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Uncertainty Quantification applied to SOLPS-ITER

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Chosen to broaden the topic: not just UQ for SOLPS-ITER, but a look at the sources of uncertainty

- **Sources of uncertainty**
- **How can we deal with this uncertainty?**
- **Applying UQ methods**

Sources of uncertainty

- SOLPS-ITER essential solves a set of coupled conservation equations for particles, energy and momentum (i.e. transport equations)
- $$\frac{\partial n}{\partial t} + \nabla \cdot \boldsymbol{\Gamma} = S$$
- Uncertainty arises in
  - The calculation of the fluxes, $\boldsymbol{\Gamma}$
  - The calculation of the sources, S
  - The boundary conditions
  - The initial conditions
- The plasma part of SOLPS-ITER (B2.5) implements
  - a fluid description — which might not always be valid
  - a 2D description — which might not always be valid
- The neutrals part of SOLPS-ITER (EIRENE) implements a Monte Carlo description of the neutrals

Sources of uncertainty, II

- Not further discussed in this talk, but still important
  - The numerical methods also produce some errors in the calculation
    - Finite grid sizes
    - Finite number of Monte Carlo (MC) particles
    - MC noise driving a bias when present as a source in the fluid equations
    - Stabilisation terms in the numerics can also introduce some artefacts

Sources of uncertainty: Calculation of fluxes

- B2.5 is a transport code, and the fluxes are usually given as a combination of diffusion and convective terms
  - Specified by transport coefficients
    - Radial “anomalous” transport usually specified by D’s and v’s for each of the equations
      - Not first principles — ad hoc models or varied to match experimental measurements
    - Parallel transport — at its most complete — bases on Zhdanov-Grad approach (see recent thesis of Sergei Makarov)
      - But still have flux limiters to try to capture some kinetic effects

Sources of uncertainty: Calculation of sources

- Sources arise in the B2.5 code from
  - Neutrals (and possibly test ions) treated by EIRENE
    - Particles, energy and momentum
  - Neutrals treated by B2.5 if the fluid neutral model is active
  - Ionization, recombination and possibly charge-exchange coupling different charge states of an impurity
- The neutrals that give rise to much of the sources come from
  - Recycling
  - Gas puffs
  - Sputtering
  - Ad hoc models for pellets
  - NBI (usually neglected as a volume source in the edge)
  - Volume recombination
- Need Atomic, Molecular and Surface (AMS) models to calculate these sources
  - Which have uncertainties of their own

Sources of uncertainty: Calculation of boundary conditions

- Will break the consideration of b.c. into three
  - Core plasma
    - Densities or particle fluxes?
    - Temperature or energy fluxes?
    - Parallel velocities or momentum fluxes?
  - Target boundary conditions
    - Sheath boundaries introduce a number of questions
      - Which sound speed
      - Velocity = sound speed or > sound speed (or < sound speed for highly collisional cases)
      - Secondary electron emission coefficient
    - Recycling coefficients, sputtering coefficients, ro-vib states of emitted molecules
  - Wall boundary conditions
    - Decay lengths? Loss conditions?
  - More recent extension of plasma to the wall mixes the last two b.c.

Sources of uncertainty: Specification of initial conditions

- **In some parts of parameter space, multiple solutions are possible**
  - **The final state is then often determined by the initial state**

Start by looking at uncertainty from atomic physics

- **(Slides stolen from a talk I gave for "2nd Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas, 6 – 9 December 2021")**

- Approach taken here
  - Have Rate(te, ne) from, for example, ADAS
    - Change this to Rate(Te*$\mathbf{v}_{\mathbf{Te}}$, ne*$\mathbf{v}_{\mathbf{ne}}$) * $\mathbf{v}_{\mathbf{rate}}$
      - With the **v**'s varying around 1
  - Do this for ionisation and recombination rates
  - Then solve for the coronal equilibrium average charge distribution, as a function of these varying **v**'s
- We can use the same methodology if we have better ways of parameterising the uncertainties in the atomic data

Now use the VECMA EasyVVUQ toolkit

- https://github.com/UCL-CCS/EasyVVUQ
- Suleimenova, Diana, Hamid Arabnejad, Wouter N. Edeling, David Coster, Onnie O. Luk, Jalal Lakhlili, Vytautas Jancauskas, et al. 'Tutorial Applications for Verification, Validation and Uncertainty Quantification Using VECMA Toolkit'. Journal of Computational Science, June 2021, 101402. https://doi.org/10.1016/j.jocs.2021.101402. [And references therein]
- Python package capable of running UQ "campaigns"

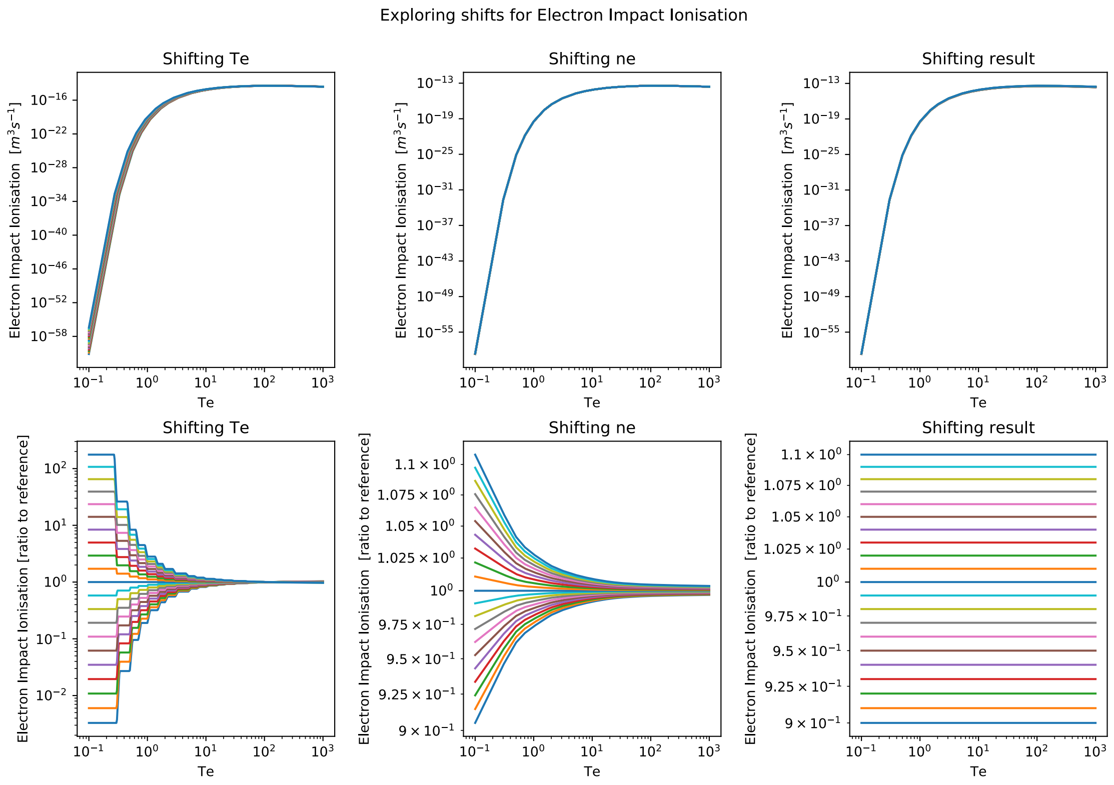
- Here we assume an uniform distribution of the **v**'s in the interval [0.8, 1.2]

