A C++ interface to nuclear databases

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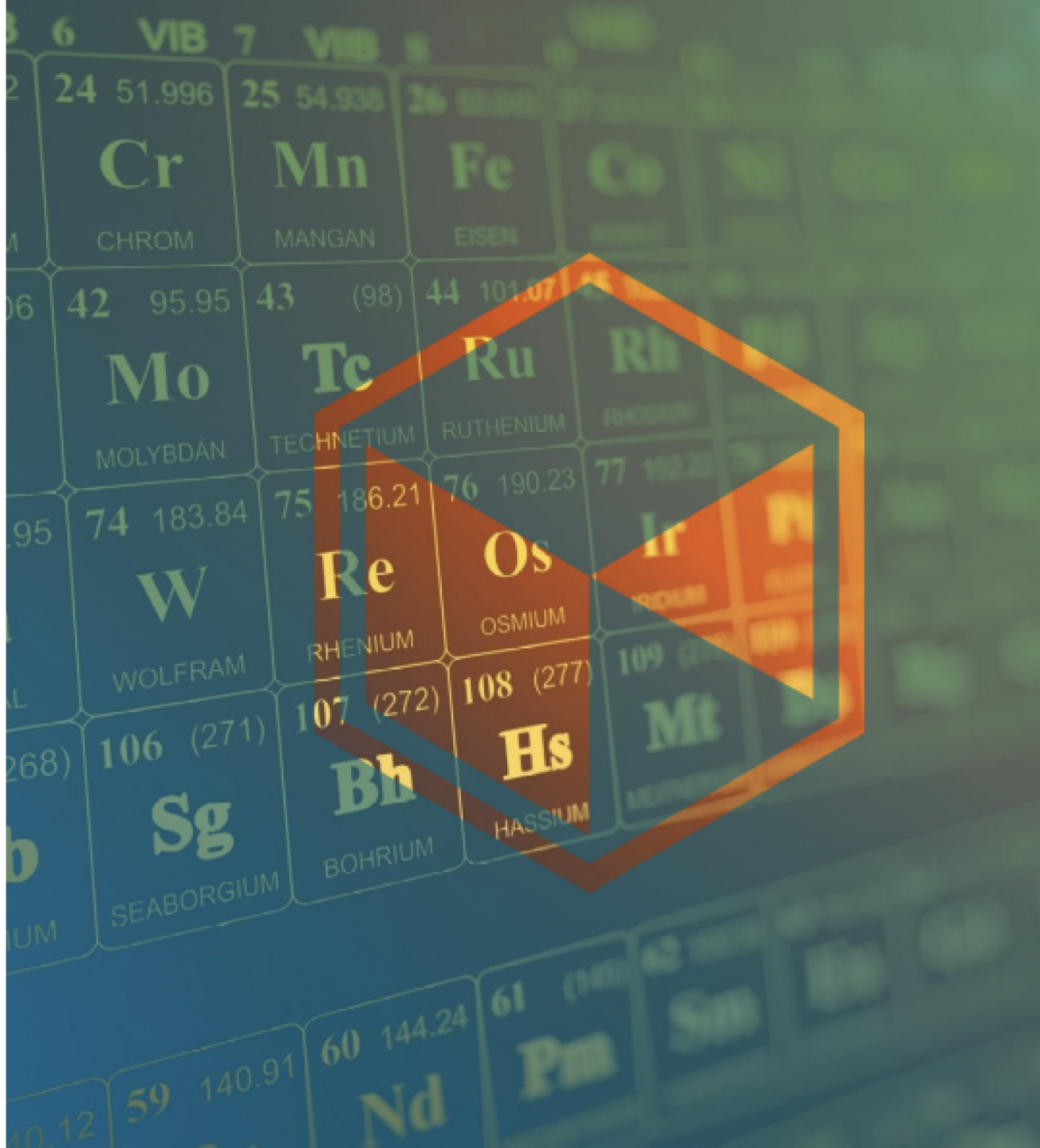
tkn.in2p3.fr
gitlab.in2p3.fr/tkn/tkn-lib

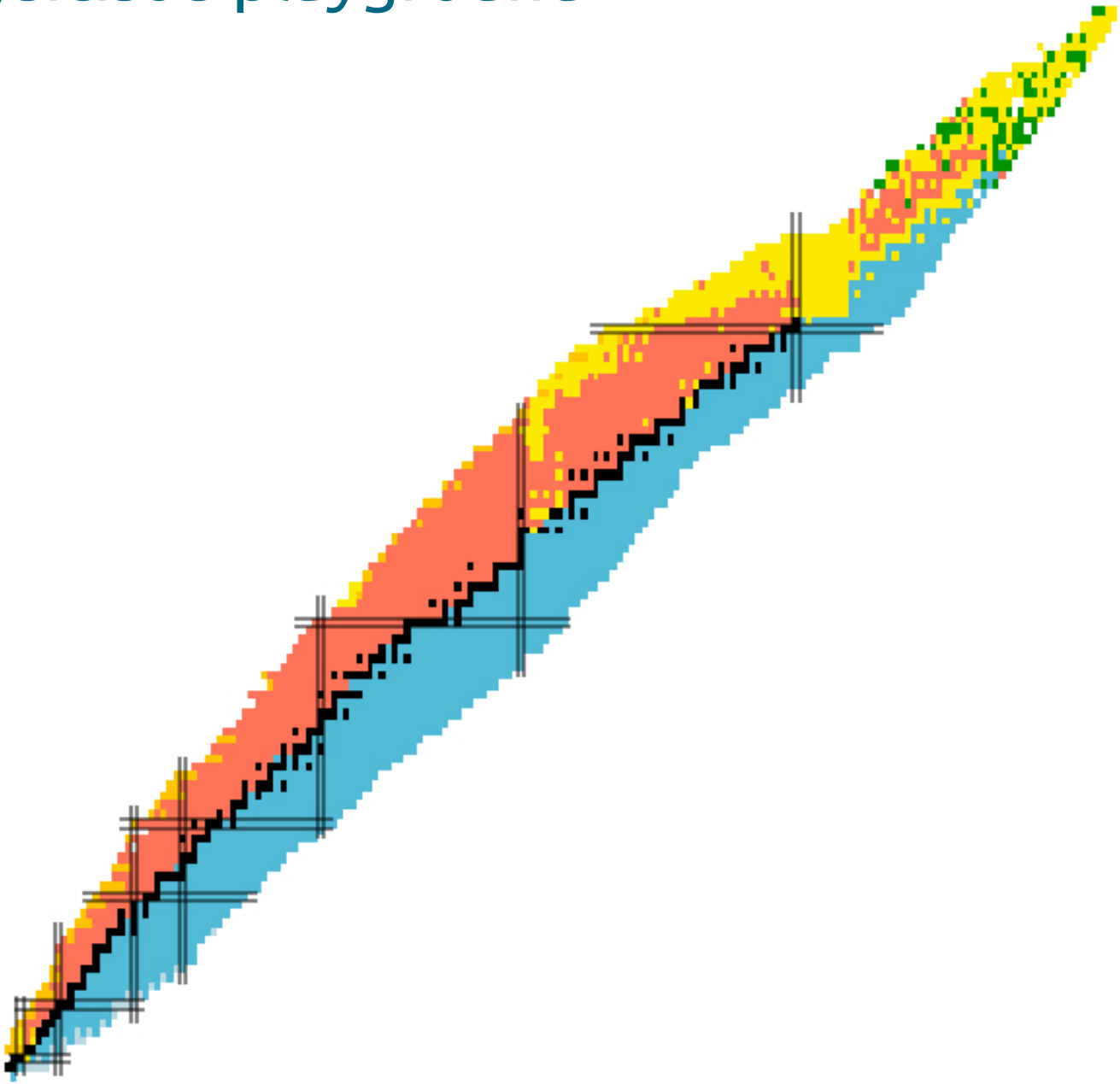
Open Science practices in Nuclear Physics
Online workshop: 5-6 December 2022



