UQ for Atomic Data

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Summary

- Apply UQ to the coronal average charge state problem
- Use 3 parameters to vary the ionisation rates and 3 for the recombination rates
- Get the rates either from the ITER AMNS library (for this data, based on ADAS) or directly from ADAS
- Explore the variance in the results and the Sobol indices which explain the variance
- Compare the variances with those arising from different ADAS data-sets

- Need a better way of parametrising the uncertainty in the atomic data
- Need better data
- Look to apply this to SOLPS runs to explore the impact of uncertainty in the atomic data
How to add UQ?

- Approach taken here
  - Have Rate(te, ne) from, for example, ADAS
    - Change this to Rate(Te*V_{Te}, ne*V_{ne}) * V_{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
Results for applying these $\mathbf{v}$’s …

- Use (here)
  - $\mathbf{v} = [0.9, 1.1]$ in steps of 0.01
Now use the VECMA EasyVVUQ toolkit

- [https://github.com/UCL-CCS/EasyVVUQ](https://github.com/UCL-CCS/EasyVVUQ)
- Python package capable of running UQ “campaigns”
Some details

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

```
vary = {
    "El_te_vary":   cp.Uniform(0.8, 1.2),
    "El_ne_vary":   cp.Uniform(0.8, 1.2),
    "El_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 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
Results for $H$, $ne=3e19$

- Similar results for the total 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
  - Also see a contribution of the Te varying RC contribution at lower temperatures
Results for H, ne=3e19

• Explanation for the difference can be seen from the second Sobols
• Largest contributions from
  • RC_te_vary / El_te_vary
  • El_te_vary / RC_te_vary
Need to check the convergence with PCE order

- Scan PCE order 1..5
- The Sobols seem to converge quite well, and order 3 seems to be a good compromise between accuracy and speed
  - Order 3 requires 4096 samples
  - Order 5 requires 46656 samples
Now consider the results for W

- Average charge and total Sobols: $\text{El}_{\text{te\_vary}}$ dominant over most of the range except for an important $T_e$ range where $\text{RC}_{\text{te\_vary}}$ takes over …
ADAS has multiple data sets: compare UQ variation to those arising from the different data sets: H

- Different ADAS data-sets for H are very similar
- Plotting the distributions doesn’t tell us much more …
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  - Much larger than the variance coming from our choice of varying coefficients
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  - At 1000eV the average charge is somewhere between 24 and 43!
In conclusion

- Need a better prescription for how to vary the atomic physics data in order to do a sensitivity study
  - Ideally with a few parameters that can alter the information from ADAS
- While we can do a 5th order PCE campaign for the coronal cases, we want to look at the impact on edge simulations
  - 46656 samples took 10767.549 seconds (~0.23 seconds per case)
  - SOLPS run with just H might take a few hours without drifts and a week with drifts for each sample
- Can do dimension adaptive analysis, though
  - In a different context 1,048,576 samples was reduced to 1245, 40 days to 6 hours