# DETAILED CHARGE EXCHANGE NEUTRAL DISTRIBUTION MODELLING FOR THE ITER MAIN WALL

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# Rationale

- ERO2.0 requires detailed distribution of neutral particles impinging specfic „diagnostic“ surfaces, i.e. mirrors
  (c.f. today‘s talk S. Rode, IO-Contract: IO/20/CT/4300002242)

- EIRENE post-processing of S. Lisgos „repository“ of SOLPS4.3 simulations with DivIMP extension of grids up to FW

- Set of simulations based on A. Khan NME 2019 WallDYN paper

- Some modifications  in EIRENE to also have both energy and angular distributions

- Python tools for plotting & (statistical) data analysis after re-processing with EIRENE



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# Various extrapolation models for the far-SOL

**d** L-mode pedestal, low density far-SOL ($v_\perp$ = 35 m/s), low temperature far-SOL ($T_e$ = 10 eV, Ti = 20 eV)

**o** H-mode pedestal, high density far-SOL ($v_\perp$ = 100 m/s), high temperature far-SOL ($T_e$ = 20 eV, $T_i$ = 40 eV)

**g** H-mode, $v_\perp$ = 35 m/s, $T_e$ = 20, $T_i$ = 40 eV

**m** H-mode, $v_\perp$ = 100 m/s, $T_e$ = 10, $T_i$ = 20 eV

**00** no near sol flow

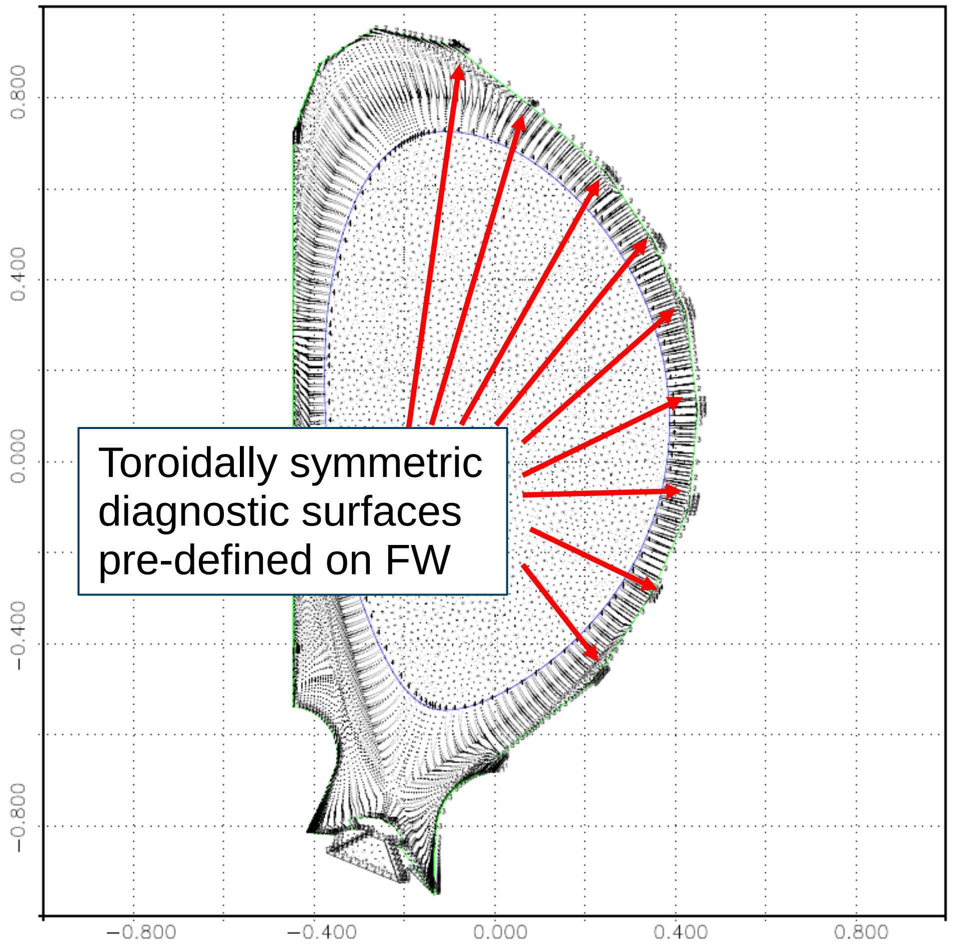
**01** near sol flow 0.5M

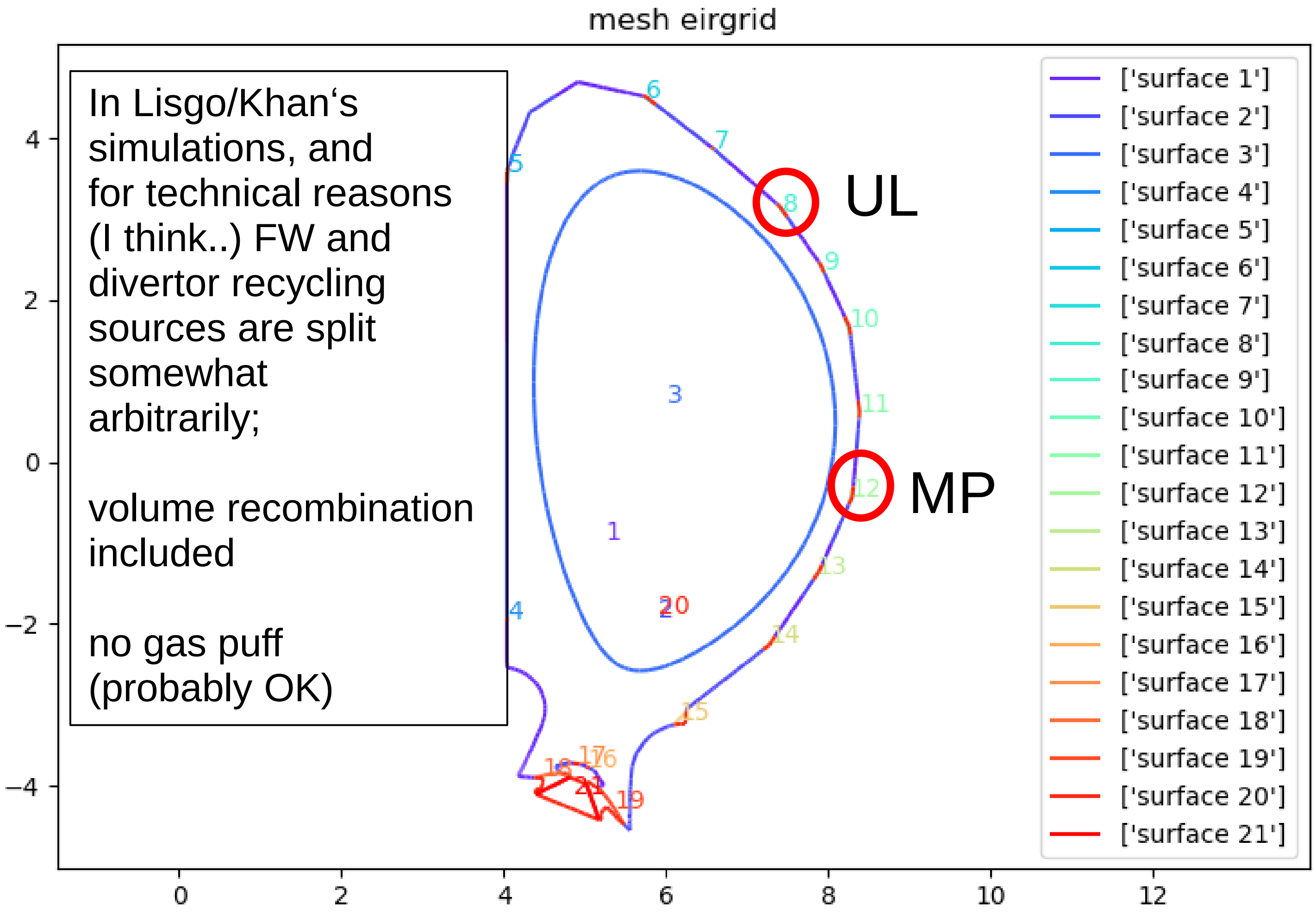
| Name<br>– | Main SOL $M_{\|\|}$<br>– | Far-SOL $v_\perp$<br>$m\ s^{-1}$ | Far-SOL $T_e$<br>$eV$ | Far-Sol $T_i$<br>$eV$ |
|---|---|---|---|---|
| 00$d$ | 0 | 30 | 10 | 20 |
| 00g | 0 | 30 | 20 | 40 |
| 00$k$ | 0 | 65 | 20 | 40 |
| 00$m$ | 0 | 100 | 10 | 20 |
| 01$d$ | 0.5 | 30 | 10 | 20 |
| 01$g$ | 0.5 | 30 | 20 | 40 |
| 01$k$ | 0.5 | 65 | 20 | 40 |
| 01$m$ | 0.5 | 100 | 10 | 20 |