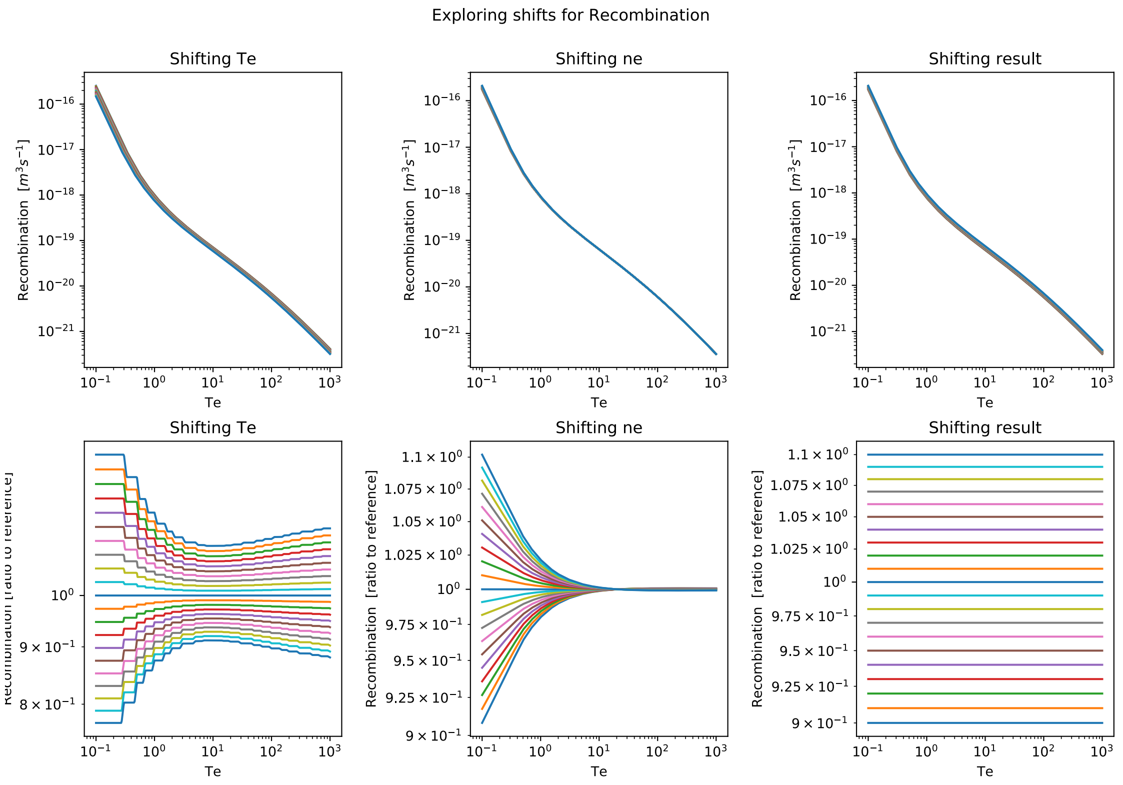
```
vary = {
    "EI_te_vary":   cp.Uniform(0.8,   1.2),
    "EI_ne_vary":   cp.Uniform(0.8,   1.2),
    "EI_rate_vary": cp.Uniform(0.8,   1.2),
    "RC_te_vary":   cp.Uniform(0.8,   1.2),
    "RC_ne_vary":   cp.Uniform(0.8,   1.2),
    "RC_rate_vary": cp.Uniform(0.8,   1.2)}
```

- Use Polynomial Chaos Expansion with varying order to evaluate the statistical information

