Towards DRAGON Version4

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What is Version4?

Version4 is a new distribution of the reactor physics computer codes at GAN. Its components are:

- `DRAGR` module in NJOY and Python script `PyNjoy.py`
- Ganlib tools (CLE-2000, LCM/XSM API)
- Modules (calculation operators) of the following codes:
  - Dragon: lattice code
  - Trivac: reactor (full core) code
  - Donjon: simulation of reactor operation – end of 2006
  - Optex: reactor design optimization – current 2007
- Configuration scripts (sh), non-regression tests, JEF2.2/XMAS standard library, LaTeX documentation, etc.

Version4 is not a complete replacement for Version3.

What is Version4?

Motivations for building this distribution are:

- We want to introduce support for cross-section library production with NJOY.
- State-of-the-art ACR1000 modelization needs some advanced capabilities not available in Version3.
- We want to avoid duplication of similar capabilities and improve interoperability
- We want to adopt a more consistent development model for our reactor physics computer codes
- After 12 years of development, the Dragon flow diagram needs some cleaning
- We did our best to avoid changing anything in the user's interface.

Advanced capabilities in Version4 1

- Jef-2.2 XMAS (172-group) Draglib-formatted libraries
- capability to produce Dragon libraries with NJOY
- NXT: module (2D/3D new-generation Excell tracking)
- self-shielding USS: module based on the subgroup equations
- isotropic streaming model ECCO in FLU: (for space-dependent diffusion coefficient calculations)
- asymptotic SPH method for reflector model
- SPH method with simplified PN Thomas-Raviart finite elements in 2D

Advanced capabilities in Version4

- multi-parameter COMPO database (creation and interpolation)
- simplified PN Thomas-Raviart finite elements in 3D for full core models in Trivac (Cartesian 3D)
- capability to use the characteristic method for self-shielding, leakage, flux and SPH calculations
- availability of the double-heterogeneity model (Bihet) with Sybil, Excell (PIJ) and NXT (PIJ)
- discrete ordinates capabilities in 1D and 2D geometries (new SNT: module)
- availability of the current iteration method with the interface current (IC) method in Sybil

Capabilities under active development 1

- `NXT:` geometries
  - MERG GEOM (equigeom) capability
  - mergings
  - cylindrical boundaries and hexagonal geometries

  Developed in Version3 and copied in Version4
- `NXT:` inline tracking with the method of characteristics (available with `EXCELT:` in Version3)
- Thomas-Raviart-Schneider (i.e., hexagonal) simplified PN capabilities in 3D (for the qualification of some ZED2 experiments)

Avoiding duplication

- Donjon-Dragon duplication

Version3	Version4
`GEOD:` in Donjon, `GEO:` in Dragon	`GEO:` in Dragon
`MACD:` in Donjon, `MAC:` in Dragon	`MAC:` in Dragon
`BIVACT:` in Donjon and Dragon	`BIVACT:` in Dragon

- Duplication of flux solution modules (power iteration)

Version3	Version4
`FLU:` P_{ij} and IC	`FLU:` all methods
`MOCC:` cyclic characteristics in 2D	(based on `MOCC:`)
`MCU:` characteristics in 3D	

Avoiding duplication

- Duplication of system matrix assembly modules

Version3	Version4
`ASM:` P_{ij} and IC `EXCELL:` 3D P_{ij} (in-line tracking)	`ASM:` all types of assemblies

Improving interoperability

resonance self-shielding

Version3	Version4
`SHI:` Stamm'ler model • P_{ij} and IC (non-iterative)	`SHI:` Stamm'ler model • P_{ij} and IC (non-iterative) `USS:` subgroup model • P_{ij} and IC (iterative or not) • characteristics • SN

Improving interoperability

Streaming models (space-dependent diffusion coefficients) in module FLU:

Version3	Version4
Isotropic streaming:	Isotropic streaming (ECCO):
• not available	• P_{ij} and IC (iterative or not) • SP_n approximation • characteristics • SN
Anisotropic streaming (HETE):	Anisotropic streaming (HETE):
• P_{ij} in Excell and NXT	• P_{ij} in Excell and NXT

