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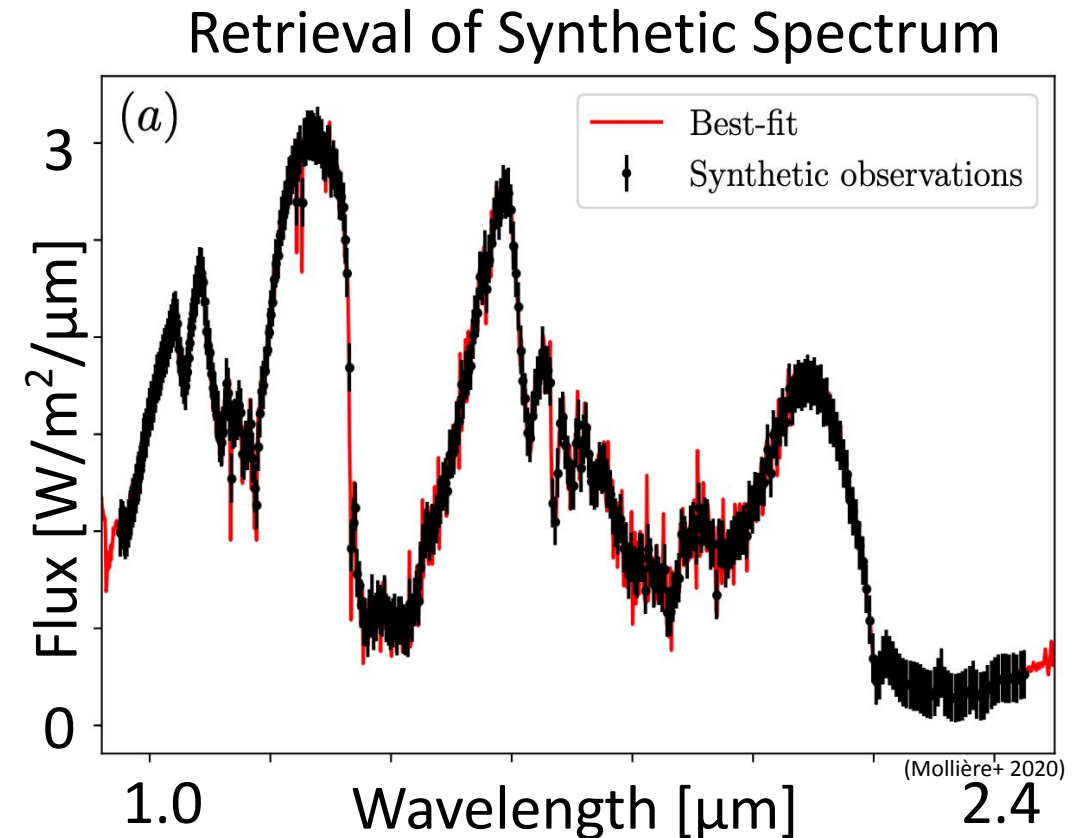
# RACER

(**RA**pid Calculation of **Exo**planetary  
**R**adiative opacities)

