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 in ITER, i.e. mirrors
  (c.f. THU talk Ch. Baumann, W-erosion in EU-DEMO)

- EIRENE post-processing of S. Lisgo's ITER „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 ITER 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

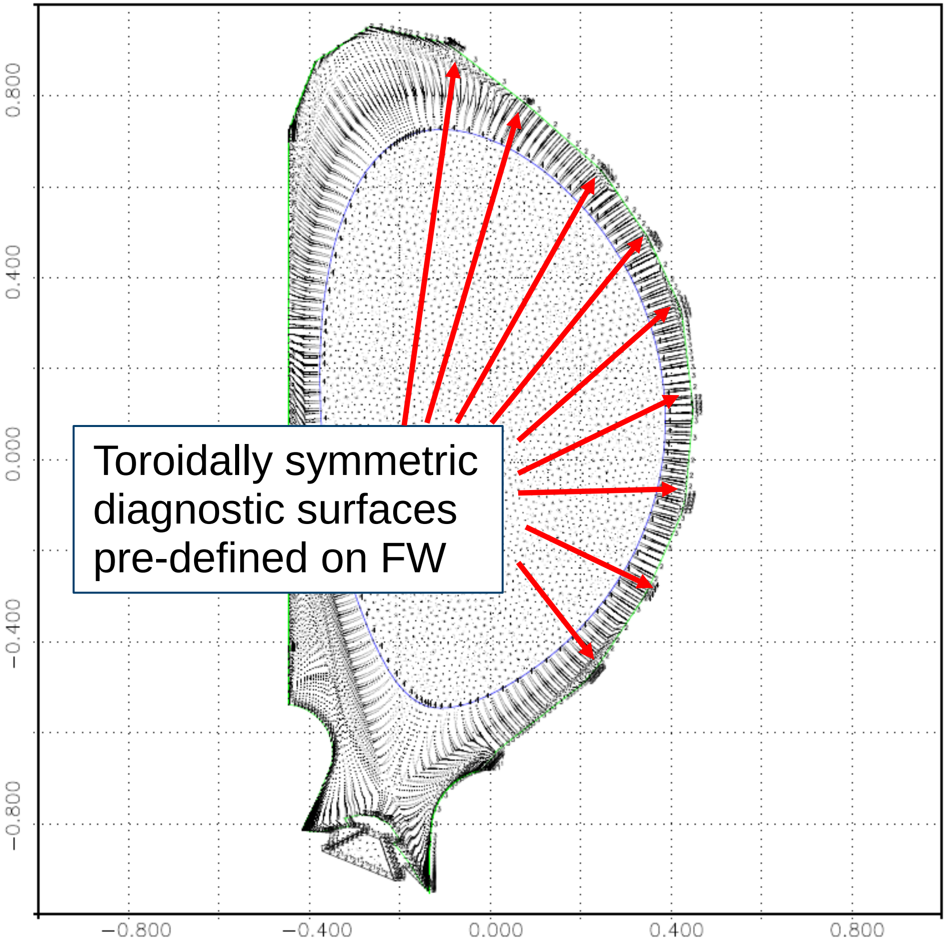
01 near-SOL flow 0.5M

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

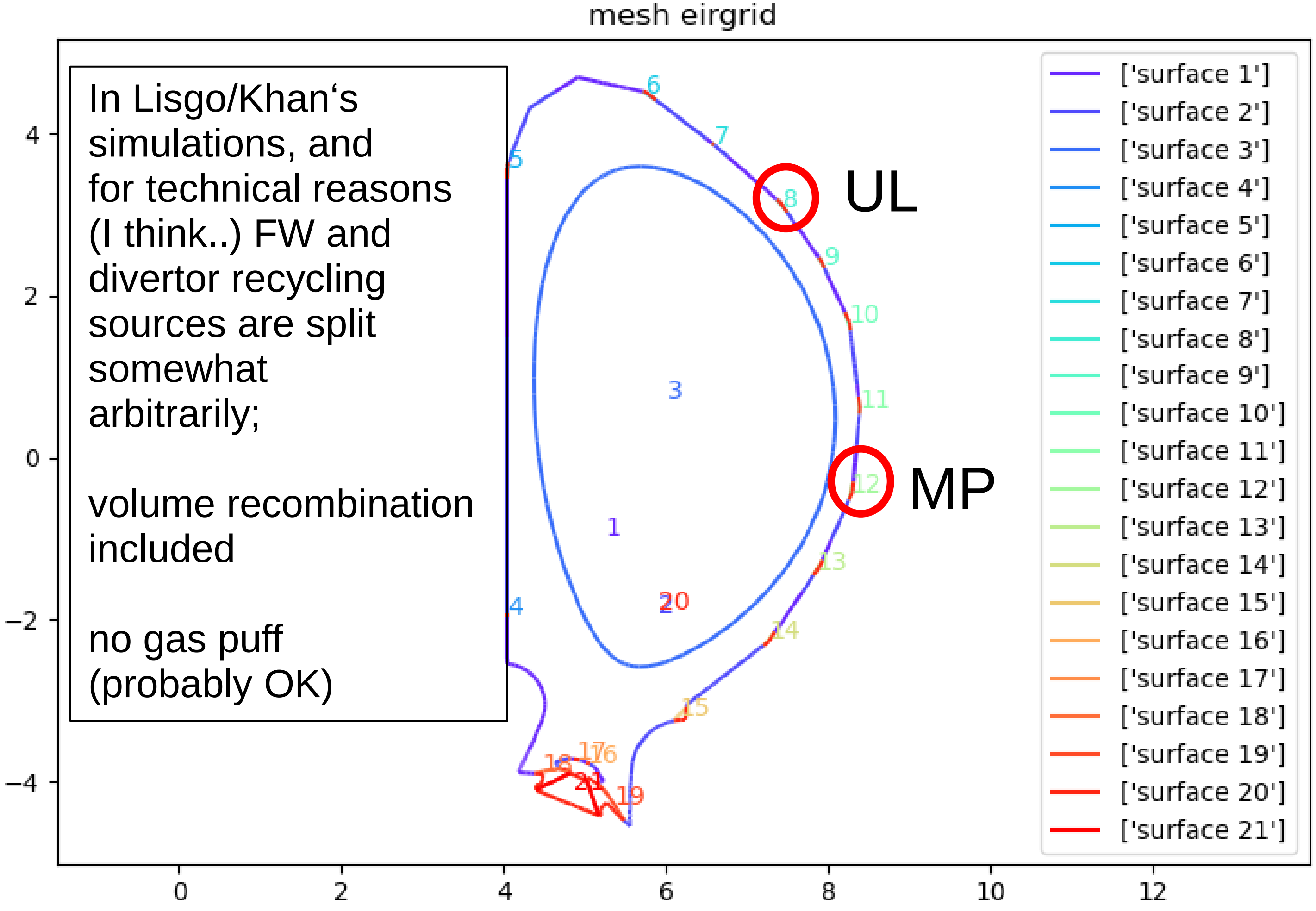
Concentrate on case series 2258_00*

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

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



Toroidally symmetric diagnostic surfaces pre-defined on FW



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)

