The University of Texas at Austin

Bayesian inference of excited state population densities and equilibrium temperatures in argon plasmas using emission spectroscopy

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Dan Fries, Ruairi O’Connor, Todd A. Oliver, Noel T. Clemens, Philip L. Varghese

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Low-temperature plasma science, engineering, technology, and applications - Measurement and diagnostic techniques

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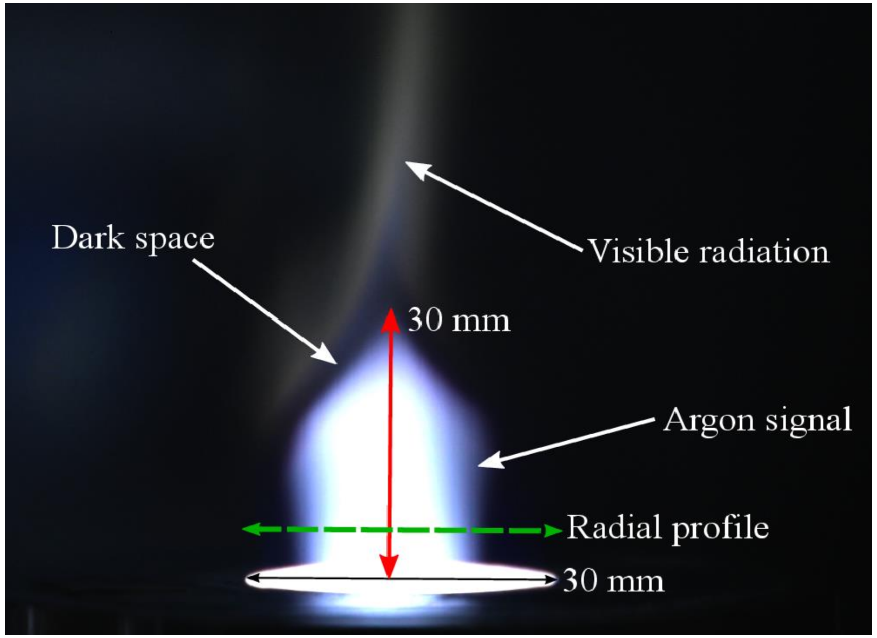
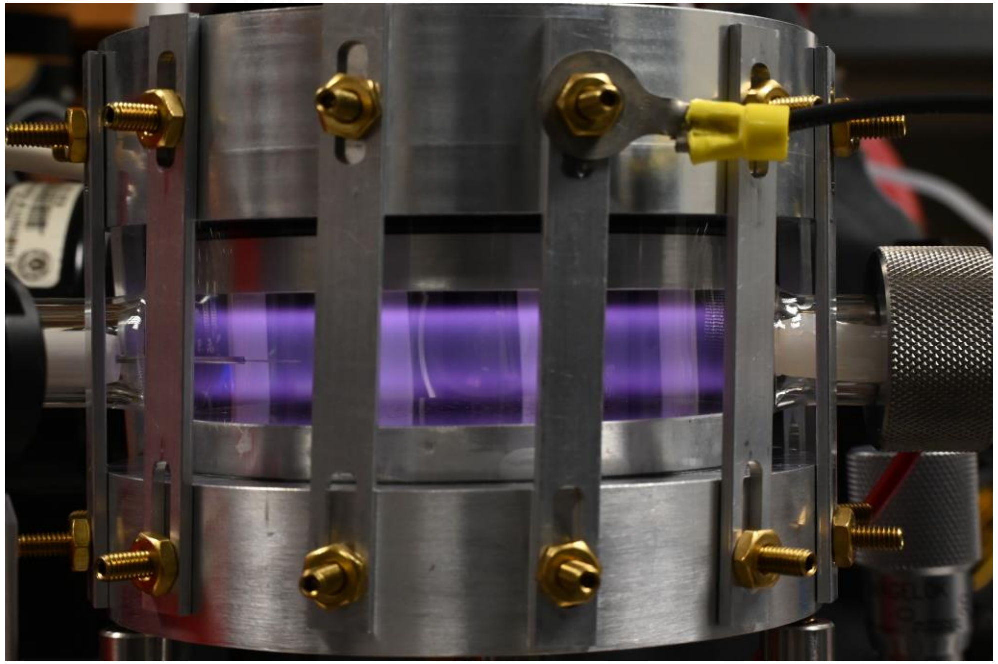
PSAAP III

Motivation

- Plasmas are relevant in material processing, medicine, energy production, hypersonics, and space propulsion.
- Complex chemistry and non-equilibrium states: **challenging for predictive modeling efforts**.
- Argon plasma: well known but limited diagnostic approaches.
- **Emission spectroscopy** both simple and applicable but **many uncertain parameters.**
- Bayesian inference for **UQ and higher fidelity results:**
  - →Has been done for singular transition in fusion device [1,2].
  - →Extract information over a larger spectral range.
  - →Include knowledge about transition parameters.
  - →Extract temperature and excited species number densities.