# Opacities are Important



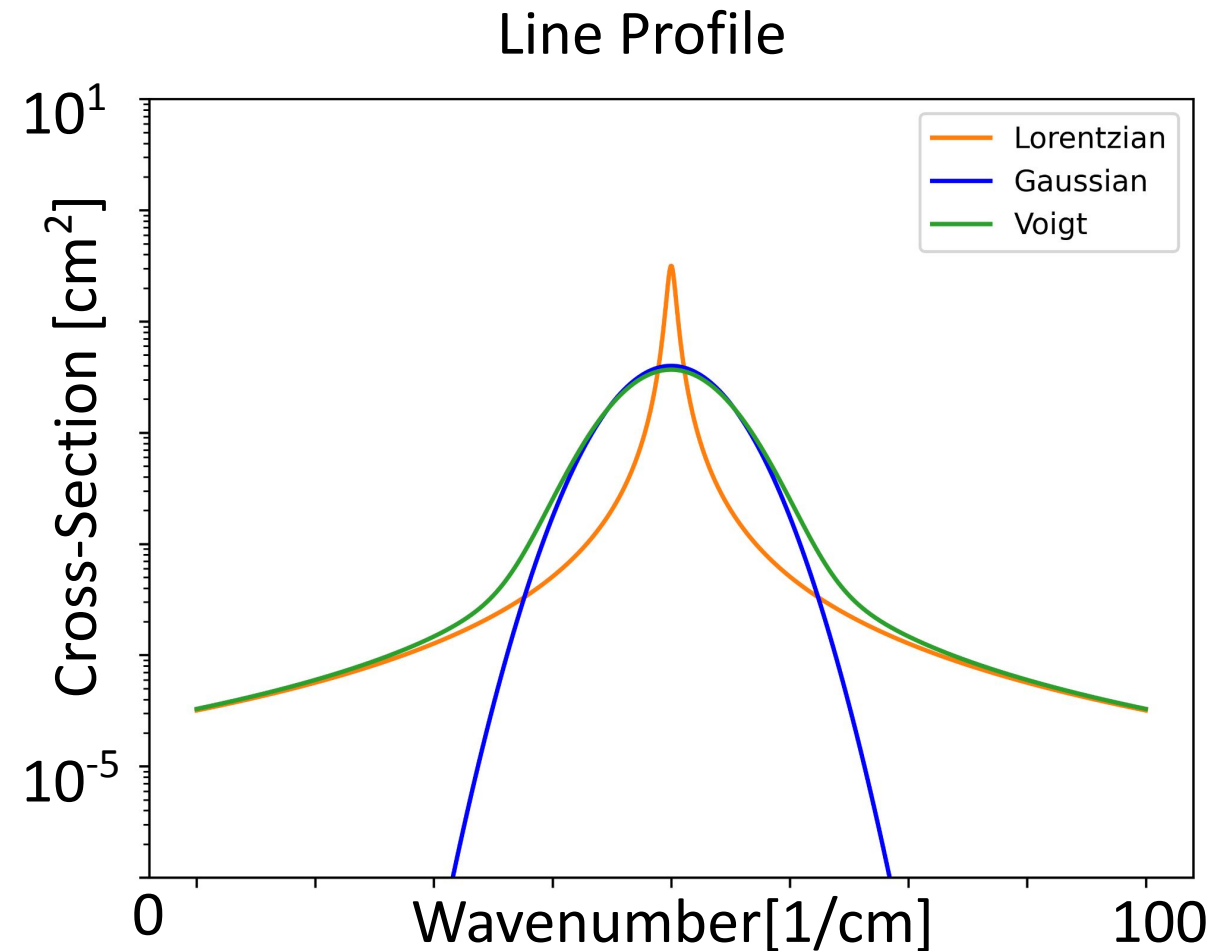
- Lines are transitions of quantum states
  - Electronic, vibrational, rotational
- Opacities important for atmospheric analysis
- Higher resolution → better constrained opacities
- Growing molecular and atomic line lists  
( $5 \times 10^{10}$  lines) → fast calculation