Improving interoperability

SPH equivalence in module `EDI`:

Version3	Version4
Types of macro-calculations: • P_{ij} and IC (non-iterative) • diffusion approximation	Types of macro-calculations: • P_{ij} and IC (iterative or not) • diffusion approximation • SP_n approximation • characteristics • SN

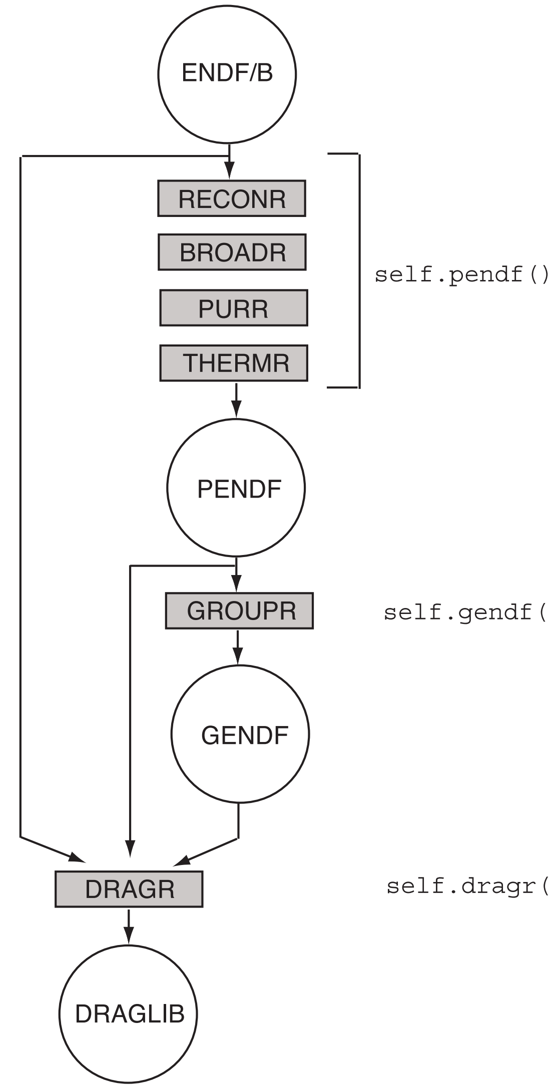
A more consistent development model 1

- Version control of the project components
  - A single Subversion repository holds the complete project
  - The repository contains sources, configuration scripts, non-regression tests, $\LaTeX$ docs and issue-tracking info.
  - LGPL subsets are available for download
- Issue tracking and spiral development management
  - the issue-tracking data is kept in the Subversion repository
  - pre- and post-commit Python scripts are hooked in the repository to help issue-tracking
  - a web/CGI tool is available to all users for submitting issues
- Configuration management of the codes Njoy, Dragon, Trivac, Donjon and Optex.
  - simple UNIX install scripts are used
  - PCs are supported through Cygwin

Draglib production with NJOY

The system is made of 3 components:

- DRAGR, a post-treatment Fortran 77 module
- PyNjoy.py, a Python script encapsulating NJOY modules
- one data-file per evaluation/library



Draglib production with NJOY

1. Instantiating an object:

```
from PyNjoy import *
jef2p2 = PyNjoy()
```

2. Defining instance variables:

```
jef2p2.evaluationName = "Jef2.2"
jef2p2.nstr = 22
jef2p2.iwt = 4
jef2p2.legendre = 1
jef2p2.hmat = "U238"
jef2p2.mat = 9237
jef2p2.evaluationFile = "$HOME/evaluations/Jef2.2/tape7"
jef2p2.fission = 2 # fission with delayed neutrons
jef2p2.ss = (2.76792, 1.22773e5)
jef2p2.potential = 11.1710
jef2p2.dilutions = ( 1.e10, 94.5, 56.3, 33.6, 20.0, 11.9, 7.1, 4.2 )
jef2p2.temperatures = ( 293., 550., 900., 1200. )
```

