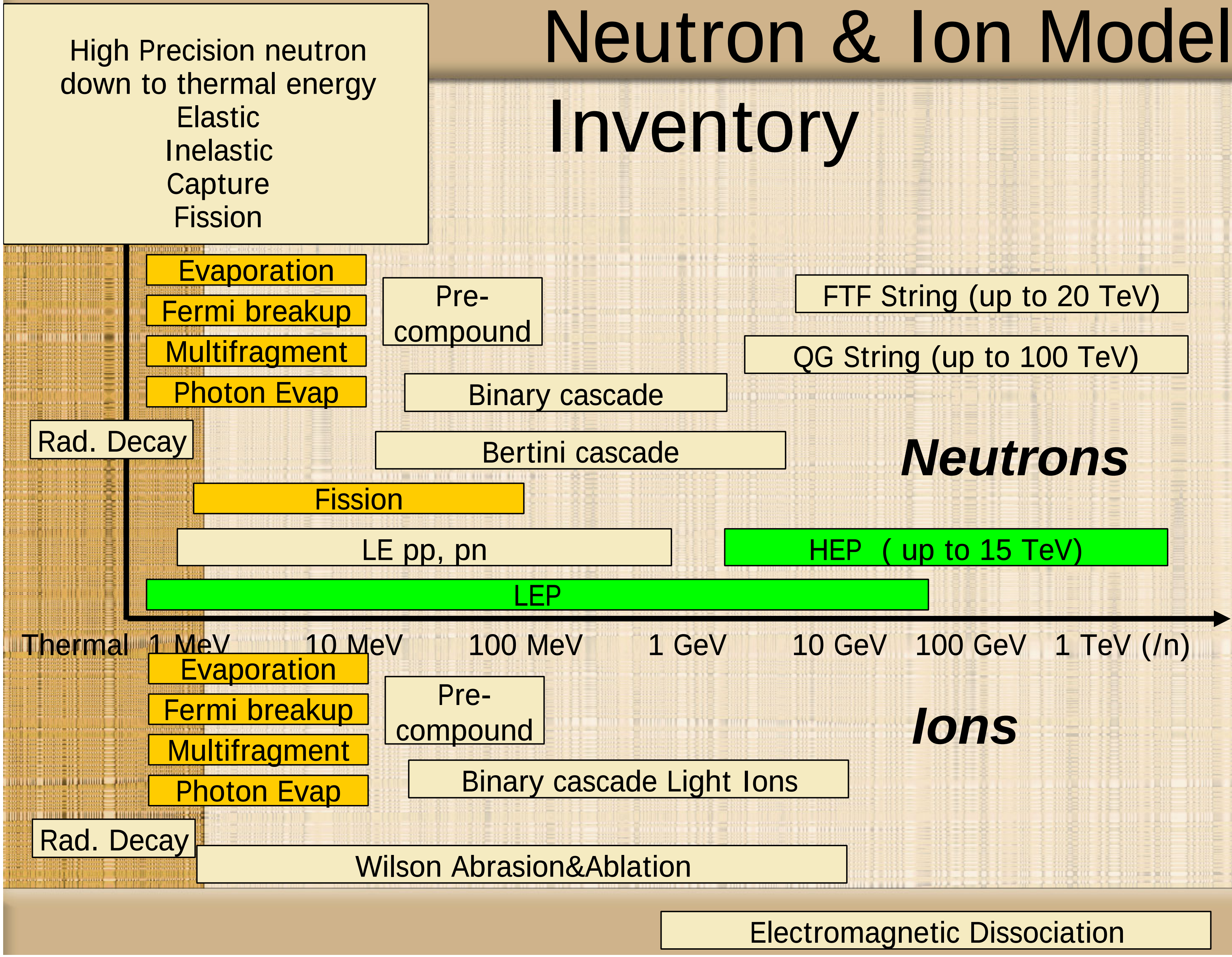
Geant4 Physics Verification and Validation
Low Energy Neutron Related Efforts ~Microscopic Levels~

Koi, Tatsumi SLAC/SCCS

Outline

- Overview of Neutron Interaction in Geant4
  - High energy neutrons interaction
  - Low energy (<20 MeV) neutrons interaction
    - G4NDL
    - Neutron High Precision Models
    - NeutronHPorLEModel
    - Thermal neutron scattering S(α , β) Models
- Verification Strategy