# How to Calculate the Lines

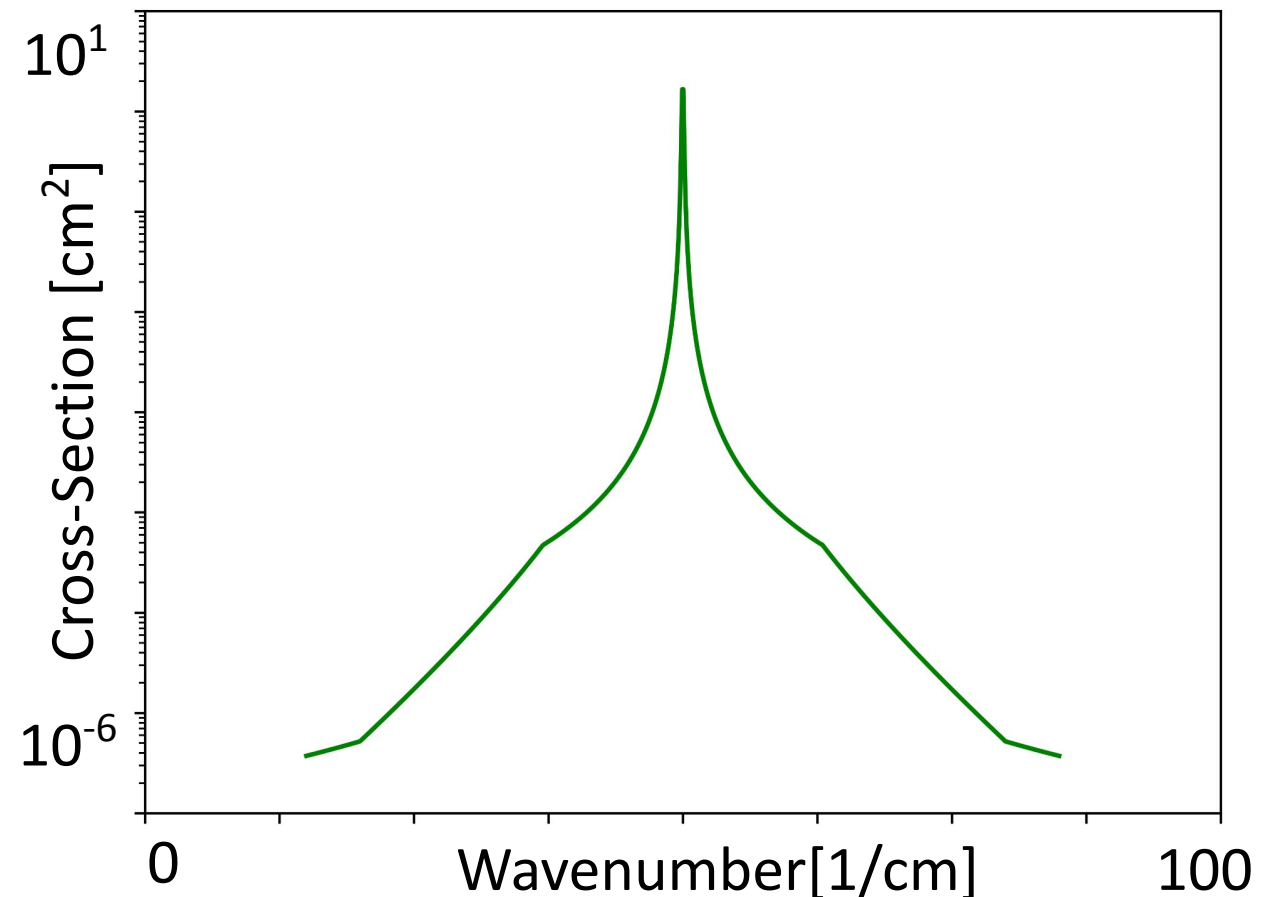
- Heisenberg (1927): Absorption line energies are not a delta function
- Additionally broadened by
  - Collisions (Lorentzian)
  - Relative velocity (Gaussian)
- Computationally expensive