3. Invoking a method:

```
jef2p2.pendf()
```

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Cross section library treatment

- Improved DRAGLIB library support
  - in-house library creation with NJOY99 and DRAGR
  - contains detailed isotopic depletion data (with reaction-wise energy components)
  - contains autolib data for the Riemann integration and Ribon extended methods.
  - contains delayed neutron data
  - no pseudo fission products
- WIMS-D4 and MATXS library support (available in V3.05)
- NDAS library support (not available in the LGPL subset)
  - use of certified AECL libraries
  - required to improve the quality of our validation studies

Resonance self-shielding models

- Models based on the Generalized Stamm'ler method (`SHI:` module)
  - without distributed self-shielding effects (available in V3.05)
  - with Nordheim distributed self-shielding model (new)
  - with Riemann integration method (new)
- Models based on the subgroup method (`USS:` module) (new)
  - with physical probability tables (aka WIMS-7 and HELIOS)
  - Ribon extended method (with or without a model to represent mutual shielding effects)

Improved isotopic depletion

- Take into account energy produced by
  - fission (aka Dragon V3.05)
  - radiative capture (important in gadolinium and dysprosium) (new)
  - radioactive decay (important when the fuel is out-of-core) (new)
- Use a linear variation of $\langle \boldsymbol{\sigma_x} \, \phi \rangle$ in time. NOTE: Version 3.05 is assuming a linear variation of $\langle \phi \rangle$ in time.
  - possibility to extrapolate from the preceding time step (new)
- Availability of a saturation model for small-halflive isotopes (aka Dragon V3.05)

Method of characteristics 1

A new set of solvers based on the method of characteristics:

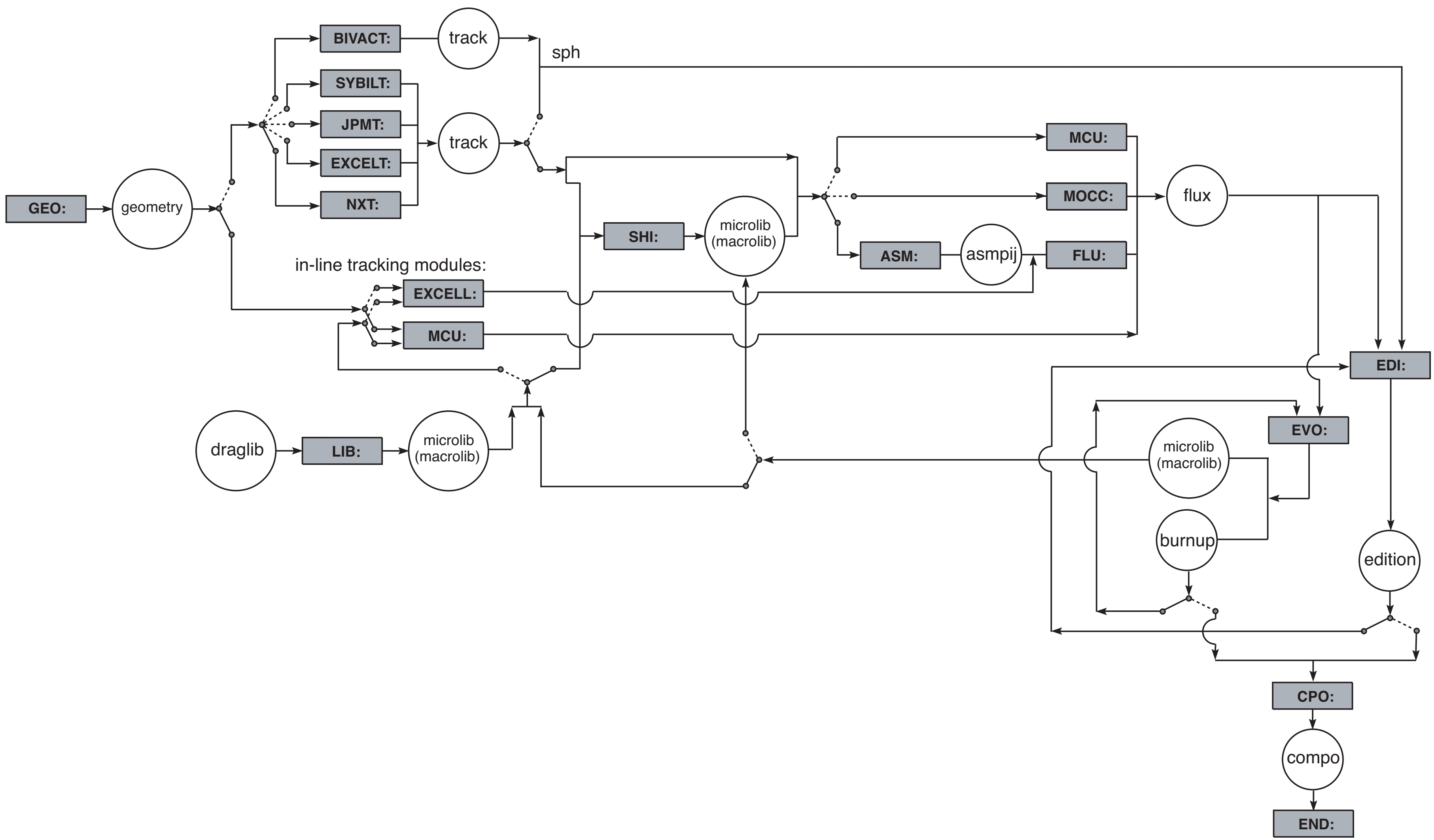
- 2D/3D `EXCELT:` and `NXT:` geometries
- 2D/3D isotropic or 2D specular (aka `MOCC:`) boundary conditions
- scattering anisotropy to arbitrary P_n order
- algebraic collapsing acceleration (ACA)
- compatible with the flux solution module used for PIJ calculations
- use of vectorial doors (`DOORAV` and `DOORFV`)