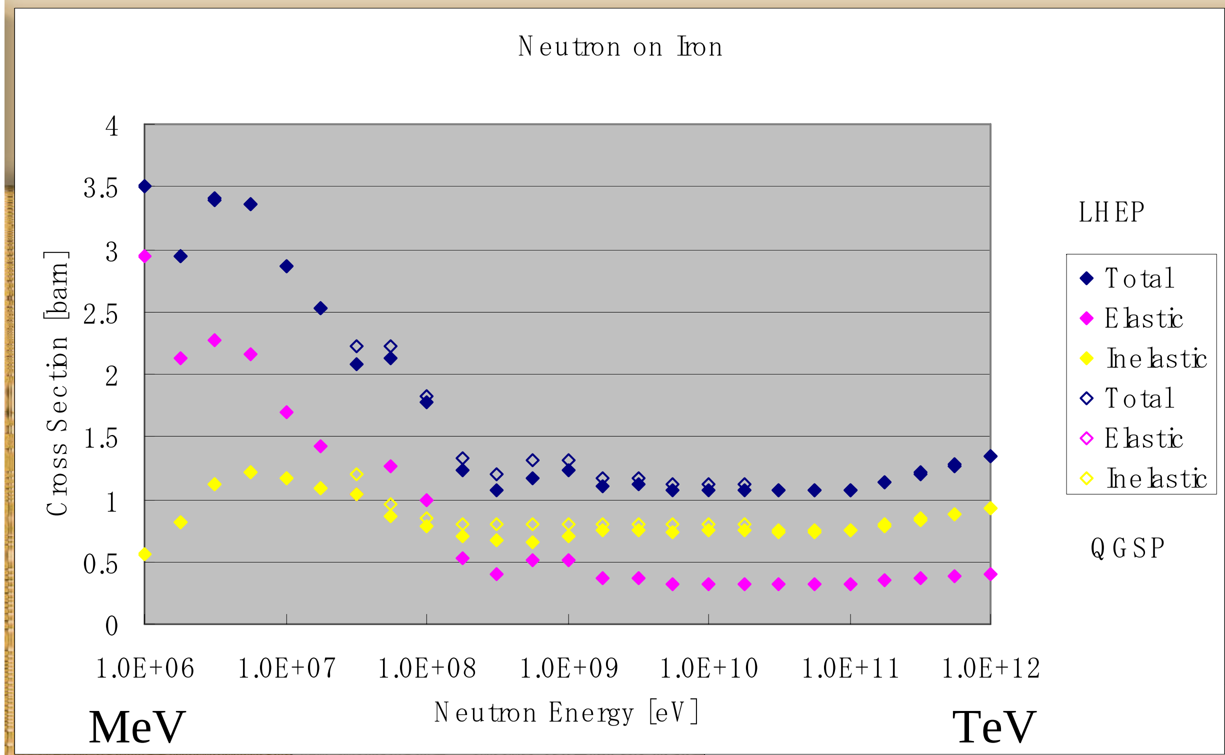
Neutron & Ion Models Inventory



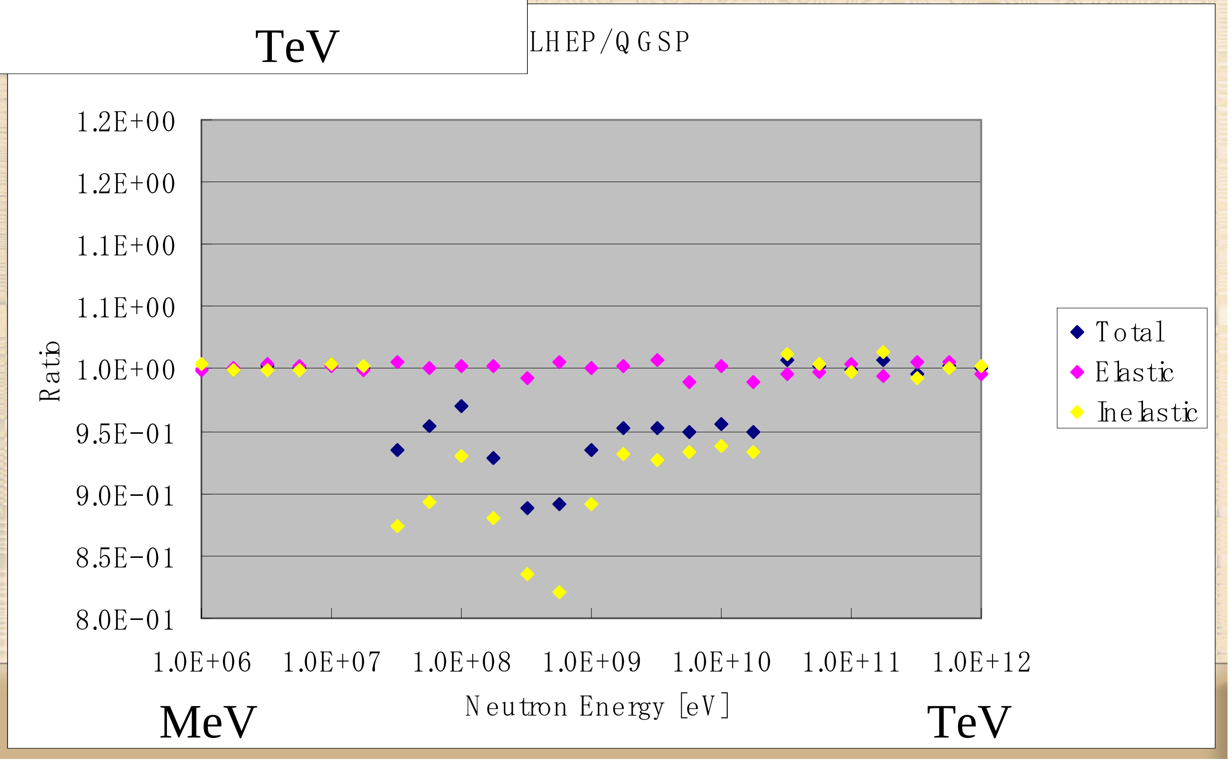
High energy neutron physics

- Parameterized models
  - LEP 0~30 GeV
  - HEP ~15 GeV up to 15 TeV
  - a re-engineered version of GHEISHA
  - Elastic, Inelastic, Capture and Fission
- Theory driven models
  - Cascade Models
    - Binary Cascade < 3 GeV
    - Bertini Cascade < 10 GeV
  - High Energy Models ~15GeV < E < ~15 TeV
    - Quark-Gluon String (QGS)
    - Fritiof fragmentation (FTF)

Cross Section Comparison between Physics Lists (Geant4 v8.1)



Neutrons on Iron



Low energy (< 20MeV) neutrons physics

- G4NDL (Geant4 Neutron Data Library)
- High Precision Neutron Models
  - Elastic
  - Inelastic
  - Capture
  - Fission
- NeutronHPorLEModel(s)
- Thermal neutron scattering S(α , β) Models

G4NDL (Geant4 Neutron Data Library)

- The neutron data files for High Precision Neutron models
- The data are including both cross sections and final states.
- The data are derived evaluations based on the following evaluated data libraries (in alphabetic order)
  - Brond-2.1
  - CENDL2.2
  - EFF-3
  - **ENDF**/B-VI.0, 1, 4
  - FENDL/E2.0
  - JEF2.2
  - JENDL-FF
  - JENDL-3.1,2
  - MENDL-2
- The data format is similar ENDF, however it is not equal to.
- After G4NDL3.8 we concentrated translation from **ENDF** library.
  - No more evaluation by ourselves.
- NDL3.9 is latest
  - Adding requested elements
  - Replace incorrect data

Low Energy Neutron: Elastic

- The final state of elastic scattering is described by sampling the differential scattering cross-sections