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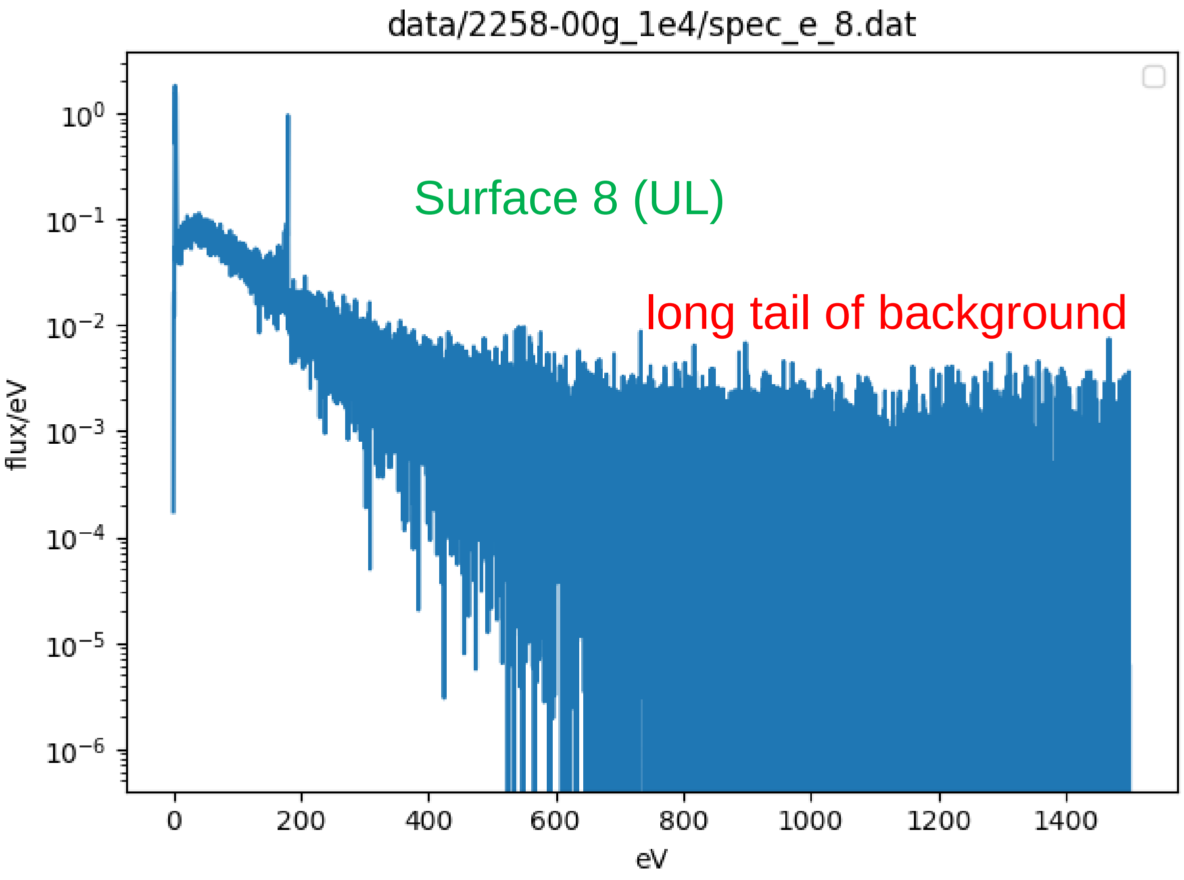
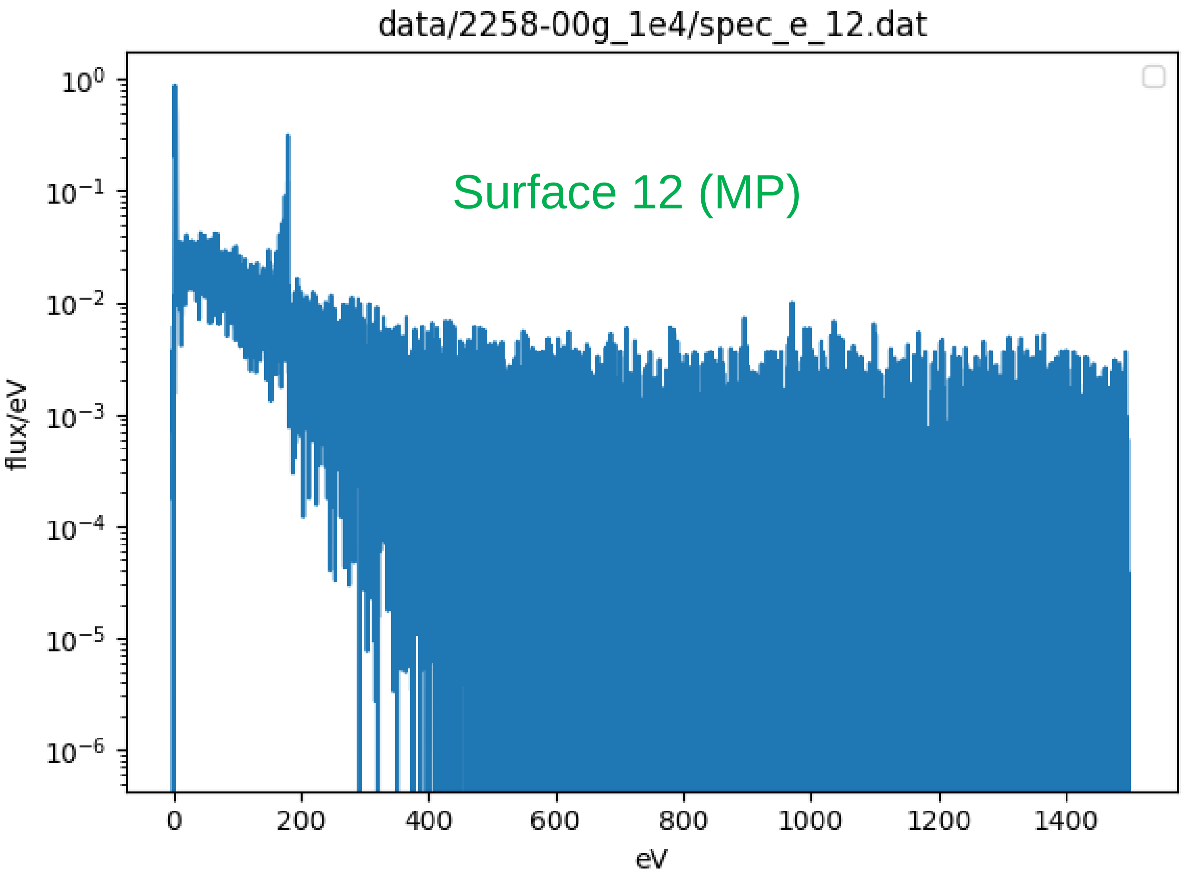
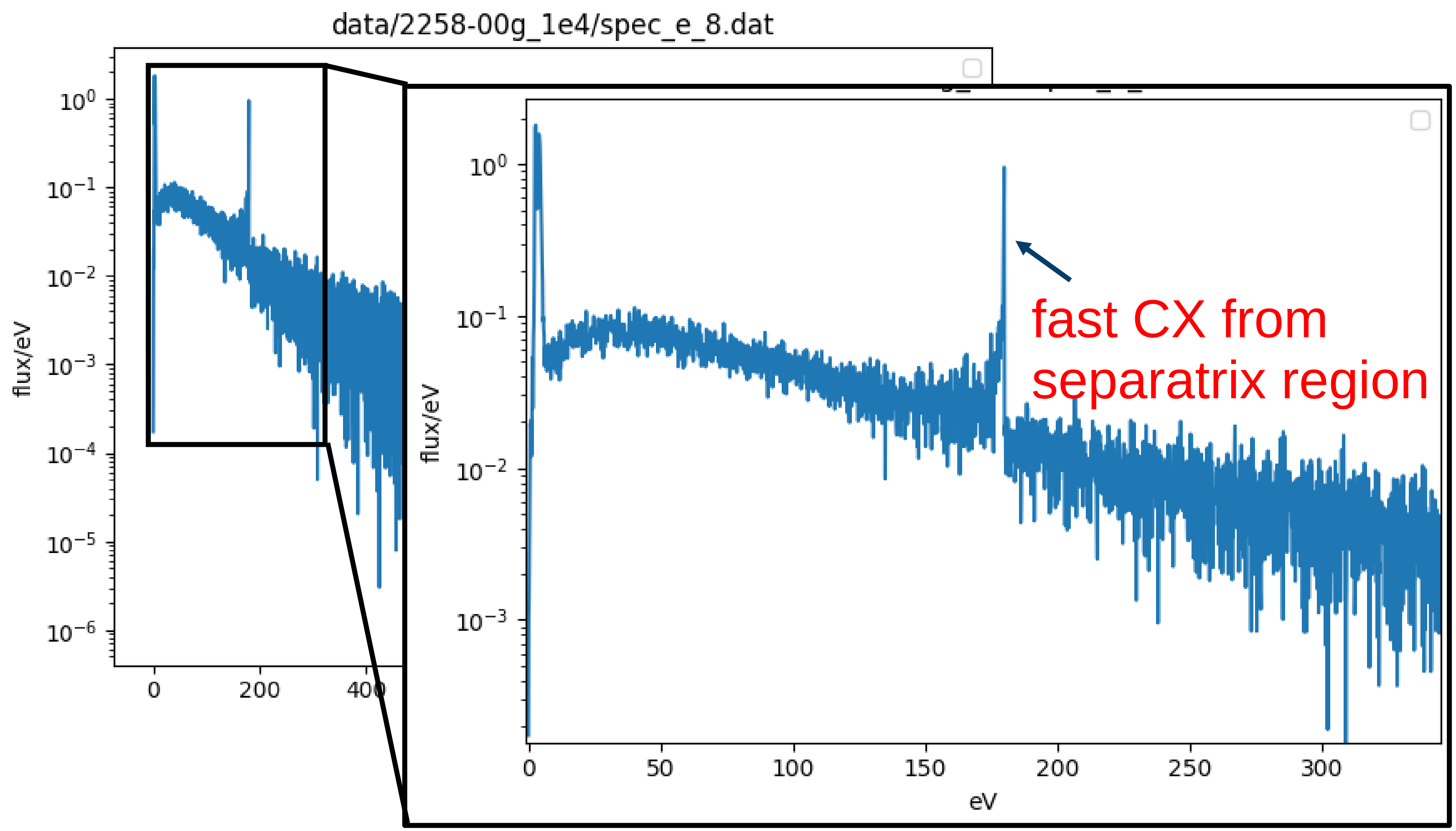
2258_00g D^0 energy spectra