# RACER: Calculating Line Profiles from Line Lists

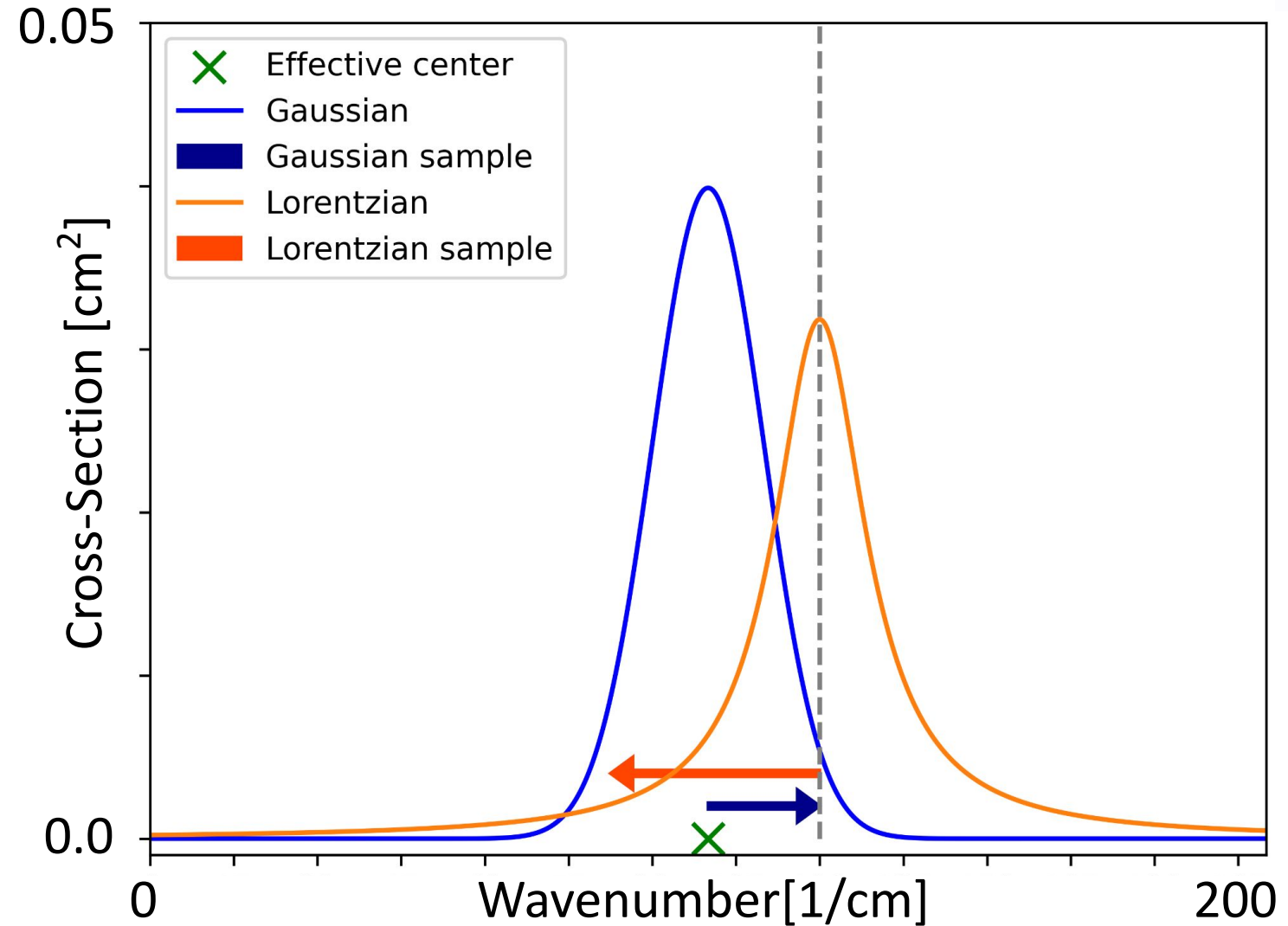
- Opacities for petitRADTRANS (Mollière+ 2019)
  - Why another code? → flexibility
    - Adapt to the latest line lists
    - Broadening parameters
    - Line wing treatment
- Line Profile + cutoff + sub-Lorentzian treatment





