# Accurate neutron elastic resonant scattering in heavy nuclei: implementation of the Doppler Broadening Rejection Correction

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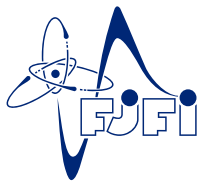


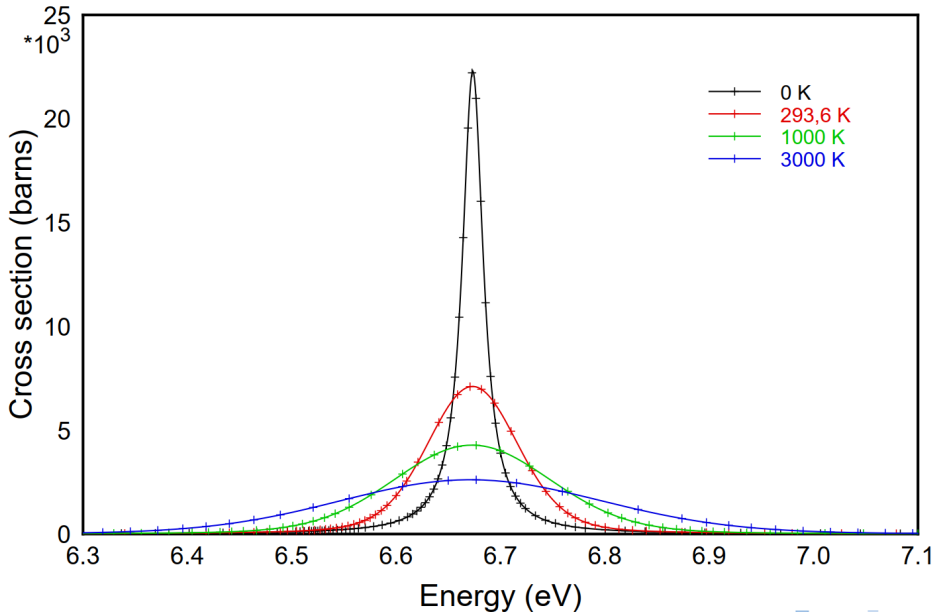


# Outline

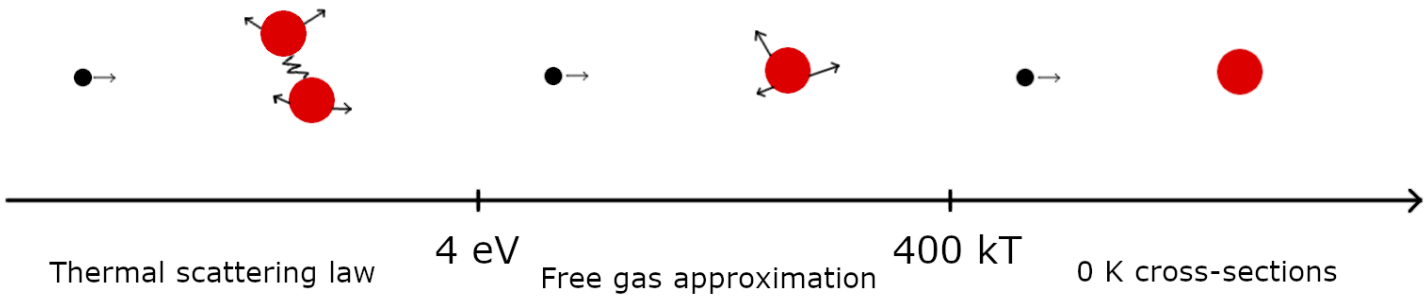
# Effect of the thermal motion

- Doppler broadening of cross sections

$$\sigma_T(v) = \frac{1}{v} \int v_r \sigma_0(v_r) P(\mathbf{V}, T) d\mathbf{V}$$




- Final states - elastic scattering kernel



# Final states - scattering kernel

$$p(V,\mu)dVd\mu = \frac{v_r\sigma_0(v_r)P(V,T)dVd\mu}{2v\sigma_T(v)}$$

assumption $\sigma_0(v_r)$ is constant $\Rightarrow$ Sampling of the Velocity of the Target nucleus method

Solutions:

- S$(\alpha,\beta)$ tables
- Weight Correction Method (WCM)
- Doppler Broadening Rejection Correction (DBRC) method

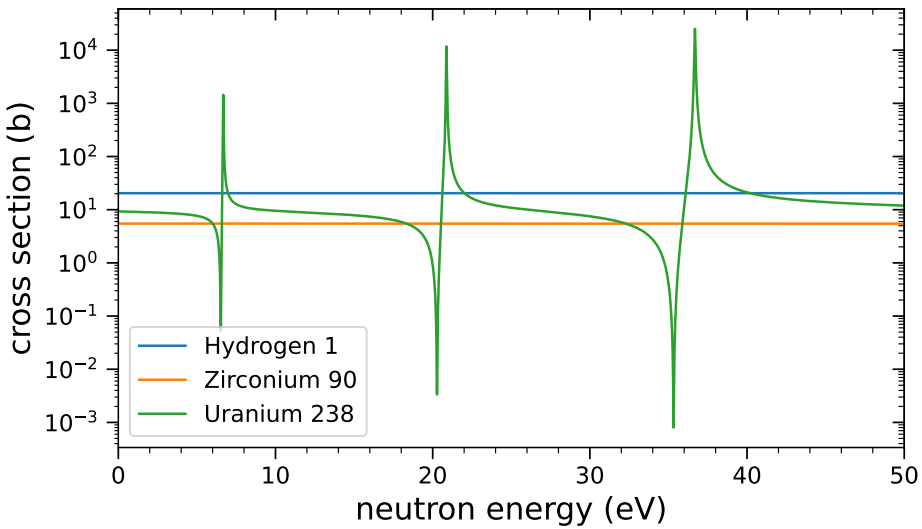



Figure: Comparison of elastic cross sections for different isotopes - DBRC important for heavy nuclei.

# Doppler Broadening Rejection Correction

$$p(V,\mu) = C \underbrace{\left(\frac{\sigma_0(v_r)}{\sigma_{\max}(v_\xi)}\right)}_{(A)} \underbrace{\left(\frac{v_r}{v+V}\right)}_{(B)} \underbrace{\left(\beta^3 v V^2 e^{-\beta^2 V^2} + \beta^3 V^3 e^{-\beta^2 V^2}\right)}_{(C)} \quad (1)$$

1. Sample $\mu$ from (-1,1) uniformly.
2. Sample $V$ from (C).
3. Accept $(\mu, V)$ with probability (B).
4. Accept $(\mu, V)$ with probability (A).

