The low energy neutron (particle) project of LLNL/SLAC G4LEND-GIDI

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Low energy nuclear data

- Nuclear data for reaction of projectile hitting a target
  - Example: n + 16O ⇒ n + p + 15N
- Most data are
  - For neutron as projectile
  - Low projectile energies: 10E-11 to 20 MeV
- In legacy formats
  - ENDL (Evaluated Nuclear Data Library)
    - Developed at LLNL ~1960
  - ENDF (Evaluated Nuclear Data File)
    - Developed by international committee ~1964

Issues with legacy formats

- Have a fixed number of supported reactions
  - The following reaction is not support

    $n + {}^{79}Kr \Rightarrow 2H + n + 3H + {}^{74}Se$
  - Fixed precision format
- Very difficult to read – try reading ENDF formatted data
- Format does not represent physics
- New format and infrastructure are designed to solve many issues

No more punch cards

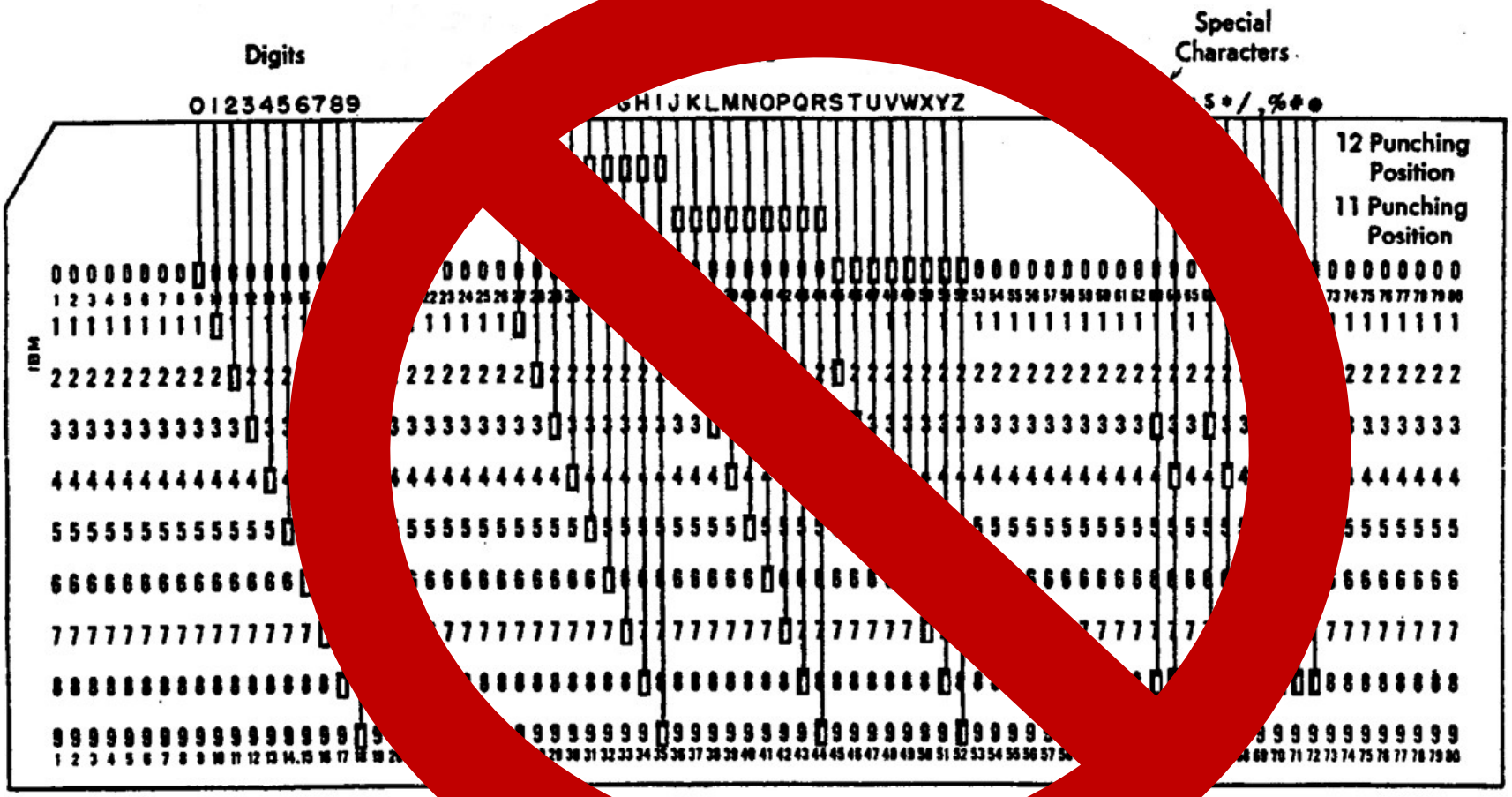


Figure 2. Punching Positions in Card

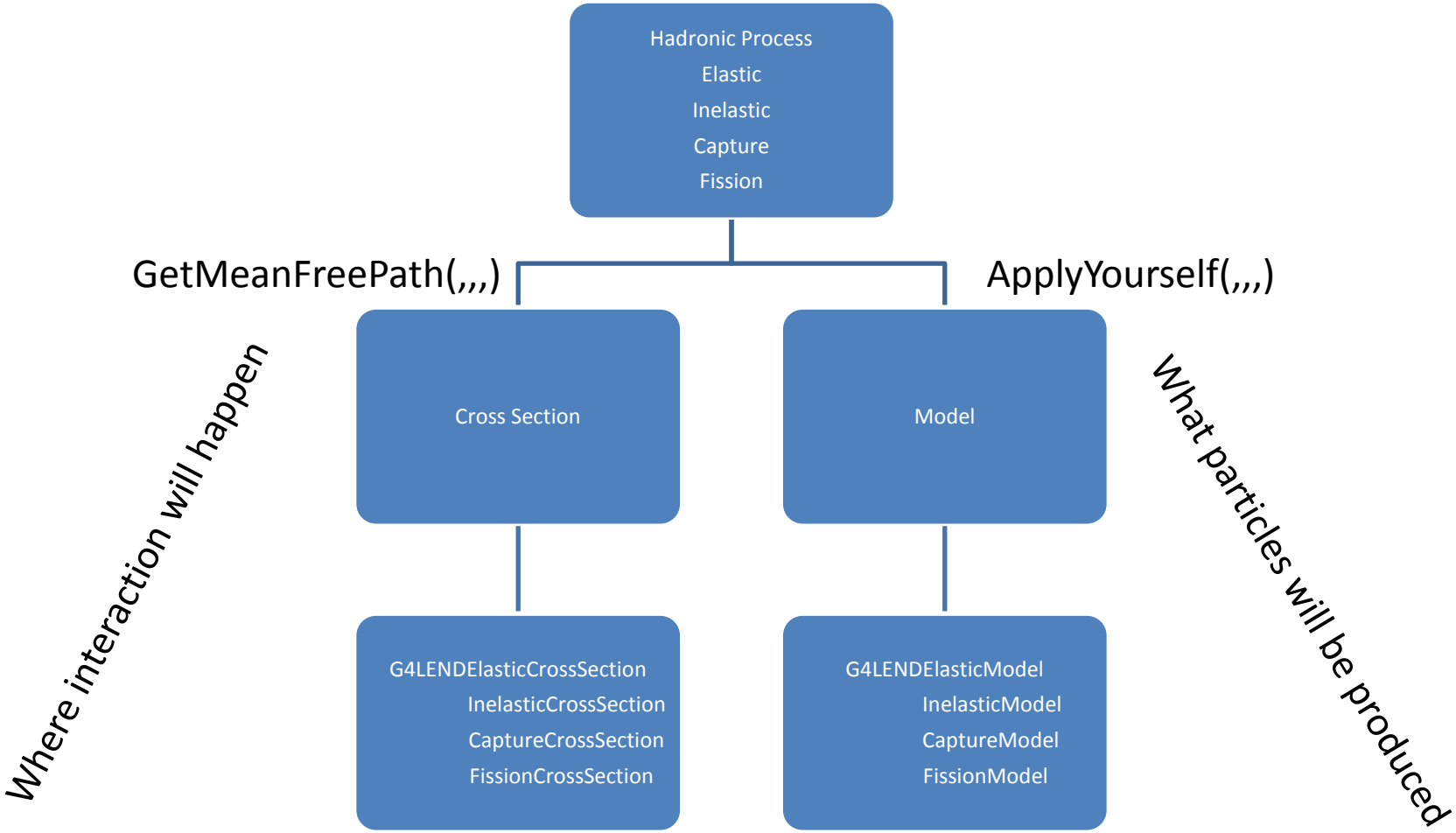
General Interaction Data Interface (GIDI) and Geant4 Low Energy Nuclear Data (G4LEND)