normalised „EIRENE-units“ Amp/eV

2258_00g D^0 energy spectra



normalised „EIRENE-units“ Amp/eV

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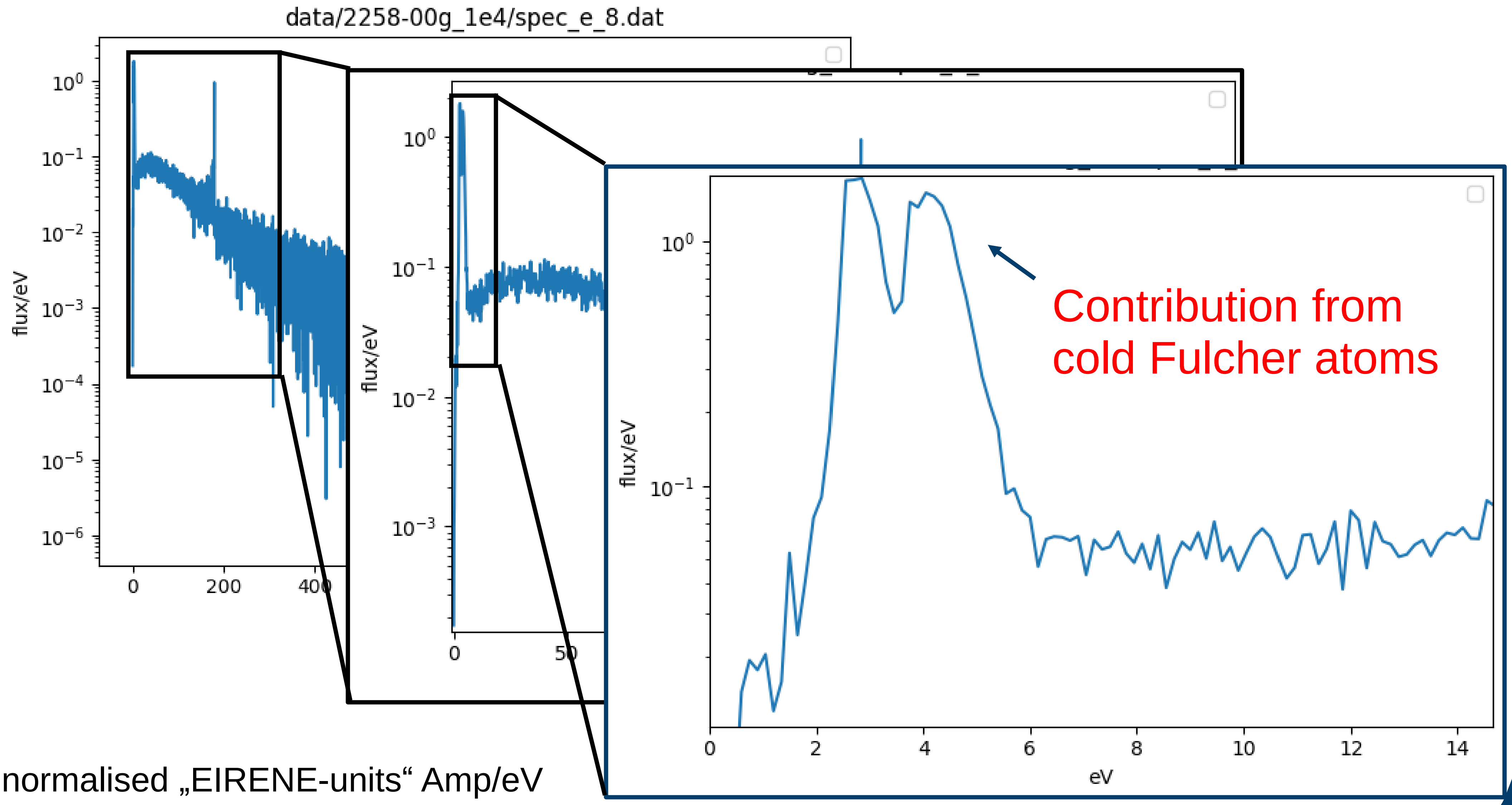
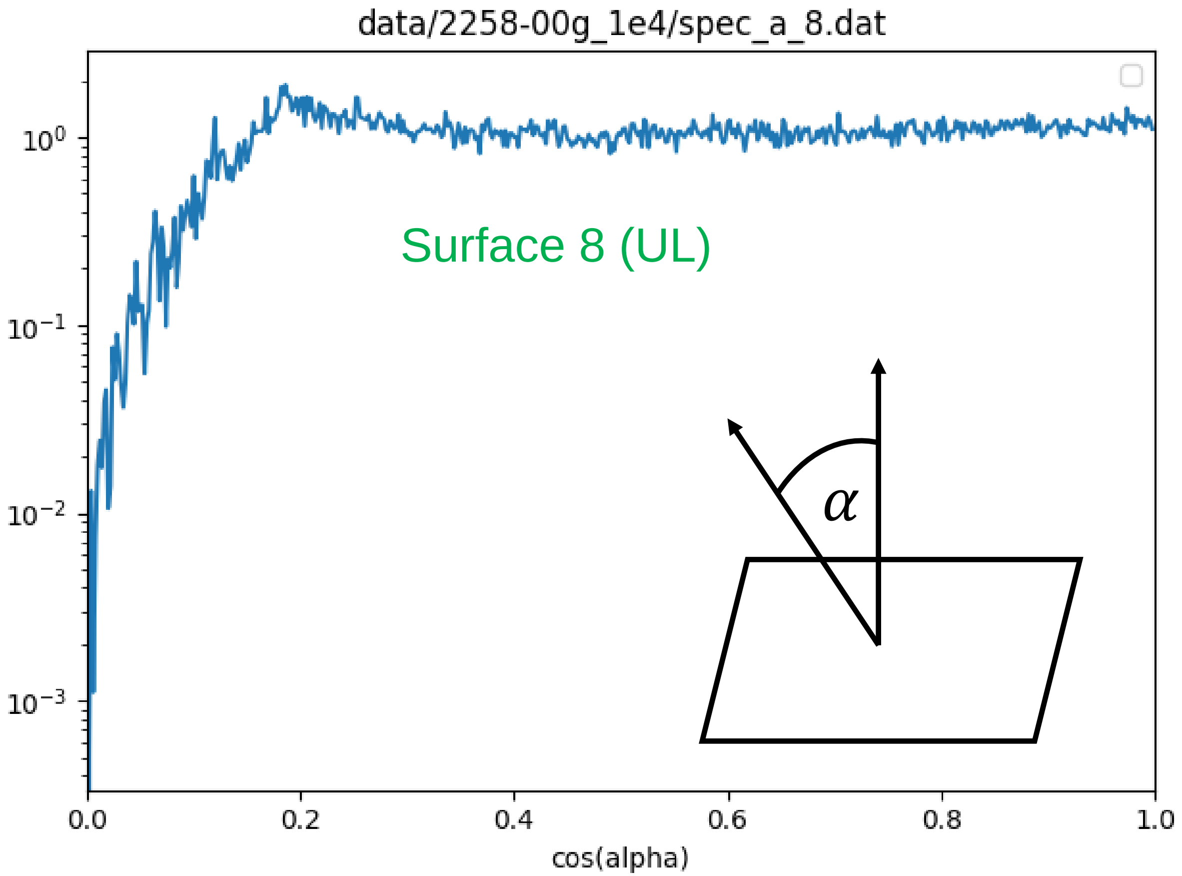
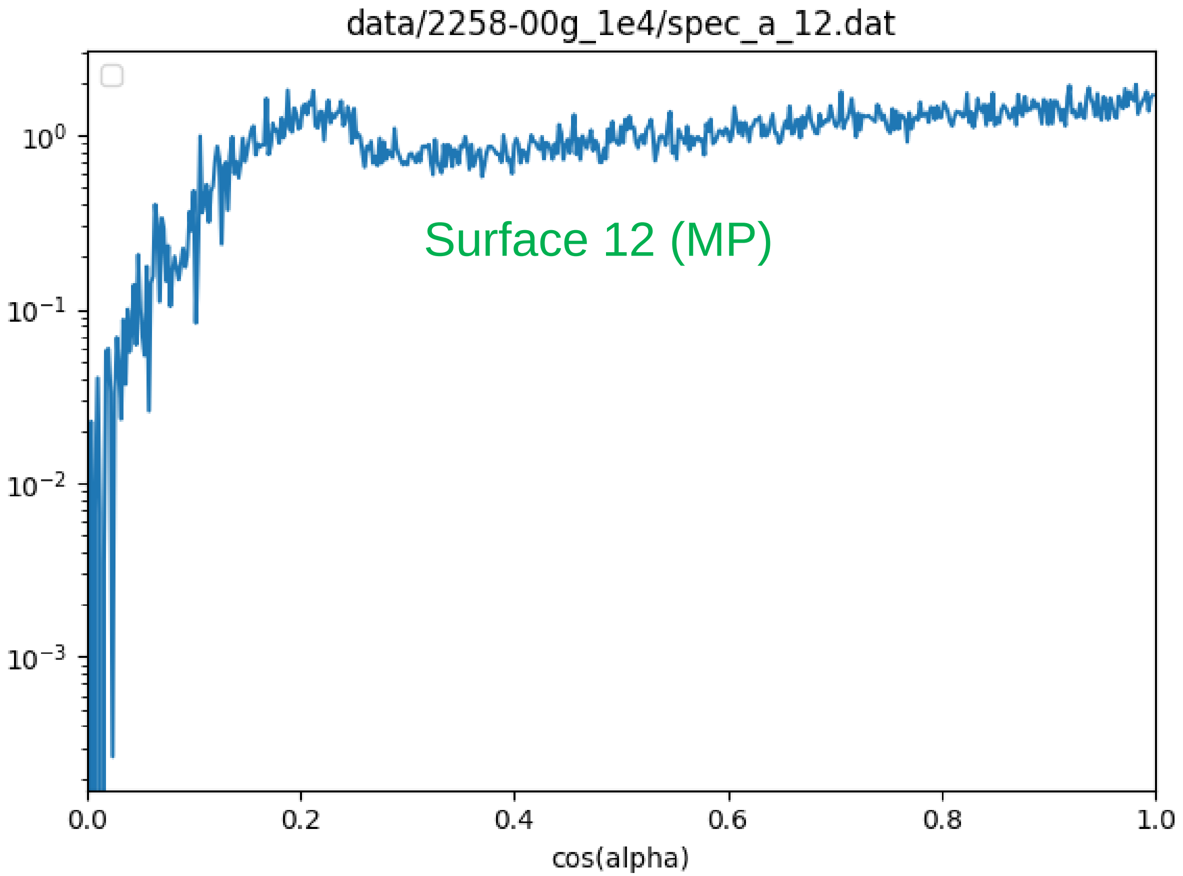
2258_00g D^0 energy spectra



