codes.
- **HXS** (Mochi, 2011): (**H**and **XS**): Macroscopic XS library manager. This program is

the interface between Cell code and Core code. It has the capability to import XS from different cell codes, and export them to different core codes.

- **POSLIB (**Mochi, 2011**)**: This program is used to generate CITATION (Fowler T; Vondi D, 1969) microscopic XS libraries from the CONDOR outputs.
- **HGEO (**Mochi, 2011**):** (**H**and **GEO**metries) This program is a visual pre processor to generate the geometrical input for CITVAP **(**Mochi, 2011**).** It also has the capability to generate PUMA (Grant C., 1980) geometrical input.
- **CITVAP (**Mochi, 2011**)**: This is the core code performing burnup-dependent calculation of nuclear reactor cores, calculating the nuclear parameters associated with several states of the reactor taking into account the feedback of many thermal-hydraulic parameters.
- **NDDUMP (**Mochi, 2011**): (N**umerical **D**ensities **DUMP)** This utility is capable to generate burnup dependent numerical densities to be used by MonteCarlo codes such as MCNP (Brown F., Kiedrowski B., Bull J., 2010) or SERPENT (Leppänen J, 2013) codes.
- **ARCANE (**Villarino E., 2013a**): (A**dvance **R**eactor **C**ore **AN**alysis **E**nvironment: enhancing the esoteric art of reactor design**):** This is a very important analysis tools to perform numerical calculations and verifications with the core or cell code calculated parameters.
- **POS_CON (**Mochi, 2011**)**: This is a graphical post processor of the CONDOR code.
- **FLUX (**Mochi, 2011**)**: This is a graphical post processor of the CITVAP code.

It should be noted that INVAP develops the graphical post-processors with a key concept based on its past decades experience: Graphical interfaces must be an engineering analysis tool not just visualization tools.

The most relevant codes of the calculation system are introduced in the following sections following the step during the calculation process.

### 1.3 Utilization and Validation

This calculation system has been used by INVAP and several of its clients for the design, optimization and follow-up of several reactors throughout the world obtaining optimum results:

- RA6: RR in Argentina, in operation (1982)
- NUR: RR in Argentina, in operation (1988)
- RA-8: Critical facility in Argentina, criticality (1997).
- ETRR2: Multipurpose RR in Egypt, in operation (1998)
- OPAL: Multipurpose RR in Australia, in operation (2006)
- CNA II; NPP in Argentina, in operation (2014).
- CAREM: Small NPP in Argentina, under design.
- RA-10: Multipurpose RR in Argentina, under design.
- RMB: Multipurpose RR in Brazil, under design.

These codes are also used by nuclear engineering students, master's and doctoral thesis students of the Balseiro Institute, performing a large number of calculations for different reactor types such as MTR, PWR, BWR, PHWR, TRIGA, FBR, ADS and Homogeneous

reactors.

### 1.4 Programming

All the codes and utility programs were developed using FORTRAN programming language. This ensures the scalability of all the software in the calculation system, making it easy for INVAP to update, combine or improve any single piece of the package in a fairly independent manner.

Besides, several standards are applied to link most key programs of the Calculation Line. The most relevant example of this criterion is the database architecture. This architecture is being changed in the versions under development in order to homogenize the interaction of all the programs with a single proprietary database access library that will provide fast (indexed) access to the information as well as great potential for further development. The current version of the database is STORM v2.0 (Villarino E., 2013b).

To improve the performance of the calculation line, the core code CITVAP was parallelized using the OpenMP directives. In this frame, two additional improvements are planned: Parallelize CONDOR code and integrate CONDOR and CITVAP codes using MPI.

The graphic pre and post processors are also programmed in FORTRAN language and currently use a commercial graphic development library for generating and managing the GUIs which has proven to be both programmer and user-friendly.

All the software is compiled (and has been successfully tested) for use in Microsoft Windows and Linux systems. Furthermore, the database files are fully portable between these two platforms. INVAP maintains only one source code for both platforms. As an example, one of INVAP customers runs the Calculation Line in a Sun Cluster, with Solaris Operating system.

### 1.5 Project Objectives

The calculation line is developed not only to have high performance and modeling calculation capabilities, but also to be properly used in the frame of a reactor project. The project management requirements can be summarized as follows:

- Minimize data errors.
- Minimize interfaces errors.
- Use the same calculation methodology
- Traceability of the results

To fulfill these objectives the calculation line facilitates sharing the data, models and calculation procedures. Additionally, the calculation line benefits from the following value added:

- Share experience between users.
- Ease the review of the input / output files.
- Backup system.
- Generate modeling and calculation knowledge

Summarizing, the INVAP calculation line fulfills the following key concept in the frame of a management of a project: *"Share between different analysts, designers, reviewers and approvers a single set of tools, data, procedures and validated documents"*

## 2 NUCLEAR DATA LIBRARY

Currently INVAP use a customized nuclear data library for each project. For most of the MTR projects they are based on the WIMS 69 group's library (Askew, Fayers and Kemshell, 1967), including several improvements in some isotopes, and adding new ones according to the needs of the project. The source of these new isotopes could be from ENDF/B (Chadwick M B, et al., 2006) using NJOY (Macfarlane R E and Muir D W, 1994), or from WLUP (IAEA, 2003) or HELIOS library (Ferri et al, 1997).