The nuclear physicist's playground

Many objects

- 118 chemical elements
- ~ 3000 nuclei
- ~ 200 000 excited states
- ~ 500 000 nuclear decays



The nuclear physicist's playground

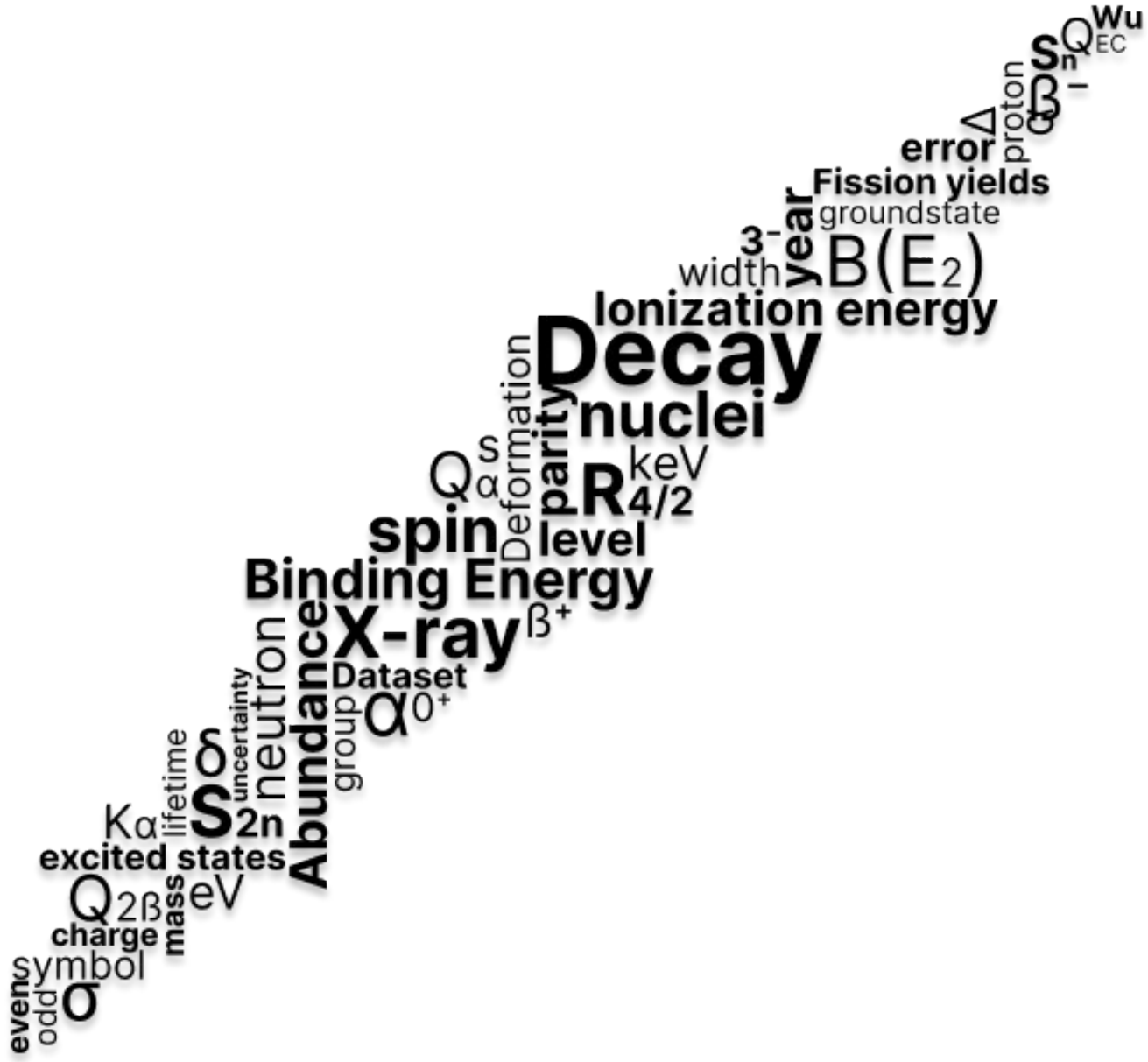
Many objects

- 118 chemical elements
- ~ 3000 nuclei
- ~ 200 000 excited states
- ~ 500 000 nuclear decays

Each with multiple properties

- energies
- lifetimes
- Q-values
- binding energies
- ...