Results for applying these v’s …

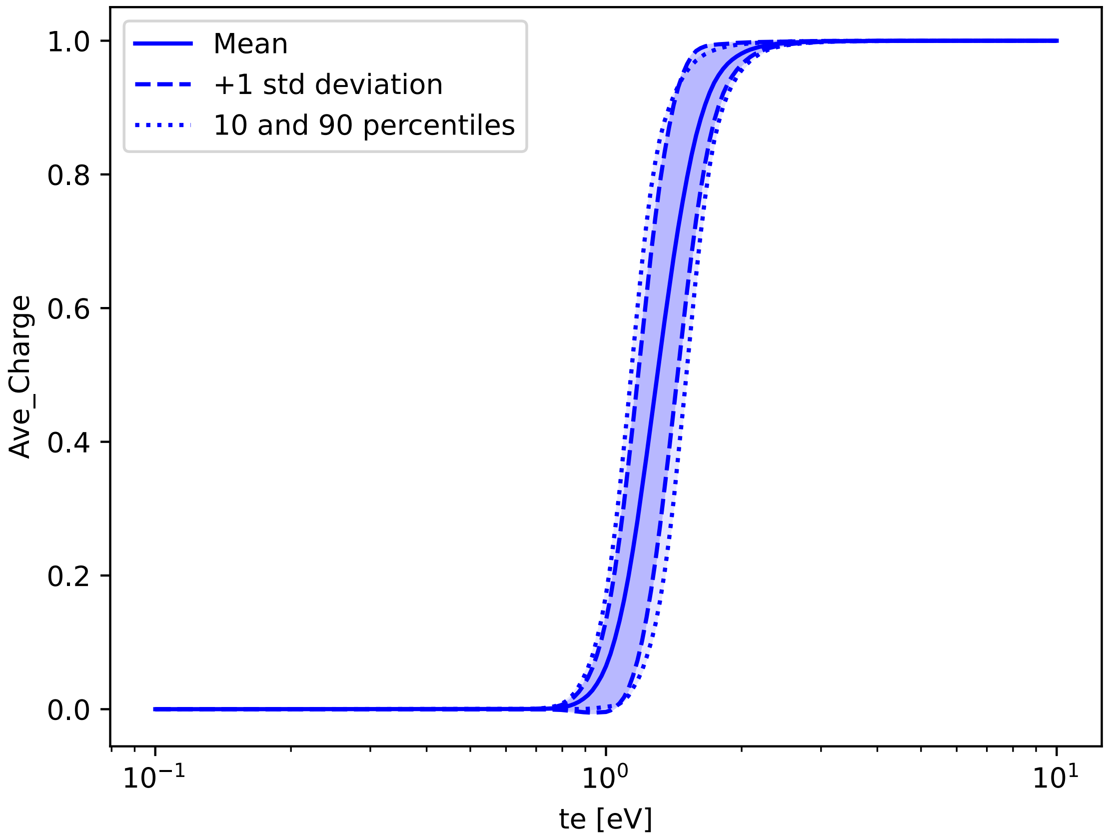
- Use (here)
  - **v** = [0.9,1.1] in steps of 0.01





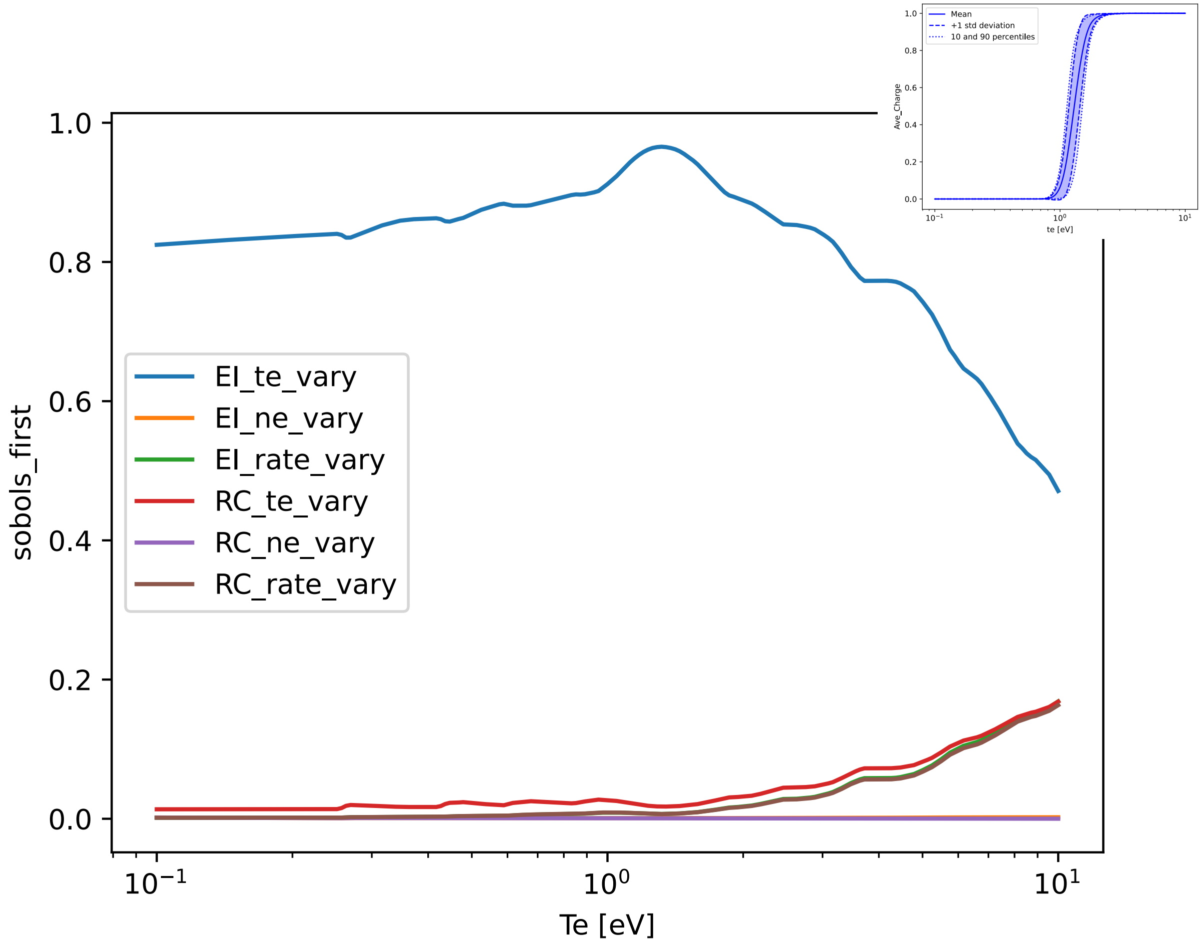
Apply EasyVVUQ: Results for H, ne=3e19

- Mean average charge as a function of Te
- With + and - 1 standard deviation
- And the 10 and 90 percentiles
- To understand where the variance is coming from, we need to look at the Sobol indices …



Results for H, ne=3e19

- For the first Sobol
  - We see that over the whole domain, contribution of varying the Te argument to the EI rate is the most important
  - At higher temperatures, we start to see increasing contributions from the RC variation: the Te argument variation and the variation in the rate