- GIDI is a newly developed data format for nuclear data
  - More modern design than current nuclear formats established in the 1960'
- GIDI also provide access routines for the data
- Conversion of the current nuclear data bases such as ENDF(USA), JEFF(Europe), JENDL(Japan), ENDL(LLNL) are on going
- LEND is Geant4 interface for GIDI

G4LEND

- Geant4 interface to GIDI
- Follows Hadronic Framework of Geant4, separated cross section and model as final state generator
- Manage target nuclei data in GIDI
- Pre-calculated data for certain temperatures are used.
  - 300, 1160 and 3590 K
- An alternative to the low energy neutron package (NeutronHP) in Geant4

Geant4 Hadronic Framework



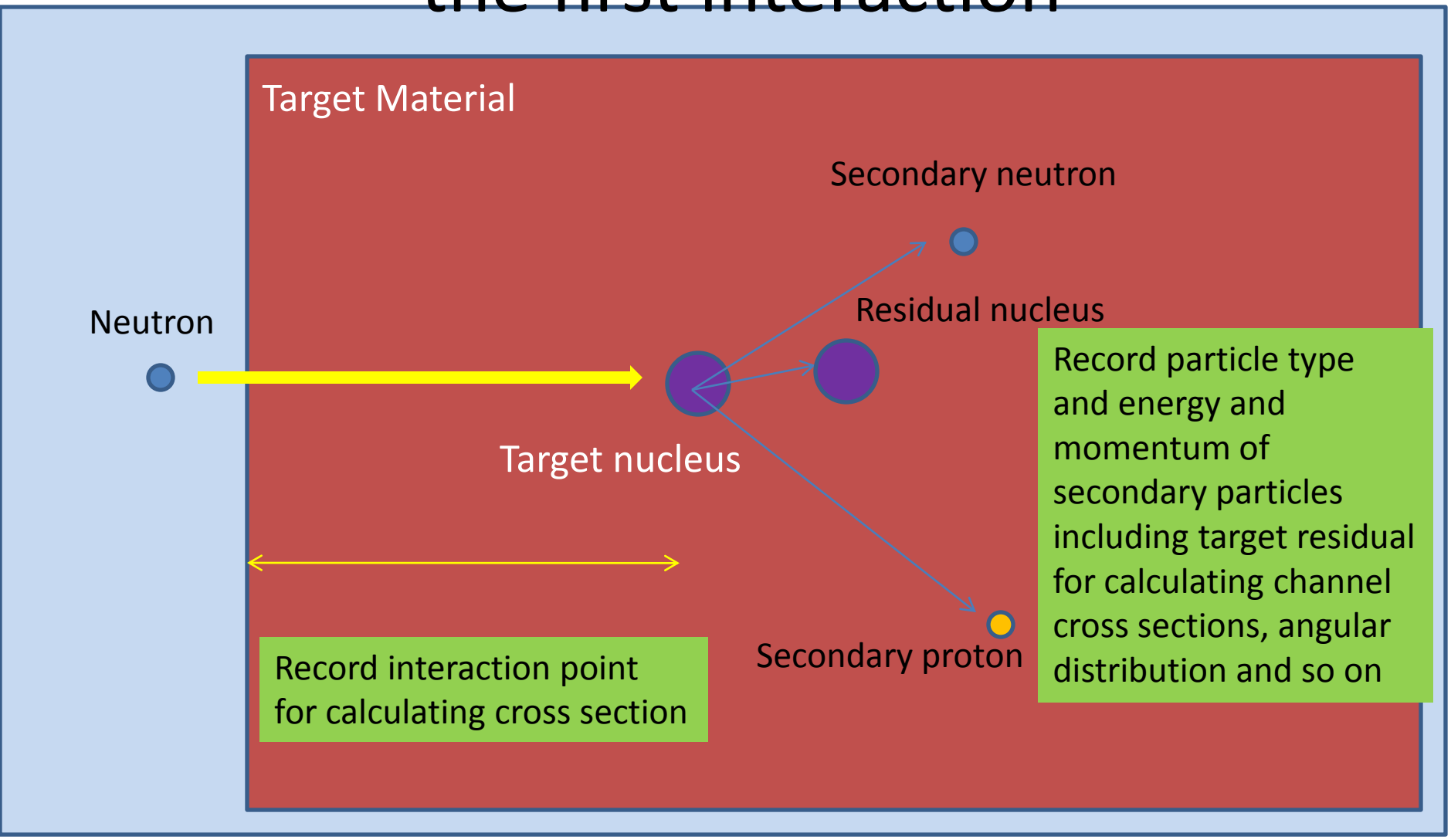
ENDL99

- ENDL99 is the nuclear database used at LLNL for long time.
- 109 isotopes data from H to Cf, including 27 natural abundance element
  - See next slide for full list
  - Total size 240MB in xml format. (unzipped)
- Select as the first dataset converted to the GIDI format
- The original converter to new nuclear format does not written ENDF format.
- Energy range
  - From 20MeV down to thermal energy (10E-4)

Full list of target isotope (element) of ENDL99

n_1	Si_natural	Zr_natural	Au_197	Pu_237
H_1	P_31	Nb_93	Hg_natural	Pu_238
H_2	S_32	Mo_natural	Pb_natural	Pu_239
H_3	Cl_natural	Ag_107	Bi_209	Pu_240
He_3	Ar_natural	Ag_109	Th_231	Pu_241
He_4	K_natural	Cd_natural	Th_232	Pu_242
Li_6	Ca_natural	In_natural	Th_233	Pu_243
Li_7	Ti_natural	Sn_natural	Pa_233	Am_241
Be_7	V_51	Sb_natural	U_233	Am_242_m
Be_9	Cr_natural	I_127	U_234	Am_243
B_10	Mn_55	Xe_134	U_235	Cm_242
B_11	Fe_natural	Xe_natural	U_236	Cm_243
C_12	Co_59	Ba_138	U_237	Cm_244
C_13	Ni_58	Eu_natural	U_238	Cm_245
N_14	Ni_natural	Gd_natural	U_239	Cm_246
N_15	Cu_natural	Ho_165	U_240	Cm_247
O_16	Zn_natural	Hf_natural	Np_235	Cm_248
F_19	Ga_natural	Ta_181	Np_236	Bk_249
Ne_20	As_74	W_natural	Np_237	Cf_249
Na_23	As_75	Re_185	Np_238	Cf_250
Mg_natural	Y_88	Re_187	Np_237	Cf_251
Al_27	Y_89	Pt_natural	Np_238	Cf_252