In V3.05, only the specular 2D and isotropic 3D options with P_0 scattering are available in specific flux-solution modules (`MOCC:` and `MCU:`).

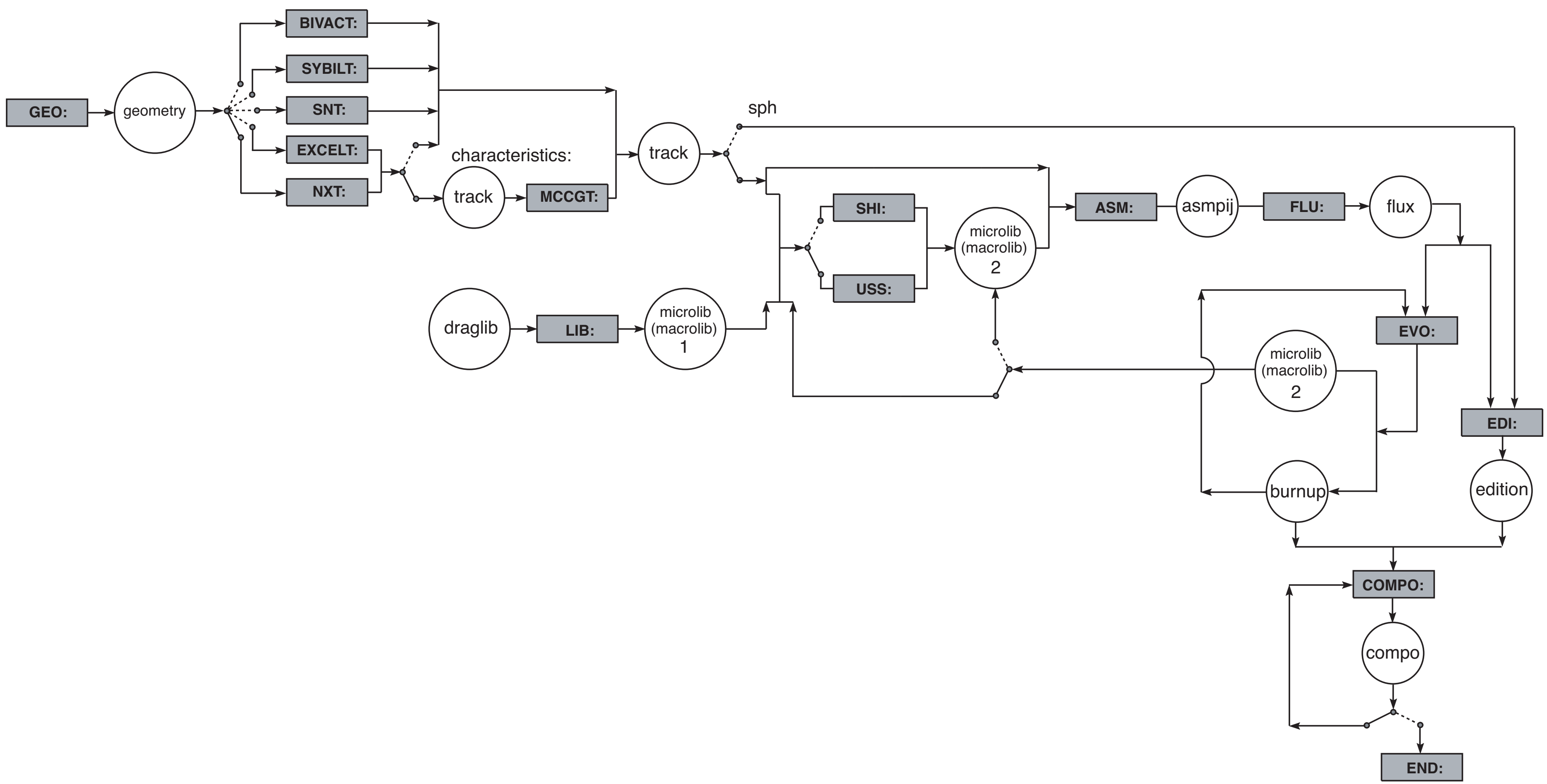
SPH model improvements

- A greater variety of macro-calculation techniques:
  - 1D, 2D and 3D collision probabilities (PIJ)
  - 1D, 2D and 3D method of characteristics (new)
  - 1D and 2D diffusion theory
  - 1D and 2D SP_n method (new)
  - 1D and 2D discrete ordinates method (new)
- Availability of the asymptotic normalization
- Use of vectorial doors (DOORAV, DOORPV and DOORFV)

Flow diagram of Dragon Version3