➥ Millions of nuclear properties published



The nuclear physicist's nightmare

Data accessibility often non-trivial

- PDF file decoding
- web page parsing
- old database format decoding

➥ Each nuclear physicist has already created her/his own macros, physics case dependant

```
12C   L 0          0+               STABLE
12C 2 L ISPIN=0 $G=2.0010415963 45 (2002Be82)
12C 3 L XREF=ABDEGHIKMNOPTUWXZacdefijklmopqstuvwxyz123456789
12C   L 4439.82   212+               10.8E-3 EV6
12C 2 L %IT=100 $ ISPIN=0 $MOME2=6 3 (1983Ve01)
12C 3 L XREF=ABDEGHIKMNOPTUWXYacdefijklmopqstuvwxyz12346789
12C  cL E$From average of values given in (1967Ch19, 1967Ko14, 1971St22,
12C 2cL 1974Jo14, 1974No07, 2016Mu06).
12C 3cL The value is dominated by E|g=4438.91 keV {I31} in (1967Ch19).
12C  cL WIDTH$From average of (1958Ra14,1967Cr01,1968Ri16,1970Co09,1970St10).
12C   G 4438.94      100      E2
12C 2 G WIDTHG=10.8E-3 EV 6$BE2W=4.65 26
12C   L 7654.07   190+               9.3 EV    9
12C 2 L ISPIN=0 $ %IT=4.16E-2 $ %A AP 100
12C 3 L XREF=ABDEGHIJKMNOPTUVWXacdefijklnopqruvwxyz1234789
12C  cL E$See discussion in (1976No02). Note: E{-x}=7657.8 keV {I10} is
12C 2cL obtained from analysis of |g rays measured in (2016Mu06).
12C  cL WIDTH$Using |G{-|p}/|G=(6.7 {I6})|*10{+-6} (average of
12C 2cL 1972Ob01,1977Ro05,1977Al31) and |G{-E0}=|G{-|p}=(62.3 |meV {I20})
12C 3cL (see discussion in 2010Ch17,2011Vo16).
12C  cL $|G{-rad}/|G=(|G{-|g}+|G{-|p})/|G=(4.16 {I11})|*10{+-4}.
12C 2cL From 10{+4}|*|G{-rad}/|G=3.3 {I9} (1961Al23), 3.5 {I12} (1964Ha23),
12C 3cL 4.20 {I22} (1974Ch03), 4.4 {I2} (1975Da08), 4.15 {I34} (1975Ma34),
12C 4cL 4.09 {I27} (1976Ob03), 3.87 {I25} (1976Ma46).
12C 5cL The value from (1961Al23) has sometimes been miscopied as 3.4, but
12C 6cL it has no impact on the average. The value of (1975Da08) has been
12C 7cL corrected, as indicated in (1976Ob03). The value (2.82 {I29})|*10{+-4}
12C 8cL (1963Se23) is a statistical outlier; including this value yields
12C 9cL the average (3.99 {I18})|*10{+-4} that is the weighted average
12C acL using the external uncertainty. The value in (1990Aj01) did not
12C bcL use the corrected (1975Da08) value. In (2014Fr09), the
12C ccL value (4.19 {I10})|*10{+-4} is deduced by rounding the above
12C dcL values to the nearest tenth.
12C  cL $|G{-rad}=3.87 meV {I39} and |G{-E2}=|G|{-|g}=3.81 meV {I39}
12C  cL $Decay mechanisms were analyzed in (2017Sm03);
12C 2cL the decay is >99.92% via sequential |a-decay to {+8}Be{-g.s.}
12C 3cL and <0.047% via direct decay into 3|a-particles.
12C 4cL This is relevant for the astrophysical 3|a rate, via detailed balance.
12C 5cL  Also see
12C 6cL (2011Ra43, 2012Ma10, 2012Ki07, 2013Ra20, 2014It01, 2016Mo05, 2017De25)
12C   G 3213.79      100      E2
12C 2 G FL=4439.82
12C 3 G WIDTHG=3.81E-3 EV 39$BE2W=8.26 85
```

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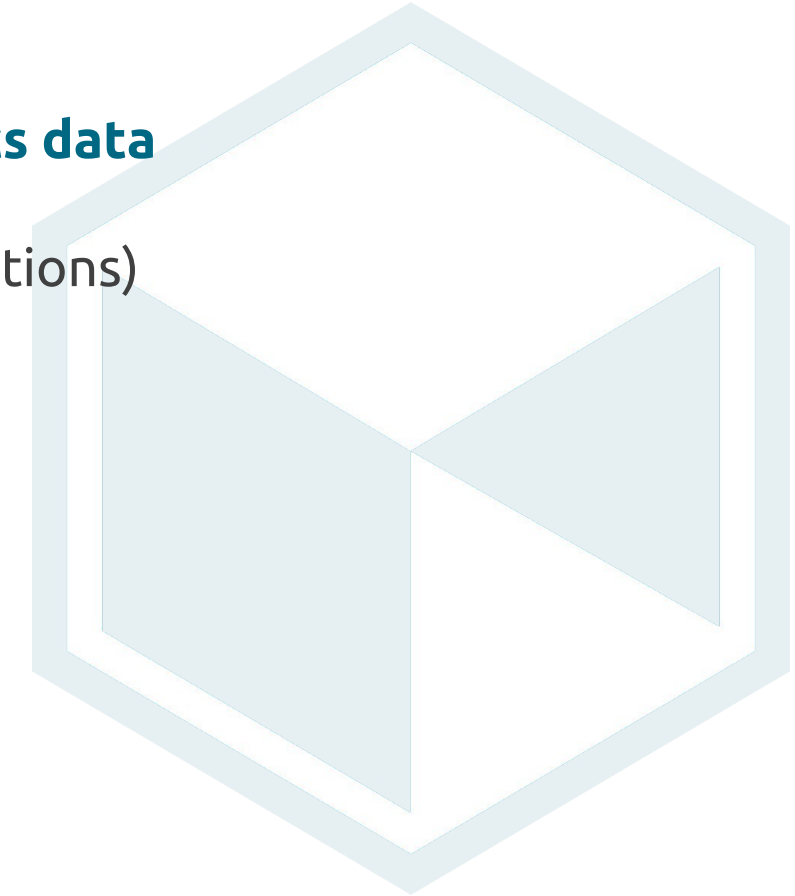
➥ Various software exist, with their own (partial) database implementation

* Only software with nice logo have been selected

The TkN (Toolkit for Nuclei) project

TkN specifications

- Light **C++ library** giving access to **published nuclear physics data**
- Regularly **updated** database
- **Fast** database access (for integration in Monte-Carlo simulations)
- **Easy to link** to any project
- **Open source** (CECILL-B CNRS licence)
- Fully **documented** software



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TkN prerequisites

- **git** to download the source code
- **cmake** to configure the TkN compilation (at least version 3.5)
- a compiler supporting **C++17** (patch available for c++11)
- if linked with **ROOT**, a ROOT version at least version 6.20