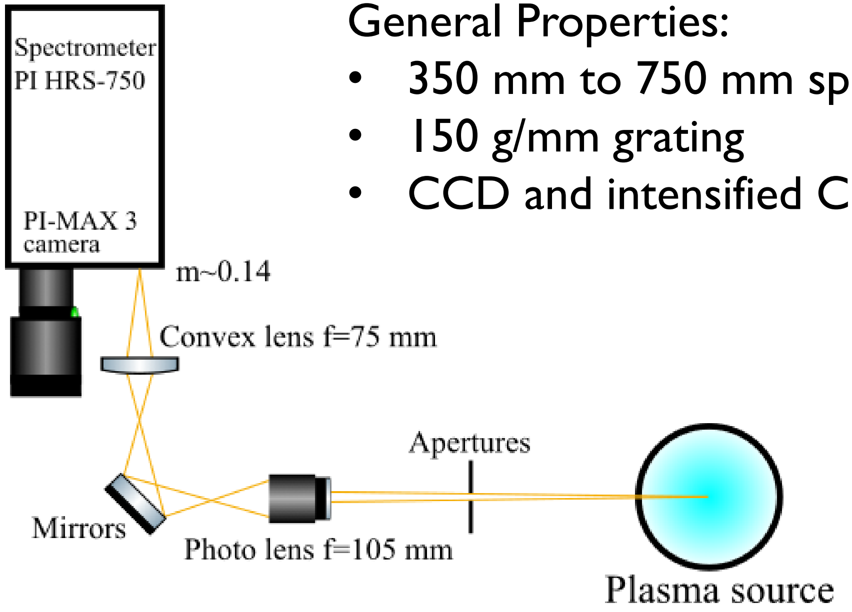




[1] Kwak et al., "Bayesian modelling of the emission spectrum of the Joint European Torus Lithium Beam Emission Spectroscopy system", *Rev. Sci. Inst.* (2016)
[2] Kwak et al., "Bayesian electron density inference from JET lithium beam emission spectra using Gaussian processes", *Nucl. Fusion* (2017)

Experimental Setup

Argon spectroscopy



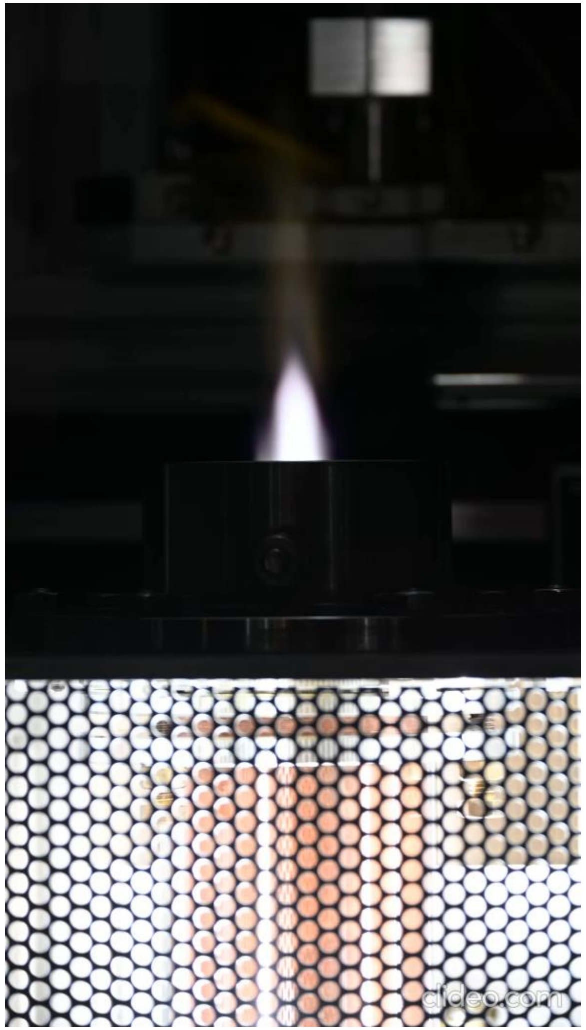
General Properties:

- 350 mm to 750 mm spectrometer
- 150 g/mm grating
- CCD and intensified CCD cameras

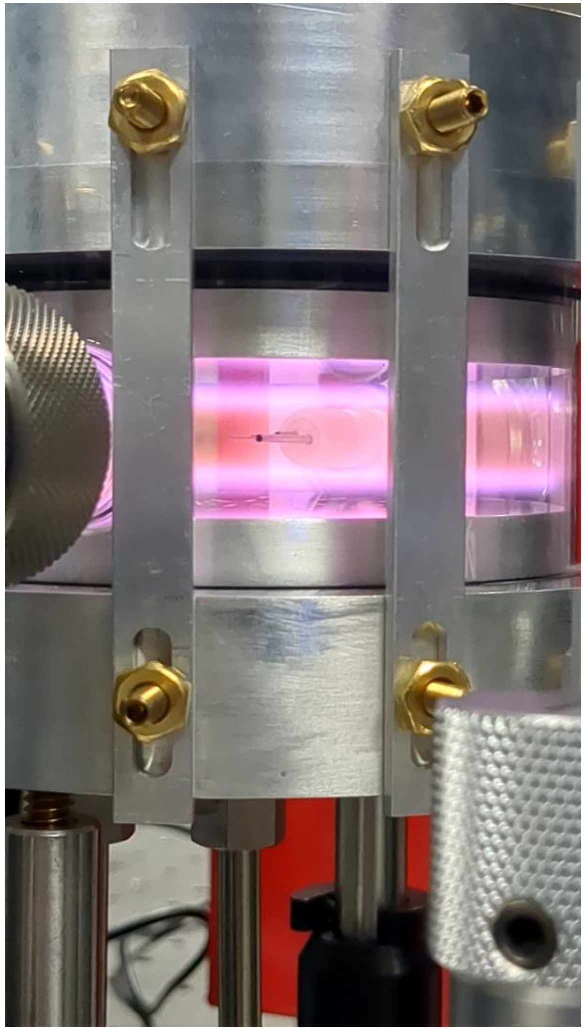
Measured signal counts

$$S(\lambda) = \int_A \eta_\lambda \tau_\lambda \frac{\Omega}{4\pi} \int_{\Delta L} \sum n_j A_{ji} \frac{hc}{\lambda_{ji}} \varphi(\lambda_{ji}, w)\ dl\ dy \frac{d\lambda}{dx} dx$$