  - tabulation of the differential cross-section

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(\cos\theta, E)$$

  - a series of Legendre polynomials and the Legendre coefficients

$$\frac{2\pi}{\sigma(E)}\frac{d\sigma}{d\Omega}(\cos\theta, E) = \sum_{l=0}^{n_l}\frac{2l+1}{2}a_l(E)P_l(\cos\theta)$$

- Will add combination usage in order to integrate JENDL-HE files

Low Energy Neutron: Inelastic

- Currently supported final states are (nA) n γ s (discrete and continuum), np, nd, nt, n 3He, n α , nd2 α , nt2 α , n2p, n2 α , np , n3 α , 2n α , 2np, 2nd, 2n α , 2n2 α , nX, 3n, 3np, 3n α , 4n, p, pd, p α , 2p d, d α , d2 α , dt, t, t2 α , 3He, α , 2 α , and 3 α .
  - 36 channels
- Secondary distribution probabilities are supported
  - isotropic emission
  - discrete two-body kinematics
  - N-body phase-space distribution
  - continuum energy-angle distributions
    - legendre polynomials and tabulation distribution
    - Kalbach-Mann systematic $A + a \rightarrow C \rightarrow B + b$, C:compound nucleus
  - continuum angle-energy distributions in the laboratory system

Low Energy Neutron: Capture

- The final state of radiative capture is described by either photon multiplicities, or photon production cross-sections, and the discrete and continuous contributions to the photon energy spectra, along with the angular distributions of the emitted photons.
- For discrete photon emissions
  - the multiplicities or the cross-sections are given from data libraries
- For continuum contribution