Concentrate on case series 2258_00*

→ **Semi-detached, high-power H-mode case**

# Collector surfaces (EIRENE tallies) for extended 2258 SOLPS4.3 geometry



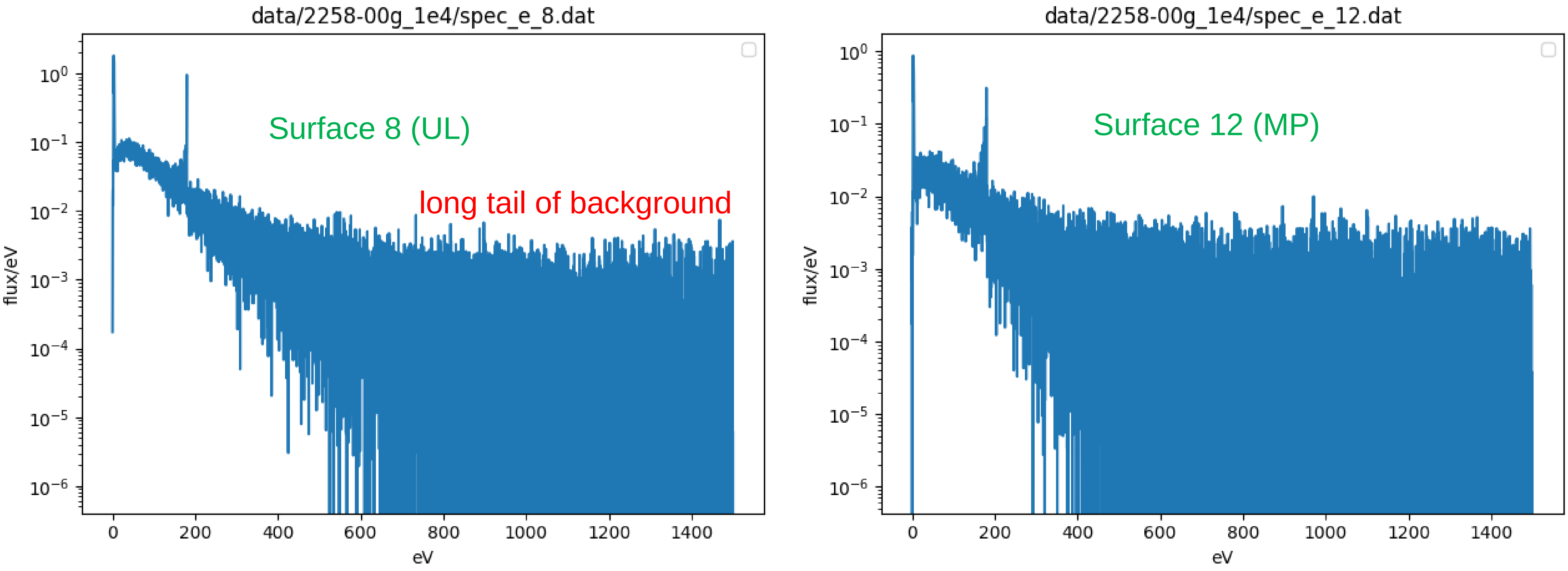




In Lisgo/Khan's simulations, and for technical reasons (I think..) FW and divertor recycling sources are split somewhat arbitrarily;

volume recombination included

no gas puff (probably OK)

# 2258_00g $D^0$ energy spectra




normalised „EIRENE-units“ Amp/eV



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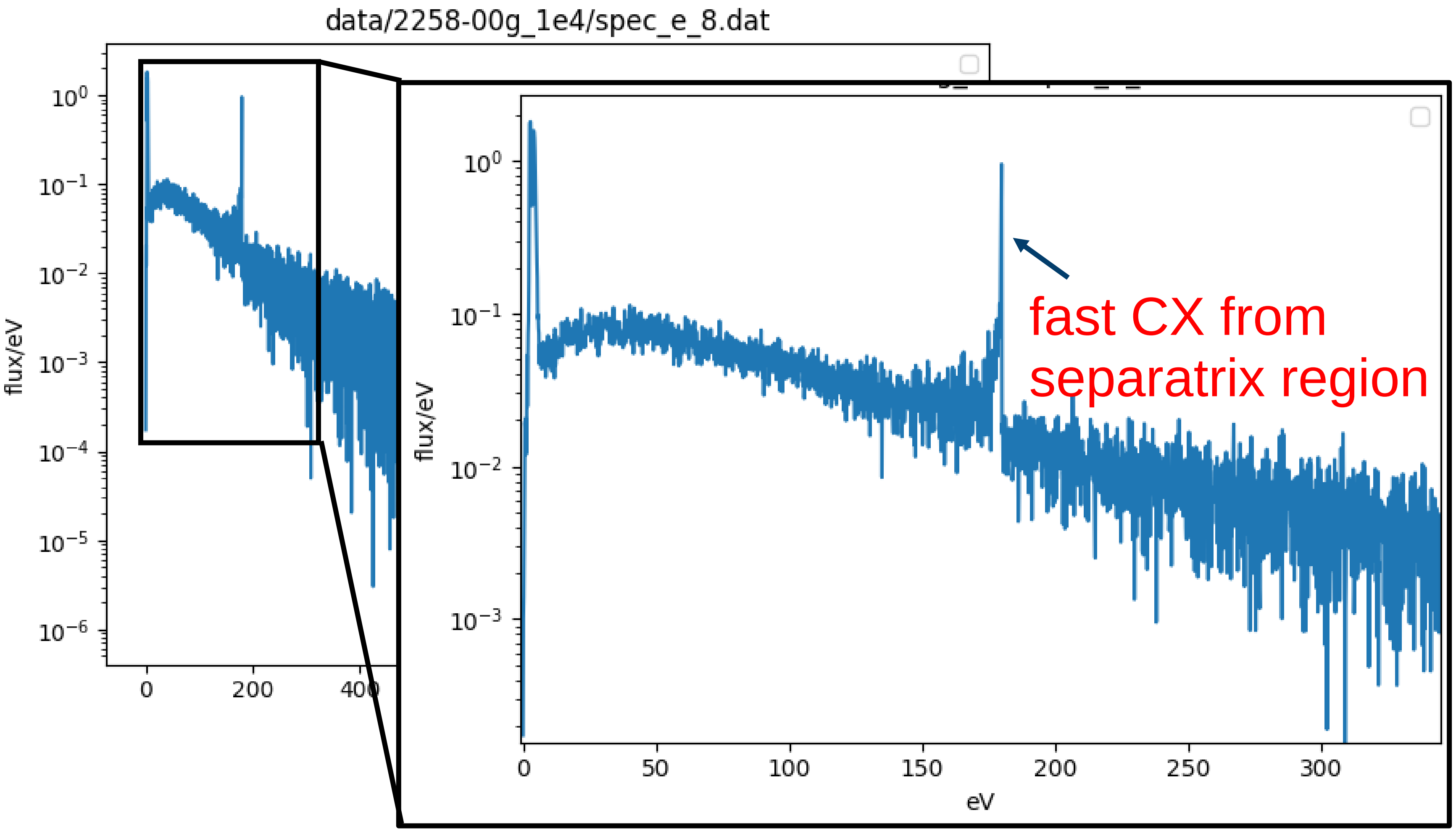
# 2258_00g $D^0$ energy spectra