# Sampling the Voigt Profile (Min, 2017)

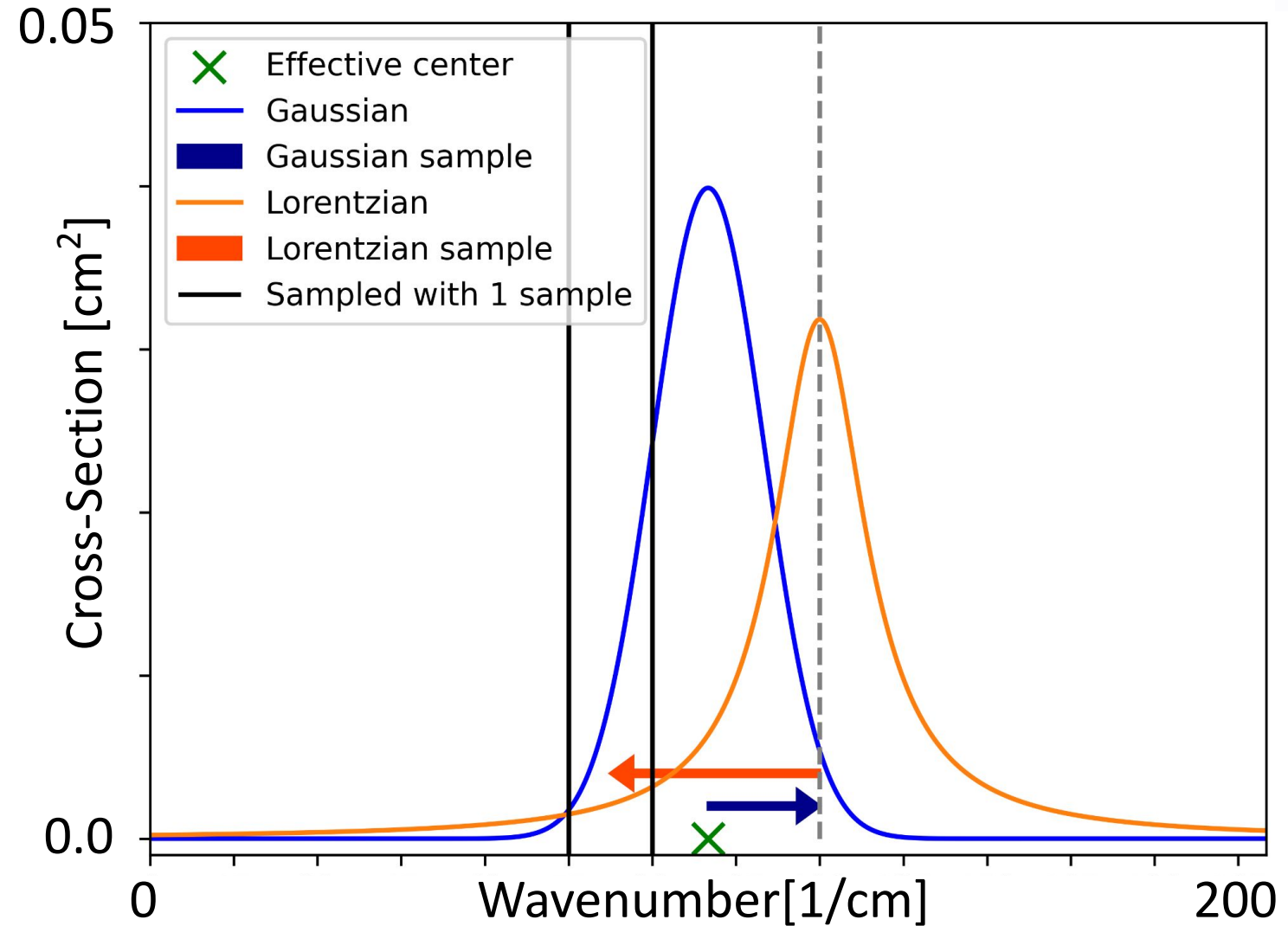
- Take a Gaussian sample
- Add the Gaussian sample to effective line center
- Take a Lorentzian sample and add it