INVAP also uses the Helios 190 group's library or WLUP (Leszczynski F, Lopez Aldama D, and Trkov, 2003) library when a project has a special requirement.

Currently, INVAP is working in the generation of a new library based on ENDF/B 7.1, with a new STORM structure adding several nuclear data to allow a significant improvement in the overall calculation capability. The microscopic XS library has a very important set of data, which couple de library with the cell calculation code.

These data are the resonant parameters, currently CONDOR code use 2 different resonance calculation methods: The integral resonant method, and the Subgroup method. Both theories requires the resonant integrals, lambda factors, but in the subgroup method, the subgroups XS and its corresponding weights need to be calculated.

Two programs are basically used for the management of the microscopic XS libraries:

- ESINLM: This program allows the generation, and modification of the ESIN libraries. It can generate the nuclear data library from different sources, like WIMDS and, HELIOS format. It can add isotopes from the NJOY output (WIMSR module), it can modify the available nuclear data, etc.
  Nowadays, a new version of the ESINLM is under development to manage the new ESIN library format.
- ESINPLOT: This is a graphic post-processor to plot microscopic XS, currently allow the comparison of different libraries, reaction types, and isotopes.

## 3 CELL CODE

Cell level calculation is a very important step in the calculation of a given reactor. This calculation is carried out with a high spatial and energy details to properly model the FA of the reactor. To perform this calculation a good transport method is needed, and the Collision Probabilities method in a multigroup scheme is an excellent choice.

CONDOR solves the transport equation in 2D general geometries using Collision Probabilities Method and the Heterogeneous Response Method. In the last method, the whole system is divided into space elements and these space elements are coupled to model the whole system where each Space element is solved by Collision Probabilities Method.

The subgroup method is used in complicated geometries to calculate effective resonance XS for the resonant isotopes. This provides an accurate method for calculating in 2D fuel assemblies, taking into account the heterogeneous character of the FA.

Accordingly, CONDOR can model in a fast and accurate way very complicated geometries needed for some FA or components of a reactor. Besides it includes several options to perform state dependent calculations to properly simulate the behavior of the reactor code. As an example, CONDOR can easily generate burnup dependent homogenized and condensed XS for the thermal-hydraulic feedback present in the nuclear power plants.

The pre-processing capabilities of CONDOR enable the use of regular expressions to create the necessary geometries in a simple way. These make easier the input preparation of complicated system. Due to this capability, and its computational efficiency, some burnup

dependent 2D full core calculations are performed.

Additionally to CONDOR code, the graphical post-processor analysis tool POS_CON is used. This program plots the system under calculation and several variables in function of Burnup, Space (1 and 2D), and Energy, where comparisons with the different calculation states or with other cases are also allowed. This pos-processing tool was designed to plot the data in floating auxiliary child windows that pops out when plotting the different type of variable in order to easy the engineering analysis. These windows can be re-located or minimized according to the required use. The program also can show burnup and energy dependent data regarding a particular point as the user hovers the 2D system plot with the pointer.

## 4 CORE CODE

Core calculation is the other key step in the calculation of a given reactor. This calculation is carried out with a high spatial volume. The Diffusion method is a proper method to solve efficiently the neutron flux.

CITVAP is a code developed from the well-known Diffusion code CITATION II (T. Fowler; D. Vondi, 1969). CITVAP greatly enhances the capabilities for design and fuel management provided by CITATION II, giving to the user an easy-to-use set of free-format keywords that provide a more intuitive input file. CITVAP can solve the following 1, 2 and 3D geometries: rectangular (XYZ), cylindrical (RθZ), triangular (TZ) and Hexagonal (HZ). It has the capability to calculate neutron flux and adjoint-flux (useful for the calculation of the kinetic parameters).

The main improvements carried out in CITVAP can be divided in two categories:

- From design point of view: Several calculation options are available like: Burnup calculation, Fuel Management, search for equilibrium cores, control rod movement strategies, Xe and Sm transients, including thermal-hydraulic feedback, calculation of feedback coefficients, including power feedback coefficient, etc.
- From reactor operation follow-up: Several administrative capabilities were added, for example: control rod movement and power changes with the operation time, fuel management with the proper fuel ID's for safeguards inventories, pool storage management, etc.

Several programs are basically used in this calculation step:

- Two of them to get the homogenized and condensed XS from the cell code (microscopic and macroscopic) and prepare them to be used for the core code:
  - HXS: This program imports the macroscopic XS generated by CONDOR code and storage in a library to be used later by CITVAP code. It can perform several administrative tasks to help a good administration of the macroscopic XS library. The information saved in the library is not only the burnup dependent XS, but they state variables like temperatures, densities, boron concentration, etc. This type of XS is the most frequently used option for core calculation.
    Additionally, this utility can import XS from other cell codes, and export to other core codes (for example PUMA).
  - POSLIB: This program imports the microscopic XS generated by CONDOR code and export them in a CITATION II microscopic library. This program can also read the burnup distribution of a core, to generate a microscopic library with better condensation spectra, and the proper numerical densities to be used in the input of

CITVAP code. This type of XS is currently used for kinetic parameter calculation.