normalised „EIRENE-units" Amp/eV



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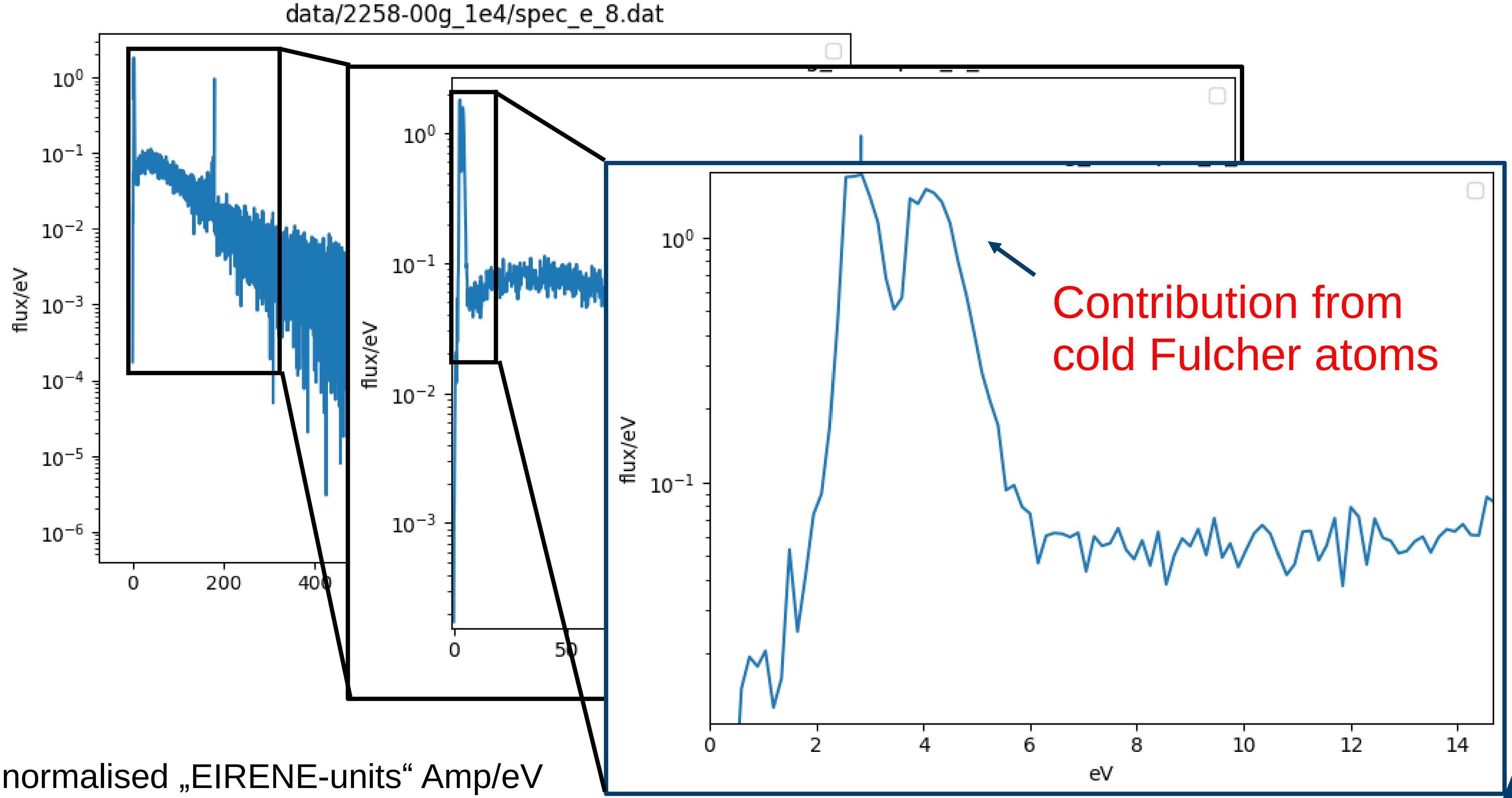
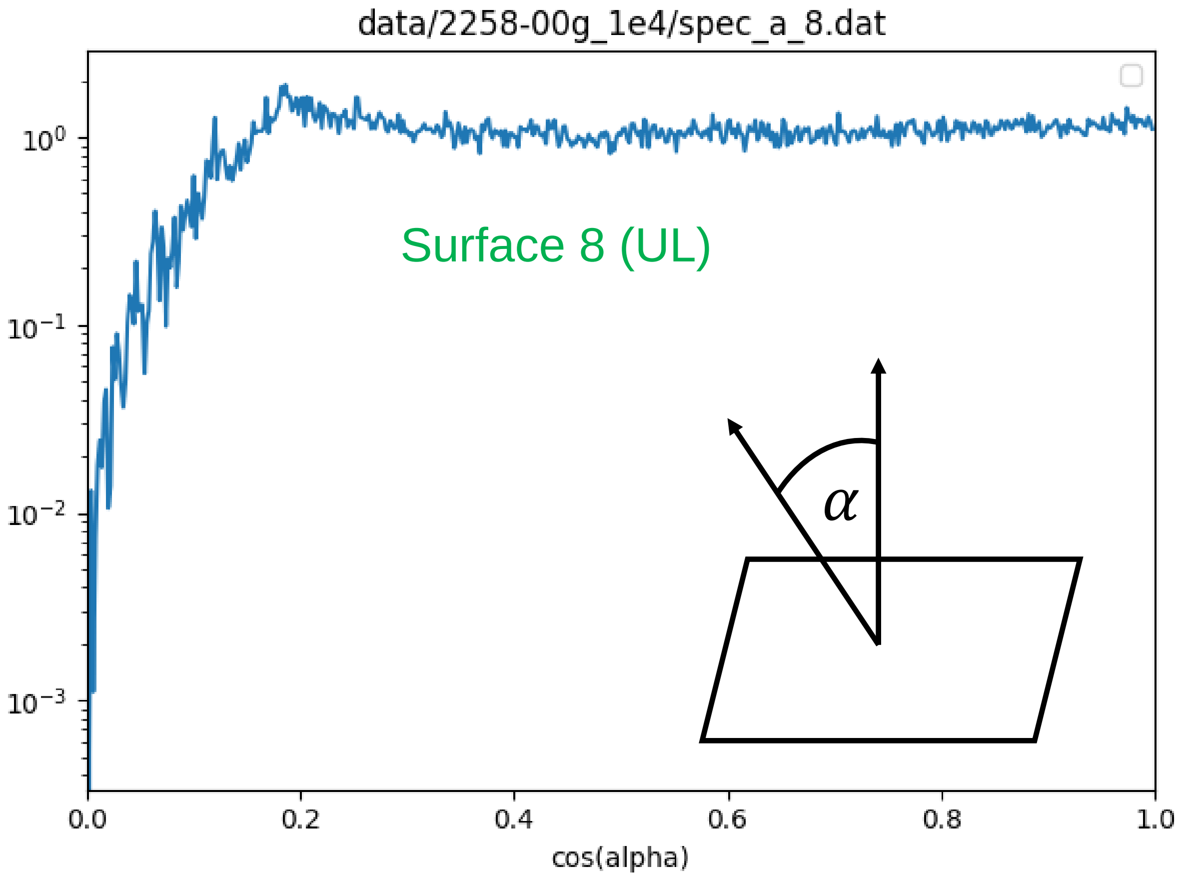
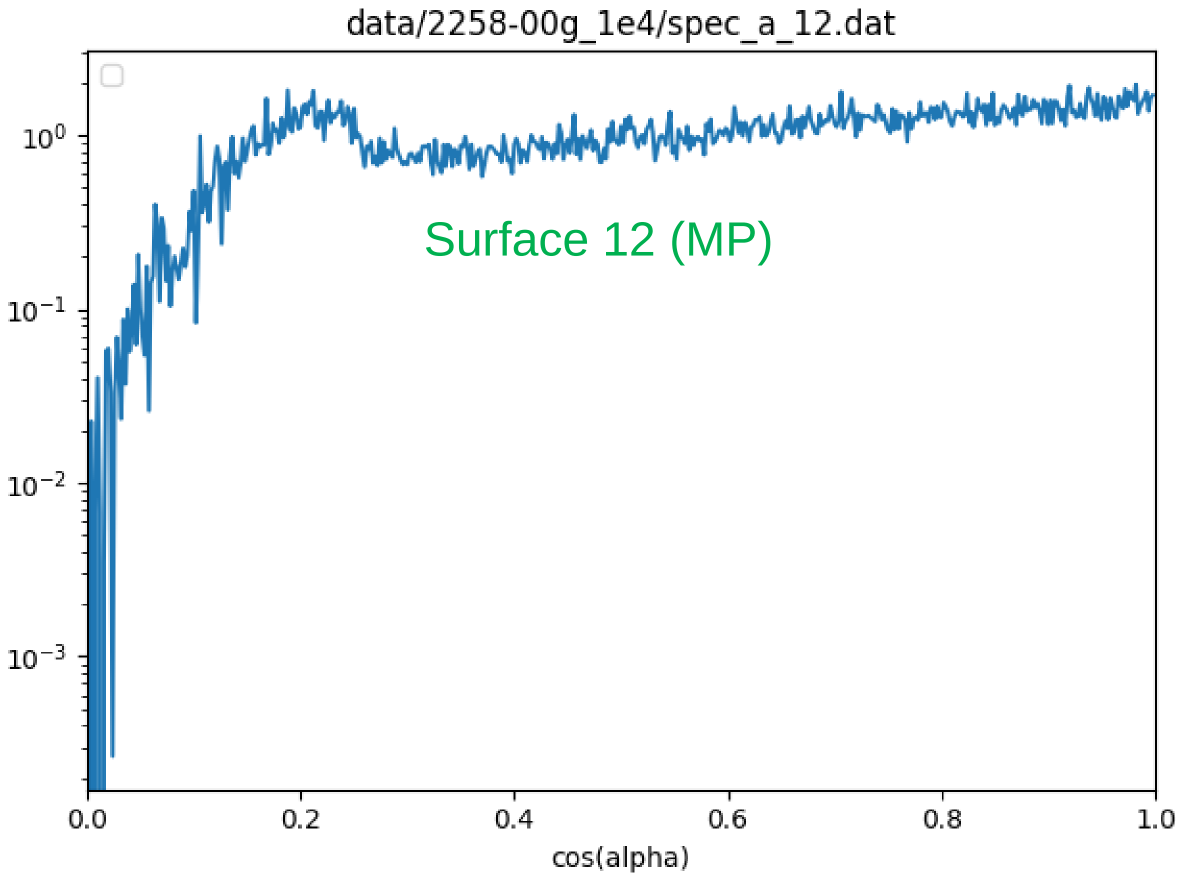
# 2258_00g $D^0$ energy spectra