ICP plasma torch



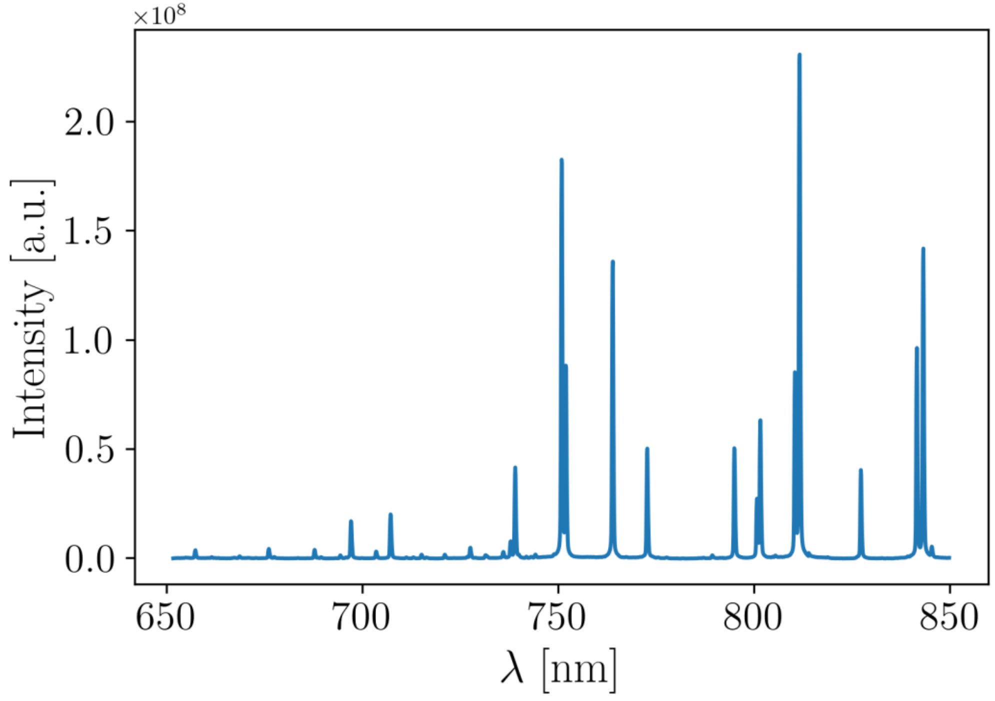
Capacitive glow discharge



Bayesian Formulation

- Bayes' theorem: $\underbrace{p(x|b)}_{\text{posterior}} \propto \underbrace{p(b|x)}_{\text{likelihood}} \cdot \underbrace{p(x)}_{\text{prior}}$
- Take x to be quantities of interest: T, n_j
- x can include additional uncertain parameters: $\Delta L, w, A_{ji}$
- b is a vector of **observations**, i.e. the data that has been collected,
  - could be raw camera counts,
  - could be intensity corrected spectra,
  - could be emission coefficients.

Observation: argon plasma spectrum



Bayesian Formulation – Population Density

Applied to capacitive glow discharge

- Measurement $\bar{\epsilon}_{ji} = \int_{\Delta\lambda} C(\lambda)\, S_{ji}(\lambda)$ and model $\widehat{\bar{\epsilon}_{ji}} = n_j\, A_{ji}\, \frac{hc}{\lambda_{ji}} \Delta L$ with

$$\bar{\epsilon}_{ji} = \widehat{\bar{\epsilon}_{ji}} + \varepsilon \text{ or more generic } b = \hat{b} + \varepsilon$$

- The error ε is additive and a combination of random and shot noise, *approximated by Gaussian PDFs* → Likelihood: multi-variate normal (MVN) distribution

$$p\left(\boldsymbol{b} \middle|\, \boldsymbol{n_j}, \boldsymbol{A_{ji}}, \Delta L = \boldsymbol{x}\right) = \frac{1}{\sqrt{(2\pi)^m \det(\Gamma_e)}}\, exp\left\{-\frac{1}{2}\left[\boldsymbol{b} - \hat{\boldsymbol{b}}(\boldsymbol{x})\right]^T \Gamma_e^{-1}\left[\boldsymbol{b} - \hat{\boldsymbol{b}}(\boldsymbol{x})\right]\right\}$$

$$\Gamma_e \approx \frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{b}_{\mathrm{ref}}^{(i)} - \bar{\boldsymbol{b}}_{\mathrm{ref}}\right)\left(\boldsymbol{b}_{\mathrm{ref}}^{(i)} - \bar{\boldsymbol{b}}_{\mathrm{ref}}\right)^T + \boldsymbol{C}\mathrm{diag}(\boldsymbol{\mu}_S)\boldsymbol{C}^T$$