UQ for linear (1D) SOLPS runs

- **(Slides stolen from a talk I gave at the 2002-07 TOK/MHD Retreat)**

SOLPS-ITER – plasma physics transport code

- **1D simulations**
  - Parallel length 50m
  - D + N, fluid neutrals
  - Boundary conditions
    - Upstream
      - Feedback on D and N densities
        D_upstream and N_upstream
      - Fixed power
        P_electron and P_ion
    - Downstream
      - Sheath boundary conditions

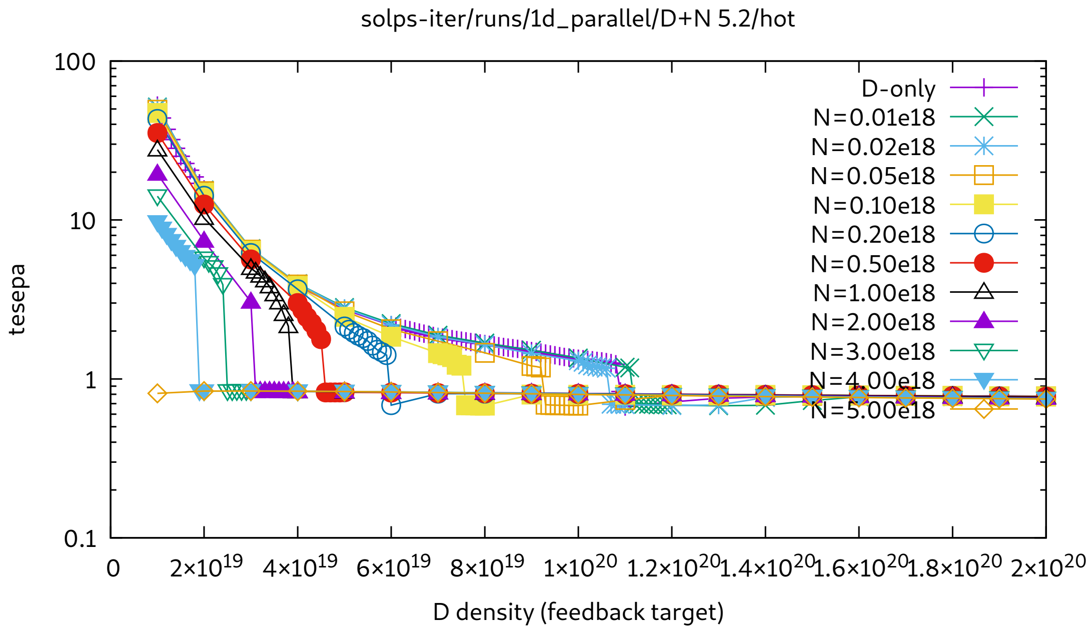
EasyVVUQ. – python framework for doing uncertainty quantification

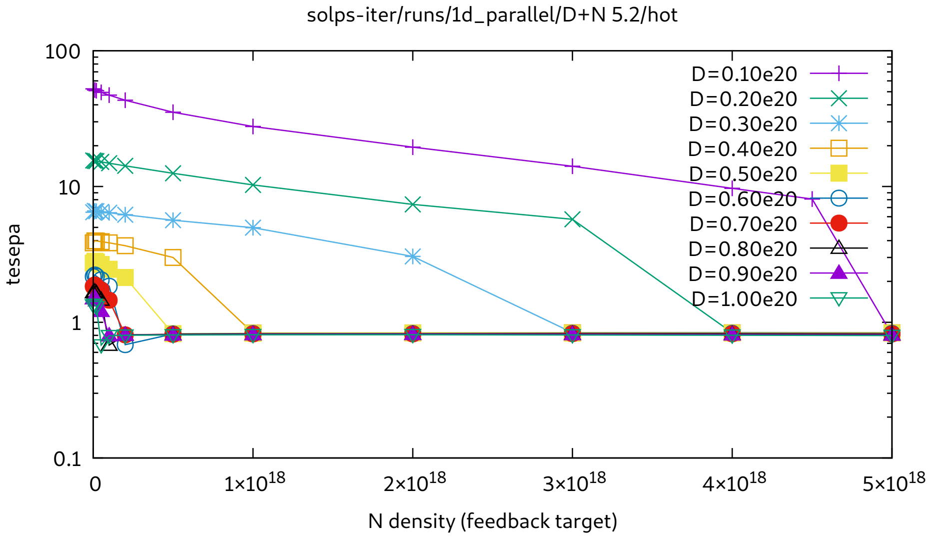
- **10 varying parameters**
  - D_upstream
  - N_upstream
  - P_electron
  - P_ion
  - RESCALE_SA – ionisation rate rescale factor
  - RESCALE_RA – recombination rate rescale factor
  - RESCALE_QA – cooling rate rescale factor
  - RESCALE_CX – charge exchange rate rescale factor
  - RESCALE_RD – line radiation rate rescale factor
  - RESCALE_BR – recombination radiation rescale factor

Leverage a set of 1D D+N SOLPS-ITER runs as a starting point

SOLPS-ITER – plasma physics transport code

- **Scans of D and N upstream densities**
- **Plots of the downstream electron temperature ("tesepa") just in front of the target**
  - As the upstream D density is increased, the downstream electron temperature drops (until it crashes)
  - As the upstream N density is increased, the downstream electron temperature drops (until it crashes)
- **Will use D=3.5e19 m^{-3}, N=5.0e17 m^{-3} as the starting point for the UQ**
  - Will also do D=4.5e19 m^{-3} and D=5.5e19 m^{-3} to see if there are changes with detachment level