normalised „EIRENE-units“ Amp/eV

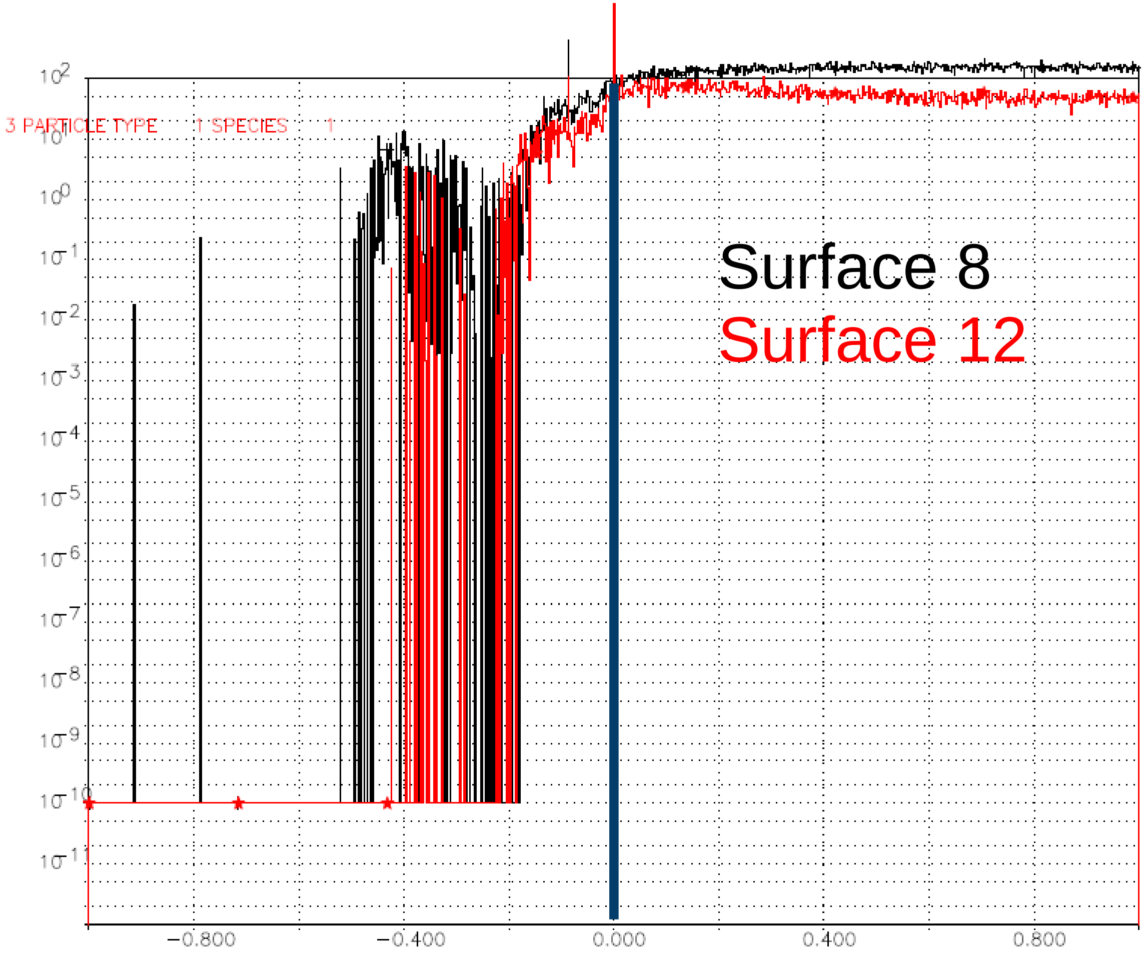
# 2258_00g $D^0$ angular distribution (polar angle only, 2D-sym)

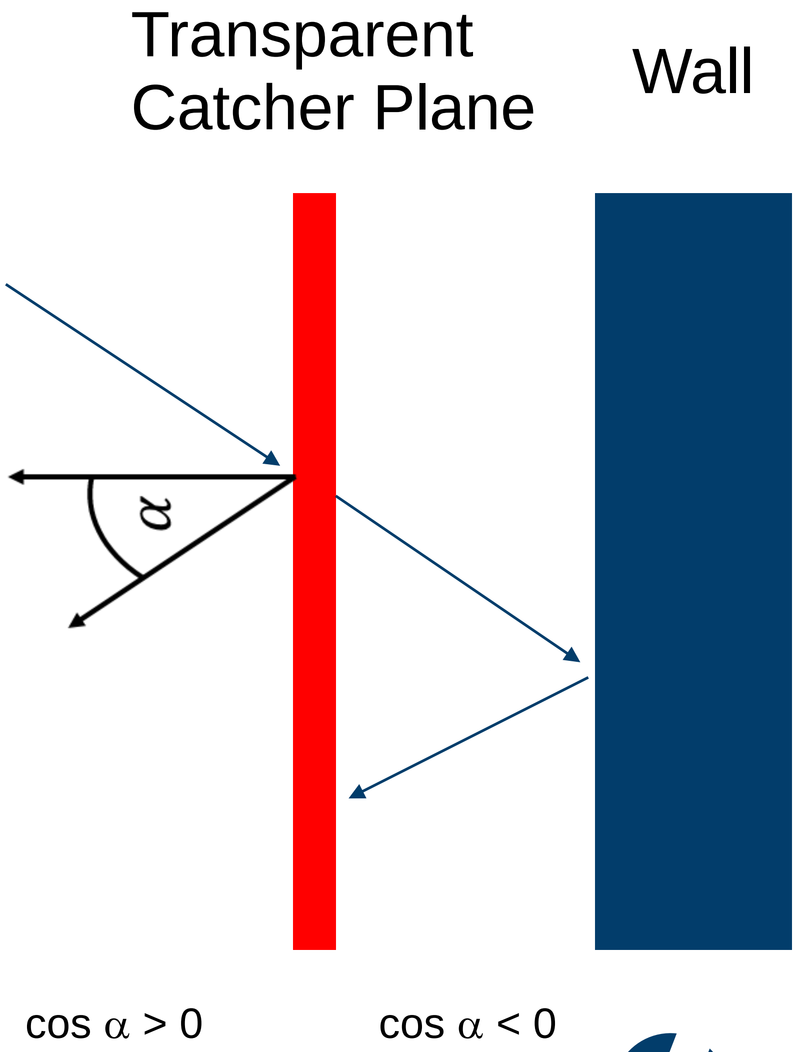



$f(\cos\alpha)$ normalised to 1

# Expert‘s advice: don‘t tally wrong..



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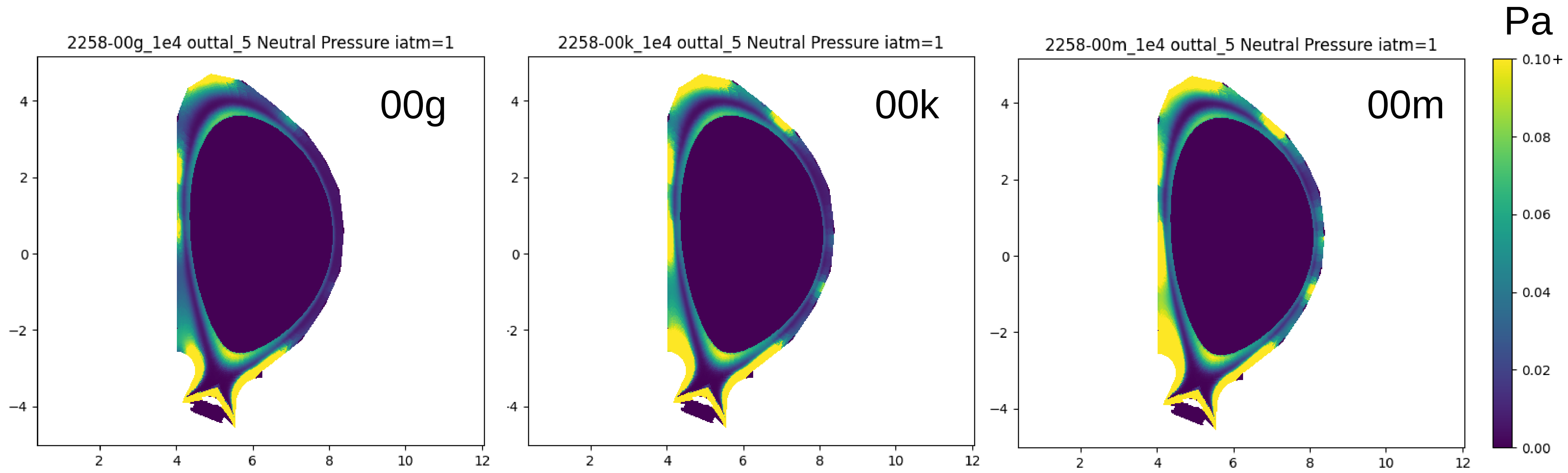
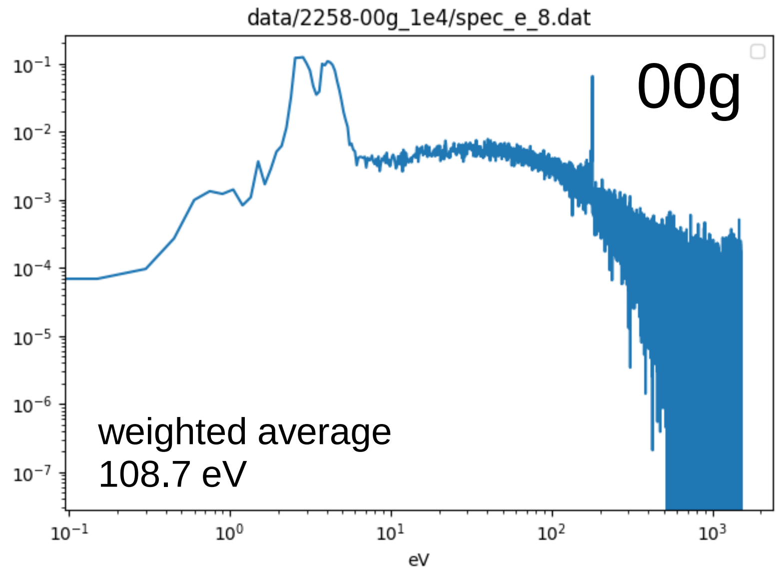
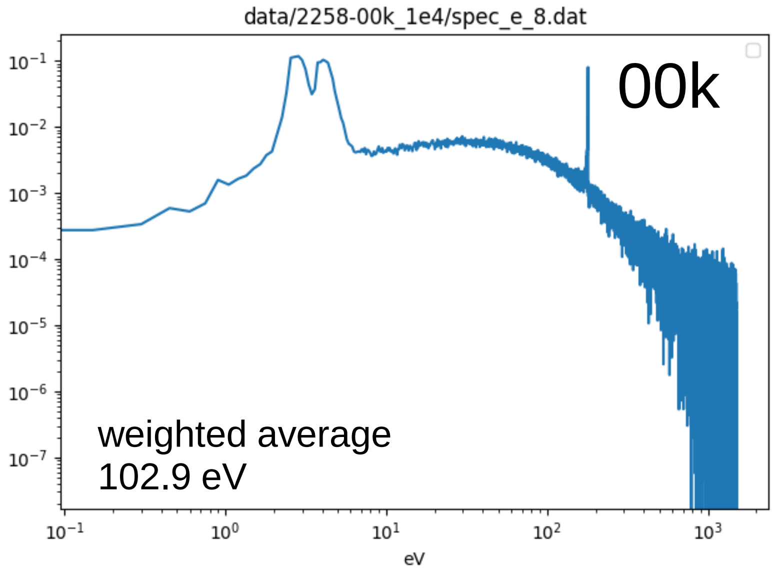
# Comparison of far-SOL assumptions: $D^0$ neutral pressure