# Implementation

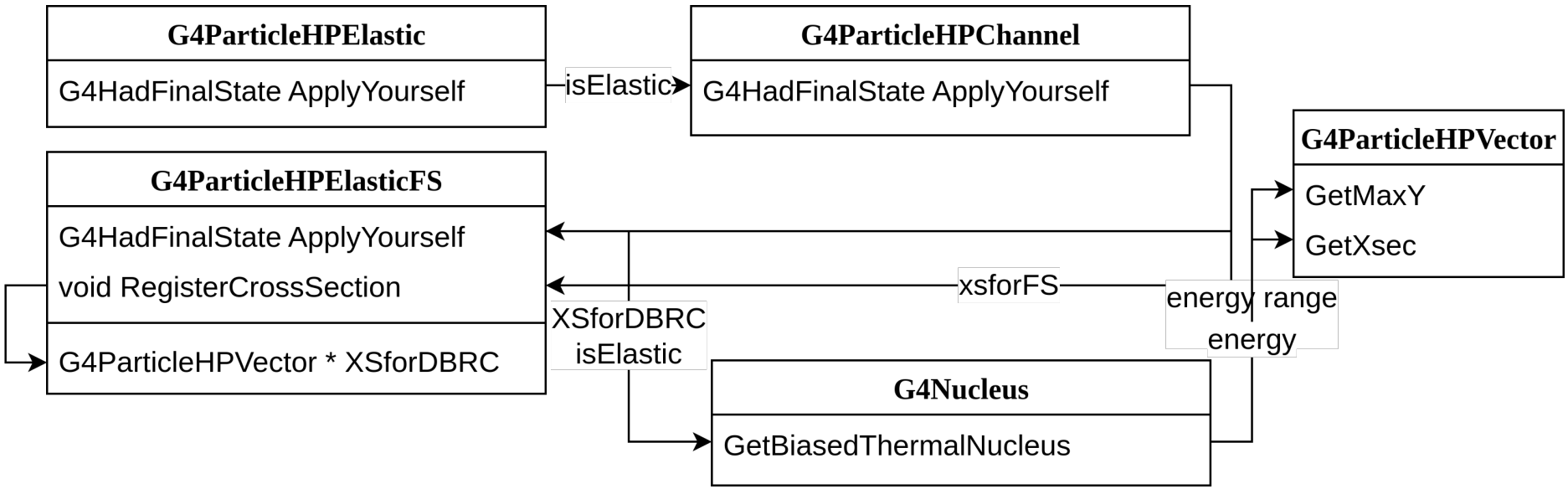
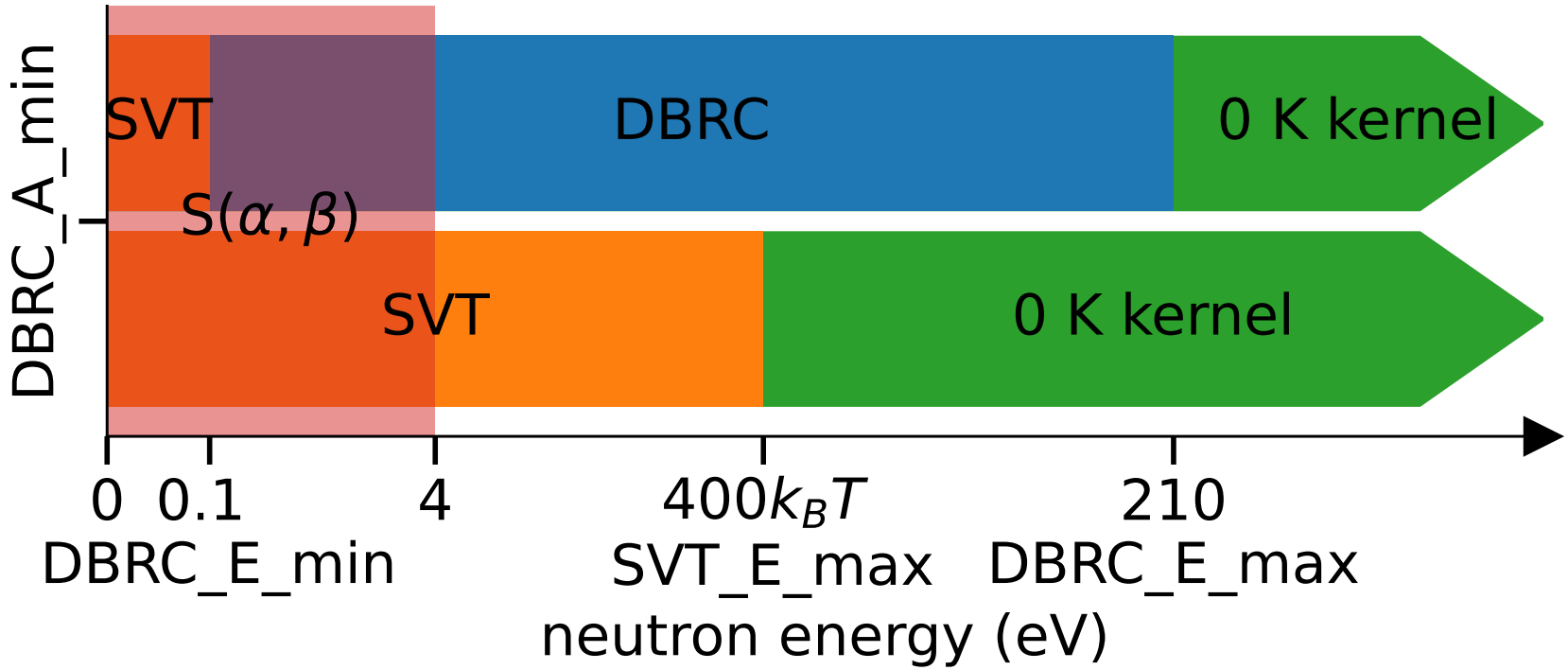



Figure: Diagram of implementation of the DBRC method.

# New flags in G4ParticleHPMessenger

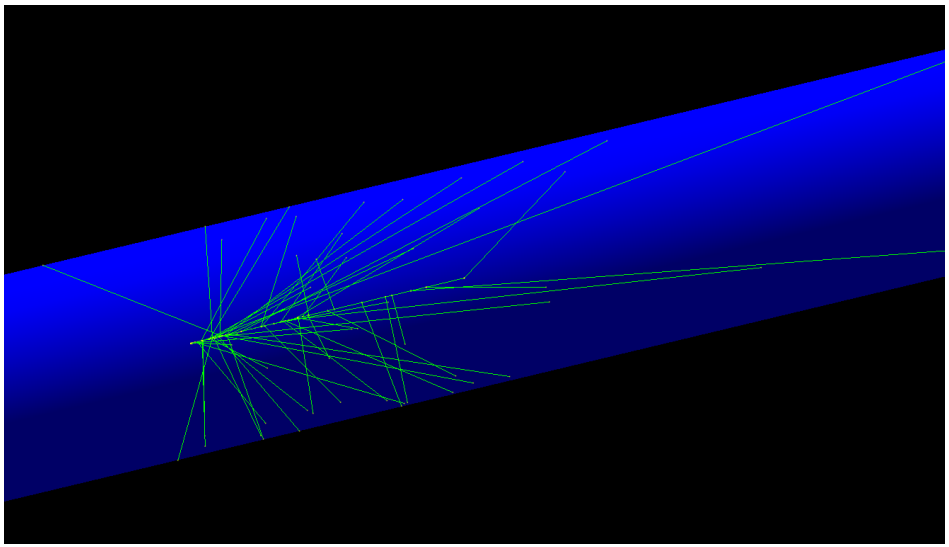
Directory /process/had/particle_hp/

- use_DBRC (false)
- SVT_E_max ($400 k_B T$)
- DBRC_A_min (200)
- DBRC_E_max (210 eV)
- DBRC_E_min (0.1 eV)