$$f(E \to E_\gamma) = \sum_i p_i(E) g_i(E \to E_\gamma)$$

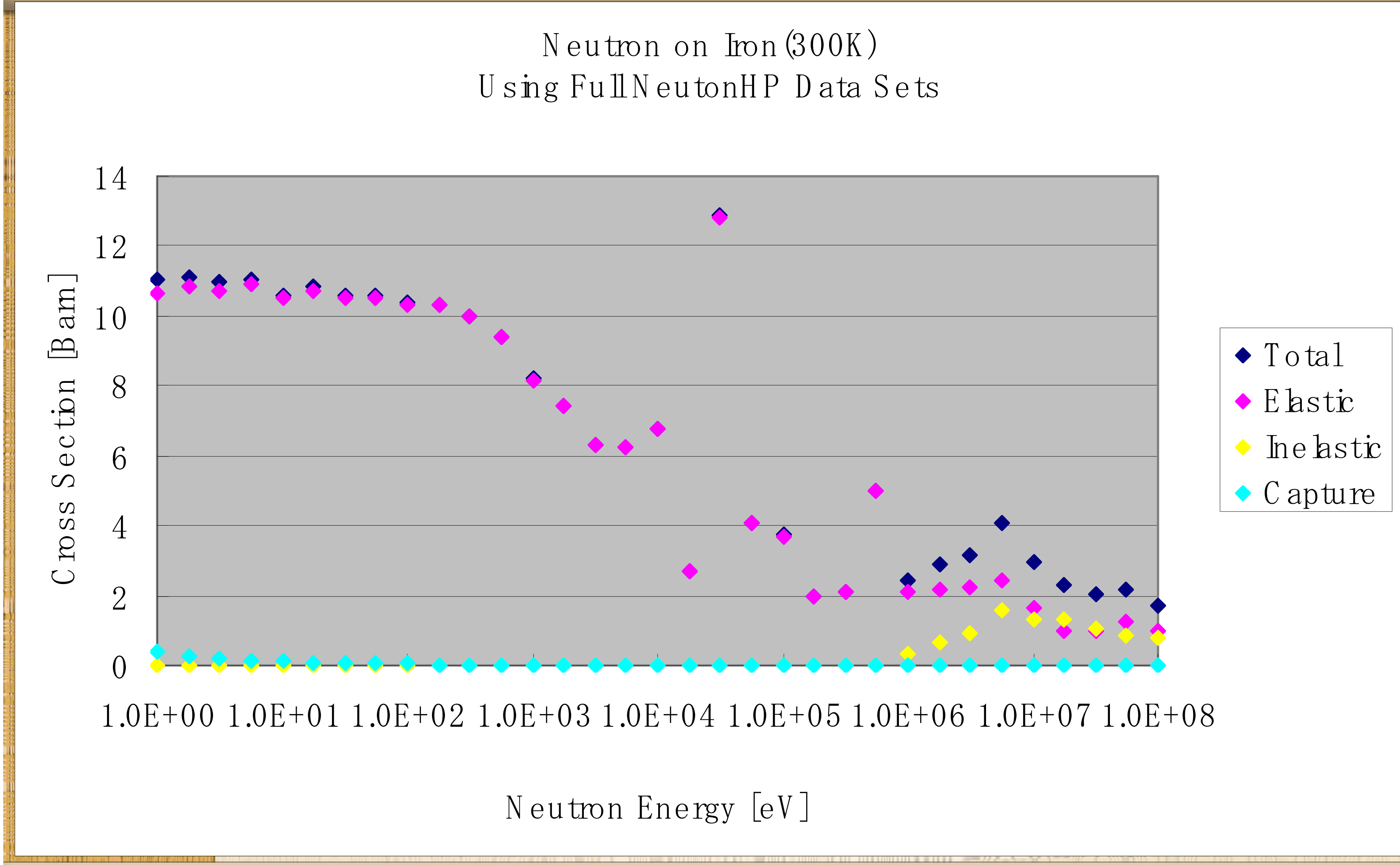
  - E neutron kinetic energy, E γ photon energies
  - pi and gi are given from data libraries
- If there is no final state data in G4NDL(means no data in ENDF file) then Photon Evaporation model of Geant4, which uses Evaluated Nuclear Structure Data File (ENSDF) create final state products including Internal Conversion electrons

Low Energy Neutron: Fission

- First chance, second chance, third chance and forth chance fission are into accounted.
- The neutron energy distributions are implemented in six different possibilities.
  - tabulated as a normalized function of the incoming and outgoing neutron energy $f(E \rightarrow E')$
  - Maxwell spectrum $f(E \rightarrow E') \propto \sqrt{E'} e^{E'/\Theta(E)}$
  - a general evaporation spectrum $f(E \rightarrow E') \propto E' e^{E'/\Theta(E)}$
  - evaporation spectrum $f(E \rightarrow E') = f\left(E' / \Theta(E) \right)$
  - the energy dependent Watt spectrum $f(E \rightarrow E') \propto e^{E'/a(E)} \sinh \sqrt{b(E)E'}$
  - the Madland Nix spectrum $f(E \rightarrow E') = \frac{1}{2}\left[g\left(E', \langle K_l \rangle\right) + g\left(E', \langle K_h \rangle\right) \right]$