- Another program needed for modeling geometrically complex systems in rectangular geometry is HGEO. This graphic pre-processor allows the user to change the free-format input file and view the changes using a very fast GUI (Graphic User´s Interface). HGEO is a program that has been greatly expanded in the past few years, taking advantages from the input processing capabilities. Some of these features allow the user to define generic templates which have several input parameters that can be used to construct arrays of complex similar objects without making the input file too hard to interpret and/or check. This program generates input files for CITVAP and PUMA codes.
- Finally the last utility needed on this calculation step is FLUX, a graphical post processor analysis tool, which has been developed in order to maximize the analysis capabilities of CITVAP. This GUI lets the user plot a wide set of variables involved in the calculation: Neutron Flux, power densities, temperatures, coolant density, fuel burn-up, control rod insertion level, selected isotopes concentration (Boron, Xenon, Samarium, Promethium and Iodine), neutronic fluence, adjoint flux, multiplication factor, reactor power, power peaking factor, fuel movements during refueling and many more. All these variables can be represented as a function of position (if applicable) and time. It also allows the user to plot these parameters following a particular fuel assembly that might be relocated several times by the refueling schedule.

  The program was designed to present most numeric data in a floating auxiliary child window that pops out when plotting a two-dimensional graph. This window can be re-located or minimized according to the required use and shows specific data regarding a particular point as the user hovers the 2D-plot with the pointer. It also shows a one-dimensional plot of the variable in the direction that is not being shown in the 2D-plot, giving the necessary information for a complete evaluation of the three-dimensional characteristics of the selected variable.

  Another very important capability is the calculation and plotting of the oxide layer growth for an MTR fuel assembly, following his historical behavior along its operating time.

## 5 UTILITIES

The INVAP has two very important tools or utilities needed for the analysis of the reactor.

### 5.1 NDDUMP

This utility is very important for the integration of the deterministic and stochastic codes. It has the capability to generate burnup dependent numerical densities (according to the reactor core state calculated by CONDOR-CITVAP codes) to be used by the stochastic codes.

The NDDUMP program read two databases:

- CITVAP database at a given state, (for example at BOC or EOC) reads burnup, coolant and fuel temperature and coolant density distribution (per FA and axial layer).
- CONDOR data base reads Fuel Assembly burnup dependent numerical densities per material.

With this information NDDUMP provide for each FA and axial layer the numerical densities for this specific condition.

The output of NDDUMP can be used in MonteCarlo codes such as MCNP and SERPENT codes.

### 5.2 ARCANE

ARCANE is a post processing environment developed under FORTRAN95 language by INVAP S.E. to perform detailed analysis of the results from codes that manage databases in STORM v2.0 format. This environment has its own language (based on FREFMT v3.3 free-format routines) that allows the user to process, operate and take decisions using data from databases in such format.

It is important to note that the current version of ARCANE code is oriented to analyze CITVAP results, thus several built-in functions are developed in such sense. Future versions of the code will be able to handle other codes databases (such as CONDOR) in an easier way.

Using this environment the user can easily:

- Manipulate and combine data from different codes like CITVAP, CONDOR, etc (with formats STORMv2.0).
- Homogenize and condensate results.
- Evaluate design parameters and/or requirements for a given reactor using data from several databases, such as shutdown margins, discharge burnup, activity, etc.
- Systematize procedures for design criteria checking.
- Facilitate the documentation of CITVAP (and other INVAP codes) results.

The user can also access to all variables from databases, thus the use of this environment is not restricted to post processing. In spite of this, the current ARCANE version includes several built-in functions, commands and automatically defined variables that are oriented to the post processing of CITVAP`s results.

## 6 CONCLUSIONS

The calculation system used by INVAP consists of a wide variety of calculation codes, utility programs and graphic processors which, coupled with third parties codes, covers the design needs for facing the near future challenges from calculation point of view and project management requirements.

This calculation line is continuously verified and validated for different applications using different tools or benchmarks:

- Against different calculation lines: WIMS-PUMA, HUEMUL-PUMA, MCNP, SERPENT, etc.
- Theoretical benchmarks: for MTR and NPP.
- Experimental benchmarks: MTR, WWER, PWR, BWR, TRIGA, Fast Reactors, Subcritical systems, etc.

It is used for different institutions like INVAP, CNEA, ARN, ANSTO, CRDN, providing a solid behavior of the calculation line under different applications and users.

It is also one of the neutronic calculation systems currently used in the Balseiro Institute for academic training of the students in the Nuclear Engineering career, and it is also used in the Degree, Master and Doctoral thesis of this Institute, showing good results and probing its user-friendly characteristics.

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