Flow diagram of Dragon Version4 1

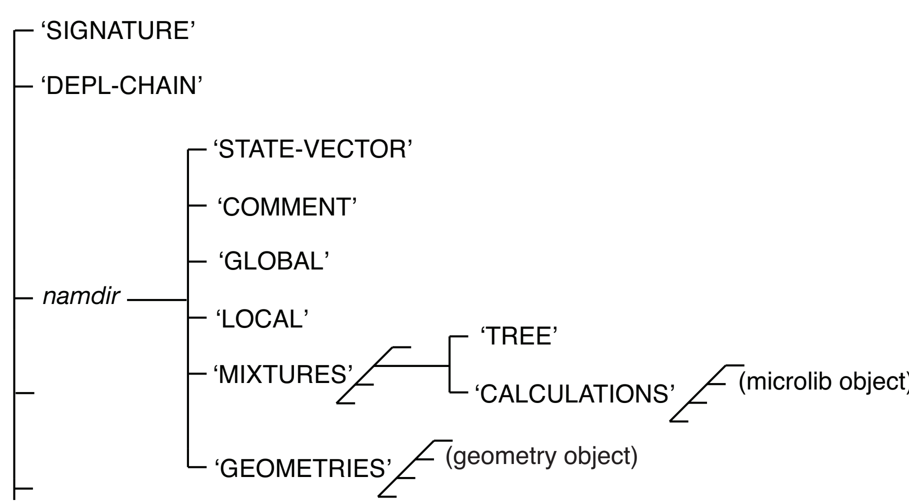


A multi-D reactor database

- We have generalized modules `CPO:` and `CRE:` to an arbitrary number of global / local parameters.
  - build a reactor database: `COMPO:` generalize `CPO:`
  - interpolate the database: `NCR:` generalize `CRE:`
- Definitions:
  - global parameter: characterize the complete lattice
  - local parameter: characterize a unique cell in a checkerboard or supercell calculation
- Compatible with micro-depletion
- Contains delayed neutron data
- Available only in Dragon Version4