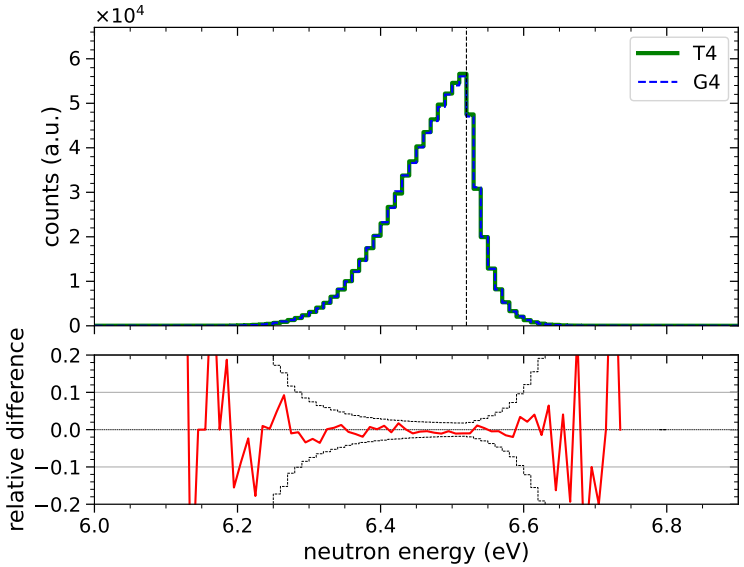


# Microscopic benchmark

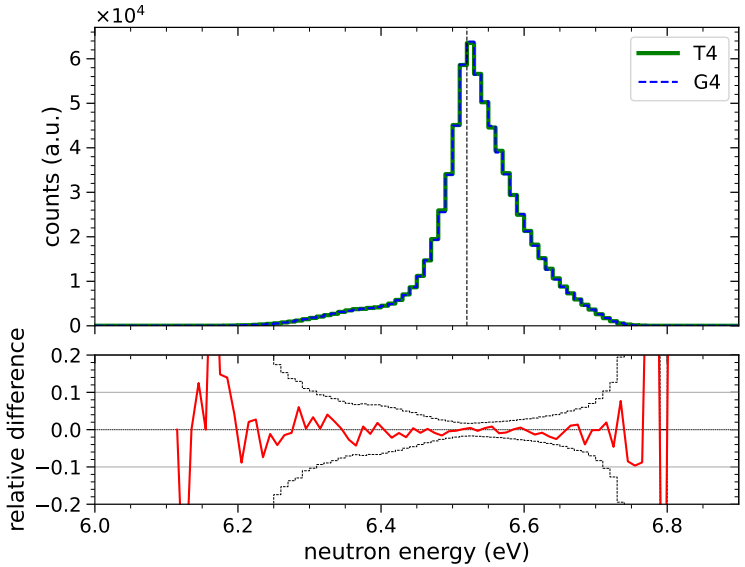
- Thin cylinder of $^{238}$U.
- Temperatures 300, 600, 1000 K energies 6.52, 20.2, 36.25 eV.
- SVT and DBRC, Geant4 and TRIPOLI-4®.
- Energy of scattered neutron.