Validation & Verification

- Comparison between thin target calculations of Geant4 and corresponding ENDF data
- Comparison between thin target calculations of Geant4 and corresponding G4NDL data
- Checking Energy and Momentum conservation levels
  - ***Neutron High Precision Model does not guarantee these conservations a priori***



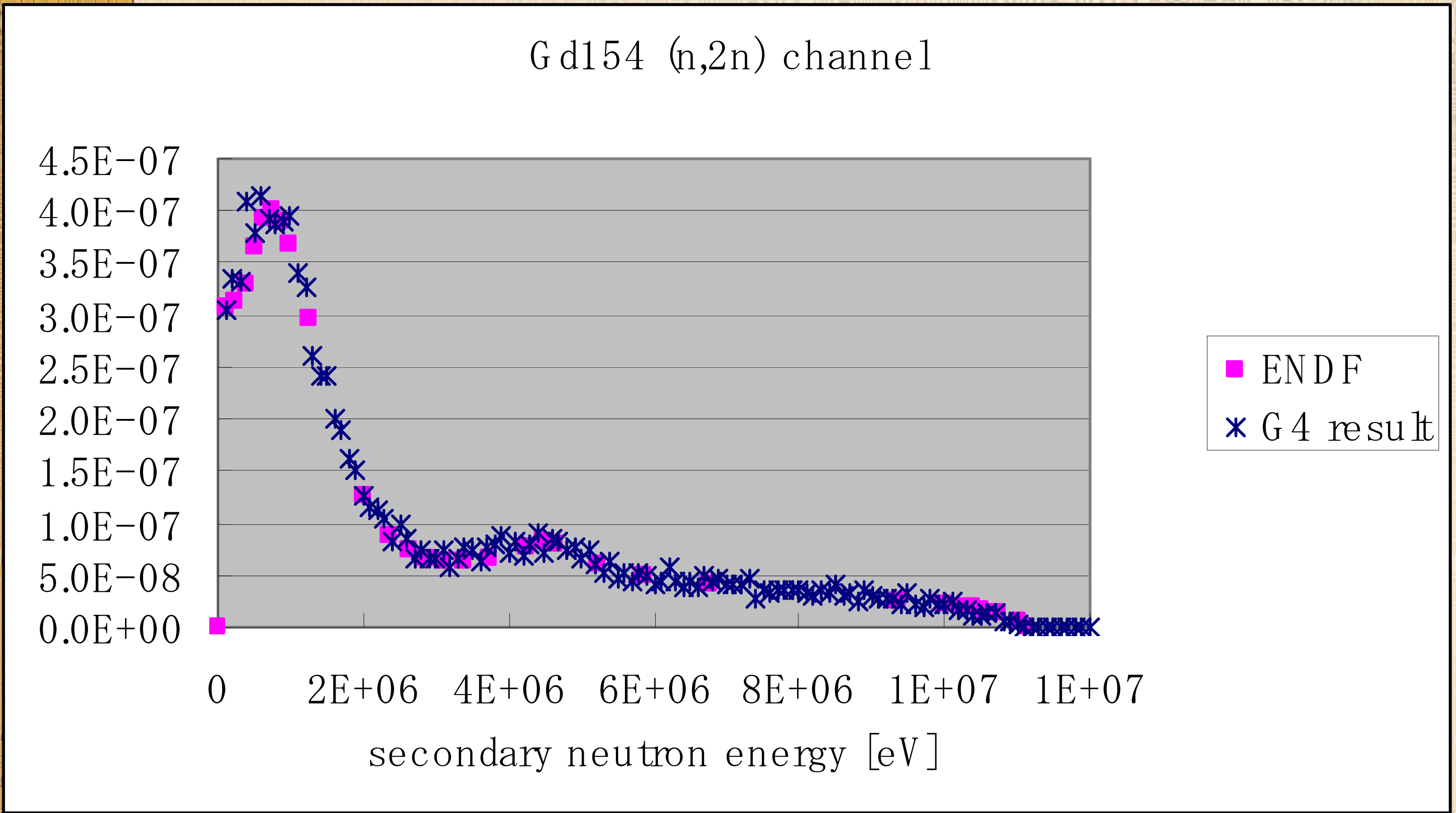
Neutron on Iron(300K)
Using FullNeutonHP Data Sets
Cross Section [Barn]
14
12
10
8
6
4
2
0
1.0E+00
1.0E+01
1.0E+02
1.0E+03
1.0E+04
1.0E+05
1.0E+06
1.0E+07
1.0E+08
Neutron Energy [eV]
Total
Elastic
Inelastic
Capture