Simulation in material up to the first interaction

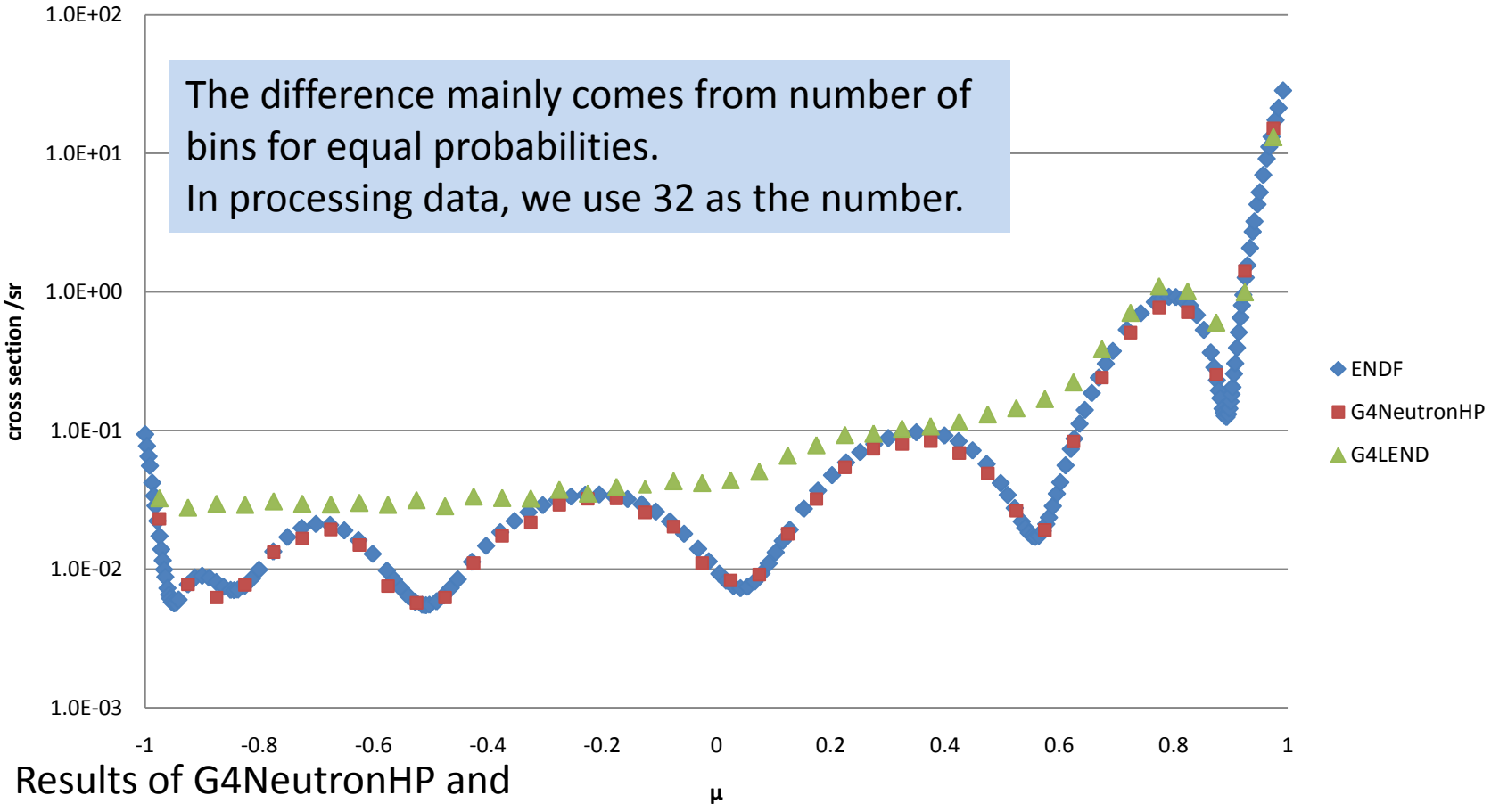


Channel Cross Section
n (16MeV) on Au

	ENDF VII	G4NeutornHP	G4LEND
Total	5.468 [barn]	5.40	5.41
Elastic	2.785	2.74	2.86
Capture	5.56e-4	9.1e-4	96.e-4
Inelastic			
(n,2n)	2.232	2.21	2.10
(n,3n)	2.75e-2	2.7e-2	2.9e-2
(n,p)	3.60e-3	3.1e-3	5.4e-3
(n,a)	1.00e-3	0.9e-3	1.4e-3

Results of G4NeutronHP and G4LEND are derived by a thin target like simulation

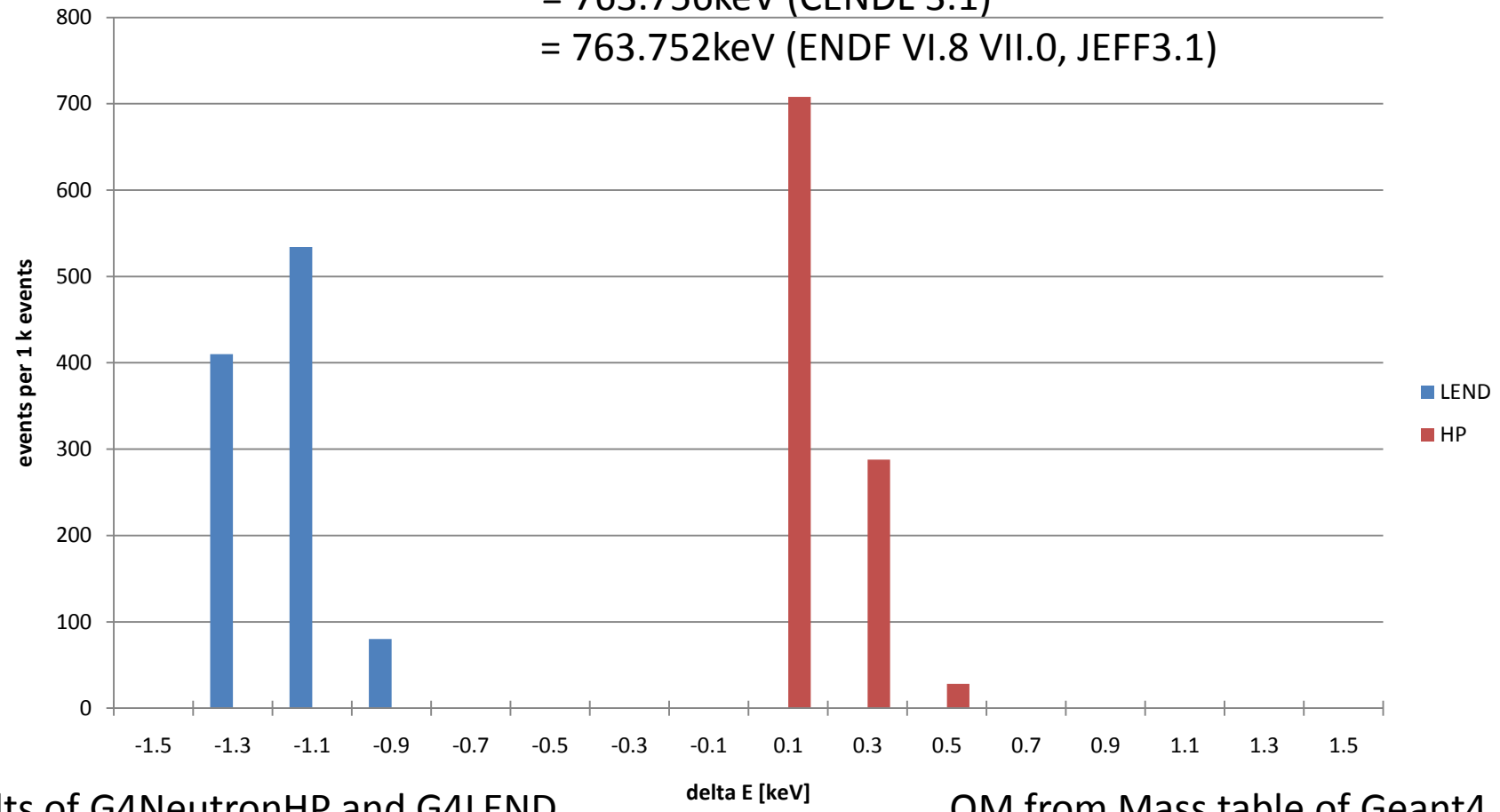
Angular Distribution of neutrons n (16MeV) on Au