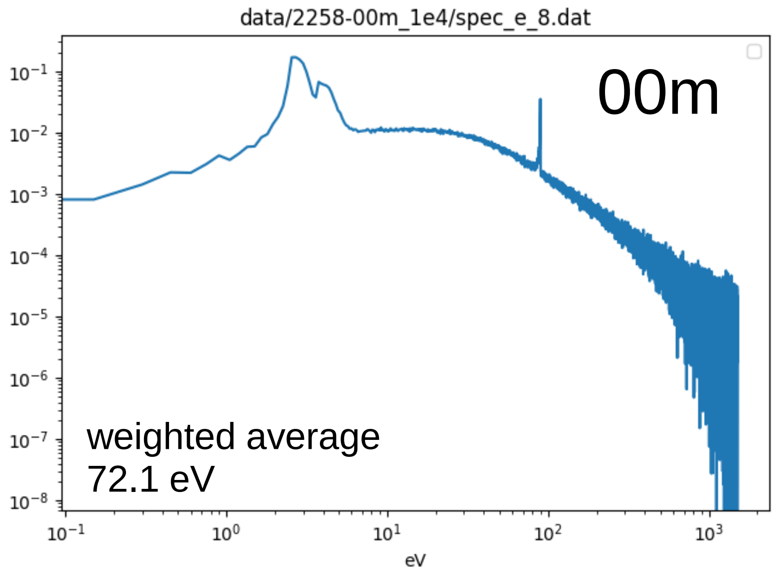


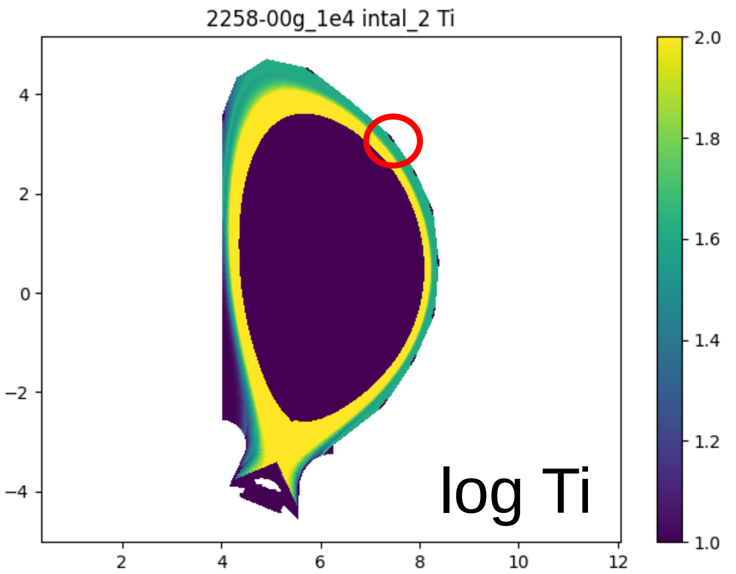

| Name<br>— | Main SOL $M_{\|\|}$<br>— | Far-SOL $v_\perp$<br>$m\ s^{-1}$ | Far-SOL $T_e$<br>$eV$ | Far-Sol $T_i$<br>$eV$ |
|---|---|---|---|---|
| 00g | 0 | 30 | 20 | 40 |
| $00k$ | 0 | 65 | 20 | 40 |
| $00m$ | 0 | 100 | 10 | 20 |

# Comparison far-SOL assumptions: $D^0$ spectra log-log (UL)



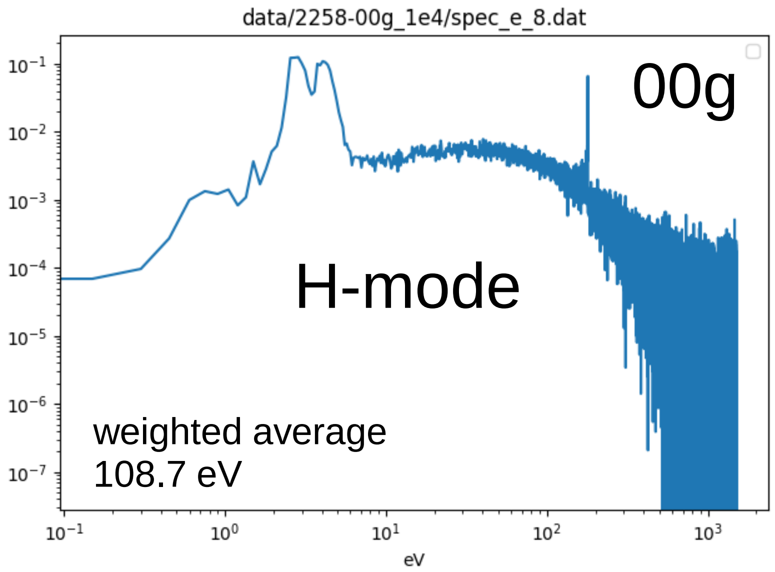



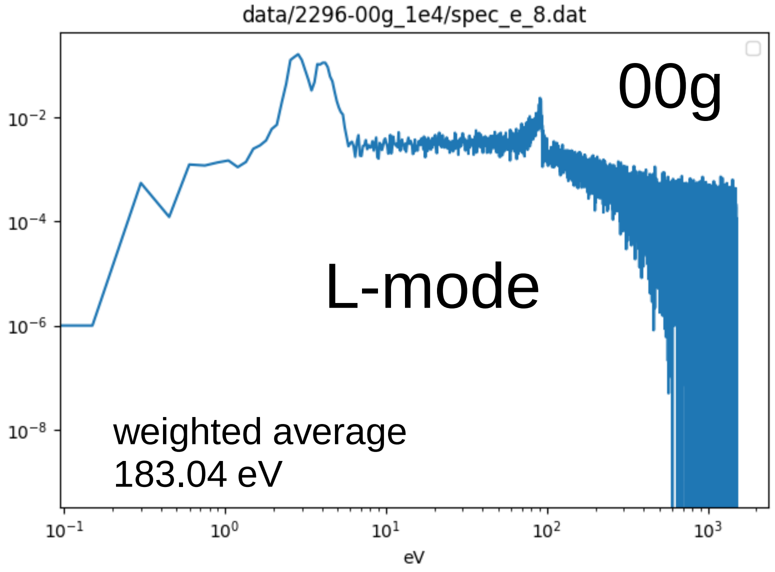




| Name | Main SOL $M_{\parallel}$ | Far-SOL $v_{\perp}$ | Far-SOL $T_e$ | Far-Sol $T_i$ |
|---|---|---|---|---|
| — | — | $m\,s^{-1}$ | $eV$ | $eV$ |
| 00g | 0 | 30 | 20 | 40 |
| 00$k$ | 0 | 65 | 20 | 40 |
| 00$m$ | 0 | 100 | 10 | 20 |