normalised „EIRENE-units“ Amp/eV

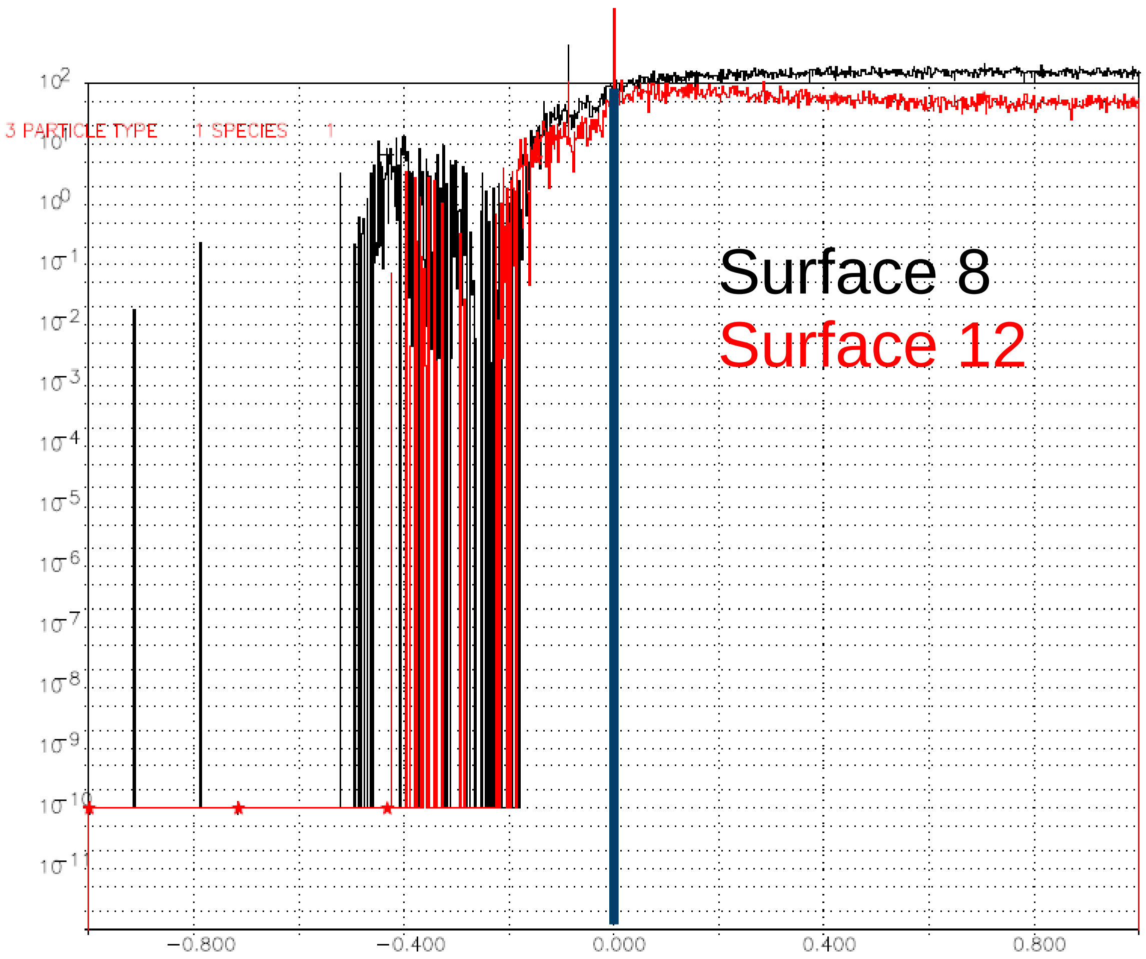
2258_00g D^0 angular distribution (polar angle only, 2D-sym)