Results of G4NeutronHP and G4LEND are derived by thin target like simulation

Level of energy conservation
n(1MeV) + 3He → 3H + 1H

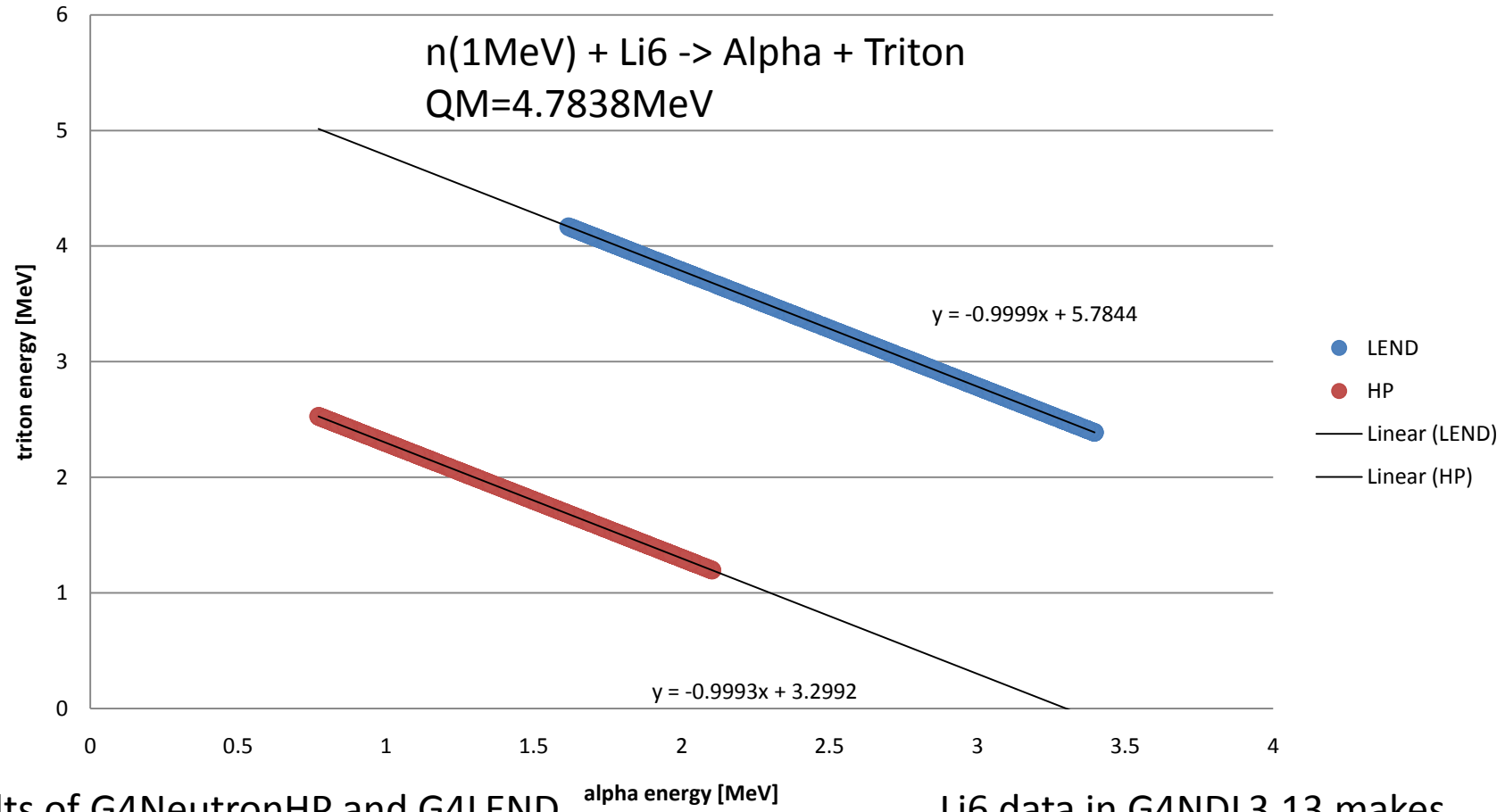
QM = 763.999keV (JENDL 3.3 4.0)
= 763.756keV (CENDL 3.1)
= 763.752keV (ENDF VI.8 VII.0, JEFF3.1)



Results of G4NeutronHP and G4LEND are derived by thin target simulation

QM from Mass table of Geant4 (AEM03 and PDG)
= 763.347keV

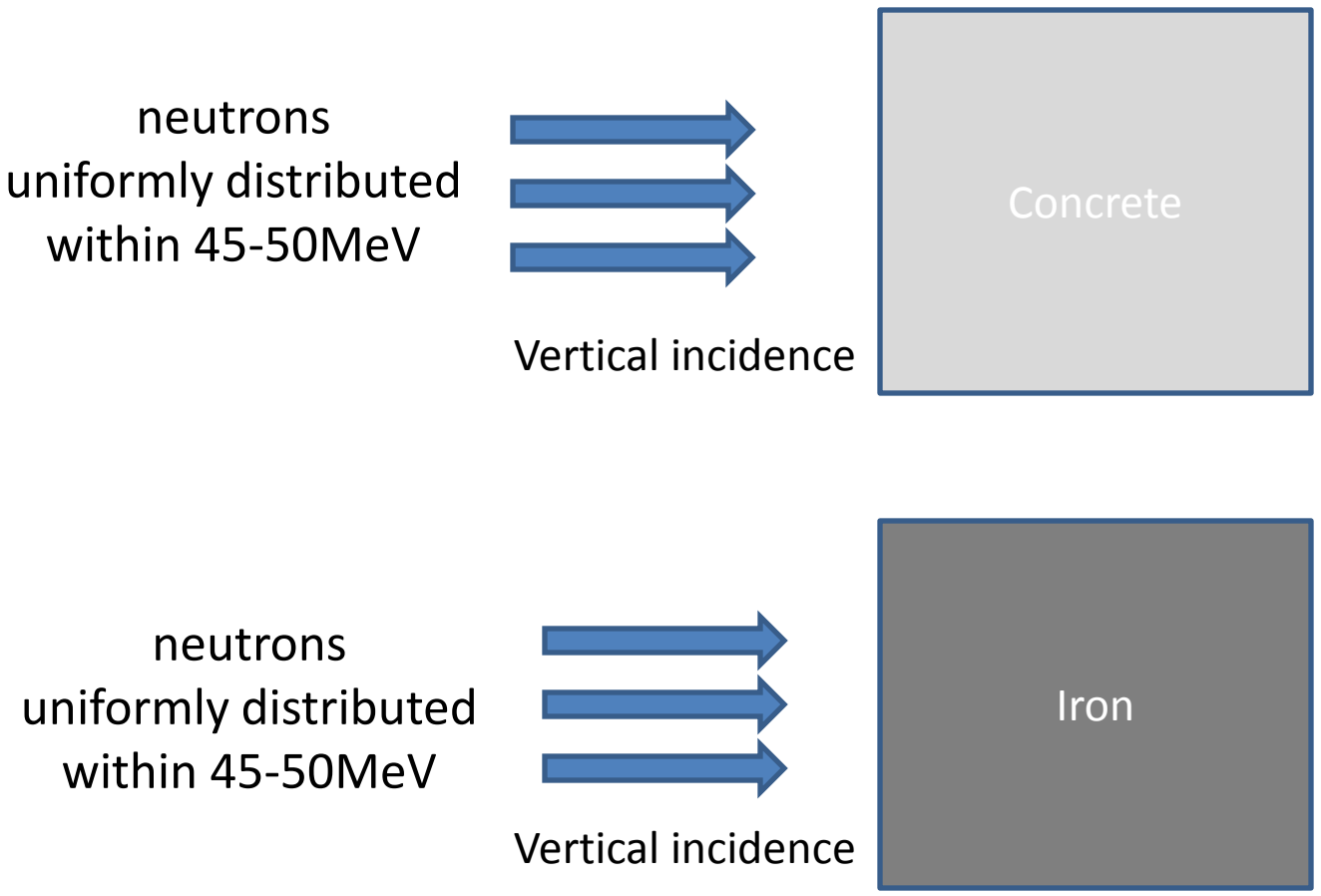
Example of problem fixed in G4NDL(v9.4)



Results of G4NeutronHP and G4LEND are derived by thin target simulation

Li6 data in G4NDL3.13 makes this trouble, and the data will be updated in the next version