Leverage a set of 1D D+N SOLPS-ITER runs as a starting point

SOLPS-ITER – plasma physics transport code

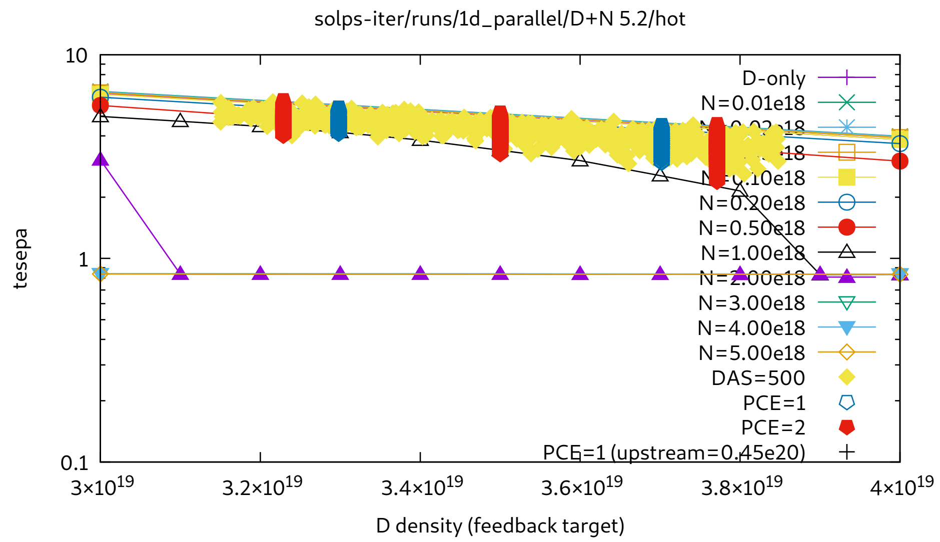
- **Will use D=3.5e19 m^{-3}, N=5.0e17 m^{-3} as the starting point for the UQ**
  - Did this for PCE=1 and PCE=2
- **Also try at higher D=4.5e19 and 5.5e19**

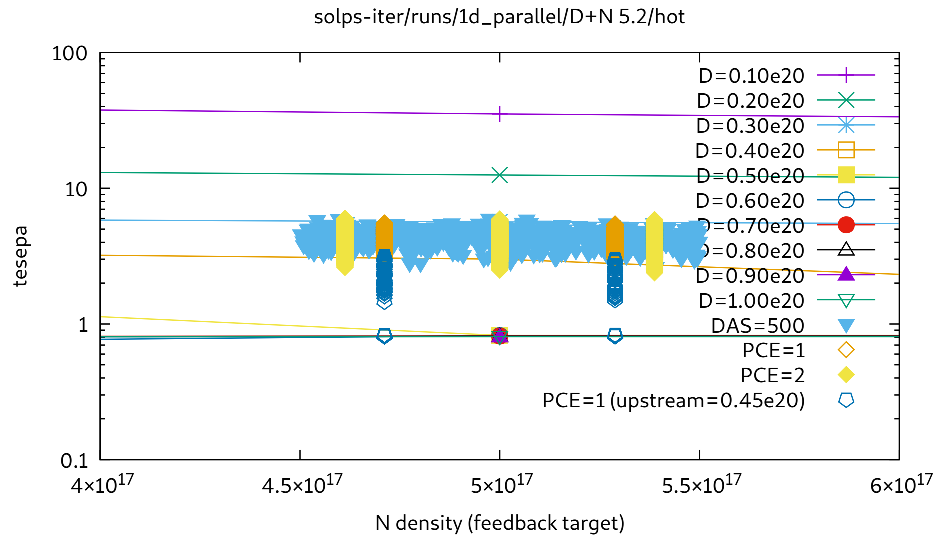
Number of SOLPS cases:

- **10 varying quantities, PCE order = 1 → 1024 cases**
- **8 varying quantities, PCE order = 2 → 6561 cases**
- **8 varying quantities, PCE order = 1 → 256 cases**