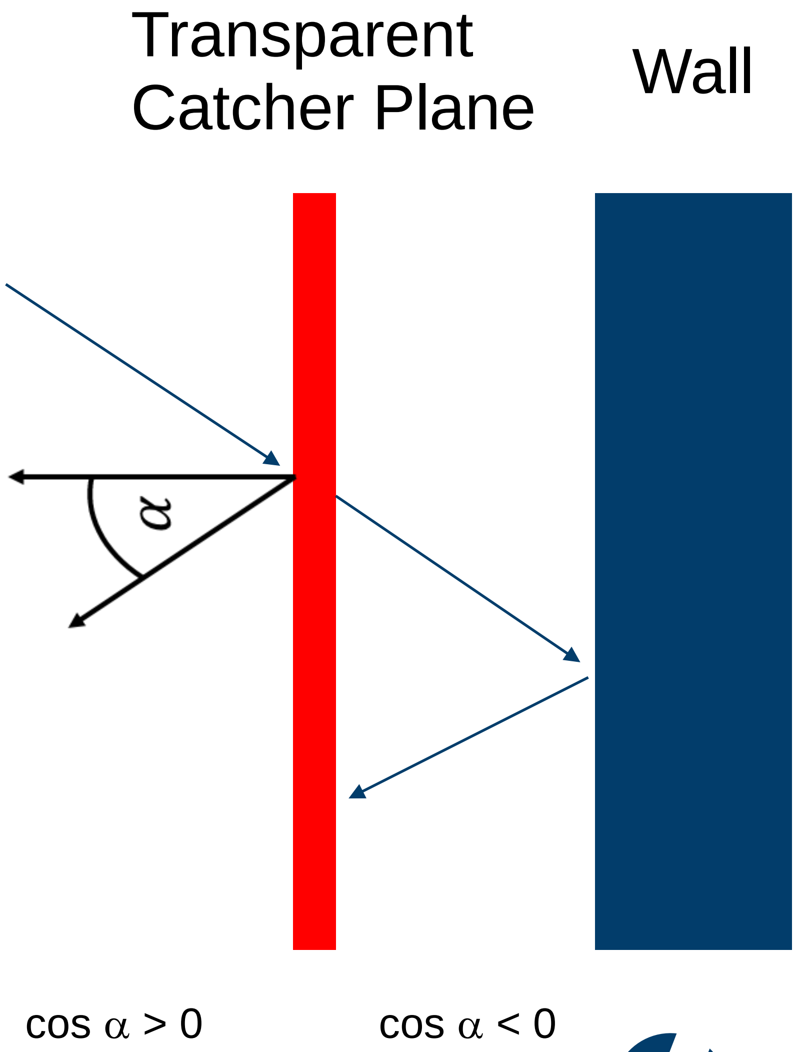




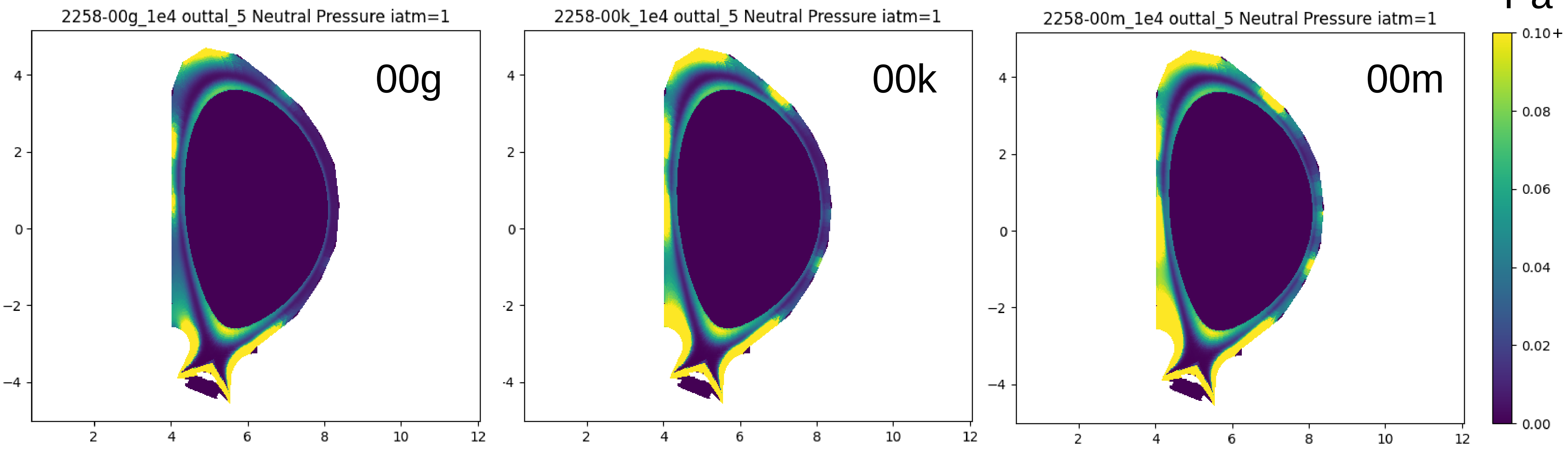
$f(\cos\alpha)$ normalised to 1

Expert‘s advice: don‘t tally wrong..





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



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—	—	$m\ s^{-1}$	eV	eV
00g	0	30	20	40
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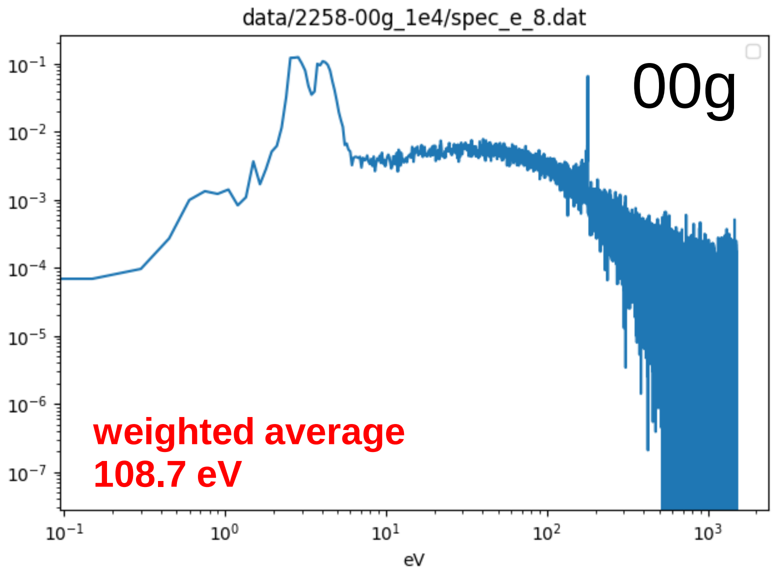
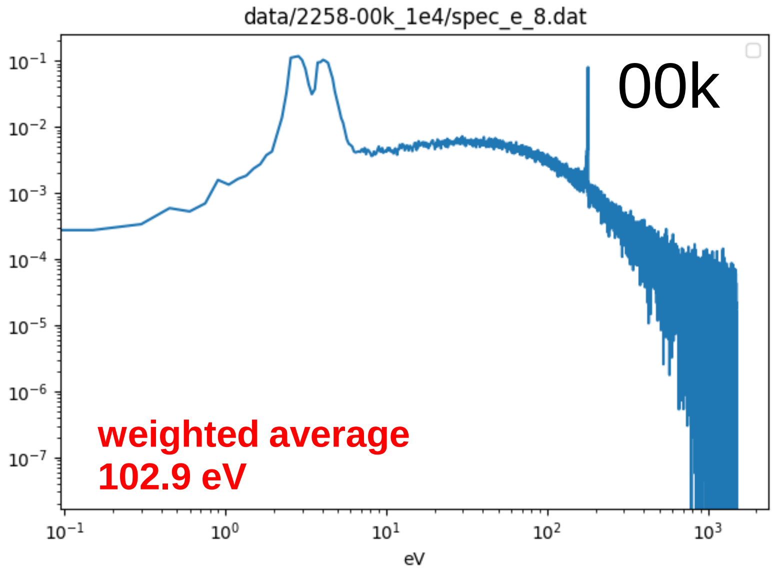
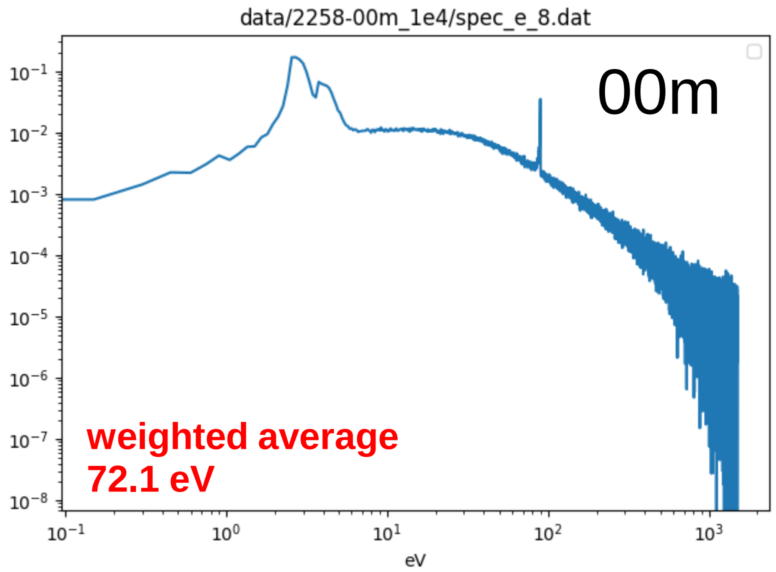
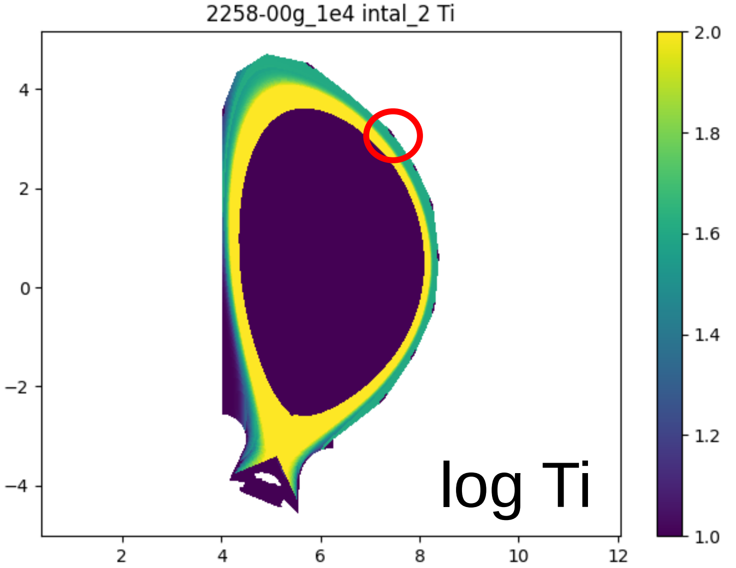
00m	0	100	10	20