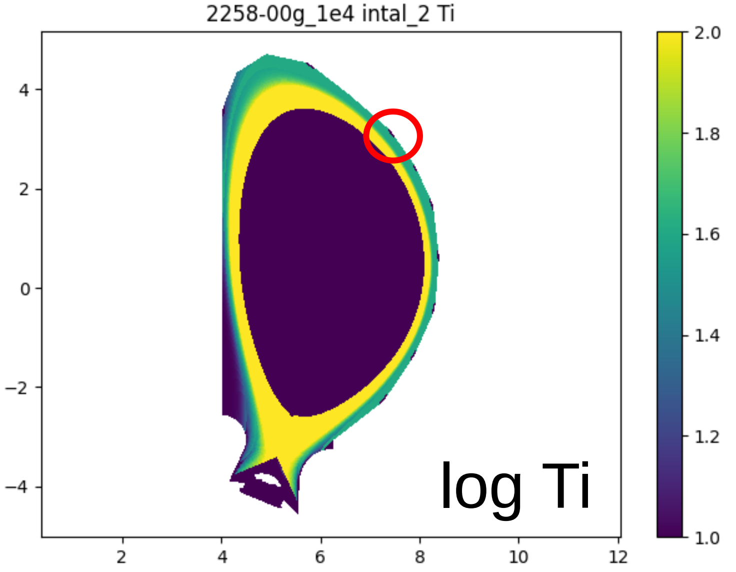
- **The "spx region peak" (CX) shifts and weighted average <E> depend on far-SOL Ti-conditions**

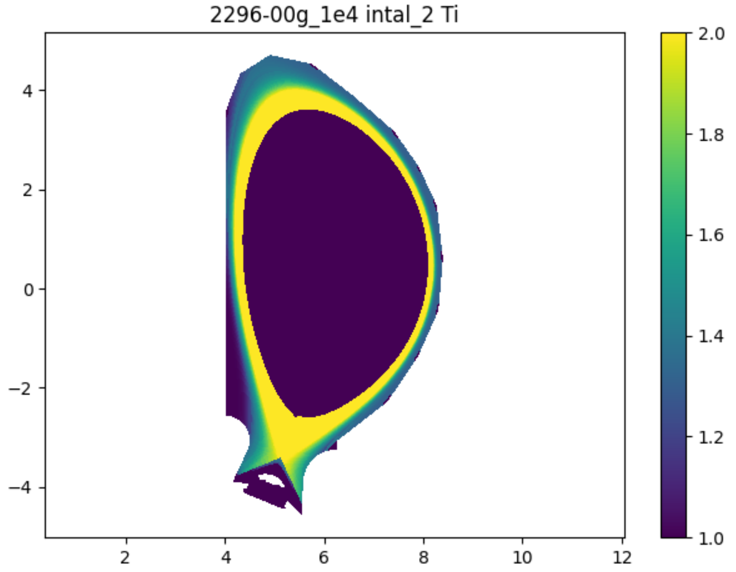
# Comparison H-mode vs L-mode (00g)




- **In L-mode the strong peak is less prominent**
- **However the average energy <E> is significantly higher than in H-mode (tail contribution)**

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# Revised H-mode (L-mode) yield estimates (00g, UL)

| | D on Be | D on W | Ne on W (*) |
|---|---|---|---|
| $Y(\langle E\rangle, \cos\alpha \equiv 1)$ | 0.025 (0.029) | 0.0 | 0.00035 |
| $\langle Y(E, \cos\alpha \equiv 1)\rangle$ | 0.015 (0.016) | 0.0003 (0.0010) | 0.00038 |
| $\langle Y(E, \cos\alpha)\rangle$ | 0.031 (0.035) | 0.0007 (0.0024) | 0.00080 |

(*) wrongly (!) assuming same spectra for Ne as for D,
and $\Gamma_{Ne0}$ = 1% $\Gamma_{D0}$
→ Need real MC calculations for Ne!

$$\langle Y(E, \cos\alpha)\rangle = \iint Y_{phys,93}^{EIRENE}(E, \cos\alpha)\, f(E, \cos\alpha)\, dE\, d\cos\alpha$$

Here: $f(E, \cos\alpha) = g(E) \cdot h(\cos\alpha)$

**Roth, Bohdansky, Eckstein (SPUTER93):**

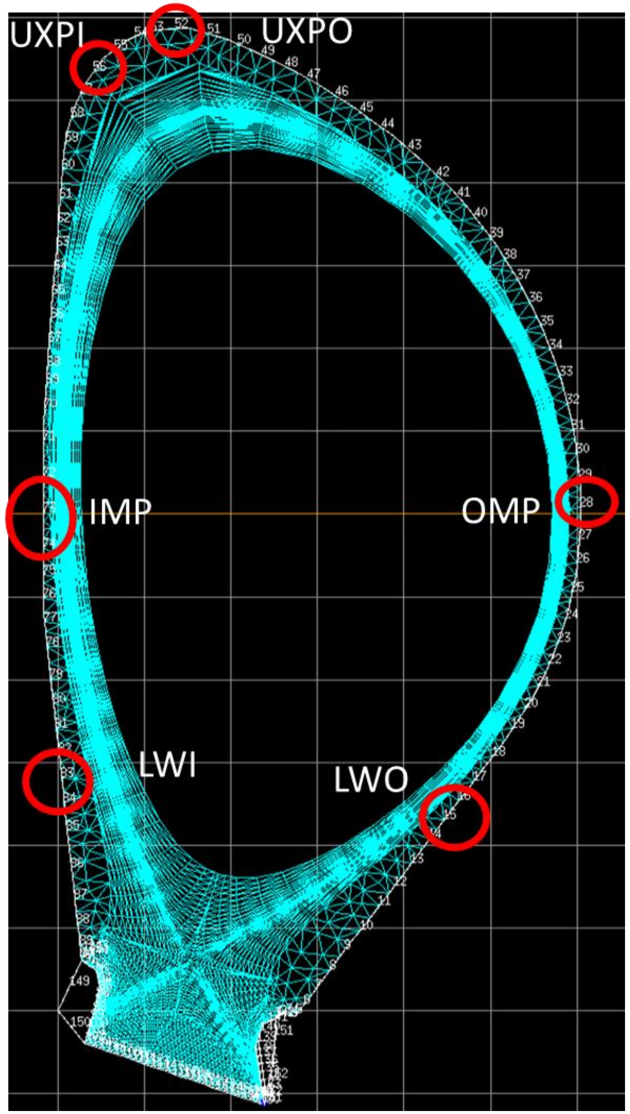
$$Y_{phys,93} = Q_p \left(1 - a^{2/3}\right)(1-a)^2 \frac{\frac{1}{2}\ln(1 + 1.2288b)}{b + 0.1728\sqrt{b} + 0.008b^{0.1504}}$$

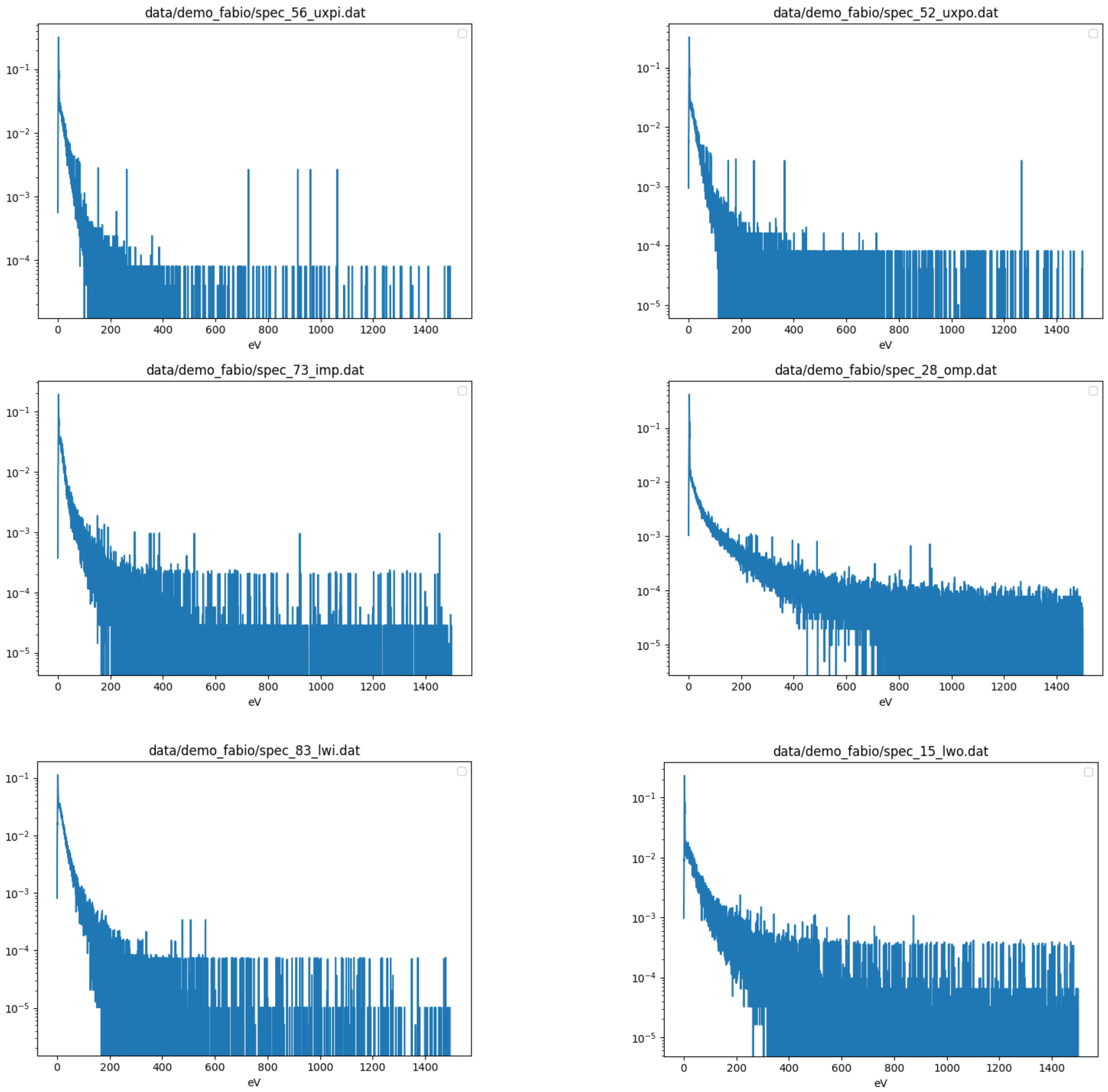
$$a = \frac{E_{th}}{E}, \mathrm{b} = \frac{E}{E_{tf}}, Q_p = const$$