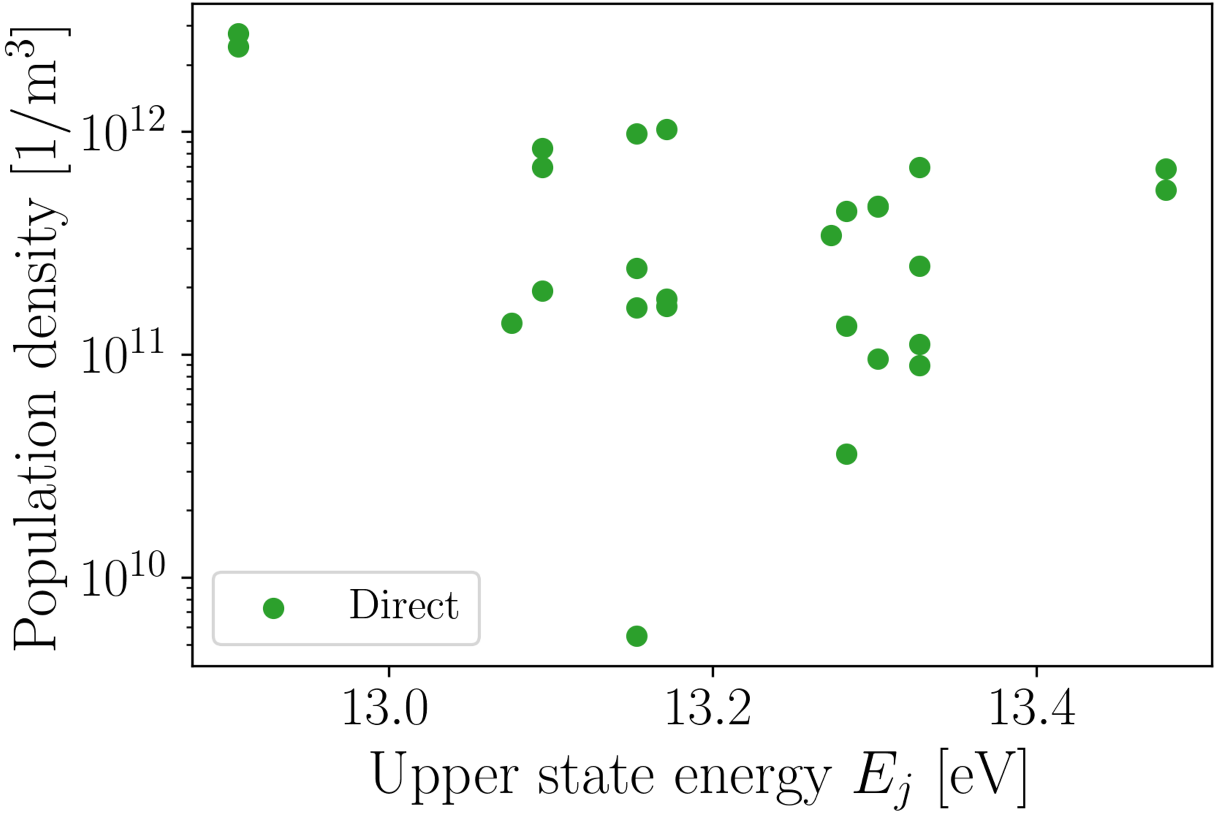
Assumptions:

- Intensity correction $C(\lambda)$ and baseline have no uncertainty
- Each measurement is completely independent
- No model uncertainty from choice of lineshape

Bayesian Formulation – Population Density

- Priors:
    - n_j: Gaussian, locally flat with very large standard deviation, mean is first guess from LSQ solution
    - A_{ji}: Gaussian, data from NIST, **marginalized out of likelihood** to reflect knowledge
    - ΔL: Gaussian, from auxiliary measurements
- Observed 26 transitions from 10 states

Direct: $\bar{\epsilon}_{ji} = n_j A_{ji} \frac{hc}{\lambda_{ji}} \Delta L$



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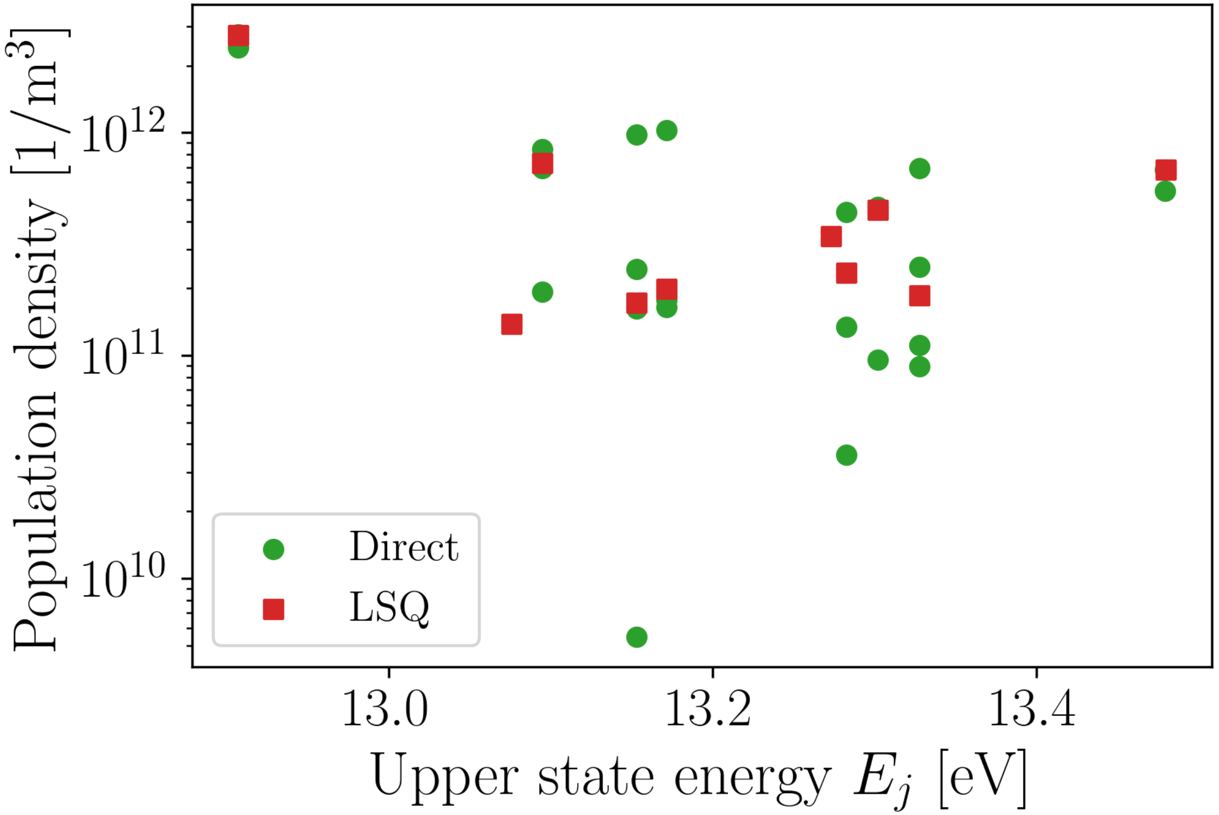
Least-squares solution: maximize unweighted likelihood