Neutron Attenuation in Iron and Concrete Slab



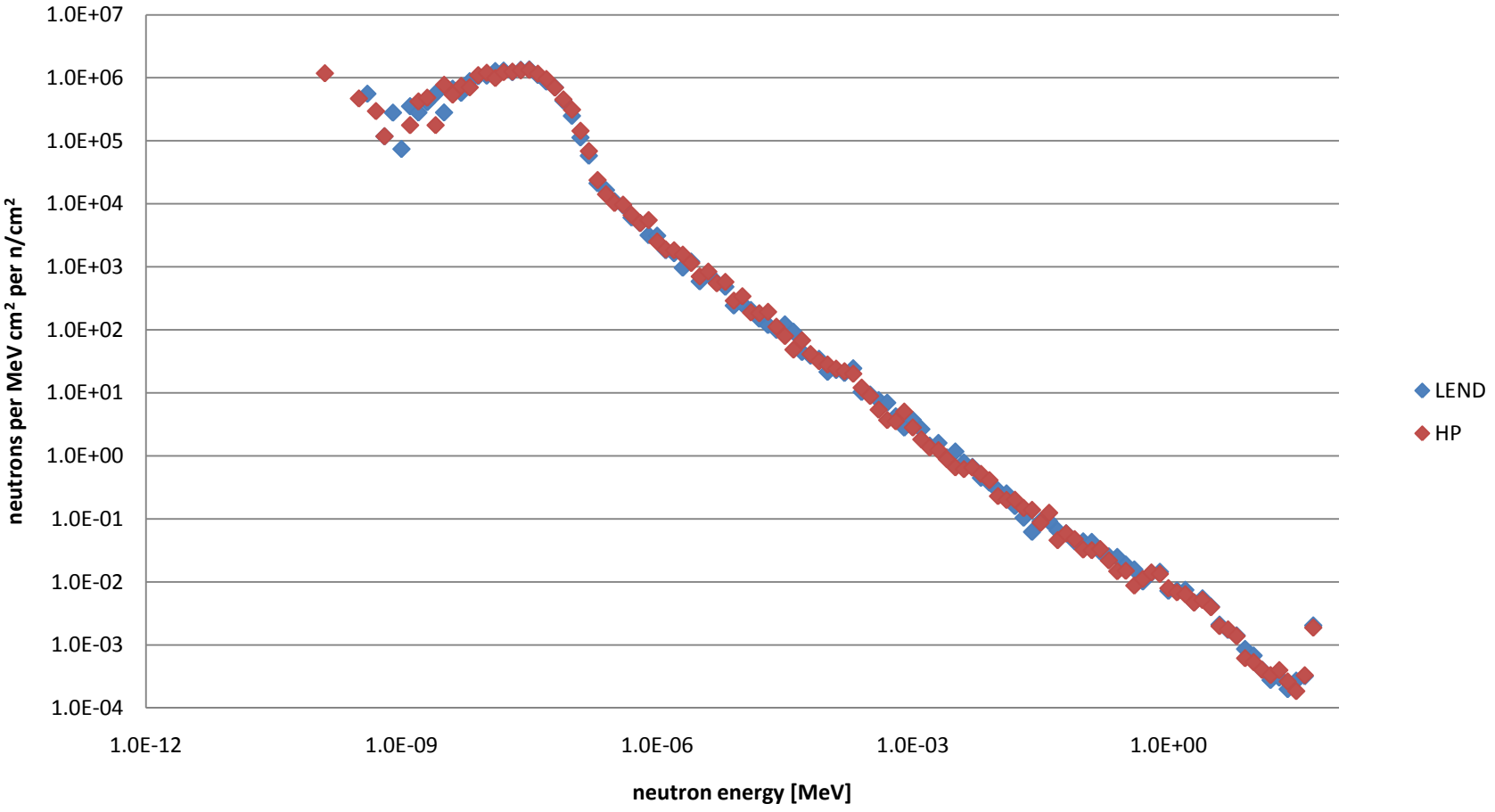
Concrete
Density 2.27 g/cm^3

Element	Weight percent
H	1.02
C	0.10
O	53.85
Mg	0.22
Al	3.44
Si	34.22
K	1.32
Ca	4.41
Fe	1.41

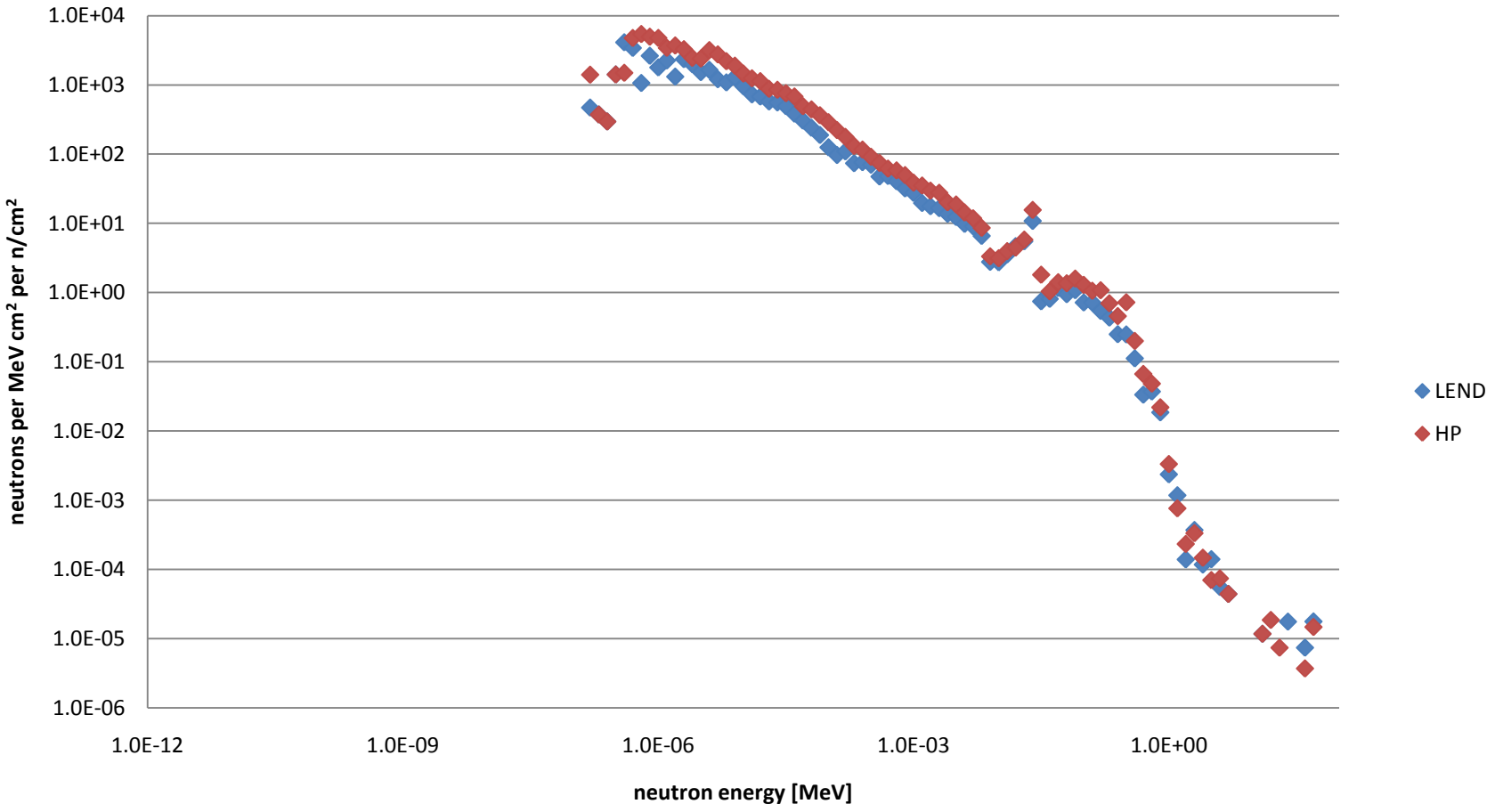
Iron
Density 7.87 g/cm^3

First and some secondaries interactions of primary neutrons are calculated by Geant4 Bertini model

45-50MeV neutrons bombarding concrete slab Neutron energy spectrum at depth of 1m