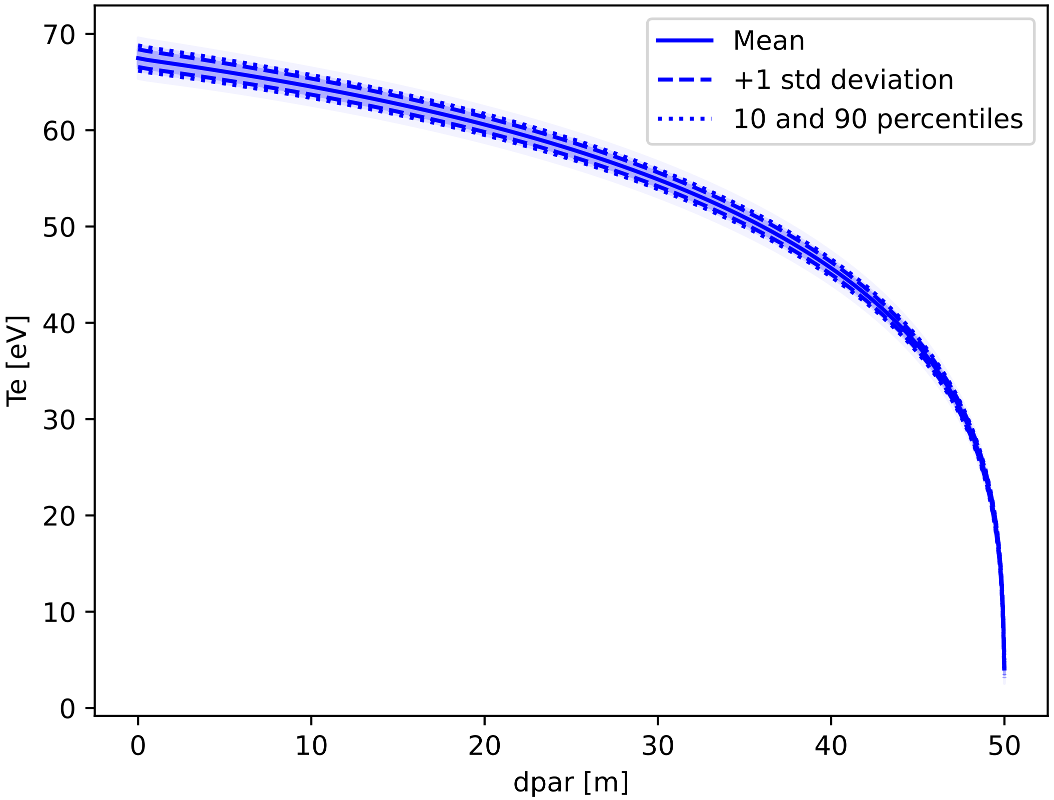
SOLPS runs stopped when

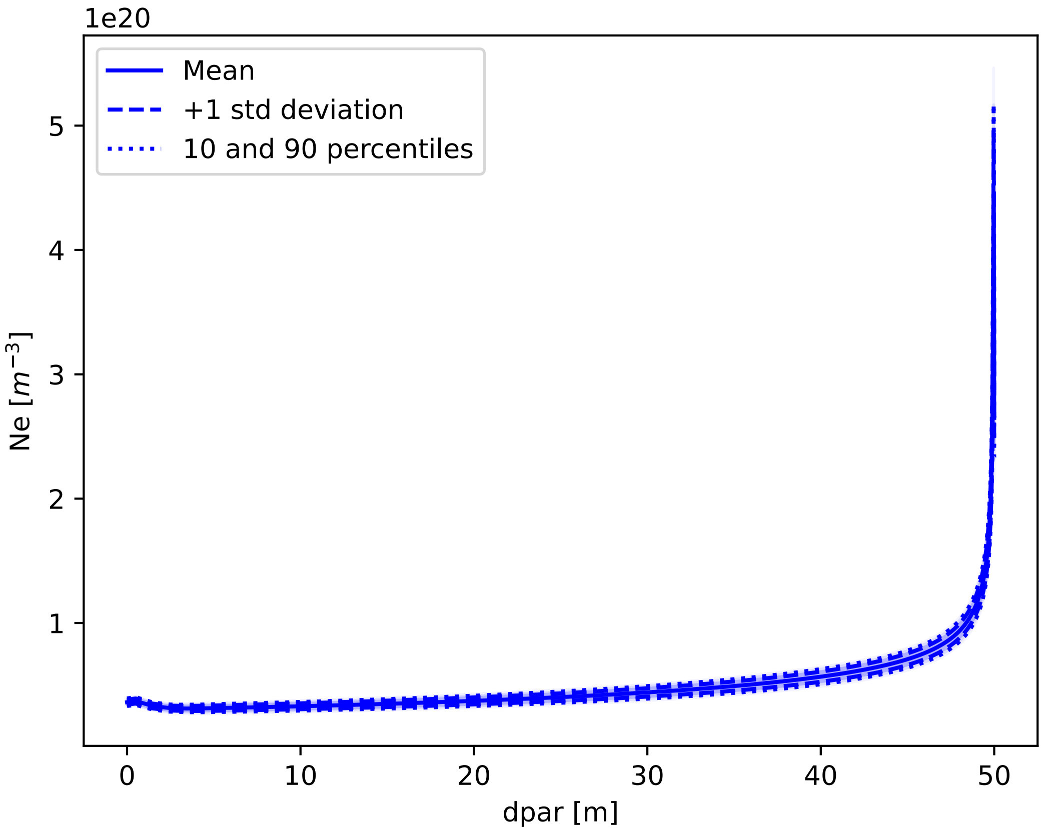
- **Key residuals < 1e-6**
- **Elapsed cpu time > 35.5 hours**
- **Then short run performed and the QOIs extracted**