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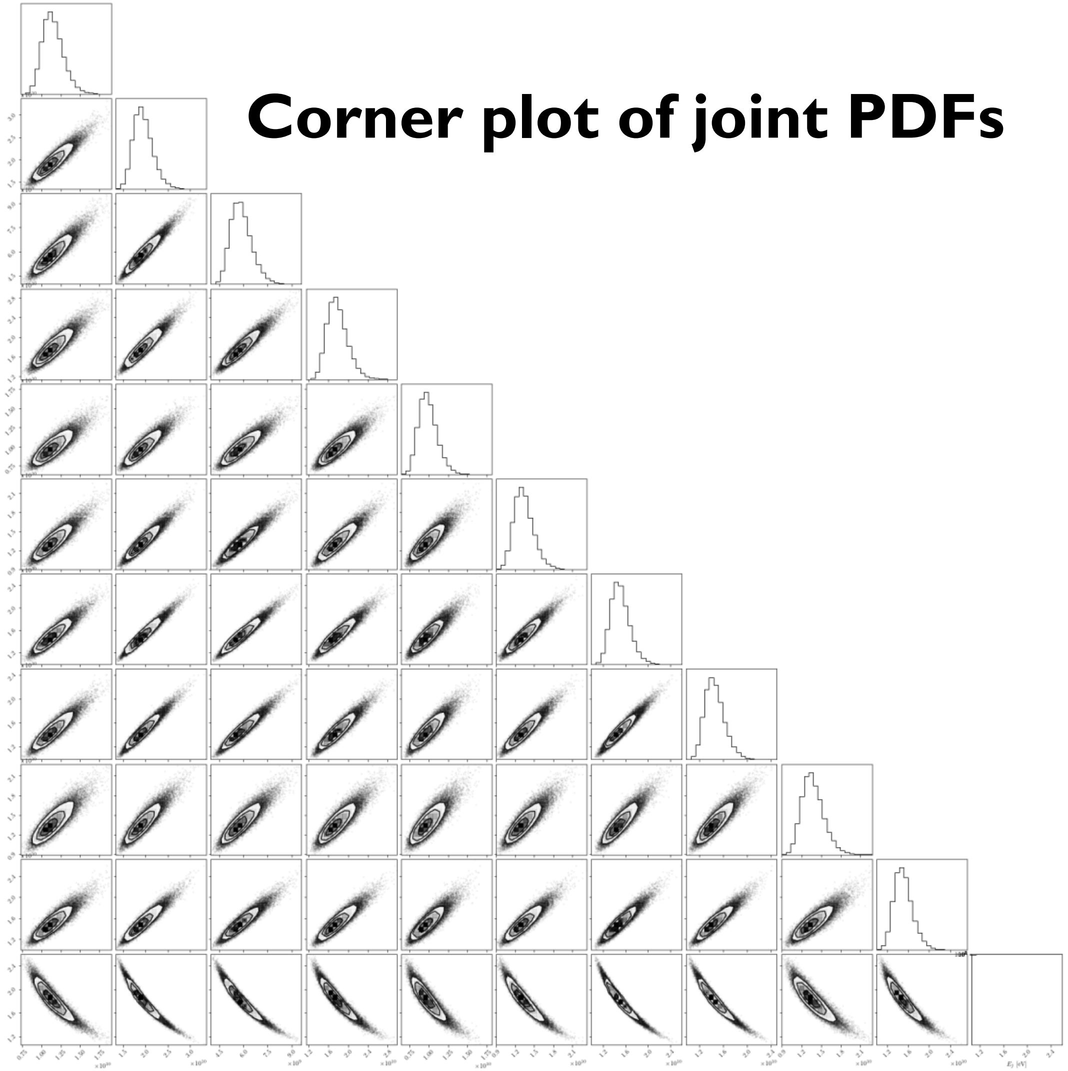

Corner plot of joint PDFs

[1] Foreman-Mackey et al., “emcee: The MCMC Hammer”, *Publ. Astron. Soc. Pac.* (2013)