45-50MeV neutrons bombarding Iron slab Neutron energy spectrum at depth of 1m



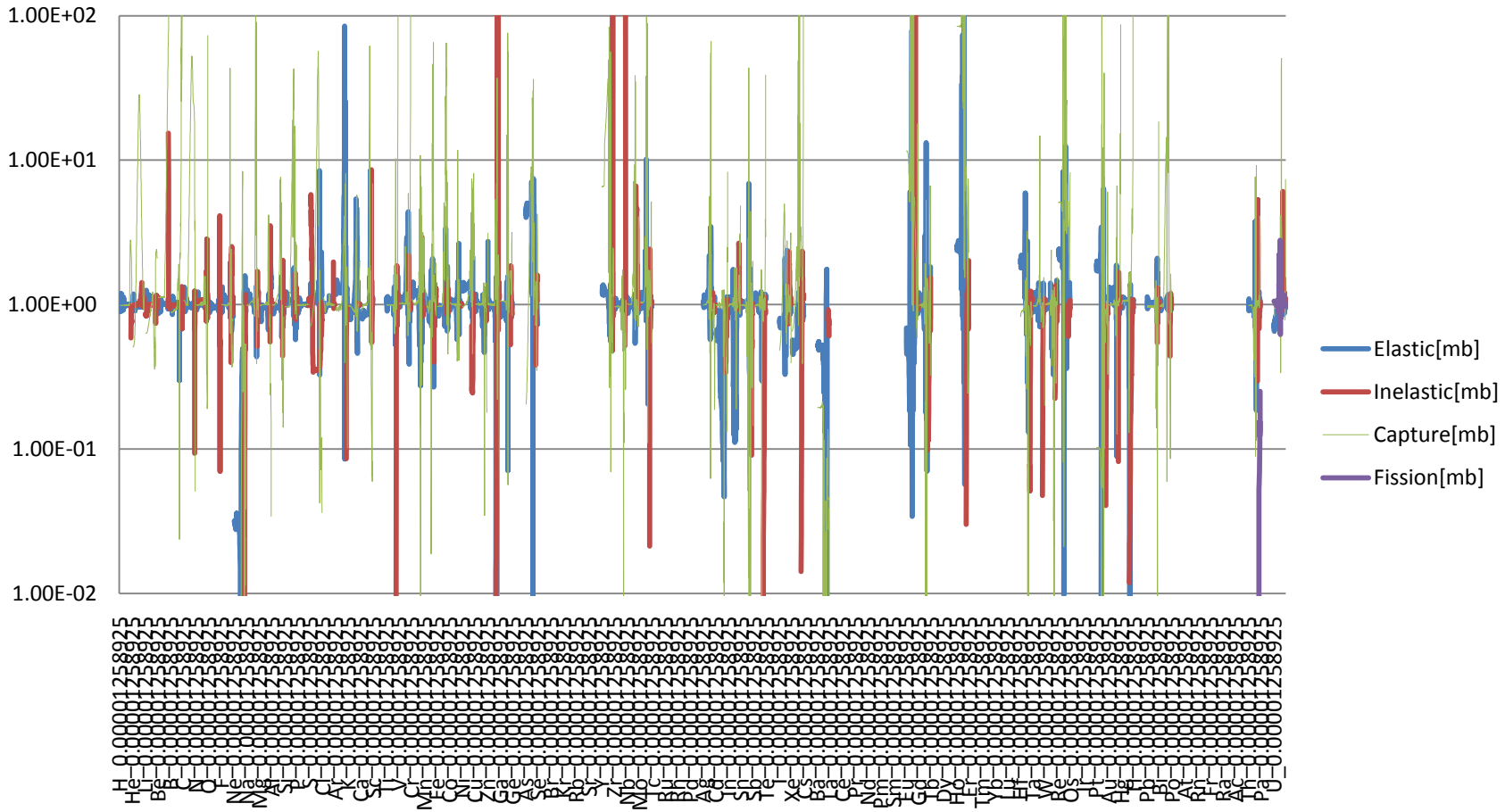
QGSP_BERT_LEND Physics List

- A proposed reference physics list which uses LEND (neutron) instead of NeutronHP
- “QGSP_BERT_LEND”
  - G4NeutronLENDBuilder
  - G4HadronElasticPhysicsLEND
  - HadronPhysicsQGSP_BERT_LEND
- Neutron time cut (10(?) micro sec)

Elemental Cross Section Check

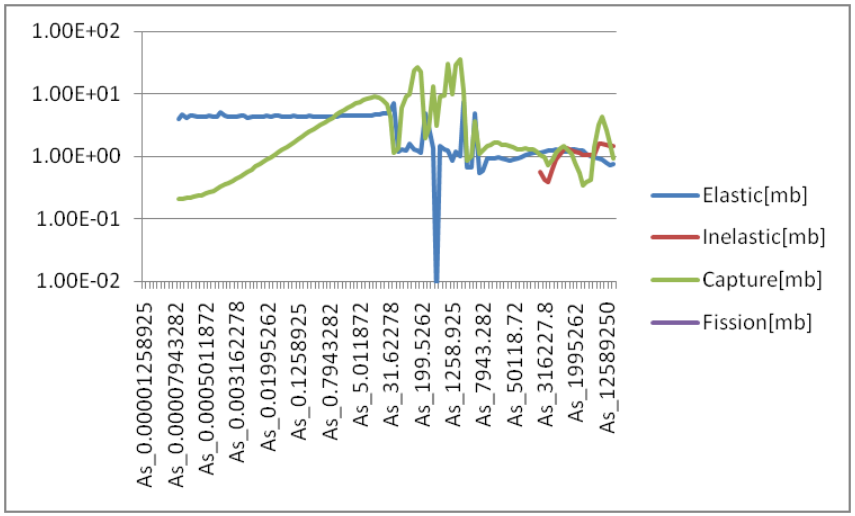
- Create G4_H to G4_U
- Configure PhysicsList
- Compare (Partial) Cross Section by
  - PROCESS->GetMicroscopicCrossSection(,,,)”
- This value is really Geant4 used in a simulation.

Checking cross section ratio HP/LEND from H to U

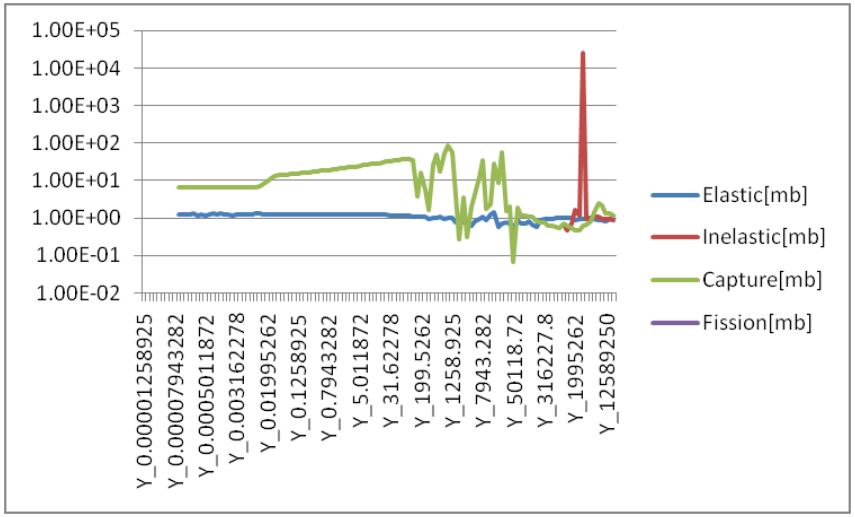


Close-up to interested element

As 75

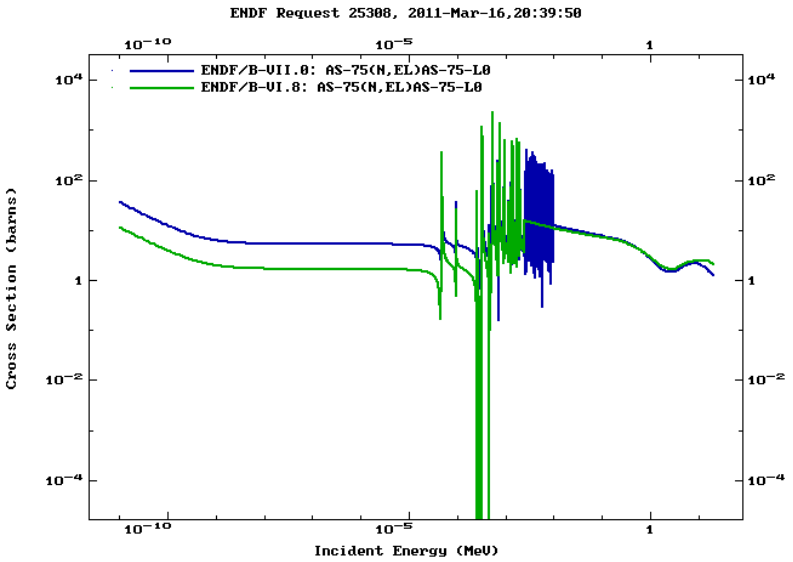


Y 89

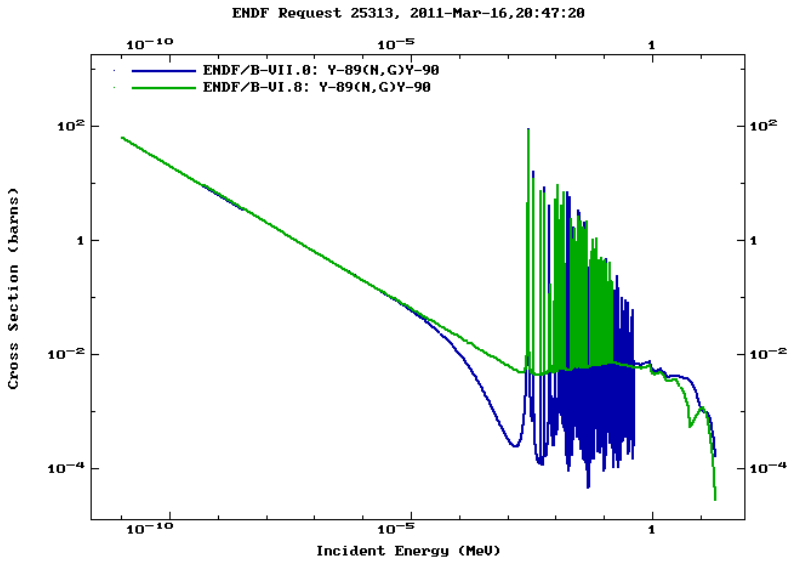


Difference in ENDF VI and VII of the elements

As 75



Y 89



ATLAS Cavern Background Simulation

- Physics List “QGSP_BERT_LEND”
- Geometry “Atlas Cavern Background Simulation”
- “ENDL99” has at least “natural element data” for the materials in the simulation