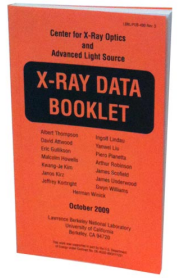
The TkN database

Data sources

- Chemical element properties
- X-ray data
- Isotopes properties
- Levels and decays properties

PubChem

NuDat 3.0



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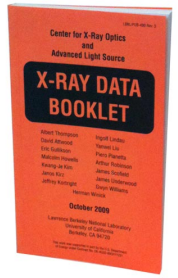


SQLite3 database

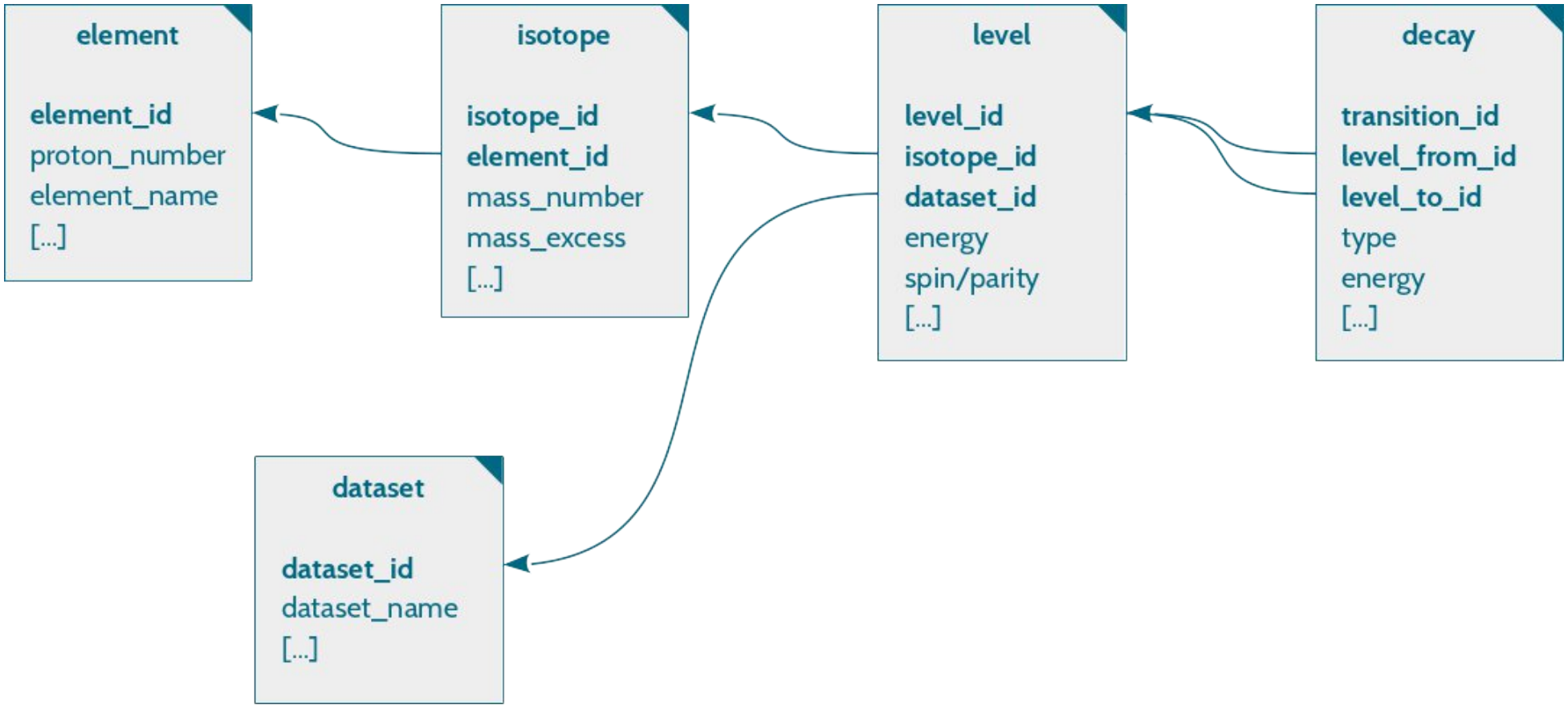
- directly **embedded** in the library
- **stable**, **cross-platform**, backward compatible (2050),
- widely used by many companies

AIRBUS

SQLite

➥ **Automatic monthly database update (stored on IP2I's servers)**

The TkN database structure



➥ **5 indexed SQL tables to avoid redundancy and for fast data access**

The TkN database content : chemical elements

element table

- charge
- symbol
- name
- group block
- standard state
- atomic mass
- electronic configuration
- atomic radius
- ionization energy
- melting point
- boiling point
- density
- year discovered
- list of X-rays

The TkN database content : isotopes

isotope table

- abundance
- binding energy per nucleon
- binding energy minus Liquid Drop model fit
- cross sections
  - thermal neutron capture cross section at 300K
  - thermal neutron fission cross section at 300K
  - decay mode
- fission yields
  - thermal neutron-induced F.Y. for 235-Uranium
  - thermal neutron-induced F.Y. for 239-Plutonium
  - spontaneous F.Y. for 252-Californium
- ground state lifetime
- ground state spin-parity
- mass excess
- pairing gap
- Q-values
  - α
  - Δα: 0.5 x (Qα(Z+2,N+2) - Qα(Z,N))
  - ß⁻
  - double ß⁻
  - ß⁺
  - electron capture
  - double electron capture
  - ß⁻ delayed neutron emission
  - ß⁻ delayed double neutron emission
  - electron capture afterproton emission
  - quadrupole deformation ß²
- separation energies
  - neutron separation energy
  - two neutron separation energy
  - proton separation energy
  - two proton separation energy

The TkN database content : nuclear exited states

level table

- energy
- life time
- spin and parity
- list of decays populating and depopulating the level

The TkN database content : nuclear decays

decay table

- energy
- relative intensity
- mixing ratio
- conversion coefficient
- electric and magnetic transition probability
- transition multi-polarity
- link to the parent and daughter levels
  - ➥ allows to determine coincident decays