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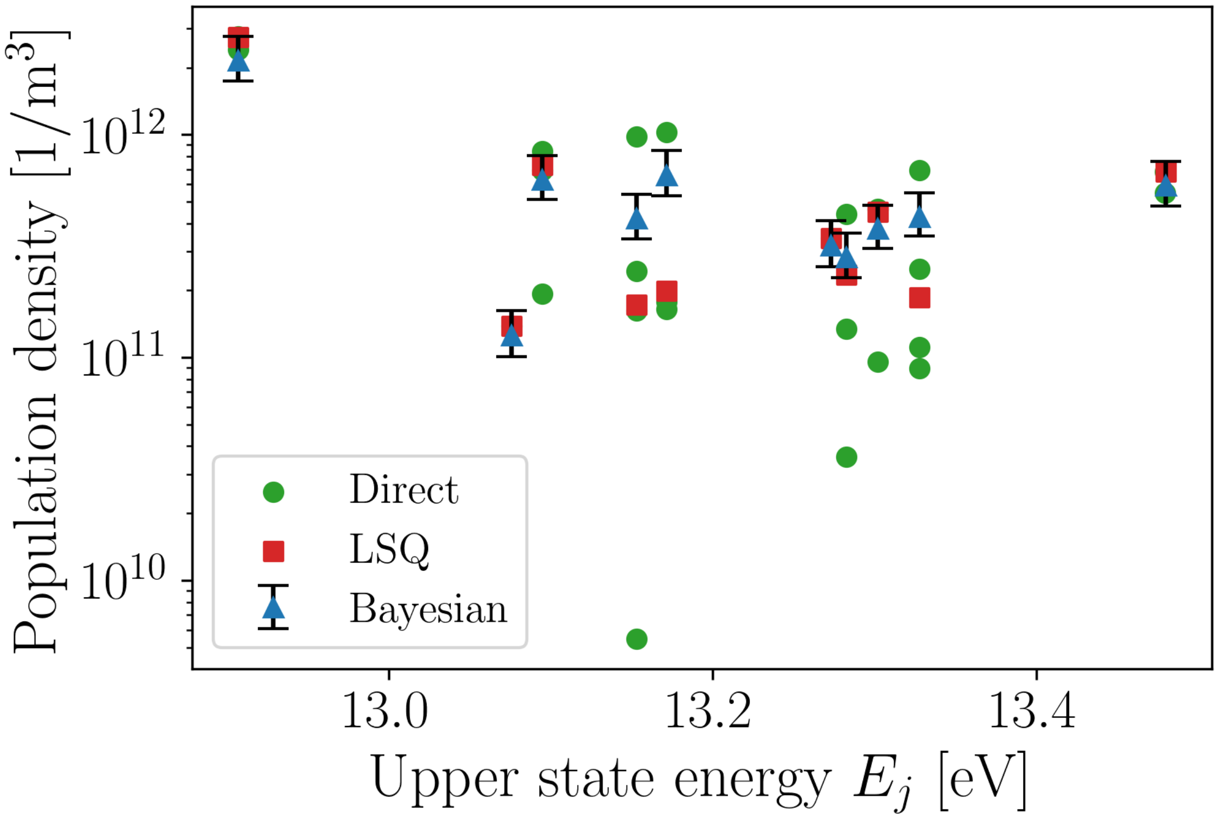
Bayesian Result



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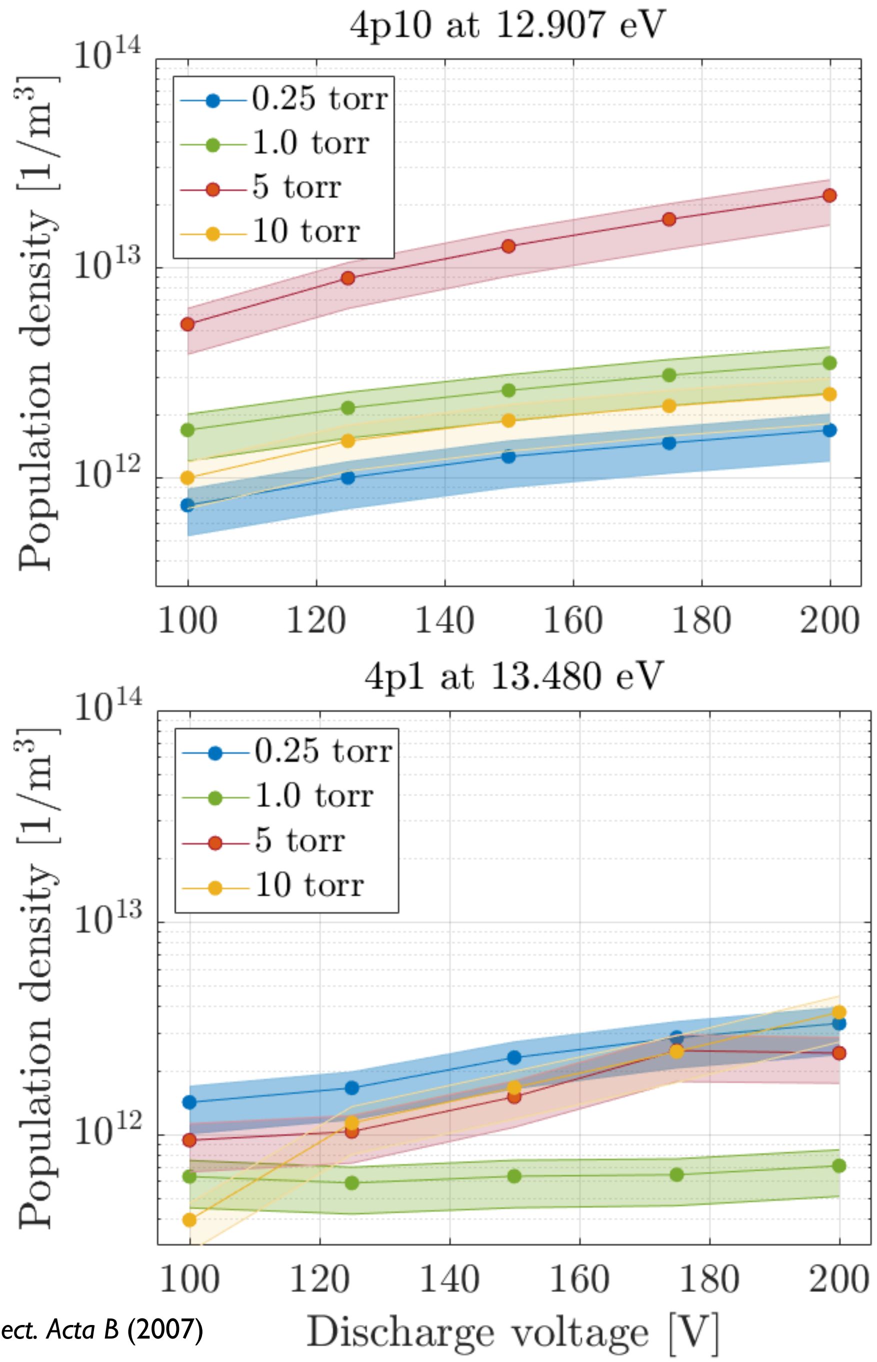
Results – Population Density