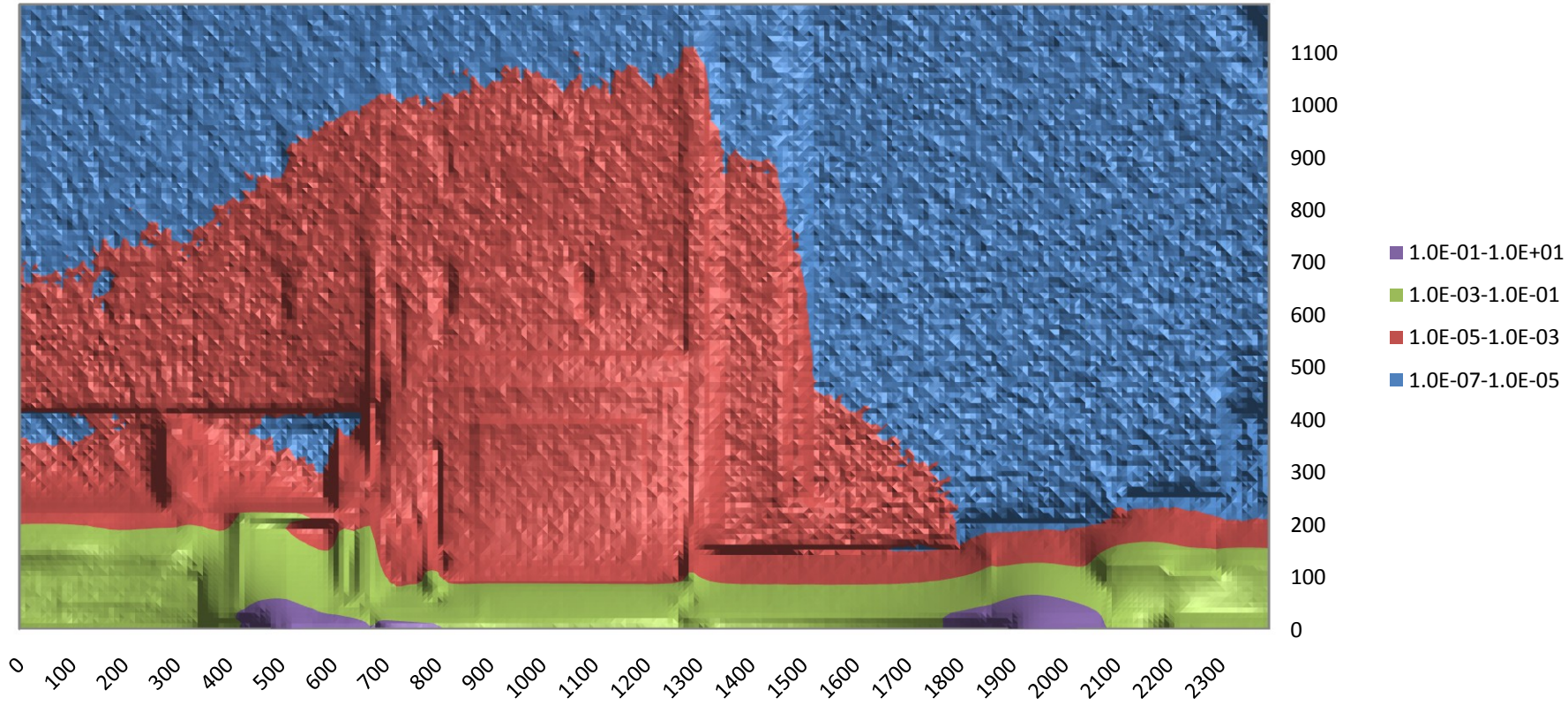
Comparison of CPU and Memory Consumption

based on ATLAS Cavern Background 64 7TeV pp events

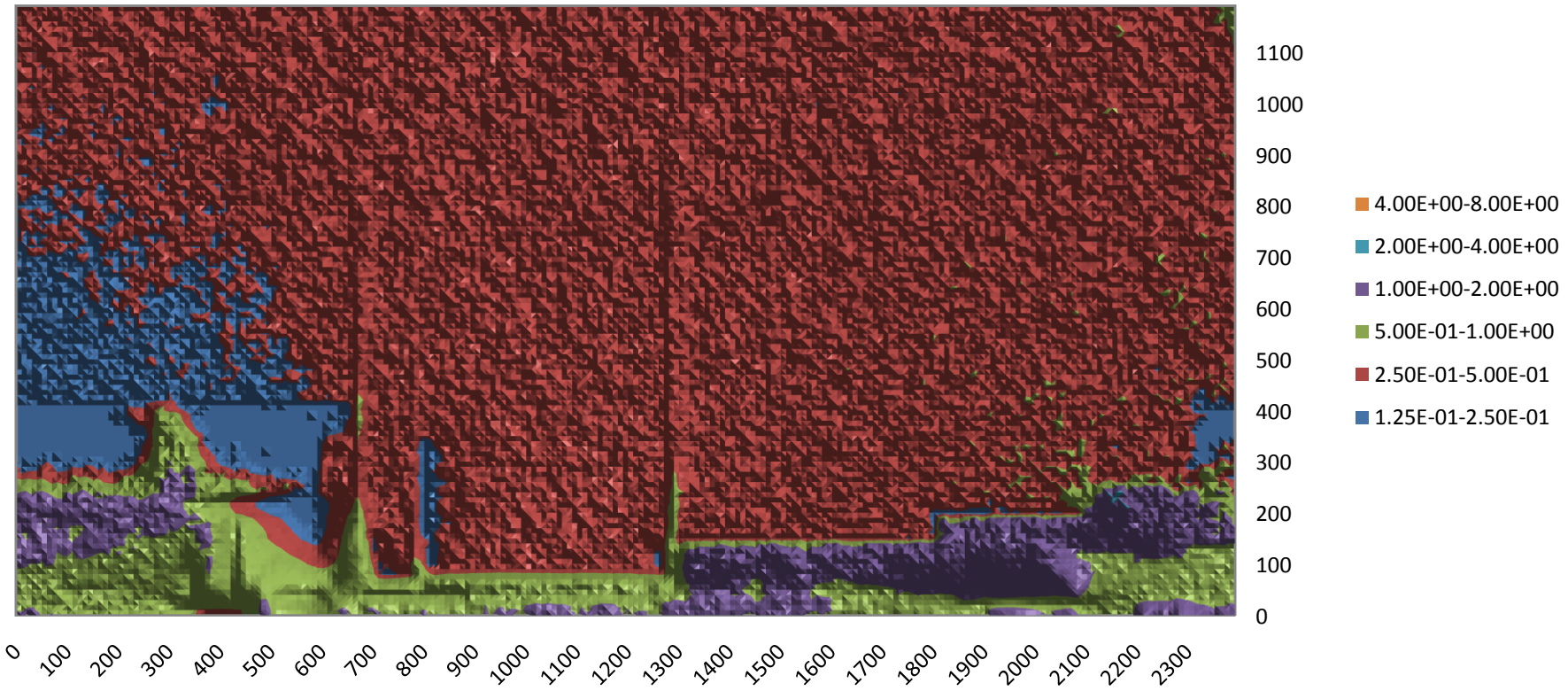
- QGSP_BERT
  - 180 sec/event, 125MB
- QGSP_BERT_HP (FULL)
  - 1,200 sec/event, 690MB (values from 16 events)
- QGSP_BERT_HP (Neglect Doppler Broadening)
  - 280 sec/event, 710MB
- QGSP_BERT_LEND
  - 300 sec/event, 160MB