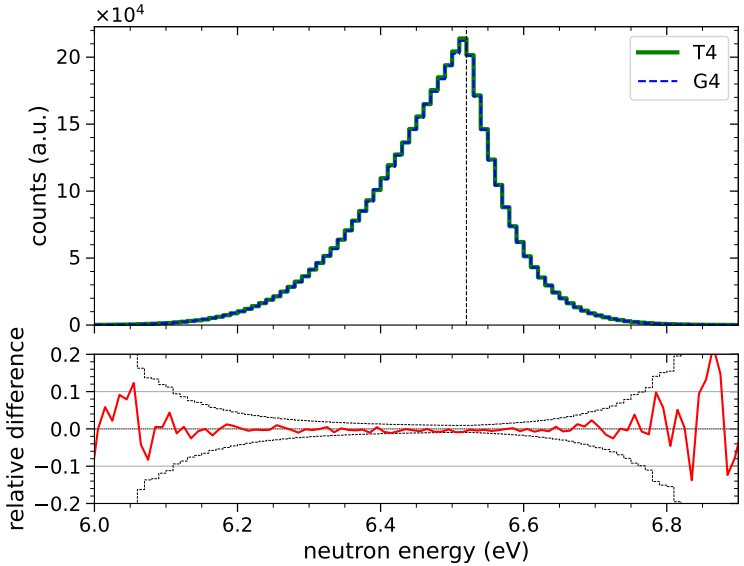
# Validation of SVT and DBRC



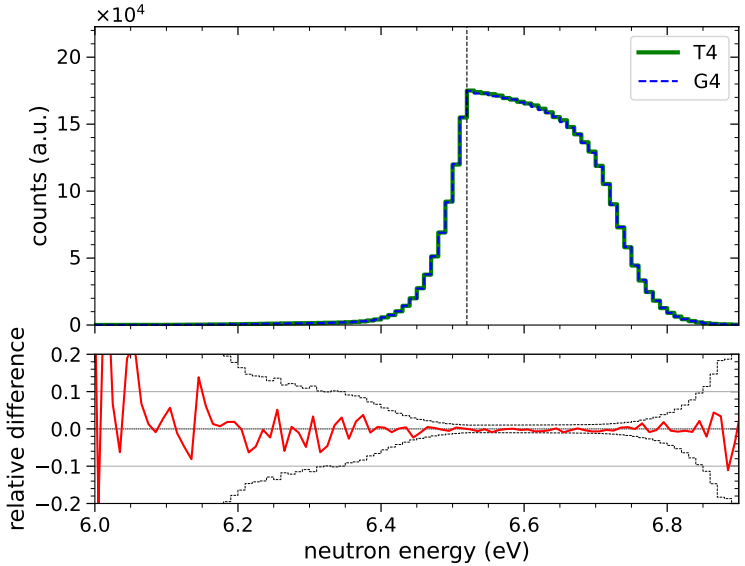

6.52 eV - 300 K - SVT




6.52 eV - 300 K - DBRC

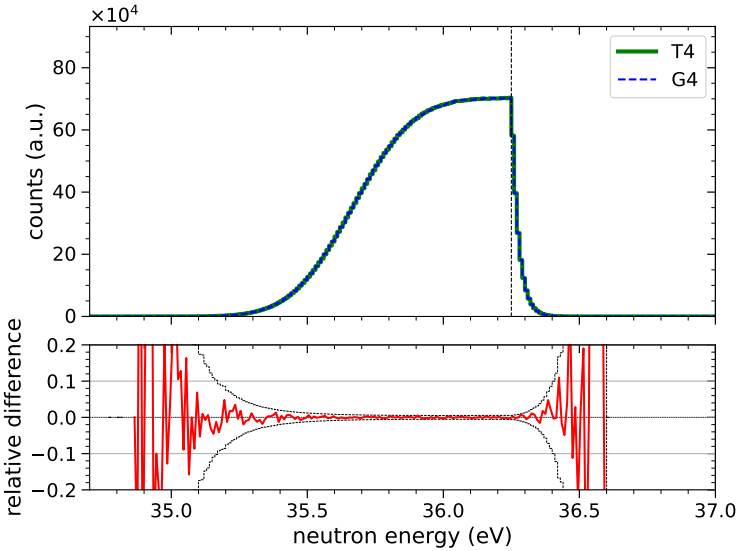



6.52 eV - 1000 K - SVT

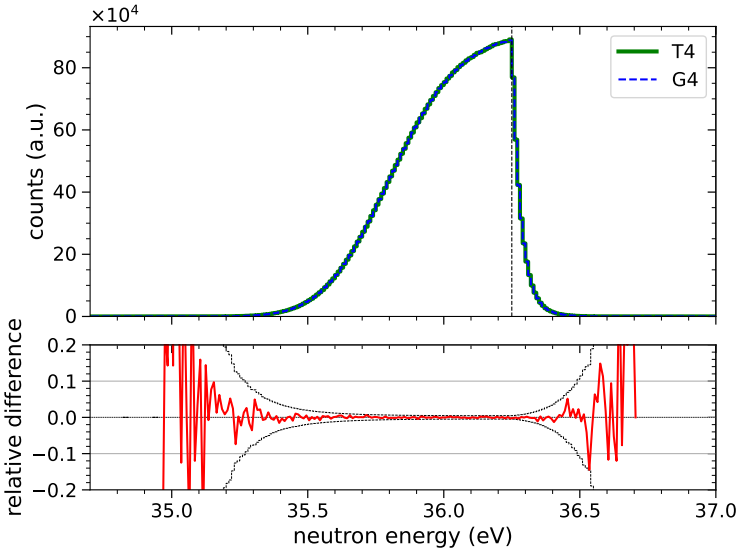



6.52 eV - 1000 K - DBRC

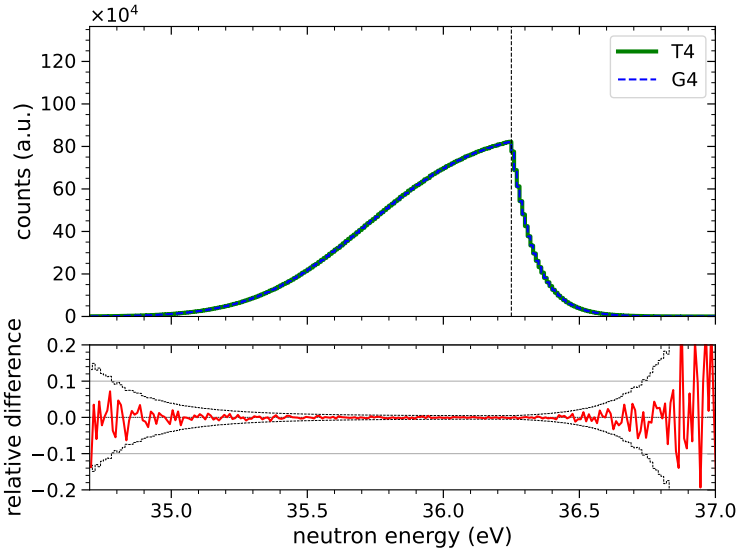
# Validation of SVT and DBRC



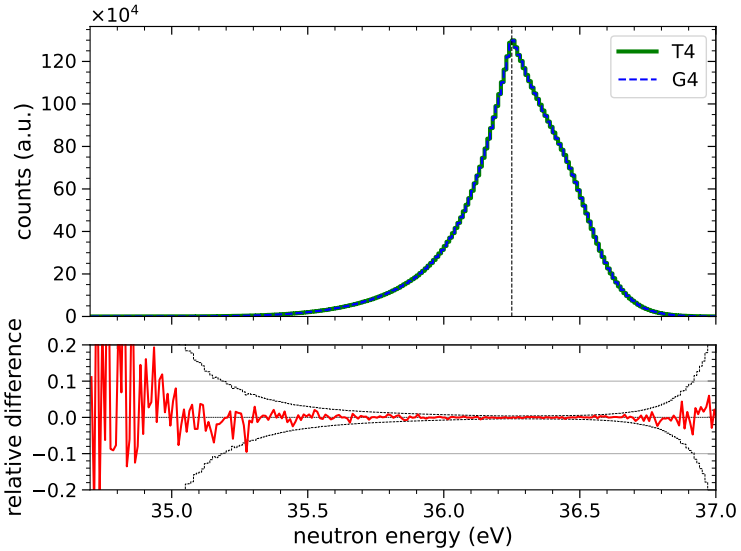

36.25 eV - 300 K - SVT




36.25 eV - 300 K - DBRC




36.25 eV - 1000 K - SVT




36.25 eV - 1000 K - DBRC

# Validation of SVT and DBRC

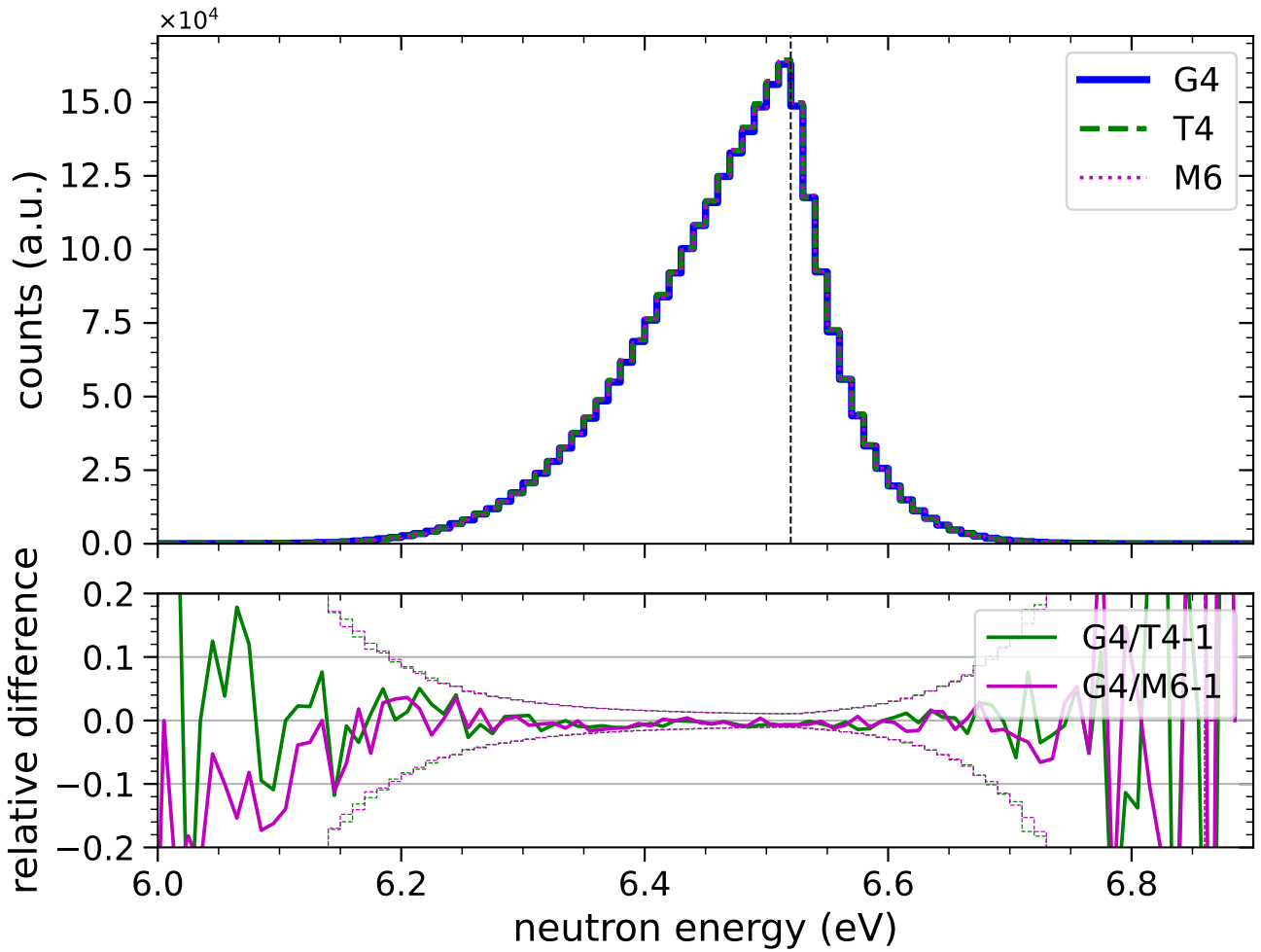



Figure: Comparison of the energy of the scattered neutrons on $^{238}$U for 6.52 eV and 600 K with only SVT method in Geant4, TRIPOLI-4®and MCNP6.2.

# Mean energy

Figure: Mean energy of the scattered neutrons in eV for different primary energies and temperatures on $^{238}$U without (SVT) and with the DBRC method in Geant4 and TRIPOLI-4® and their relative difference in $1 \cdot 10^{-3}$ %.

| E (eV) | T (K) | Geant4 SVT | Geant4 DBRC | TRIPOLI-4® SVT | TRIPOLI-4® DBRC | rel. diff. SVT | rel. diff. DBRC |
|---|---|---|---|---|---|---|---|
| 6.52 | 300 | 6.466 | 6.534 | 6.466 | 6.535 | 0.21 | -4.24 |
| | 600 | 6.466 | 6.589 | 6.466 | 6.589 | -0.16 | 0.88 |
| | 1000 | 6.467 | 6.605 | 6.467 | 6.606 | 2.75 | -3.06 |
| 20.20 | 300 | 20.031 | 19.979 | 20.030 | 19.980 | 2.47 | -3.92 |
| | 600 | 20.031 | 19.987 | 20.031 | 19.988 | 0.06 | -5.44 |
| | 1000 | 20.032 | 20.043 | 20.032 | 20.042 | 1.28 | 4.45 |
| 36.25 | 300 | 35.946 | 36.008 | 35.946 | 36.008 | -0.06 | -0.59 |
| | 600 | 35.946 | 36.128 | 35.946 | 36.128 | -0.19 | 0.37 |
| | 1000 | 35.947 | 36.256 | 35.947 | 36.256 | -0.46 | 0.09 |

# Probability of upscattering

Figure: Relative difference of the probability of elastic scattering from TRIPOLI-4®, its relative variance and the computation time of Doppler broadening for different convergence criteria and minimum number of loops.