- $\overline{\Delta L} = 1.8 \pm 0.4$ cm (compare to 10 cm diameter of glow discharge).
- 1torr results on same order of magnitude as detailed collisional-radiative model [1].
- Can use results for validation and comparison to lumped states models.



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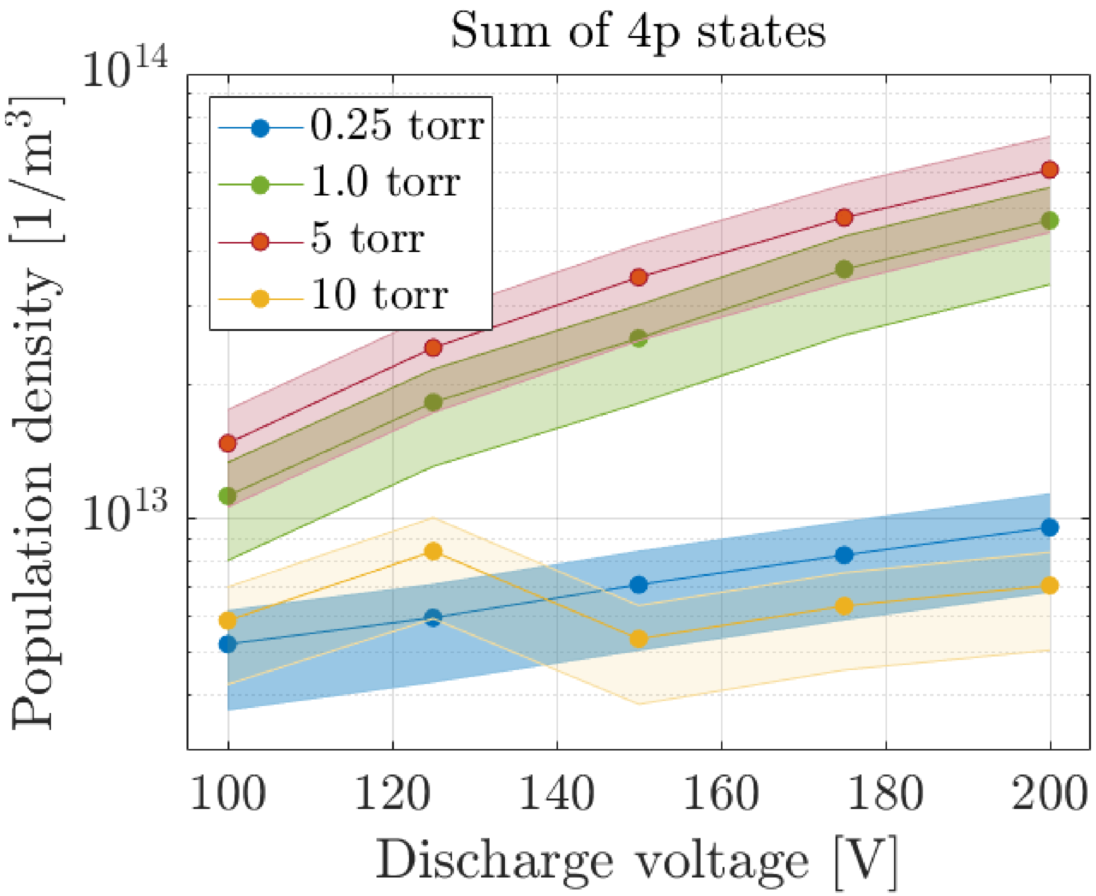

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Bayesian Formulation – Temperature

Applied to ICP plasma torch

- Measurement model in thermal equilibrium:

$$\hat{L}_{e,\lambda}(\lambda) = \sum g_j e^{-E_j/kT} \frac{A_{ji}}{\lambda_{ji}} \varphi\left(\lambda_{ji}, w\right) = \hat{b}$$