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









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

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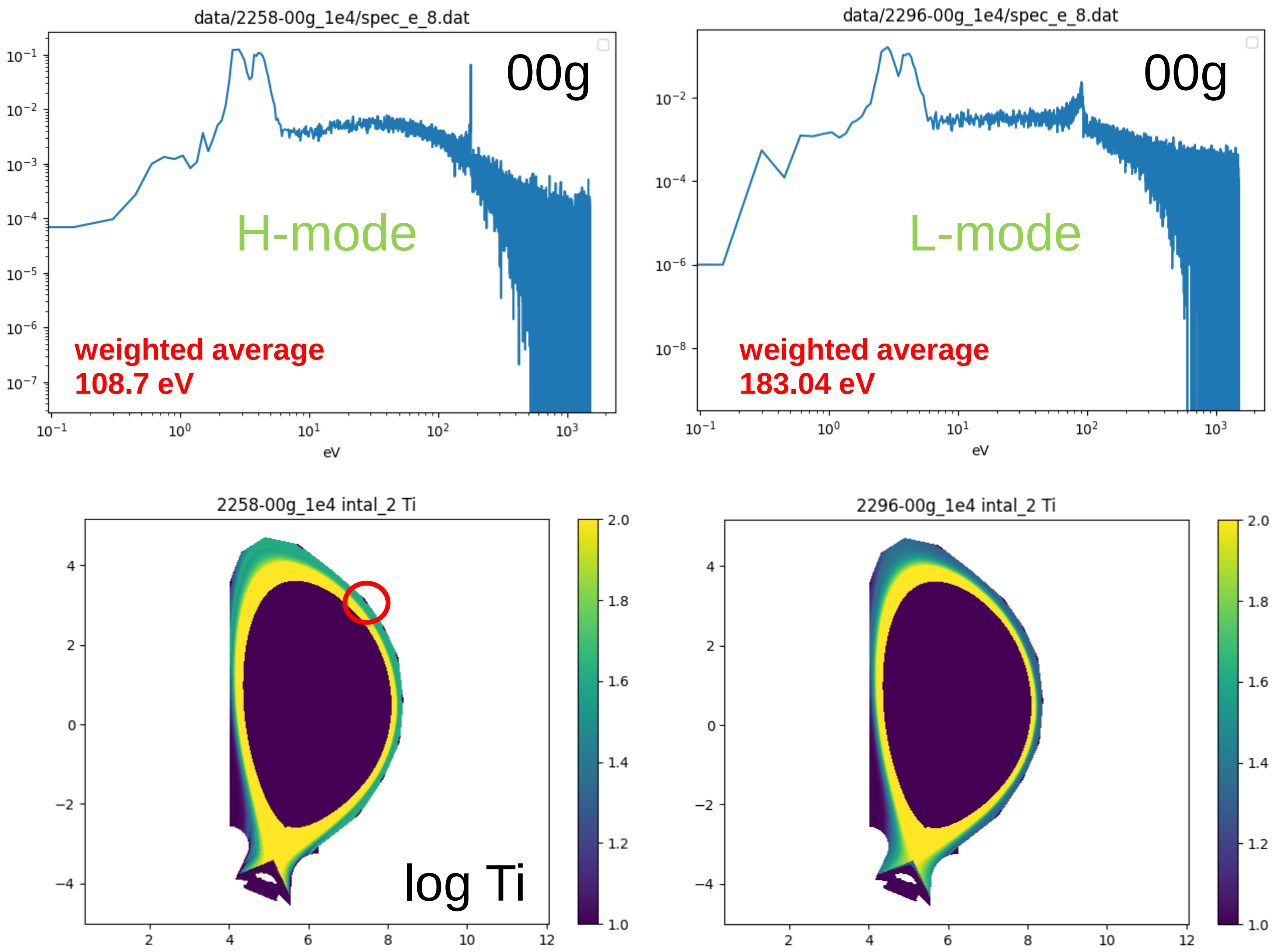
Comparison H-mode vs L-mode (00g)



- **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 Γ_{Ne0} = 1% Γ_{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):

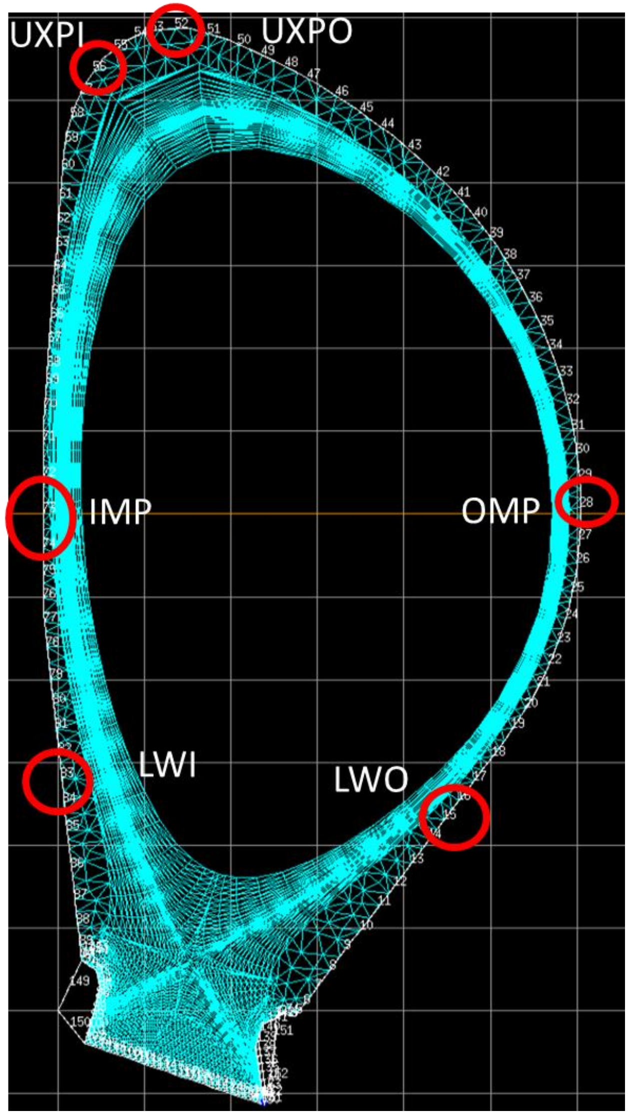
$$Y_{phys,93} = Q_p \left(1 - a^{2/3}\right)(1-a)^2 \frac{\frac{1}{2}\ln(1 + 1.2288b)}{b + 0.1728\sqrt{b} + 0.008b^{0.1504}}$$