➥ **Only gamma decays are implemented in TkN 1.0**

The TkN database content : datasets

For each nucleus, various published **datasets** are available

```
tknucleus nuc("132Sn");
nuc.get_level_scheme()->print("dataset")
```

```
[ INFO     ] Available datasets are :
[ INFO     ] 132Sn : ADOPTED LEVELS, GAMMAS (12587)
[ INFO     ] 132IN B- DECAY (0.200 S) (12588)
[ INFO     ] 132SN IT DECAY (2.080 US) (12589)
[ INFO     ] 133IN B-N DECAY (165 MS) (12590)
[ INFO     ] 248CM SF DECAY (12591)
[ INFO     ] COULOMB EXCITATION (12592)
[ INFO     ] U(N,F):IS,RADIUS:XUNDL-3 (12593)
[ INFO     ] COULOMB EXCITATION:XUNDL-4 (12594)
[ INFO     ] 133IN B-N DECAY:162 MS:XUNDL-5 (12595)
[ INFO     ] 133IN B-N DECAY:167 MS:XUNDL-6 (12596)
[ COMMENT  ] Current dataset is '132Sn : ADOPTED LEVELS, GAMMAS' (12587)
```

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[ COMMENT  ] Current dataset is '132Sn : ADOPTED LEVELS, GAMMAS' (12587)
```

→ default dataset

→ non evaluated datasets

➥ The merged dataset “ADOPTED” is selected by default, but the user can select any dataset for a given nucleus

The TkN database : summary

Database content

- 3 559 isotopes
- 22 906 datasets
- 550 080 levels
- 703 109 decays

To be added in future TkN versions

- particle decays
- charge radii
- other properties proposed by the users
- python/julia interface

Reading performances

- 1rst full database read ~ 15s
- 2nd full database read ~ 0.02s
- Extracting randomly 10^8 levels (1 thread) ~ 250s
- Extracting randomly 10^8 levels (16 thread) ~ 30s

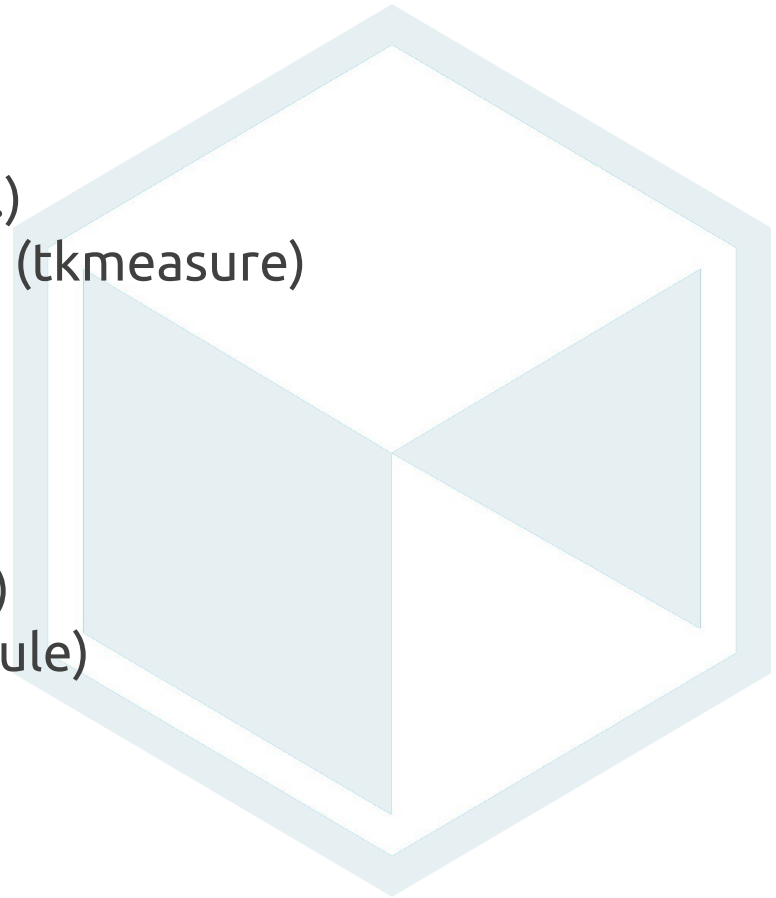
The TkN user interface

Dedicated c++ classes are provided in order to

- browse the **database** (tkmanager)
- extract the desired **properties** (tknucleus, tklevel, tkdecay...)
- handle **uncertainties**, including asymetric unc, limit values... (tkmeasure)
- handle **units** and units conversion (tkunit_manager)

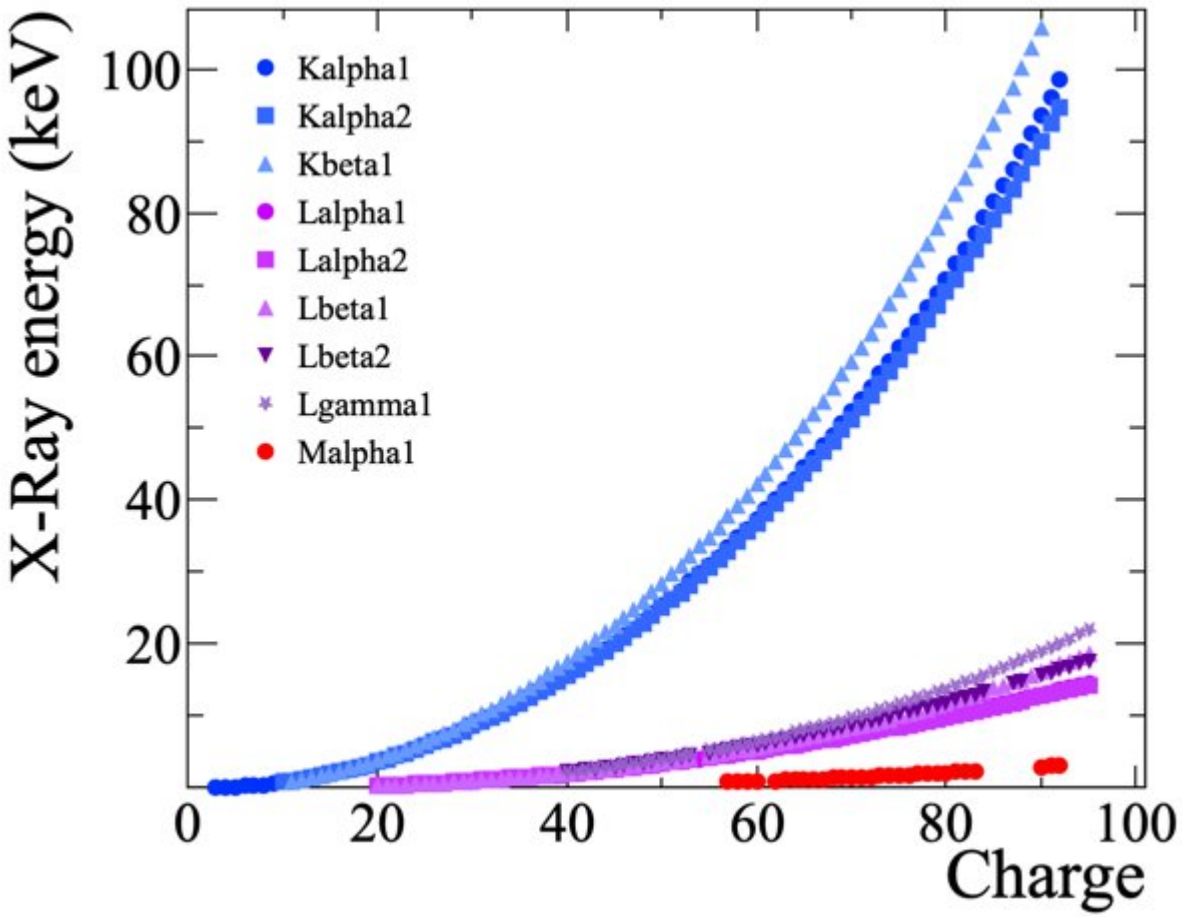
Dedicated tools are provided in order to:

- download/update the database (tkn-db-update)
- start an **interactive root** terminal with TkN linked (tkn-root)
- **link** TkN to an external project (cmake example, git submodule)



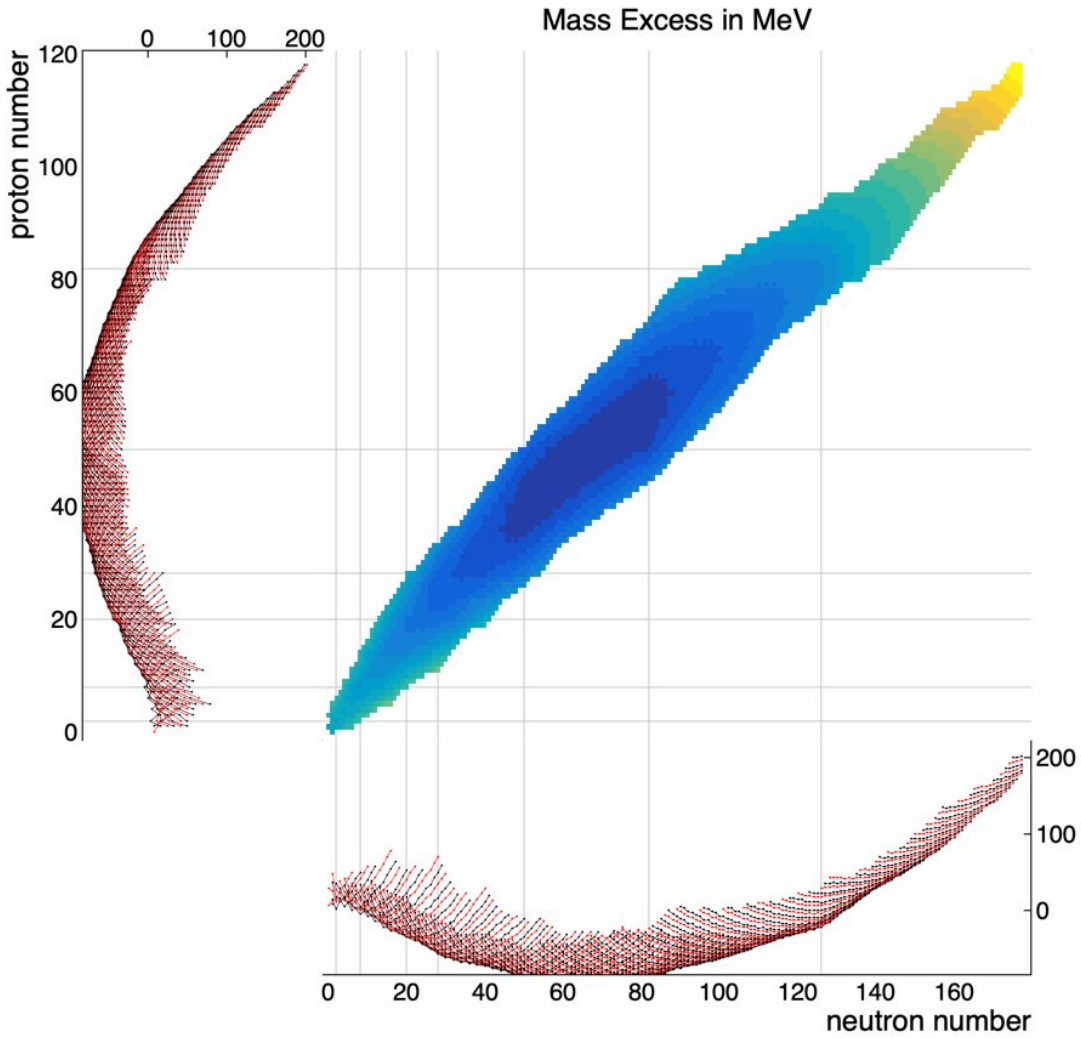
Some examples : X-ray energies