PCE=1 around D=3.5e19 m^{-3}

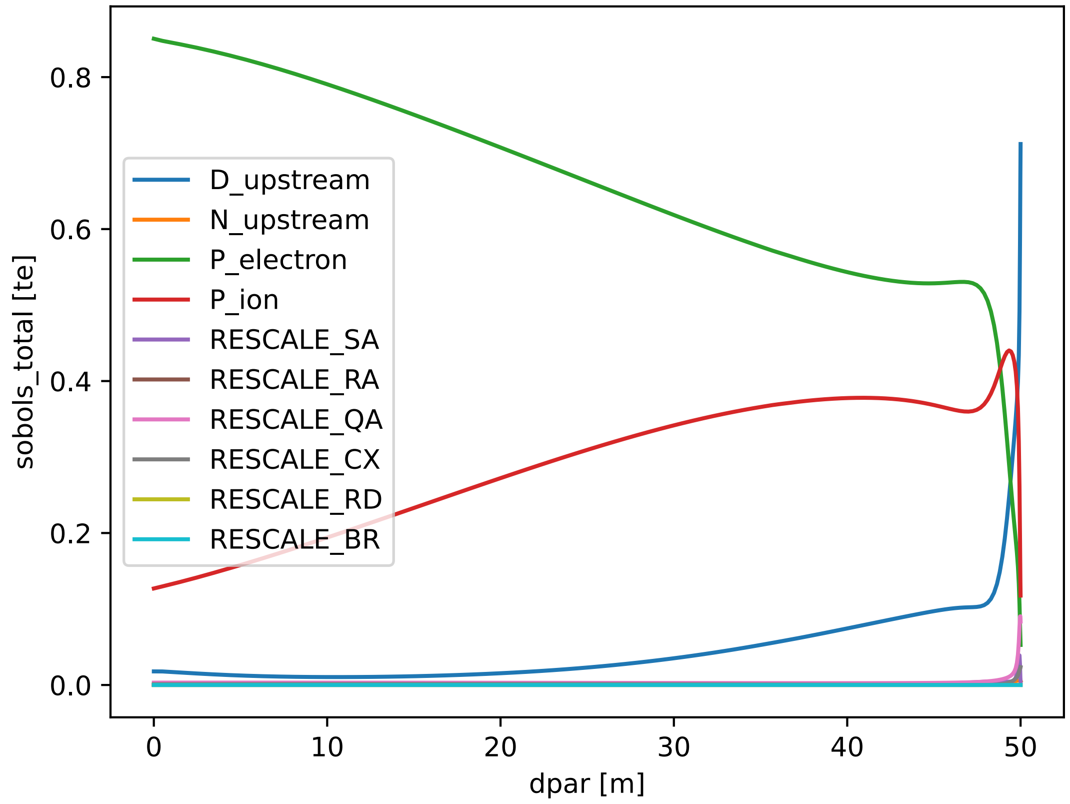


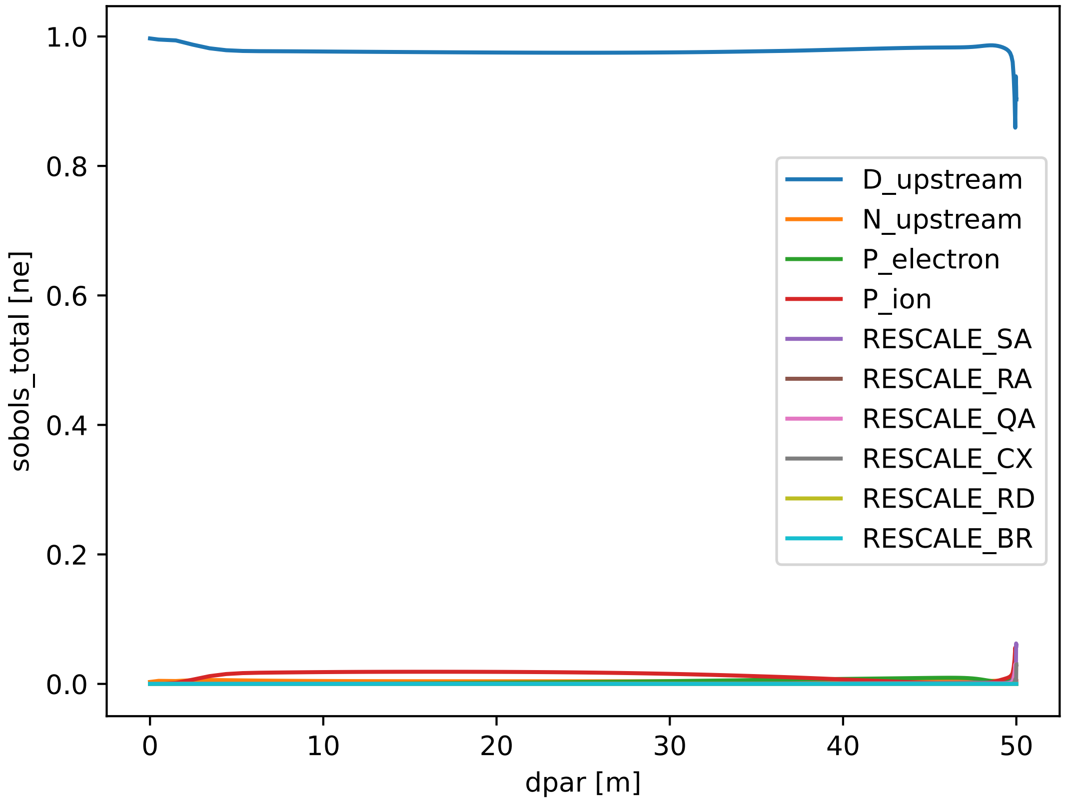


Fairly typical high recycling profiles
- Te dropping towards the target

Fairly typical high recycling profiles
- ne rising towards the target

Total Sobol indices for PCE=1 around D=3.5e19 m^{-3}





Total Sobol:

- Te variance mostly explained by variance of electron heat input, then ion heat input; near the target, upstream D density takes over in importance
- ne variance mostly from variance in upstream D density
- Almost no dependence on atomic physics

Look at the maximum (across the parallel distance) for the total Sobols

For Te

- **Most important atomic physics parameter is electron cooling rate at ~ 9%**
  - Then ionization rate at ~ 4%

For ne

- **Most important atomic physics parameter is the ionization rate at ~ 6%**

Two quantities are completely unimportant – which is good because they should have no effect on the plasma density or temperature

Drop these two and then do PCE=2

- Maximum difference in Sobol's of 0.005

Varying input	Max Total Sobol	
	Te	ne
D_upstream	0.712	0.997
N_upstream	0.00595	0.00665
P_electron	0.851	0.0201
P_ion	0.44	0.0561
RESCALE_SA	0.039	0.0625
RESCALE_RA	0.000123	3.9e-05
RESCALE_QA	0.0904	0.0303
RESCALE_CX	0.0234	0.0302
RESCALE_RD	3.19e-13	5.73e-12
RESCALE_BR	2.88e-13	1.22e-11

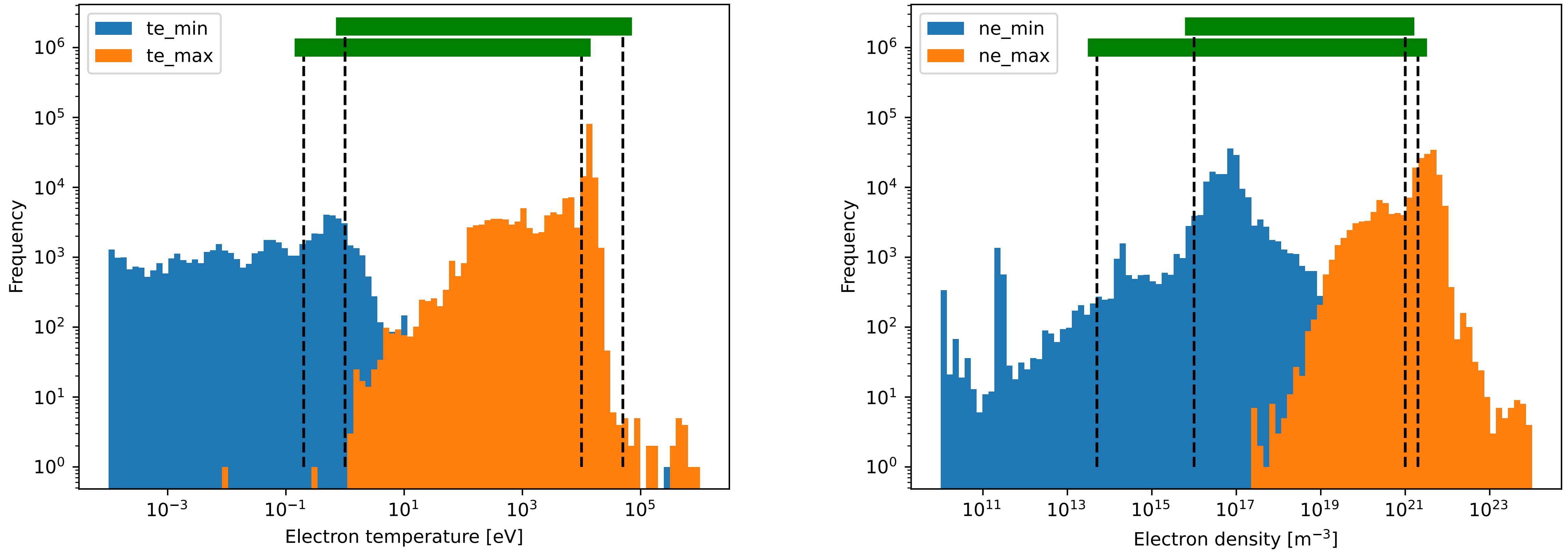
Another aspect: One of the common issues is the calculation of rates when extrapolation is needed