$$Y_{phys,93}^{EIRENE} = Y_{phys,93} \cdot (\cos\theta)^{-f} \exp\left(fc - \frac{fc}{\cos\theta}\right)$$

Yamamura-fit: $f = 2, c = 0.26$

# EU-DEMO


UXPI
UXPO
IMP
OMP
LWI
LWO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data/demo_fabio/spec_73_imp.dat
data/demo_fabio/spec_28_omp.dat
data/demo_fabio/spec_83_lwi.dat
data/demo_fabio/spec_15_lwo.dat
eV

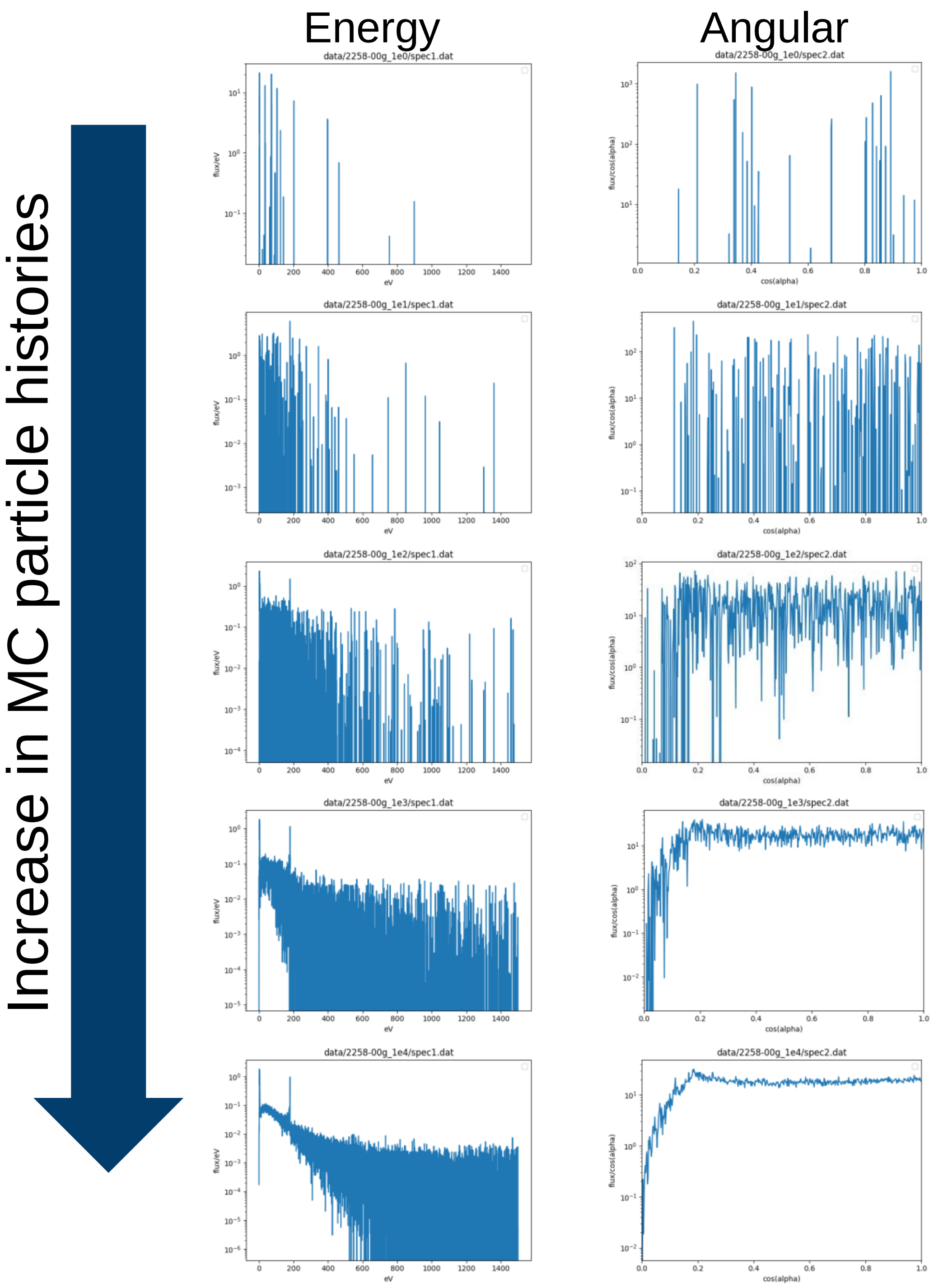
# Comments on spectral statistics

Shannon-Entropy

$$S = -\sum_k f_k \log f_k$$

| MC histories | Wall-clock time (12 CPUs) | $S(g(E))$ | $S(h(\cos\alpha))$ |
|---|---|---|---|
| 1.92e5 | < 1min | 2.409 | 2.409 |
| 1.92e6 | 7 min | 4.097 | 4.143 |
| 1.92e7 | 71 min | 5.926 | 5.792 |
| 1.92e8 | 12.5 hs | 6.819 | 6.087 |
| 1.92e9 | 72 hs | 7.083 | 6.134 |

OK, but Shannon-Entropy mixing invariant!
Need a better figure-of-merit for statistical accuracy



# Towards optimised statistics and data compression

## MaxEnt-regularised approach

**Maximise**

$$\mathcal{L} = S + \sum_{l=1}^{L} \lambda_l \left( \int_{x_0}^{x_1} x^l \rho(x)\, \mathrm{d}x - \mu_l \right).$$

- <u>Requires calculation of higher moments in EIRENE</u>

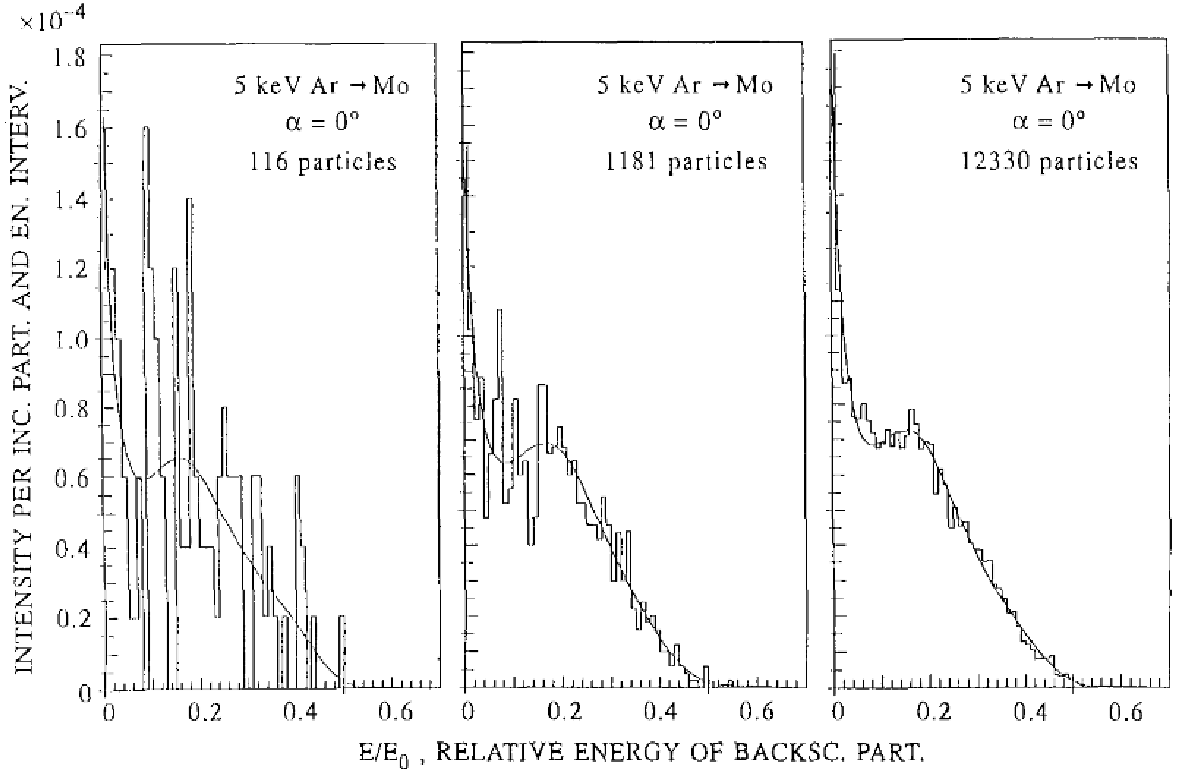
  → mean $l = 1$ & variance $l = 2$ (both done)

  to be implemented $l > 2$:
  → skewness, kurtosis, hyper-skewness, hyper-tailness, … **→ recovers local/mixing structures**

- If statistical fluctuations < evolving structures
  → stop the EIRENE run
  (implementation of a halt during run-time reqd.)