Verification of High Precision Neutron models
Channel Cross Sections

Geant4 results Derive from thin target calculations	ENDF Values Derived from data files
Ela XS 3.7104216 [barn]	3.708710 [barn]
Inela XS 1.2508858	
Inela XS F01 0.99179298	9.940940E-1
Inela XS F04 0.18413539	1.836200E-1
Inela XS F06 0.020973994	2.126800E-2
Inela XS F10 0.041302787	4.064300E-2
Inela XS F23 0.009658162	9.717300E-3
Inela XS F27 0.0030225183	3.306100E-3
Cap XS 0.0017767842	1.646330E-3

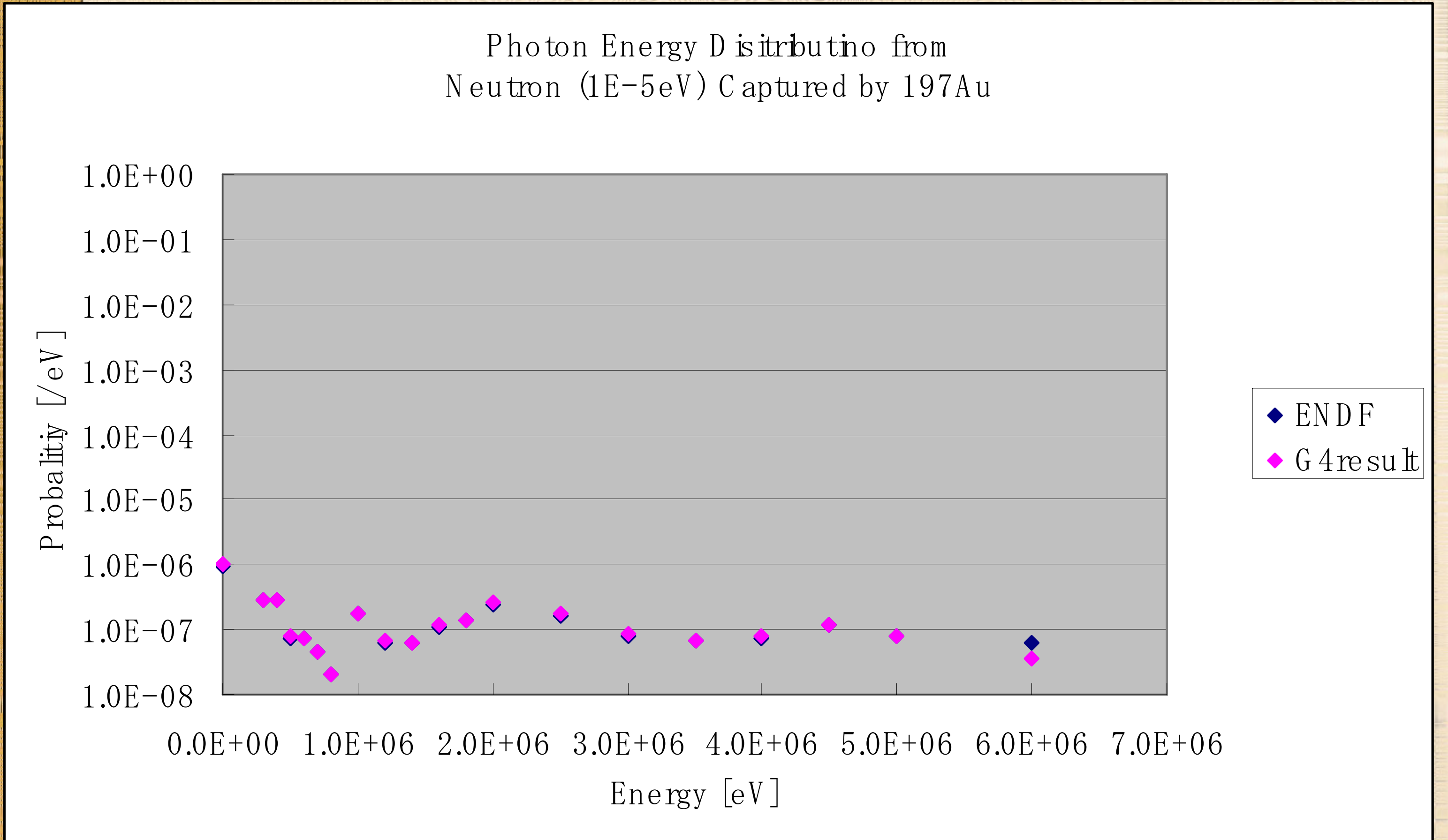
20MeV neutron on Gd157(0k)

Verification of High Precision Neutron Models
Energy Spectrum of Secondary Particles



20MeV neutron on Gd154(0K)

Verification of High Precision Neutron Models
Energy Spectrum of Secondary Particles