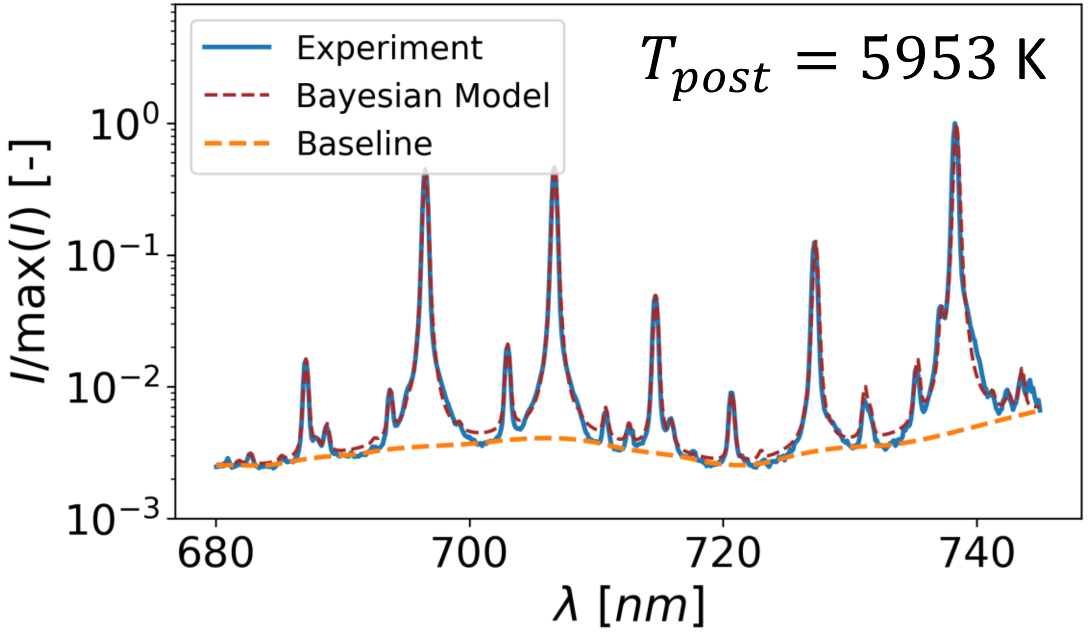
$$b = \hat{C}(\lambda) S(\lambda)$$

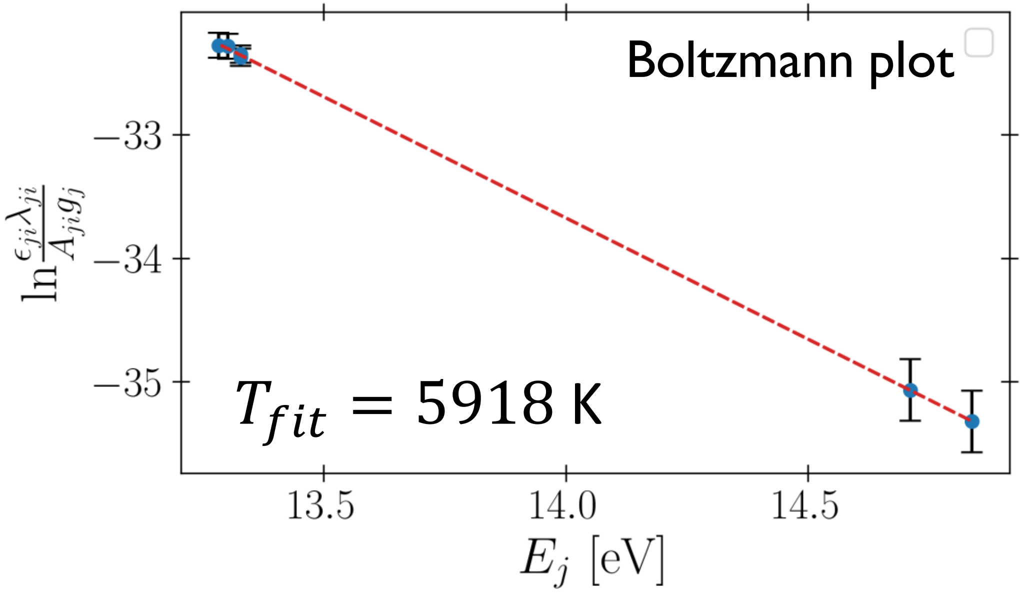
- Likelihood: assume additive error as before, $\boldsymbol{x} = (\boldsymbol{T}, \boldsymbol{w})$
- Priors:
  - T: Gaussian, locally flat with very large standard deviation, mean is first guess from LSQ solution
  - w: Gaussian, from preliminary processing tests
- Assumptions: same as in population density approach
  → marginalization in A_{ji} is *work in progress*.
- Posterior: sampled using emcee package (Markov-Chain Monte-Carlo):
  5,000 samples, mean acceptance ratio ~0.64

Results –Temperature

- Temperatures:
  - Median: 5953 K
  - 5%: 5858 K
  - 95%: 6051 K
- Voigt lineshape (w_G, w_L)
  - Median: (0.30,0.20)
  - 5%: (0.29,0.20)
  - 95%: (0.30,0.21)
- Temperature from Boltzmann plot method: 5918 ± 1000 K

→ Uncertainties in Bayesian result very low due to missing marginalization in A_{ji}.





Conclusions

- Bayesian framework to extract information from emission spectroscopic data.
- Includes a priori knowledge about spectroscopic and instrument parameters.
- Provides direct estimate of uncertainties.

Future work

- Add inference of intensity calibration and baseline.
- Unify treatment of population densities and temperature.
- Extract additional information with more complex measurement model
  - Electron number density
  - Multi-temperature EEDFs
  - Molecular Species

THANK YOU!

Questions?

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