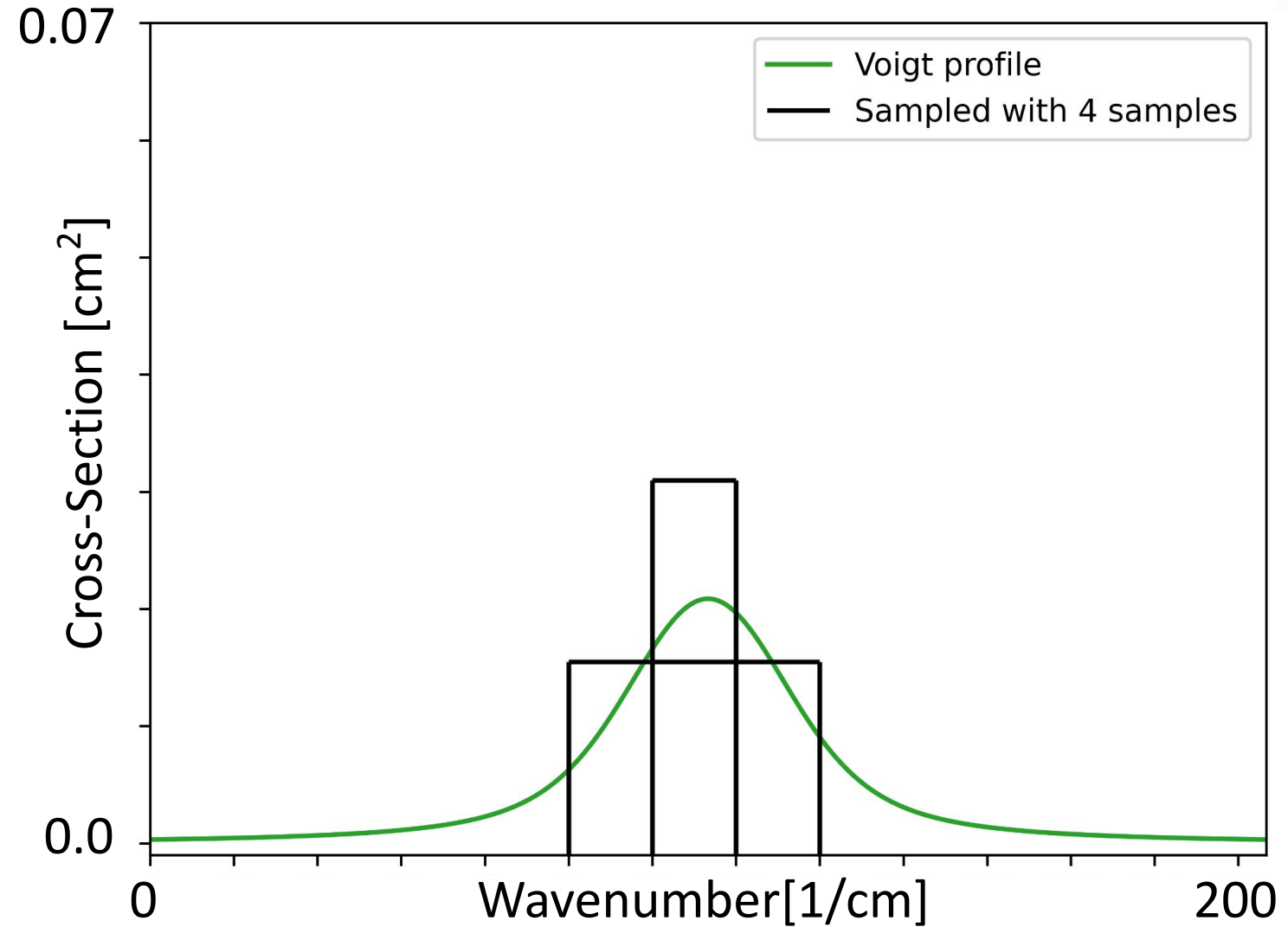


# Sampling the Voigt Profile (Min, 2017)

- At the sampled location  
add the weight to the  
bin

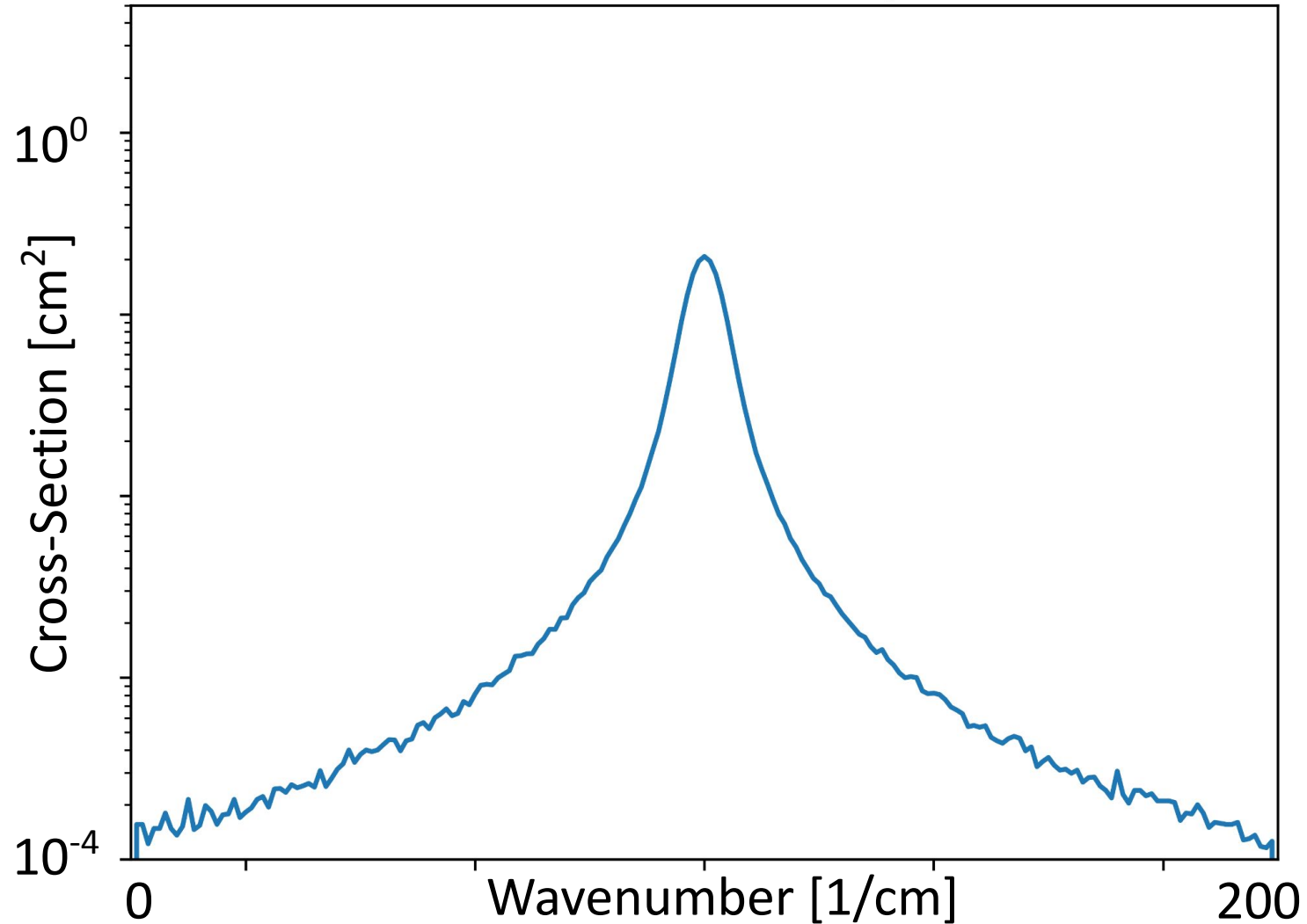


# Sampling the Voigt Profile (Min, 2017)



# Sampling