- **Bonus: moment-representation possible for spectra, data-compression rate > 100 possible**

W. Eckstein Nucl. Instr. And Meth. In Phys Res B 95 (1995)
"Efficient tabulation of plasma interaction data" (SDTrimSP)



# Summary / Conclusion

- Neutral particle energy and angular distributions $f(E, \cos\alpha)$ collected on diagnostic surfaces for ITER reference SOLPS-ITER plasmas with manually extended grid up to FW (A. Khan et al)

- **Result: detailed distributions give 2-3 larger D → W sputter yields $\langle Y(E, cos\,\alpha)\rangle$ compared to standard estimates $Y(\langle E\rangle)$, depends on far-SOL assumptions or H/L-mode, $\cos\alpha$-dependence gives a factor 2, H-mode: main contribution from tail of distribution**

- Next Step: Ne → W calculation, and compare relevance to D → W

- SOLPS-ITER with wide-grid option should provide a better picture

- Also: JET post-processing with EIRENE on-going (M. Groth et al), DEMO (Wiesen, Brenzke FZJ)

- So far only uncorrelated energy and angular distributions collected
  → extension to multi-variate distribution functions possible $f = f\big(E, cos(\alpha)\big)$
  → requires longer EIRENE run-times for improved statistics and requires large memory
  → data compression through MaxEnt regularization

- Only polar angles are collected (toroidally symmetric)
  → extension to full 3D possible (e.g. post-processing EMC3 plasma-backgrounds)



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# Backup



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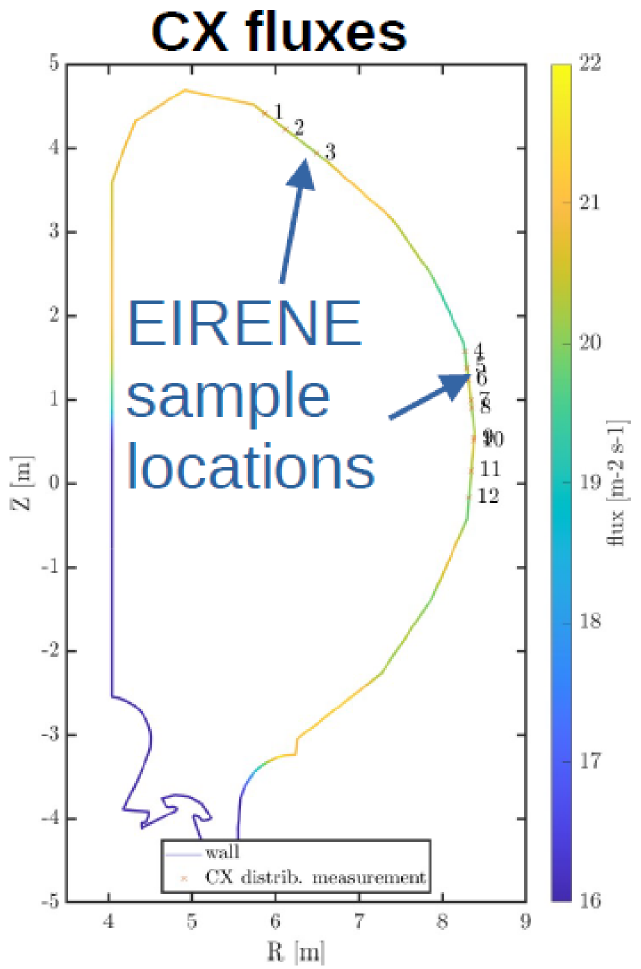
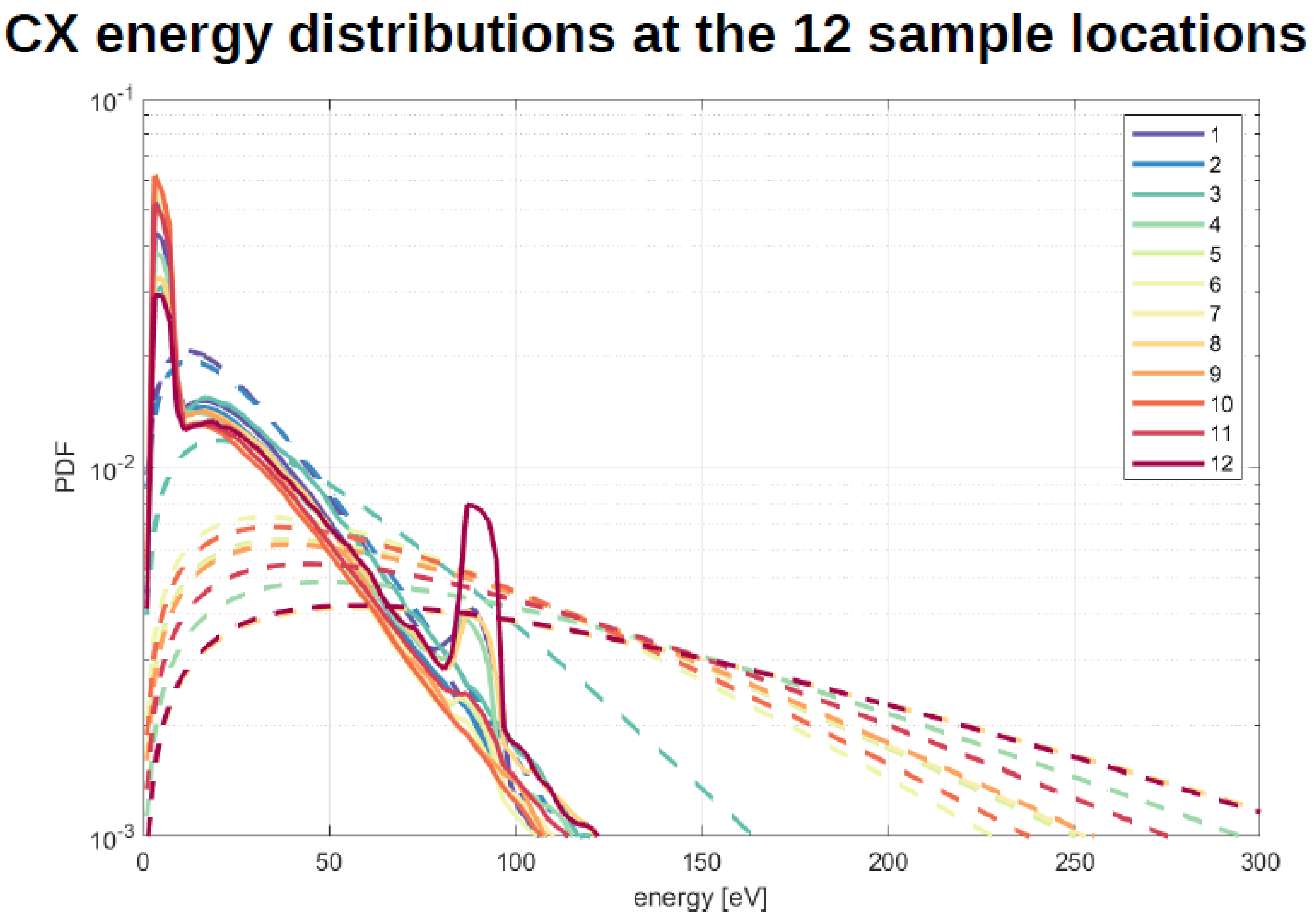
# Example: CX distributions from Steve Lisgo for ITER (case #1514)

- File name “i-cxd-0003-1514-00g.wall_energy_spectra” -> I guess that’s not a standard EIRENE output…?
- Energy distributions at 12 locations, however no angular distributions.



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# Modifications to the EIRENE code for angular distributions

- (Output/outspec)
- (Plotting/eirmod_plteir)
- Modules/eirmod_parmmod
  Modules/eirmod_cestim → introduction of ISPCOPT flag (for angular spectra)
- Scoring/update_spectrum
- Startup_routines/input.f
  Startup_routines/plasma.f
- Assistant/learca2
- Particle_tracing/folneut.f → bugfix in case of transparent srfcs