Database content

- set of elementary calculations characterized by a unique n–tuple of global / local parameters
- each of them is a microlib containing data condensed over G groups and homogenized over each local zone
- a table-of-content is used to classify the elementary calculations and to relate them to global / local parameters.



Database format

- build from
  - associative tables (aka hash tables or dictionaries)
  - heterogeneous lists (aka cell arrays) (new)
- use `LCM` (in core memory) and `XSM` (direct access file) access routines
  - available in Fortran-77 and ANSI C
- Other characteristics:
  - XSM: direct access binary format (big or little endian)
  - LCM and XSM: same auto-descriptive format (similar to XML). Can be serialized.
  - the XSM associative tables are used for the Draglib object.

Database construction in COMPO : 1

- Initialization call (at the beginning of the Dragon run)
  - define the number and types of global / local parameters
- Data gathering call (at the end of each burnup / edition step in Dragon)
  - find the values of the global / local parameters
  - store the corresponding homogenized / condensed microlib object.

Database construction in COMPO: 2

- Initialization call:

```
EVALUATE FUEL1 := 3 ;
CPO := COMPO: ::
     STEP UP fuel
     COMM  'Line of comment'  ENDC
     PARA  'BCON' VALU REAL
     PARA  'FTMP' TEMP LIBRARY <<FUEL1>>
     PARA  'BURN' IRRA
     PARA  'FLUB' FLUB
     PARA  'PUIS' POWR
     PARA  'XE1'  CONC XE135PF LIBRARY <<FUEL1>>
     LOCA  'burn' IRRA
     LOCA  'flub' FLUB    ;
```

- Data gathering call:

```
  CPO := COMPO: CPO EDIT BURNUP FLUX LIBRARY ::
     STEP UP fuel
     SET <<evoend>> DAY
     BCON <<BoronCont>>   ;
```

Database interpolation in NCR : 1

- Multidimensional interpolation based on
  - Ceschino polynomial expansions
  - cubic Hermite polynomials
- Available functionalities:
  - interpolation at a specific parameter n–tuple
  - parameter-averaging (e. g., time-averaging)
  - delta-sigma contributions
- Produce a microlib or a macrolib
- Can gather parameters values from a `map` object in Donjon
- Micro-depletion is possible from the interpolated microlib.

Database interpolation in NCR : 2

- Interpolation call:

```
MACRO2 := NCR: CPO ::
   NMIX 7 MACRO COMPO CPO fuel
   MIX 1 FROM 1 SET 'flub' 2.1248E-02 ENDMIX
   MIX 2 FROM 2 SET 'BURN' 3.7498E+01 ENDMIX
   MIX 3 FROM 3 SET 'FLUB' 2.1363E-02 ENDMIX
   MIX 4 FROM 4 SET 'burn' 3.7426E+01 ENDMIX
   MIX 5 FROM 5 SET 'flub' 2.1127E-02 ENDMIX
   MIX 6 FROM 6 SET 'flub' 2.1289E-02 ENDMIX
   MIX 7 FROM 7 SET 'BURN' 3.7498E+01 ENDMIX  ;
```

Availability

The open-source subset of Version4 (including PyNjoy, Dragon and Trivac) is available for download. Visit: `http://www.polymtl.ca/merlin`

- Actually at level v4.0.0. `NXT:` is identical to the version in v3.0.5B
- This is open-source; you can contribute with
  - improved configuration scripts
  - new or improved Fortran sources
  - bug report and/or development suggestions

  Use our issue tracking submission form!