the Voigt Profile (Min, 2017)

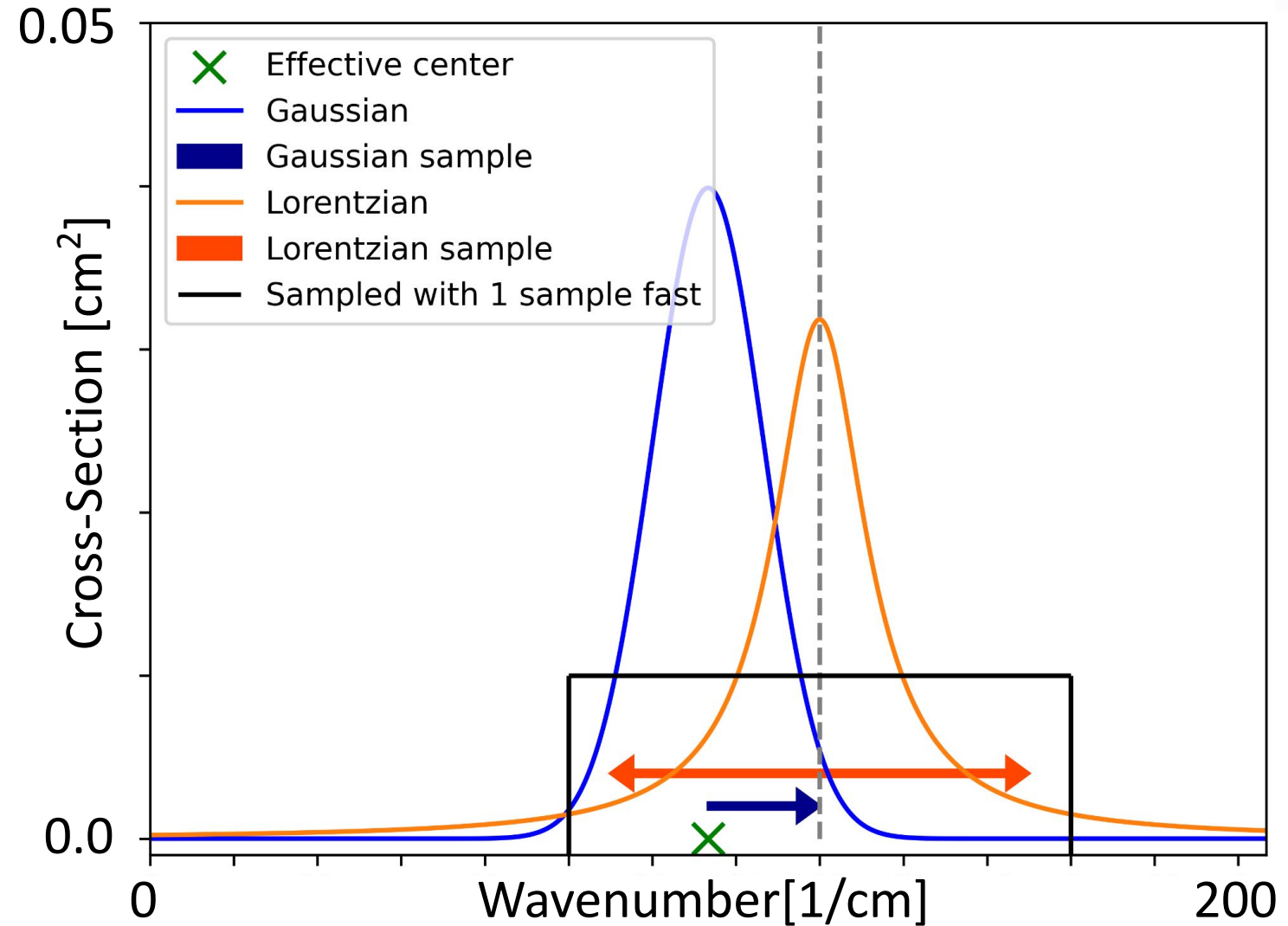
1 000 000 samples





# Sampling the Voigt Profile Faster (Min, 2017)

- Add and subtract absolute value of Lorentzian sample
- Add weight in all bins in the intervall