| E (eV) | T (K) | Geant4 SVT | Geant4 DBRC | TRIPOLI-4® SVT | TRIPOLI-4® DBRC | rel. diff. SVT | rel. diff. DBRC |
|---|---|---|---|---|---|---|---|
| 6.52 | 300 | 18.124 | 62.294 | 18.008 | 62.413 | 0.64 | -0.19 |
| | 600 | 25.452 | 82.798 | 25.354 | 82.747 | 0.39 | 0.06 |
| | 1000 | 30.407 | 84.325 | 30.229 | 84.354 | 0.59 | -0.04 |
| 20.2 | 300 | 7.499 | 5.692 | 7.435 | 5.850 | 0.87 | -2.70 |
| | 600 | 13.502 | 15.456 | 13.401 | 15.590 | 0.76 | -0.86 |
| | 1000 | 18.848 | 30.725 | 18.775 | 30.641 | 0.39 | 0.27 |
| 36.25 | 300 | 4.242 | 7.135 | 4.235 | 7.155 | 0.18 | -0.28 |
| | 600 | 8.264 | 30.658 | 8.265 | 30.630 | -0.02 | 0.09 |
| | 1000 | 12.712 | 55.275 | 12.731 | 55.284 | -0.15 | -0.02 |

# Doppler broadening overview

- Pre-prepared cross sections (NJOY).
- Interpolation between temperatures.
- Computation of integral (SIGMA-1, Gauss-Legendre quadrature, Fourrier transform, Gauss-Hermite quadrature).
- On-the-fly (OTF) methods - regression method (MCNP), multipole representation (OpenMC), rejection sampling (Serpent).

$$\sigma_T(v) = \frac{1}{v} \int v_r \sigma_0(v_r) P(\mathbf{V}, T) d\mathbf{V}$$

# Cross section Doppler broadening in Geant4

**while** $\left(\left|\overline{\sigma_T^{\mathrm{old}}(v)} - \overline{\sigma_T^{\mathrm{new}}(v)}\right| > criterion \cdot \overline{\sigma_T^{\mathrm{old}}(v)}\right)\{$

$\overline{\sigma_T^{\mathrm{old}}(v)} = \overline{\sigma_T^{\mathrm{new}}(v)}$

**while** $(counter < size)\{$

sample $\mathbf{V}$ from Maxwell–Boltzmann distribution

get $\sigma(v_r)$

$\sigma_T^{\mathrm{new}} \mathrel{+}= \sigma(v_r) \cdot \frac{|\mathbf{V}-\mathbf{v}|}{v}$

$counter++$

$\}$

$\overline{\sigma_T^{\mathrm{new}}(v)} = \frac{\sigma_T^{\mathrm{new}}}{counter}$

$size \mathrel{+}= size$

$\}$

**return** $\overline{\sigma_T^{\mathrm{new}}(v)}$

# Doppler broadening modification

Figure: Relative difference of the probability of elastic scattering from TRIPOLI-4®, its relative variance and the computation time of Doppler broadening for different convergence criteria and minimum number of loops.