- (Stolen from a talk given at the IAEA AMPMI workshop in Helsinki, 2024)
- ADAS stores the ionisation/recombination/etc. data as a table of values of the logarithm of the quantity versus the logarithm of the electron density and temperature
  - Range used differs for different cases
    - ne for ’89 data seems to start at $1*10^{14}$, $1*10^{15}$ and $1*10^{16}$ and end at $1*10^{21}$ m^{-3}
    - Te for ’89 data seems to start at 1 and ends at 50 keV
    - ne for ’96 data seems to start at $1*10^{10}$, $5*10^{13}$ and $1*10^{14}$ and end at 2, 3, 5, or 10 * 10^{21} m^{-3}
    - Te for ’96 data seems to start at 0.2 and end at either 10 or 15 keV

- EIRENE uses (in a number of places), either a nine-order polynomial of one variable, or a 9x9 order polynomial in two variables
  - Fitted over some domain
  - With (increasingly) extrapolation formulae for use outside the domain
  - Can also break down in some cases

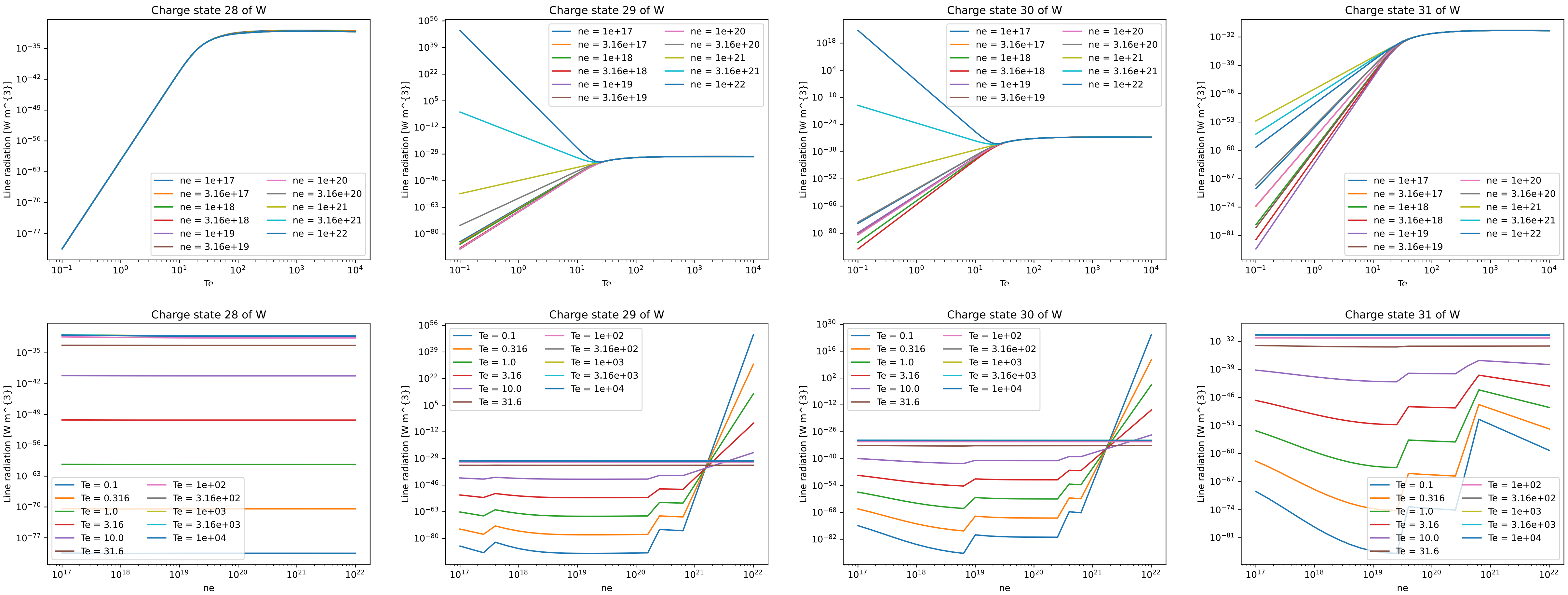
Need to think of the range of electron temperatures and densities needed: data extracted from a large set of SOLPS simulations

- Cases stored to the solps-mdsplus database (185188 cases)
- Extract the minimum and maximum electron temperature and density
- Show the ADAS adf11/scd89 and adf11/scd96 intervals



Need to make sure that the extrapolations don’t go wrong!

- Case where extrapolations for W line radiation went wrong:
  - The presence of a density dependence for some charge states resulted in very bad extrapolations



Getting back to the points raised at the beginning

- Sources of uncertainty
  - Multiple sources of uncertainty
- How can we deal with this uncertainty?
  - Know where it comes from
  - Don’t be too confident in your predictions
  - Trends are probably better predicted than point values
- Applying UQ methods
  - Can quantify which sources of uncertainty are most important
    - But only in some neighbourhood
    - Can be expensive in terms of computational demand
      - (Which is why the SOLPS-ITER runs I showed were 1D fluid neutral cases rather than drift cases with Monte Carlo neutrals)
  - Sensitivity scans are important if you can’t afford full UQ treatments