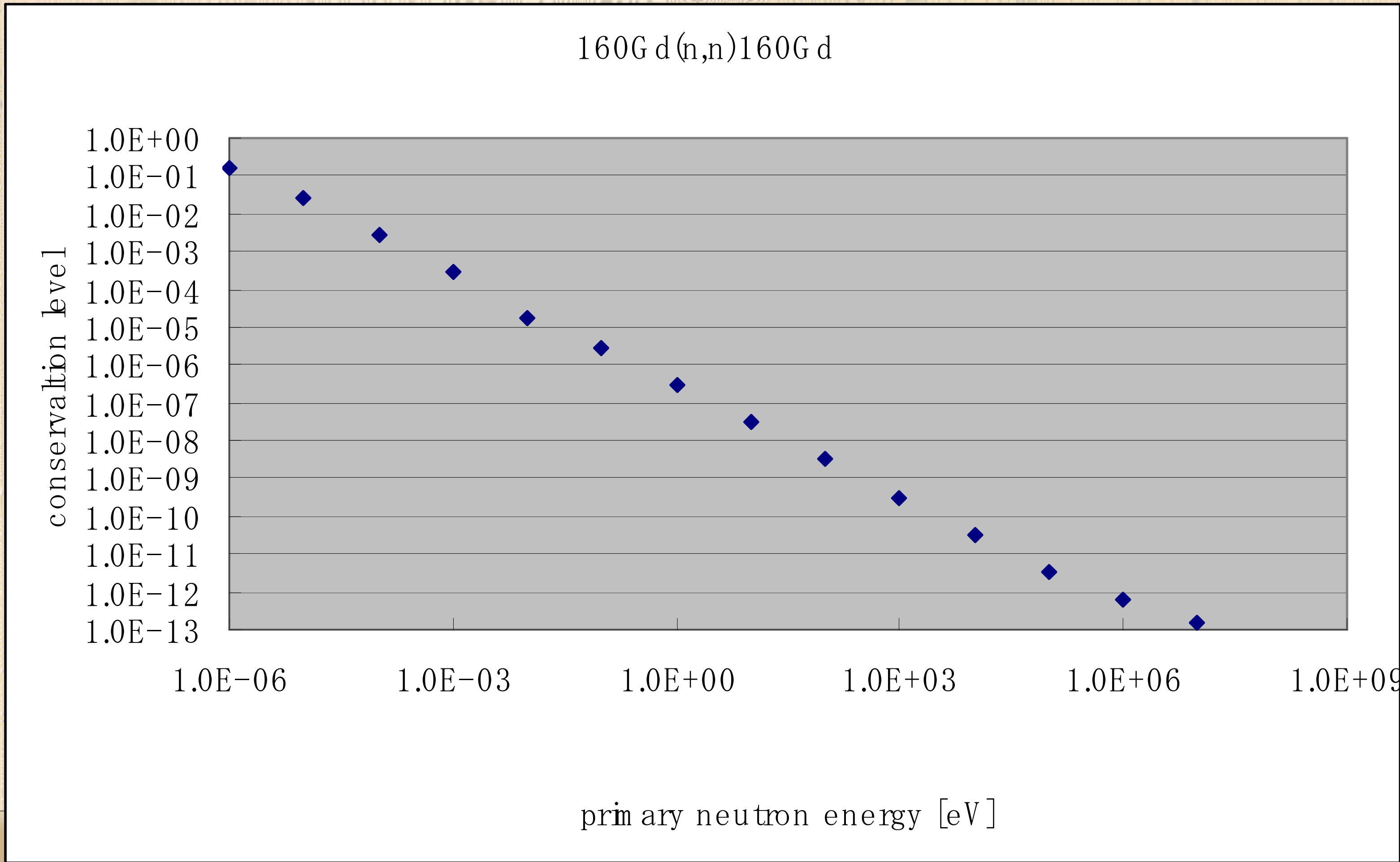


Cold Neutron Captured by 197Au (0K)

Validation of High Precision Neutron Models
Momentum conservation level of Elastic Scattering

conservation level = delta / primary

delta = primary – (scattered A + scattered B)