| convergence criterion | minimum of loops | relative difference from TRIPOLI-4® | relative variance | computation time (s) |
|---|---|---|---|---|
| 0.03 | 0 | -12.35% | 18.03% | 0.004 |
| 0.01 | 0 | 1.87% | 3.11% | 0.077 |
| 0.005 | 0 | 1.75% | 3.39% | 0.293 |
| 0.001 | 0 | -0.44% | 1.10% | 7.65 |
| 0.0005 | 0 | -0.47% | 1.11% | 31.28 |
| 0.0005 | $1 \cdot 10^6$ | -0.20% | 0.29% | 44.0 |
| 0.0005 | $5 \cdot 10^6$ | -0.26% | 0.25% | 41.8 |
| 0.0001 | 0 | -0.29% | 0.16% | 266 |
| 0.0001 | $5 \cdot 10^6$ | -0.25% | 0.04% | 272 |

# Preliminary: detailed study of DB

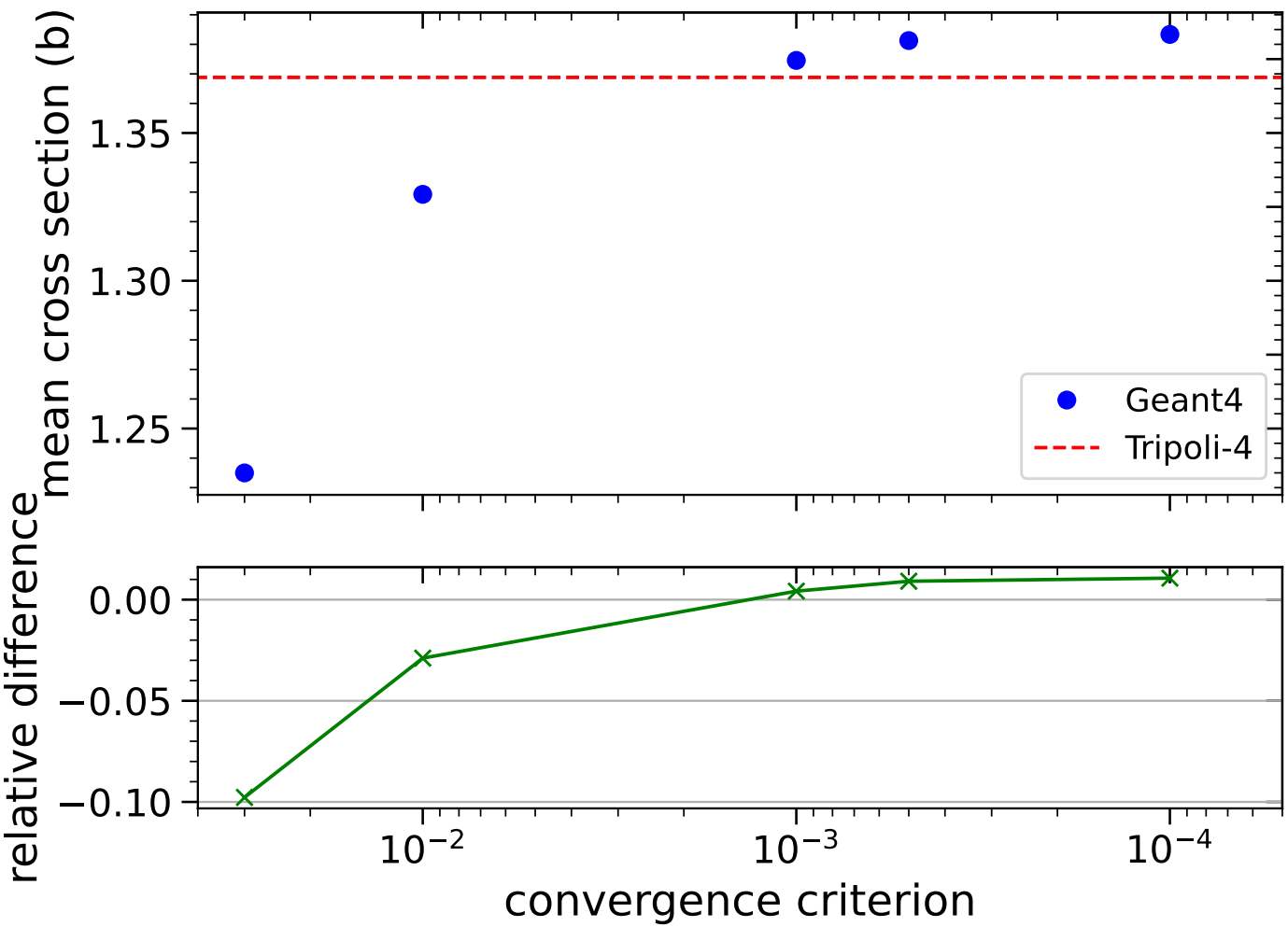



Figure: Elastic cross section of Uranium 238 and its relative difference from cross section in Tripoli-4 for different convergence criteria.