QGSP_BERT_LEND
neutorn

neutrons per cm^2 per pp event



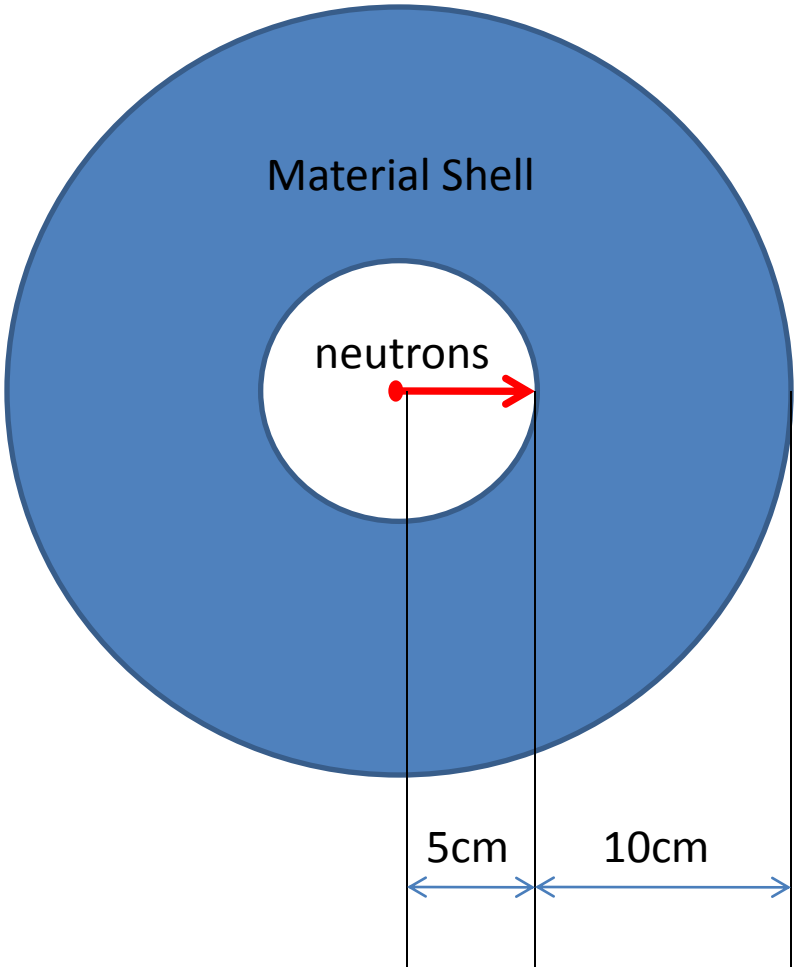
QGSP_BERT_HP/QGSP_BERT_LEND
neutorn



GAMOS comparison

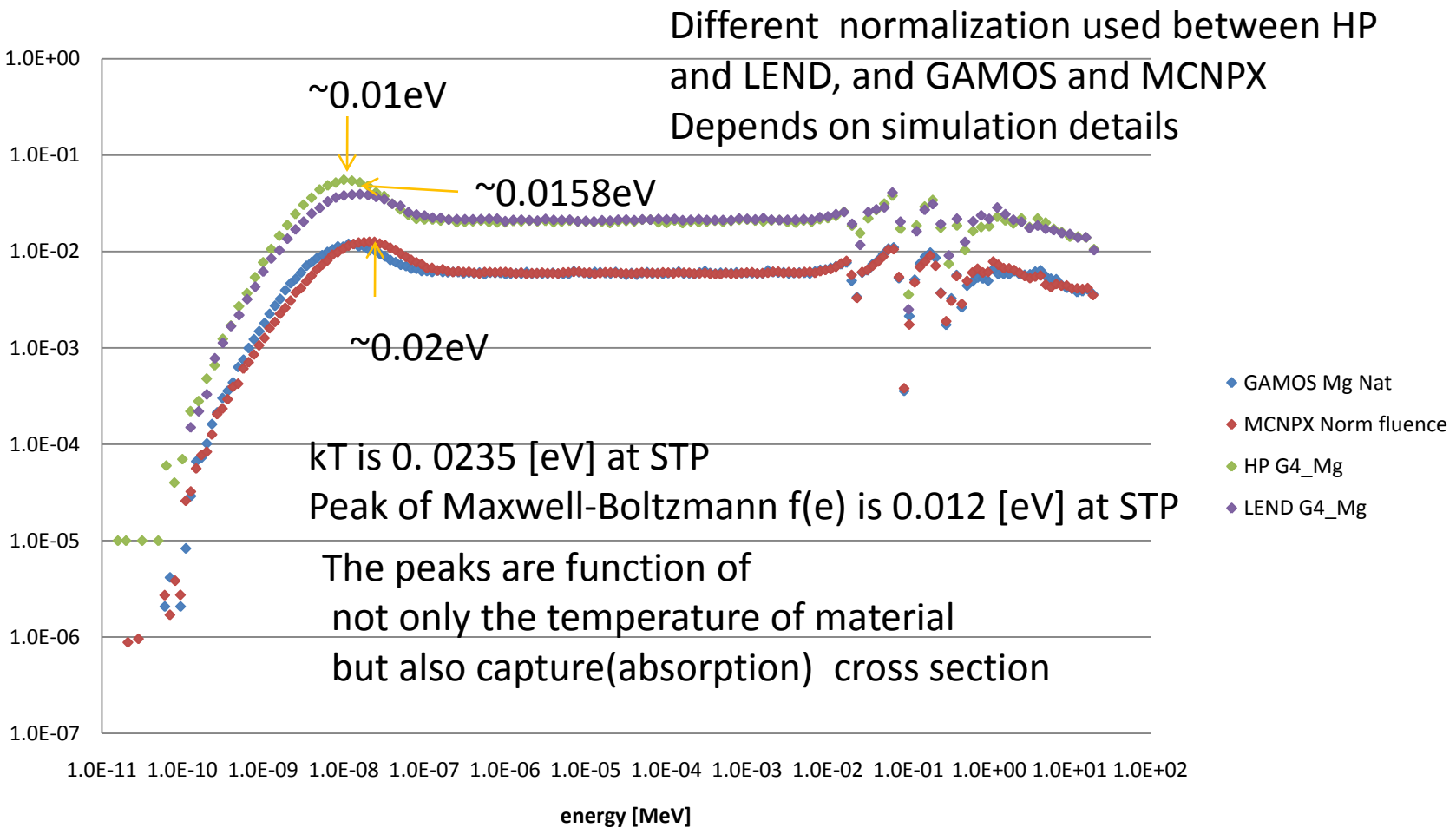
- Requested by Pedro
- Neutron energy spectrum after certain amount (10cm) of materials
- His main interest is shape and position of thermal peak.
  - In some case there are relatively large deference to MCNP result

Condition of GAMOS comparison



- Neutron from the center of the sphere.
- Energy of source neutron
  - flat in the logarithm of the energy, from 1E-11 to 19 MeV
- Material shell has thickness of 10cm
- Measure energy of neutrons at the outer surface of the shell

An example of GAMOS comparison



Same kind of plots are available for
O16 O17 Na23 Mg_nat Al27 Si28 Si29 Si30 Cl35 Cl37 K_nat
Ca_nat Fe54 Fe56 Fe57 Mn55 Pb204 Pb206 Pb207 and Pb208

How to use LEND and QGSP_BERT_LEND

- LEND and its ENDL99 is already in Geant4 repository
- Checkout trunk of “source/processes/hadronic/models/lend”
- Edit GNUmakefile“source/processes/hadronic/models”
  - Add

    SUBDIRS += lend

    SUBLIBS += G4had_lend

    at proper positions.

    You may need update of “libname.map”.
- Set environment variable of “G4LENDDATA”
- Edit GNUmakefile of you application
  - Add

    CPPFLAGS += -I$(G4INSTALL)/source/processes/hadronic/models/lend/include

    EXTRALIBS += -lexpat

    at proper positions

How to build and use LEND and QGSP_BERT_LEND (cont.)

- “QGSP_BERT_HP” is not yet in the repository.
  - Cause compile errors for who does not check out “LEND”.
- Please allow tar ball based distribution for a while.
- Unpack the tar ball at “source/physics_lists” and make.
  - You may need “make clean” at first.
- Include “QGSP_BERT_LEND.hh” in your application.
  - You cannot use the physics list through “PhysicsListFacotry”

Typical Physics List for LEND

```
#include "G4HadronElasticProcess.hh"
#include "G4LENDElasticCrossSection.hh"
#include "G4LENDElastic.hh"

*******************************************************************************
// “particle” is the particle definition of neutron (G4Neutron)
// “pmager” is the process manger of neutron (G4Neutron)

G4HadronElasticProcess* theNeutronElasticProcess = new G4HadronElasticProcess();

//setup LEND XS and model

G4LENDElasticCrossSection* endlElasticXS = new G4LENDElasticCrossSection( particle );
endlElasticXS->AllowNaturalAbundanceTarget();
//endlElasticXS->AllowAnyCandidateTarget();
G4LENDElastic* endlElasticFS = new G4LENDElastic( particle );
endlElasticFS->AllowNaturalAbundanceTarget();
//endlElasticFS->AllowAnyCandidateTarget();
theNeutronElasticProcess->AddDataSet( endlElasticXS );
theNeutronElasticProcess->RegisterMe( endlElasticFS );
pmanager->AddDiscreteProcess( theNeutronElasticProcess );
```

GIDI ver2

- We are already working for LEND-GIDI ver2.
- At this version, we will convert not only ENDL(LLNL) but also most of nuclear data libraries (ENDF(USA), JEFF(Europe), JENDL(Japan),CENDL(Chaina) ROSFOND(Russia) to the GIDI format.

Summary

- We are developing G4LEND which is Geant4 interface for the GIDI.
- This will be an alternative choice of low energy neutron transportation in Geant4
- First comparison against ENDF data and Neutron HP has reasonable agreement
- Plan is to include G4LEND in the next Geant4 beta release (June,2011)
- GIDI library and data should also to be available at that time
  - They will be separately distributed from Geant4