```
for(const auto &znucs : gmanager->get_map_of_nuclei_per_z()) {
    tknucleus nuc(znucs.first);
    auto xrays = nuc.get_xrays();
    for(const auto &xray: xrays) {
        TGraph *g = xrays_graphs[xray->get_type().copy().remove_all("XRay_")];
        g->AddPoint(nuc.get_z(),xray->get_value());
    }
}
```



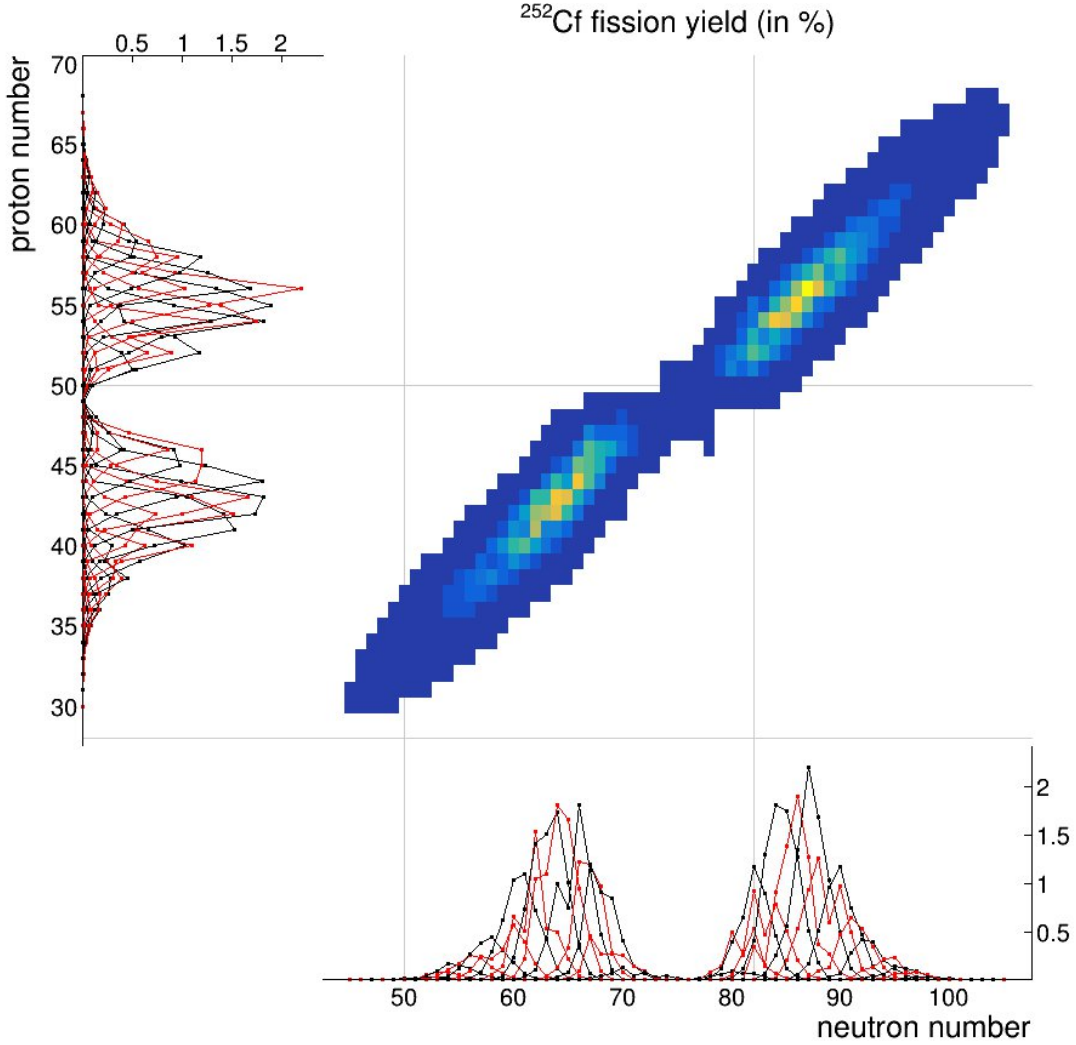
Some examples : isotope mass excess