# Preliminary: detailed study of DB

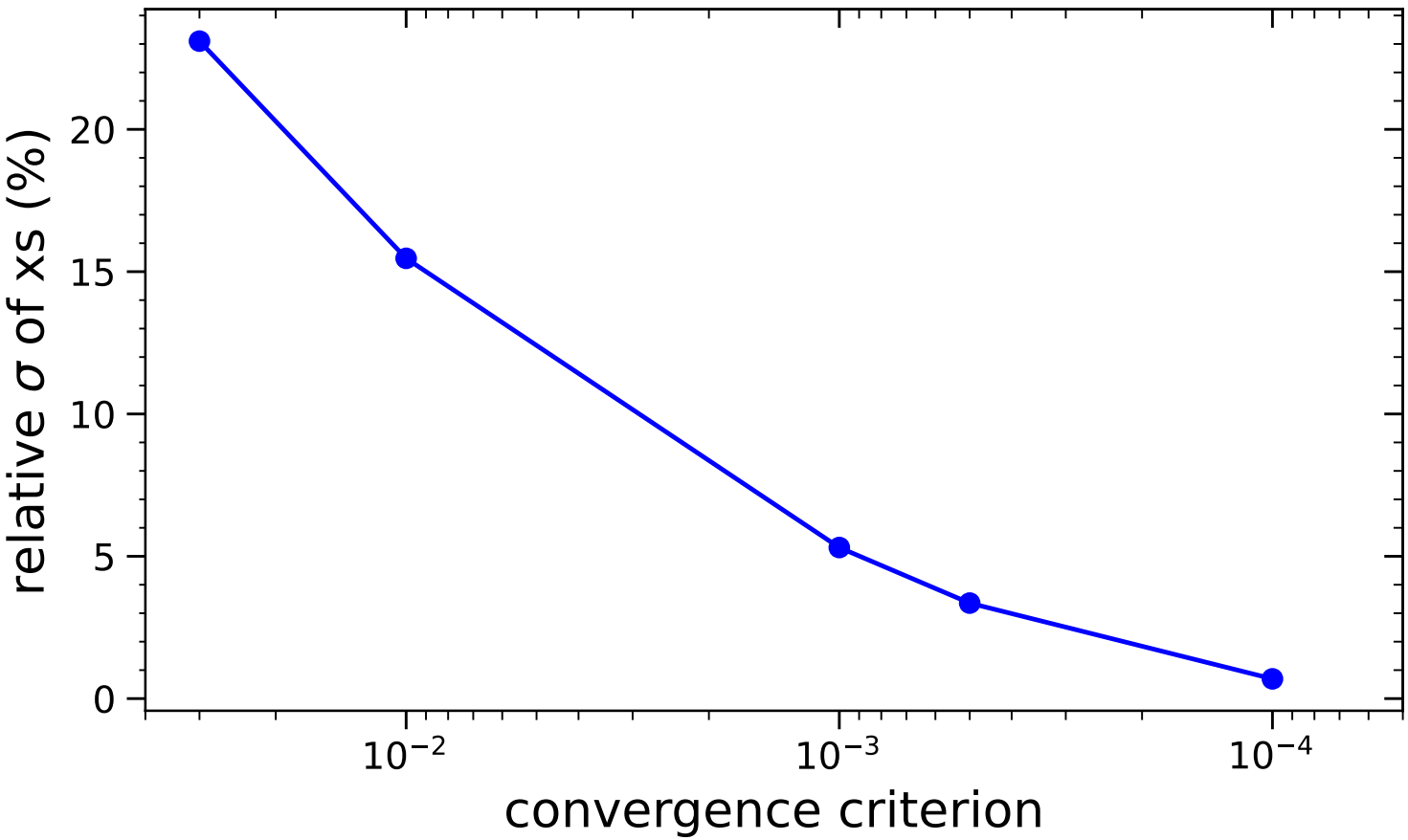



Figure: Relative standard deviation of the elastic cross section of Uranium 238 for different convergence criteria.

# Preliminary: detailed study of DB

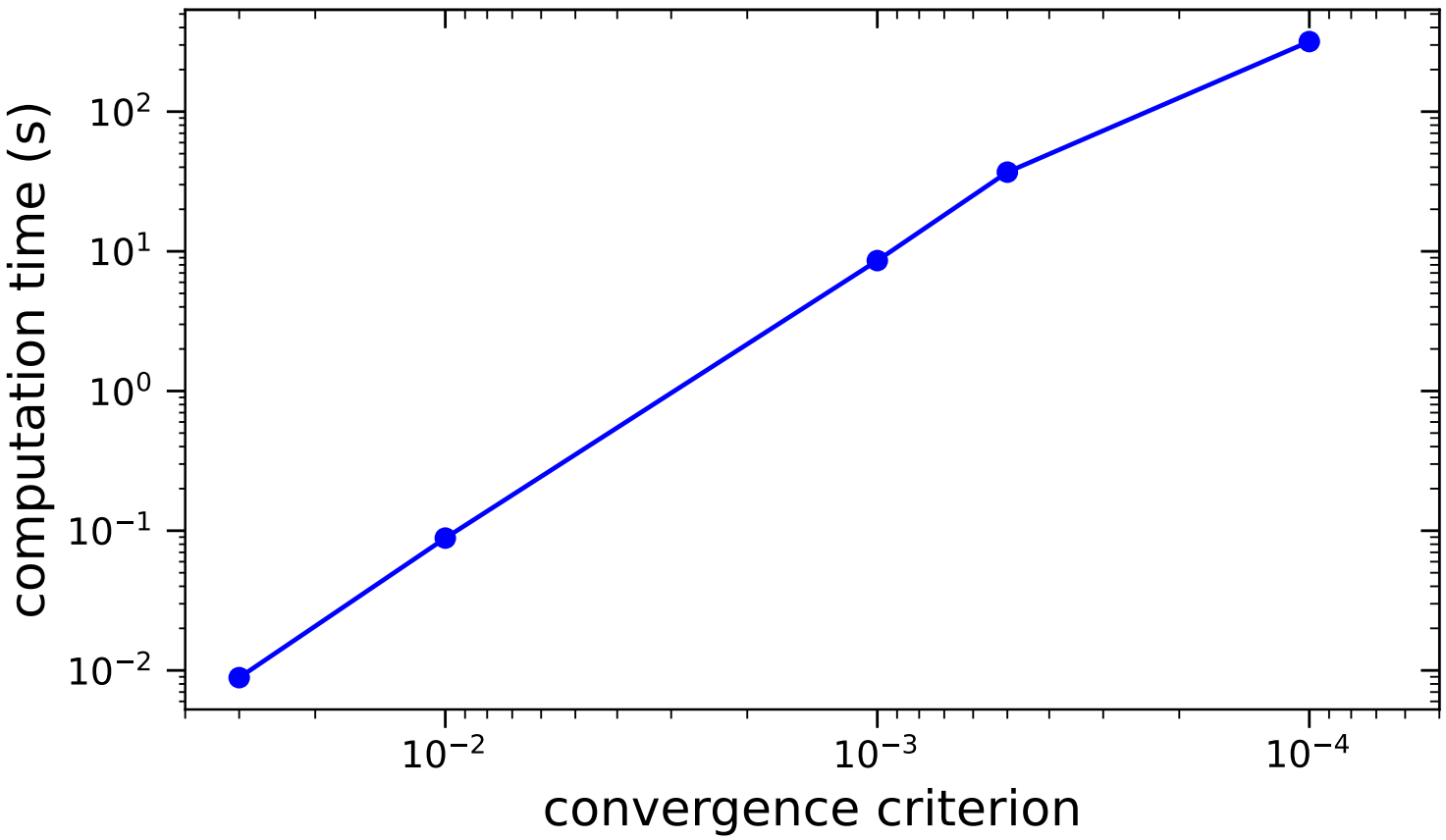



Figure: Time consumption for different convergence criteria.