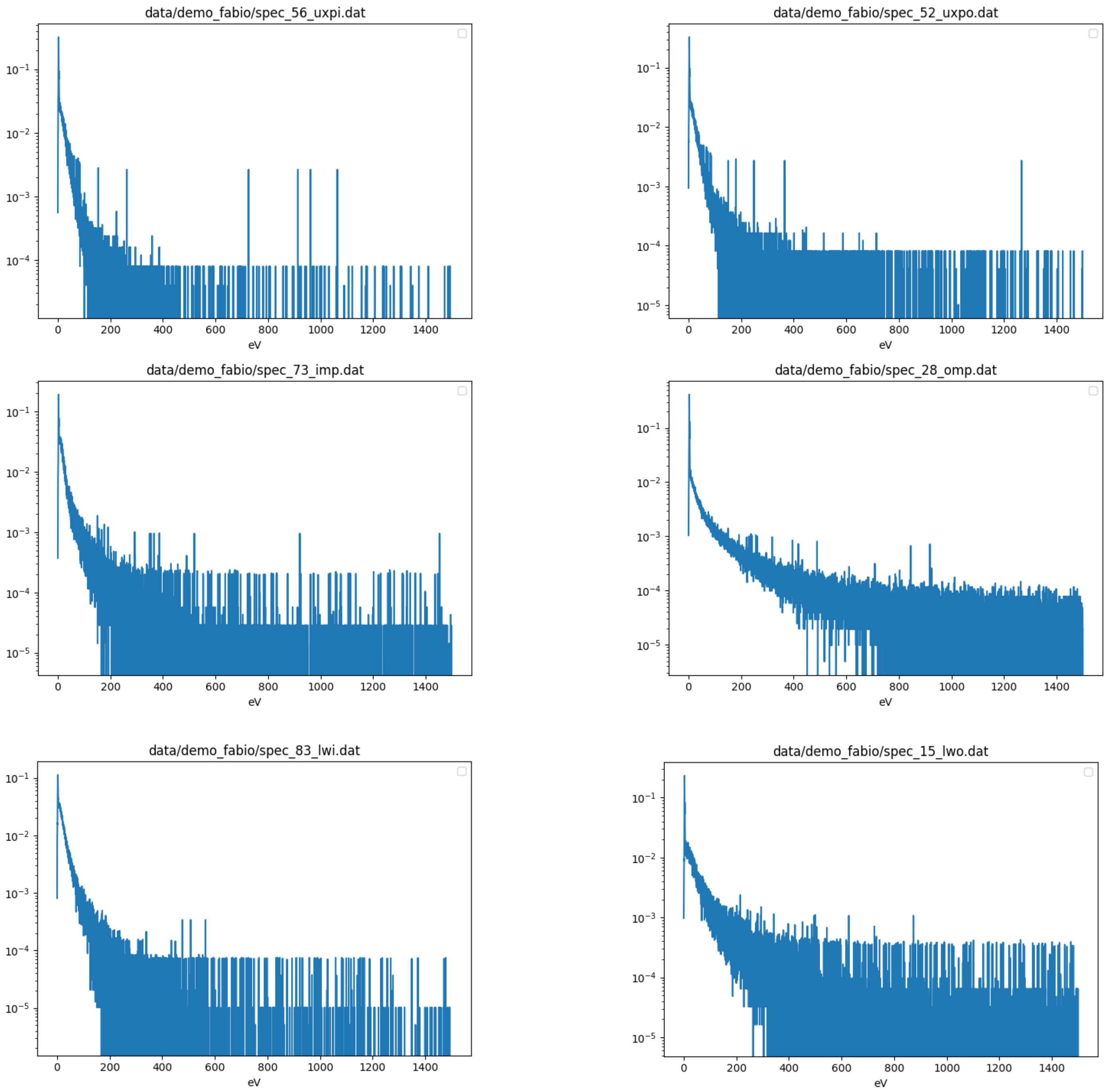
$$a = \frac{E_{th}}{E}, \mathrm{b} = \frac{E}{E_{tf}}, Q_p = const$$