```
tkn::tkmanager dtm;
auto* nn = new tknuclear_chart("Mass Excess in MeV",tknuclear_chart::kAll,true);
for(const auto &nuc : dtm.get_nuclei()) {
    double yy = nuc->get_mass_excess(tkn::tkunit_manager::units_keys::MeV);
    nn->set_value(nuc->get_z(), nuc->get_n(), yy);
}
```

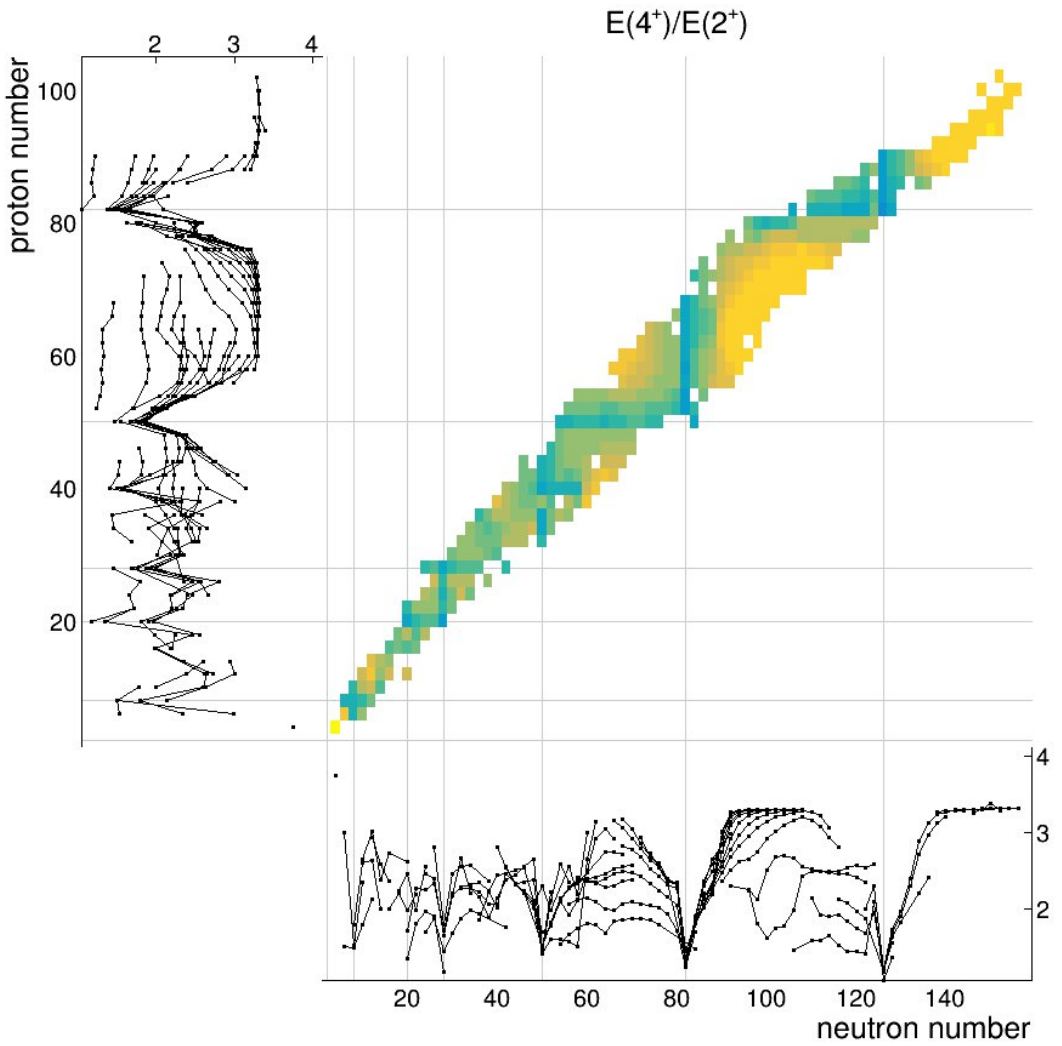


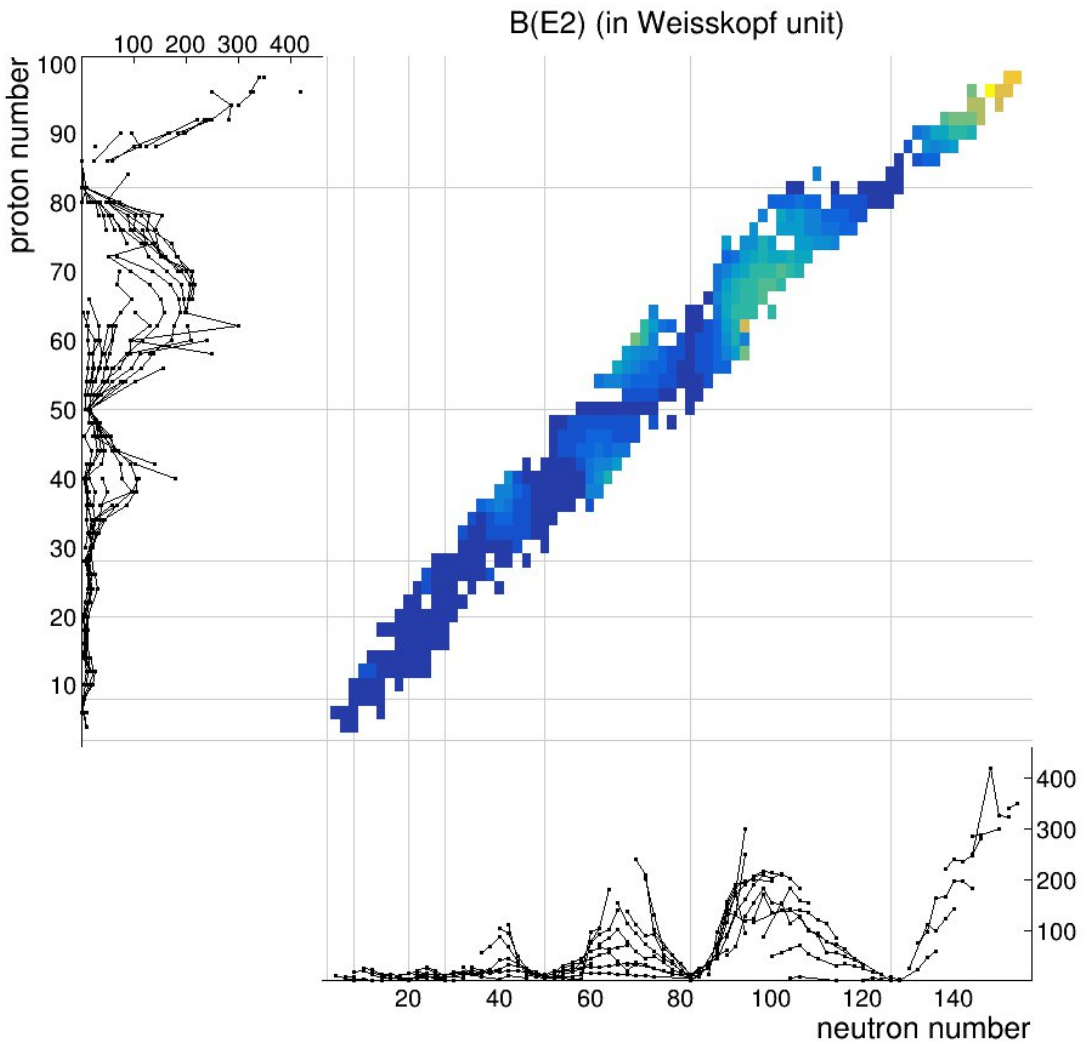
Some examples : isotopic fission yields