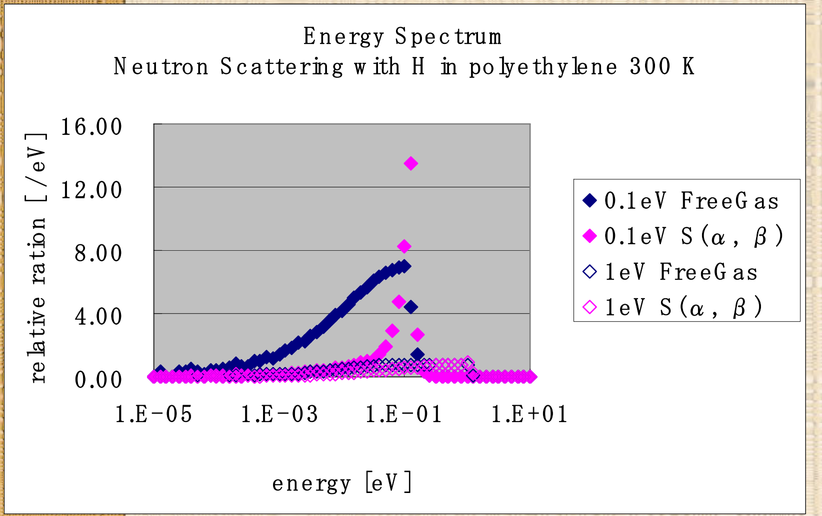
G4NeutornHPorLEModels

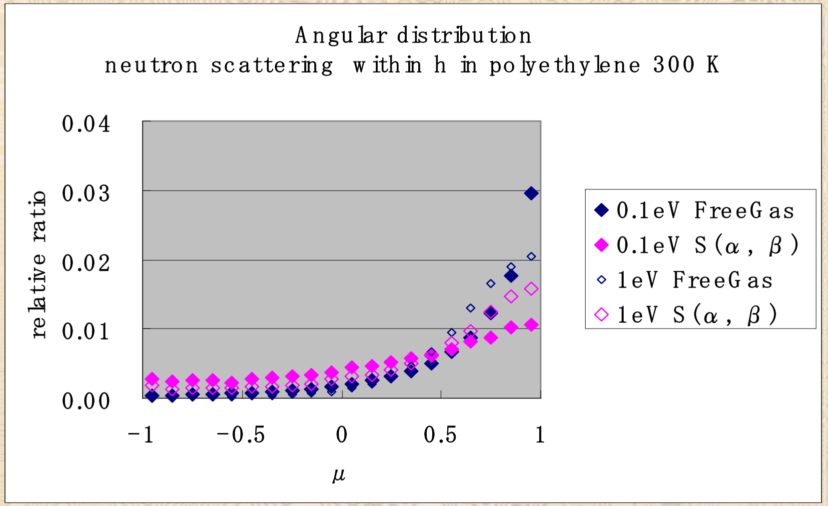
- Many elements remained without data for High Precision models.
- Those models make up for such data deficit.
- If the High Precision data are not available for a reaction, then Low Energy Parameterization Models will handle the reaction.
- Those can be used for not only for models (final state generator) but also for cross sections.
- Elastic, Inelastic, Capture and Fission models are prepared.

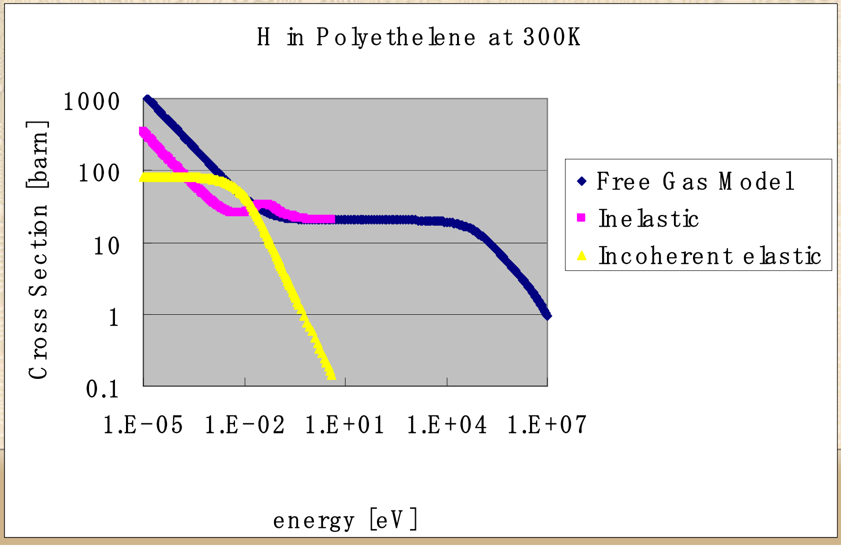
Thermal neutron scattering: S(α, β) Model

- For thermal neutron scattering from nuclei with chemically bonded atoms
- Based on thermal neutron scattering files from the evaluated nuclear data files ENDF/B-VI, Release2
- Coherent elastic, incoherent elastic and inelastic scattering are included
- Will be included release

Cross section and Secondary Neutron Distributions of S(α, β) model







Conclusions

- Geant4 has abundant processes for neutron interactions with matter from thermal energy to much above TeV energy.
- The Geant4 toolkit contains a large variety of complementary and sometimes alternative physics models covering the physics of neutrons.
- Validation and verification results show reasonable agreement with data.
- Systematic evaluations of agreement between Geant4 results and ENDF data are desirable and under investigation.
- Computing speed and memory usage could become discussion issues in the future.