# Preliminary: detailed study of DB

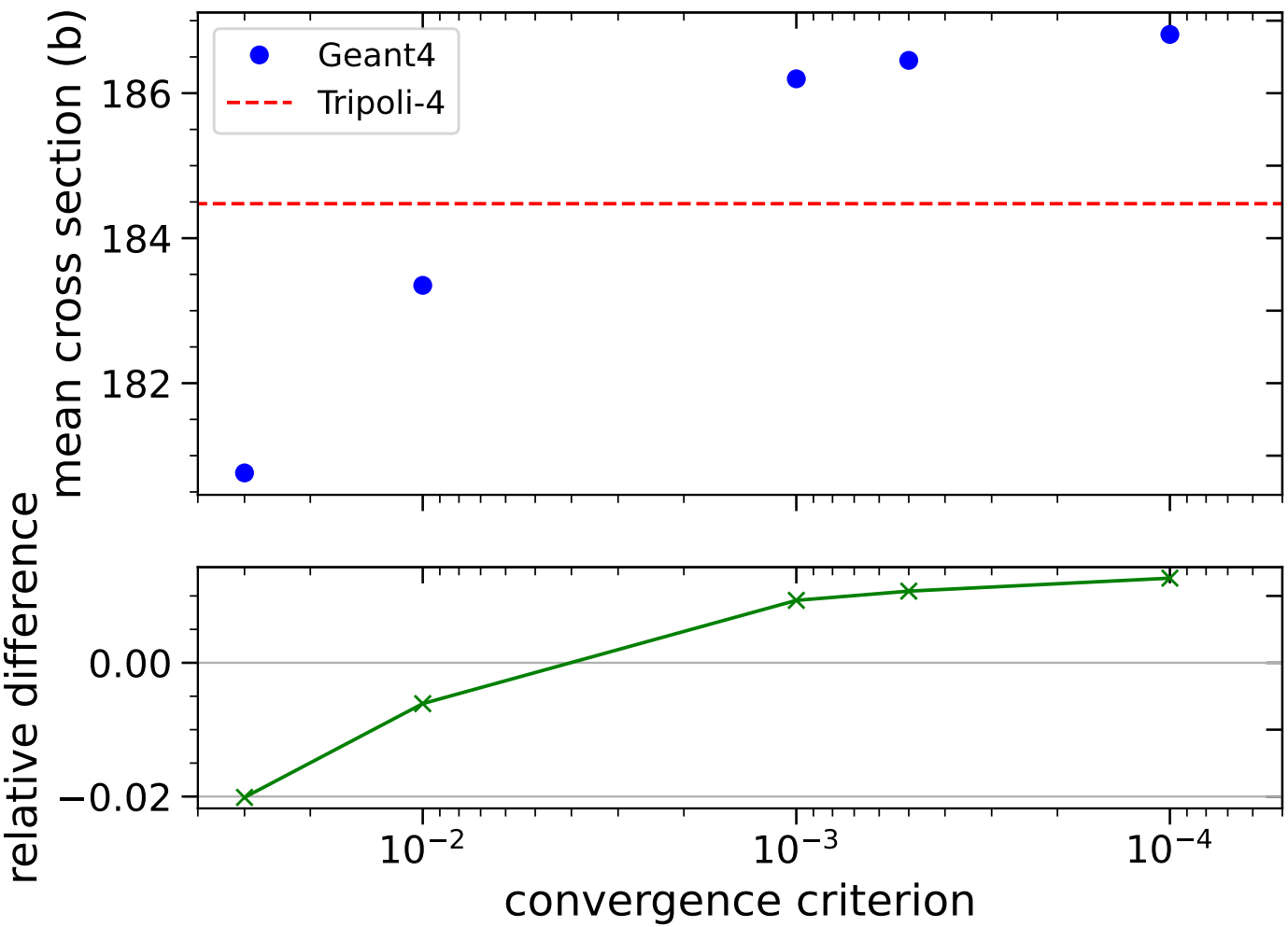



Figure: Capture cross section of Uranium 238 and its relative difference from cross section in Tripoli-4 for different convergence criteria.

# Preliminary: detailed study of DB

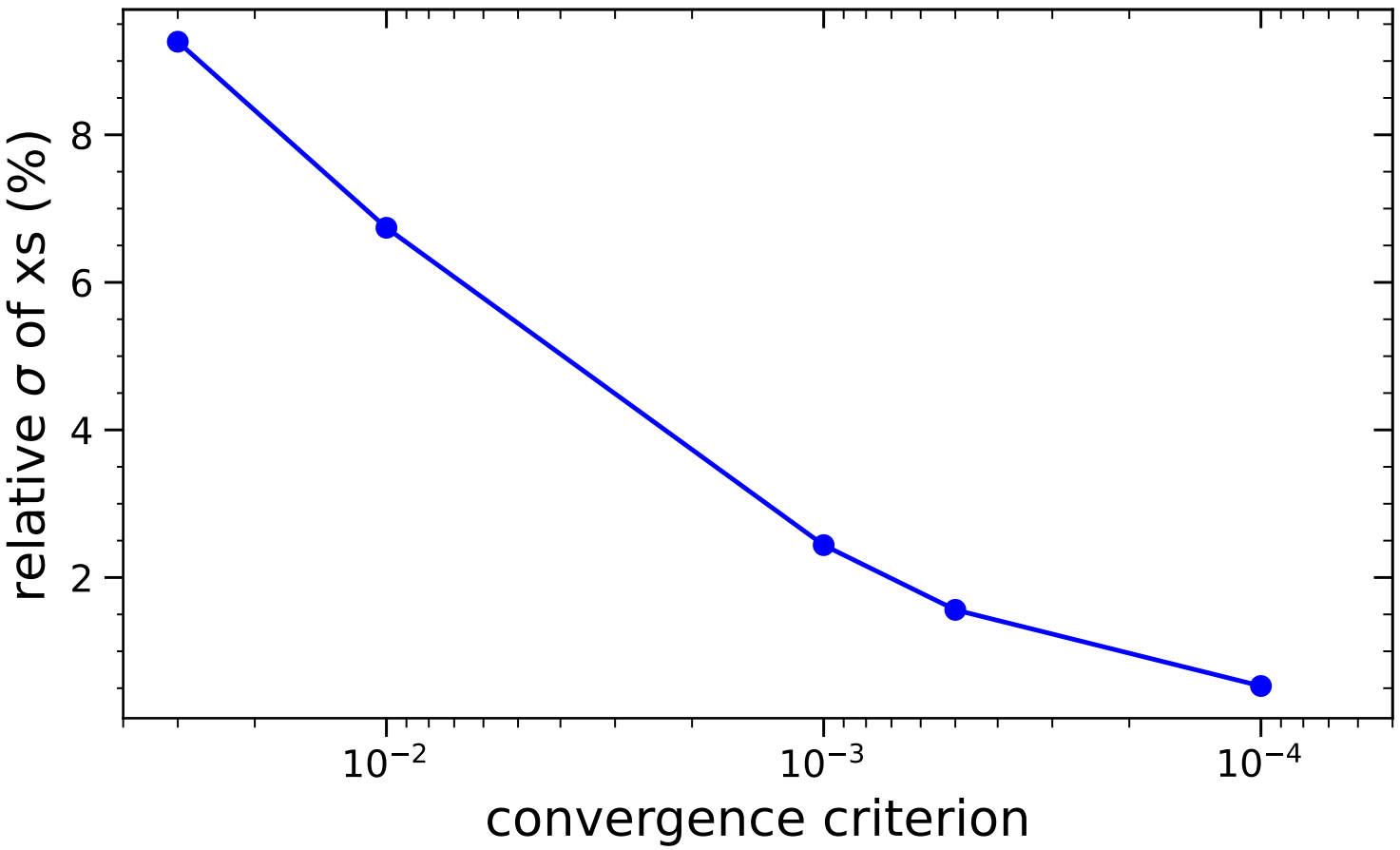



Figure: Relative standard deviation of the capture cross section of Uranium 238 for different convergence criteria.

# Conclusion

- DBRC method was successfully implemented and validated in Geant4.
- New commands in G4ParticleHPMessenger to set this method.
- Are the new flags welcomed, sufficient? Add a flag for convergence criterion in Doppler broadening of cross sections?
- A paper regarding this method will be sent to NIMA (end of January, mid-February).
- Possible revision of simplified Doppler broadening.
- On-going work on implementation of probability tables in the unresolved resonance region.

# End

Thank you for your attention!