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

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

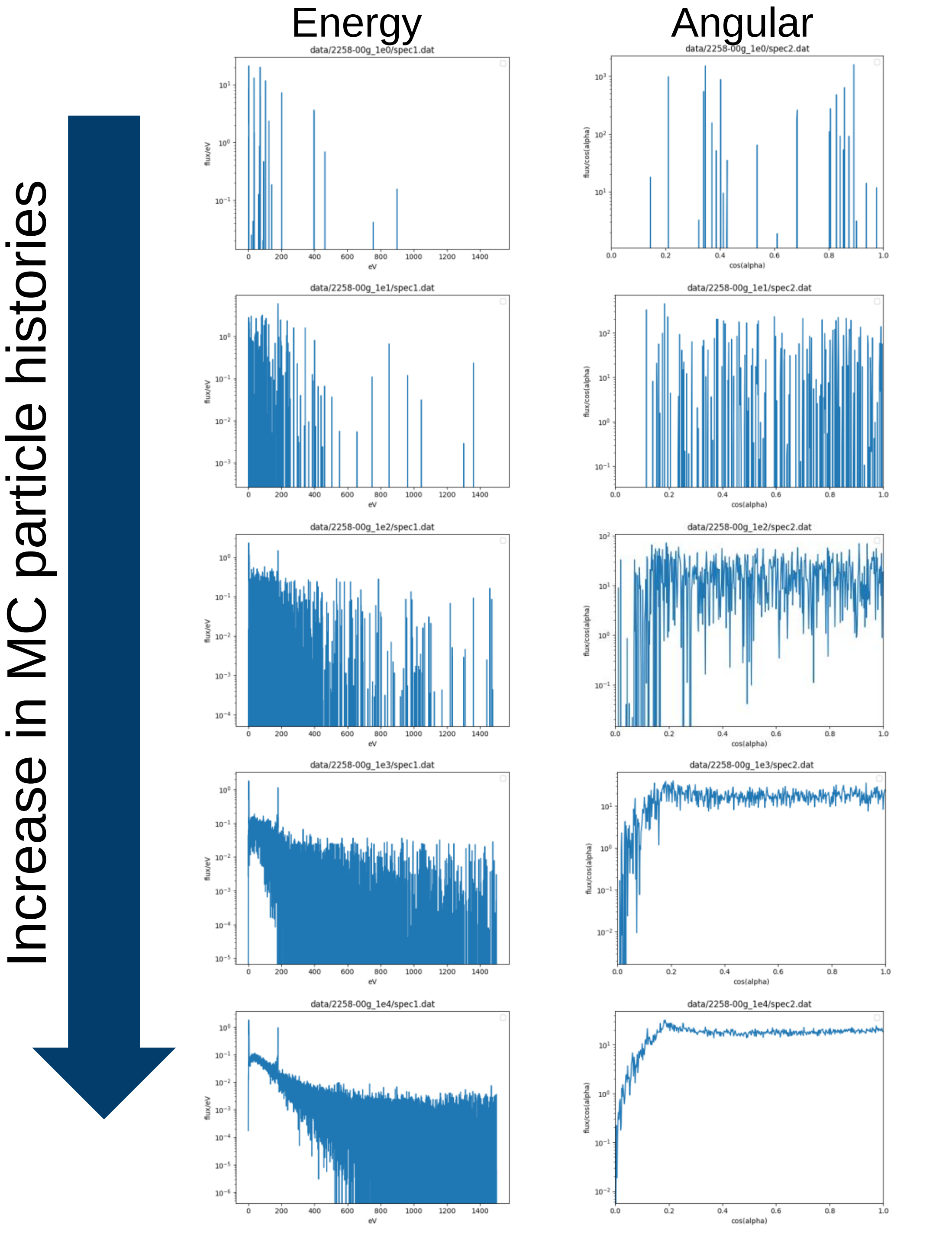
Comments on spectral statistics

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

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

- Requires calculation of higher moments in EIRENE

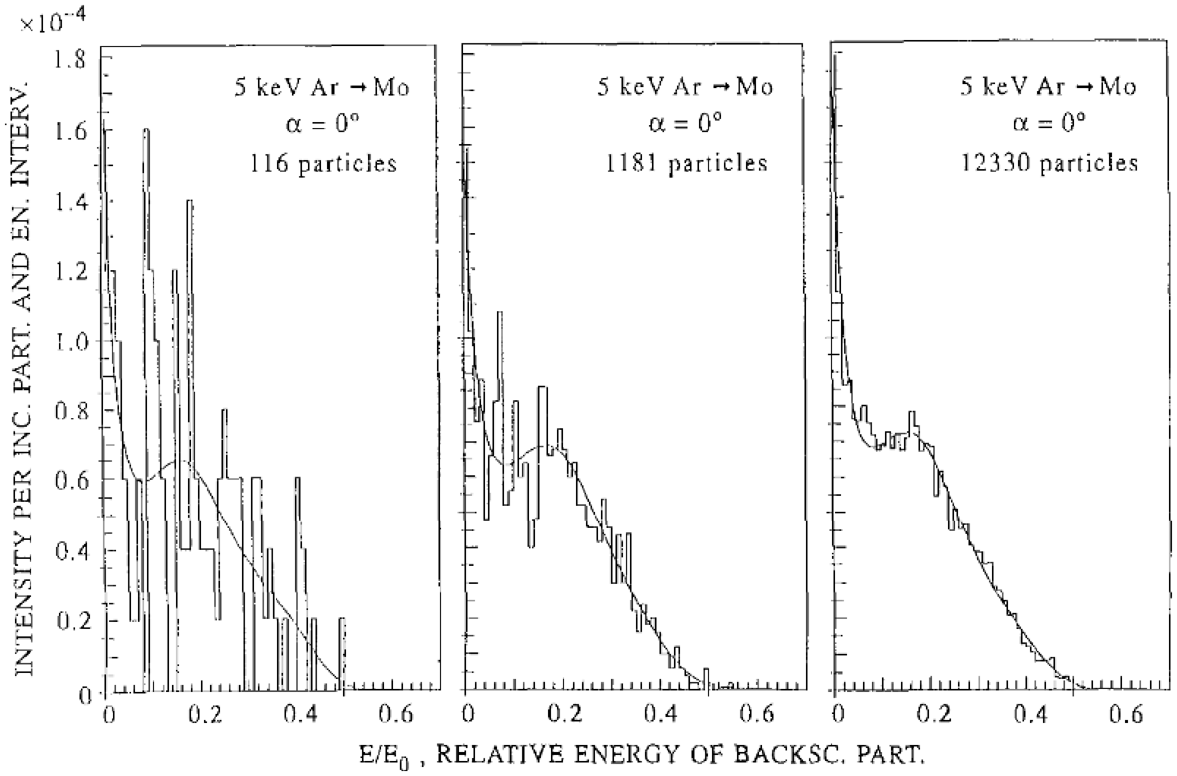
  → mean $l = 1$ & variance $l = 2$ (both done)

  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)



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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 (IO task to provide data)

- 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

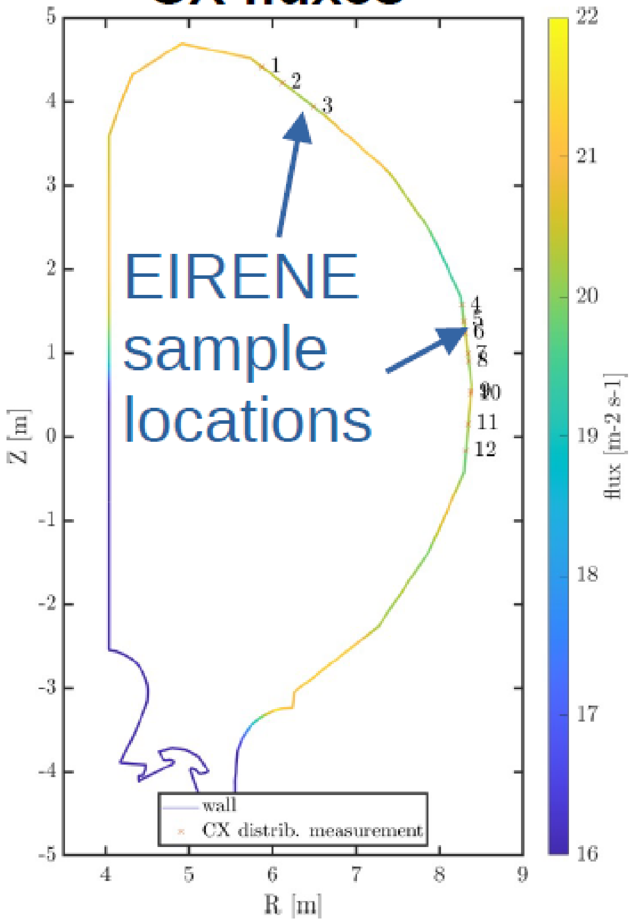
- Only polar angles are collected (toroidally symmetric)
  → extension to full 3D possible (e.g. post-processing EMC3 plasma-backgrounds)

Backup

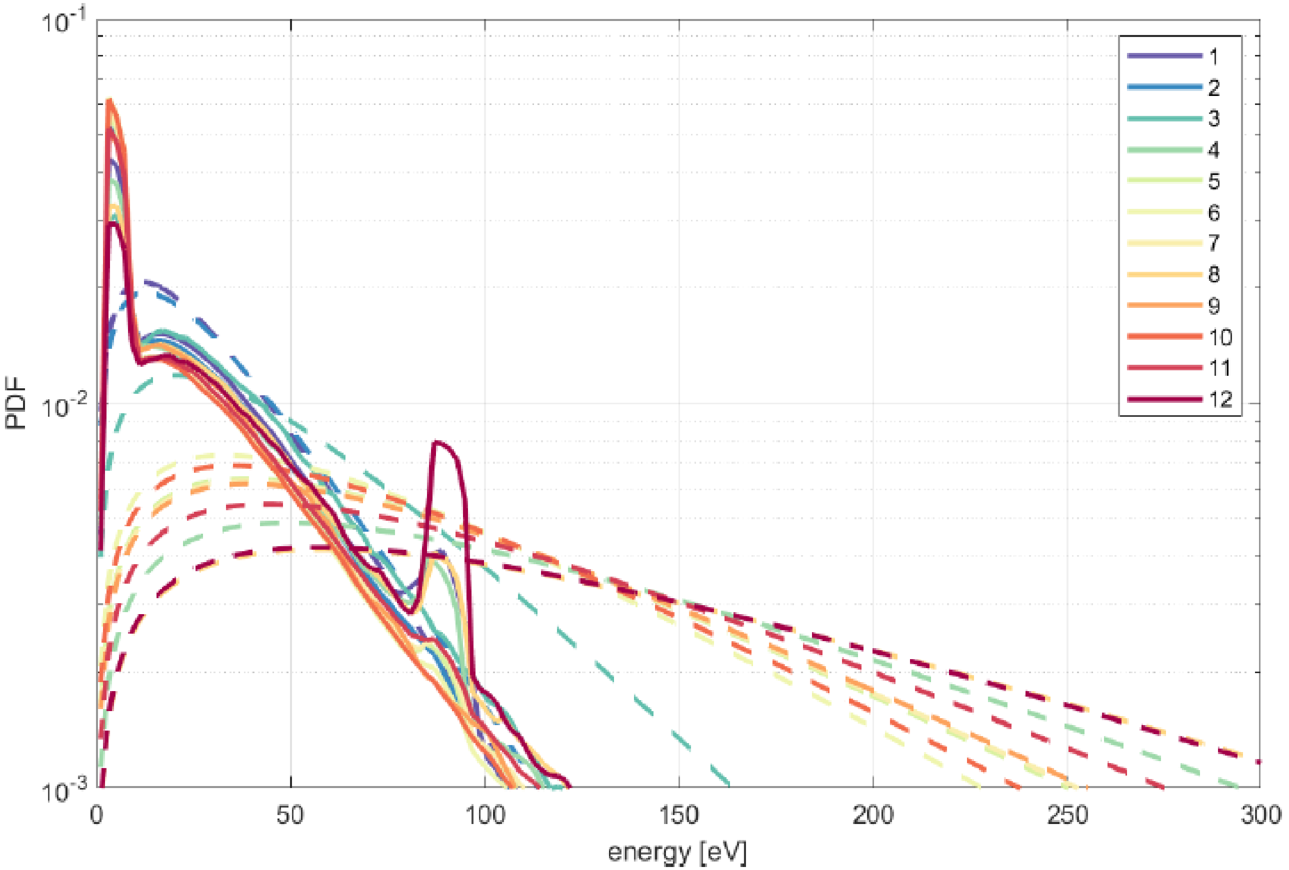
Example: CX distributions from Steve Lisgo for ITER (case #1514)

- 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.

CX fluxes



CX energy distributions at the 12 sample locations



j.romazanov@fz-juelich.de | 14.04.2021

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