```
tkn::tkmanager dtm;
auto* nn = new tknuclear_chart("^{252}Cf fission yield (in %)",tknuclear_chart::kAll,0,true);
for(const auto &nuc : dtm.get_nuclei([](auto nunu) { return nunu->has_property("FY252Cf");})) {
    double yy = nuc->get_property("FY252Cf").atof();
    if(yy>0) nn->set_value(nuc->get_z(), nuc->get_n(), yy*50);
}
```



Some examples : level and decay properties

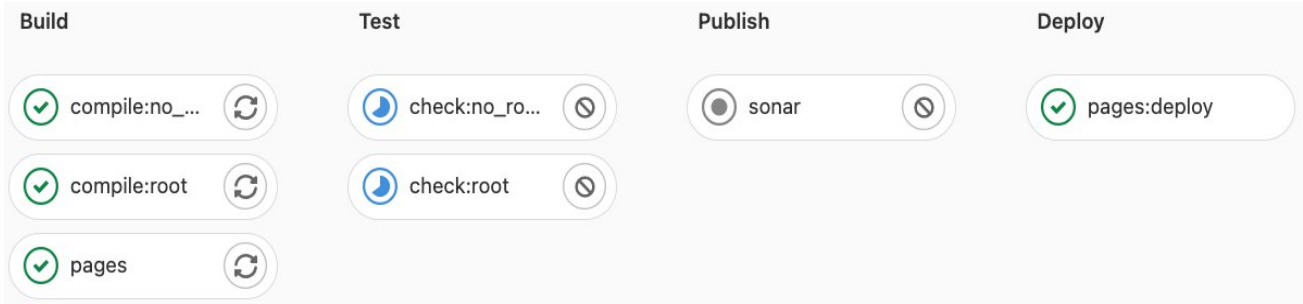




The TkN user support

Gitlab CI and documentation

- **automatic** TkN compilation, unitary tests,
  and **example execution** after each new code commit
- TkN online **documentation** https://tkn.in2p3.fr
  - install and link tutorials
  - complete **userguide**
  - code fully documented using doxygen



Human support

- TkN channel on IN2P3's Rocket.Chat
- TkN mailing list to be informed on any release or updates

tksummary

Database with many (nuclear) data
Automatic monthly **update**

C++ interface for exploring the database
Utility programs and interactive ROOT environment

Easy to link to any C++ project (cmake, submodule)
Continous integration on Gitlab

Extensive **userguide** and documenation website
Code **fully documented** using doxygen

tkn.in2p3.fr

gitlab.in2p3.fr/tkn/tkn-lib

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