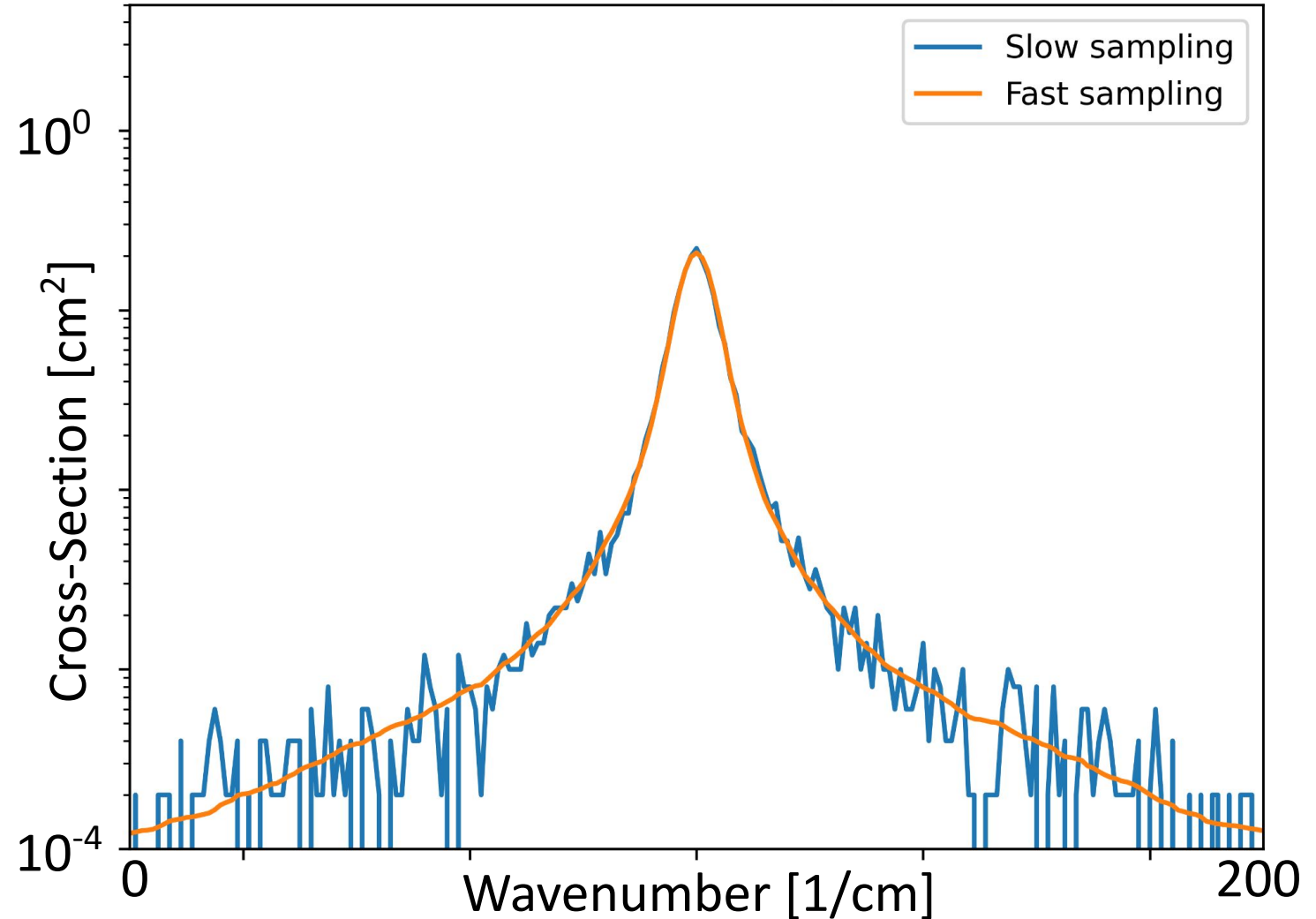
# Sampling the Voigt Profile Faster (Min, 2017)



10 000 samples

Speedup:

- Spread the sample
- Weight by the width



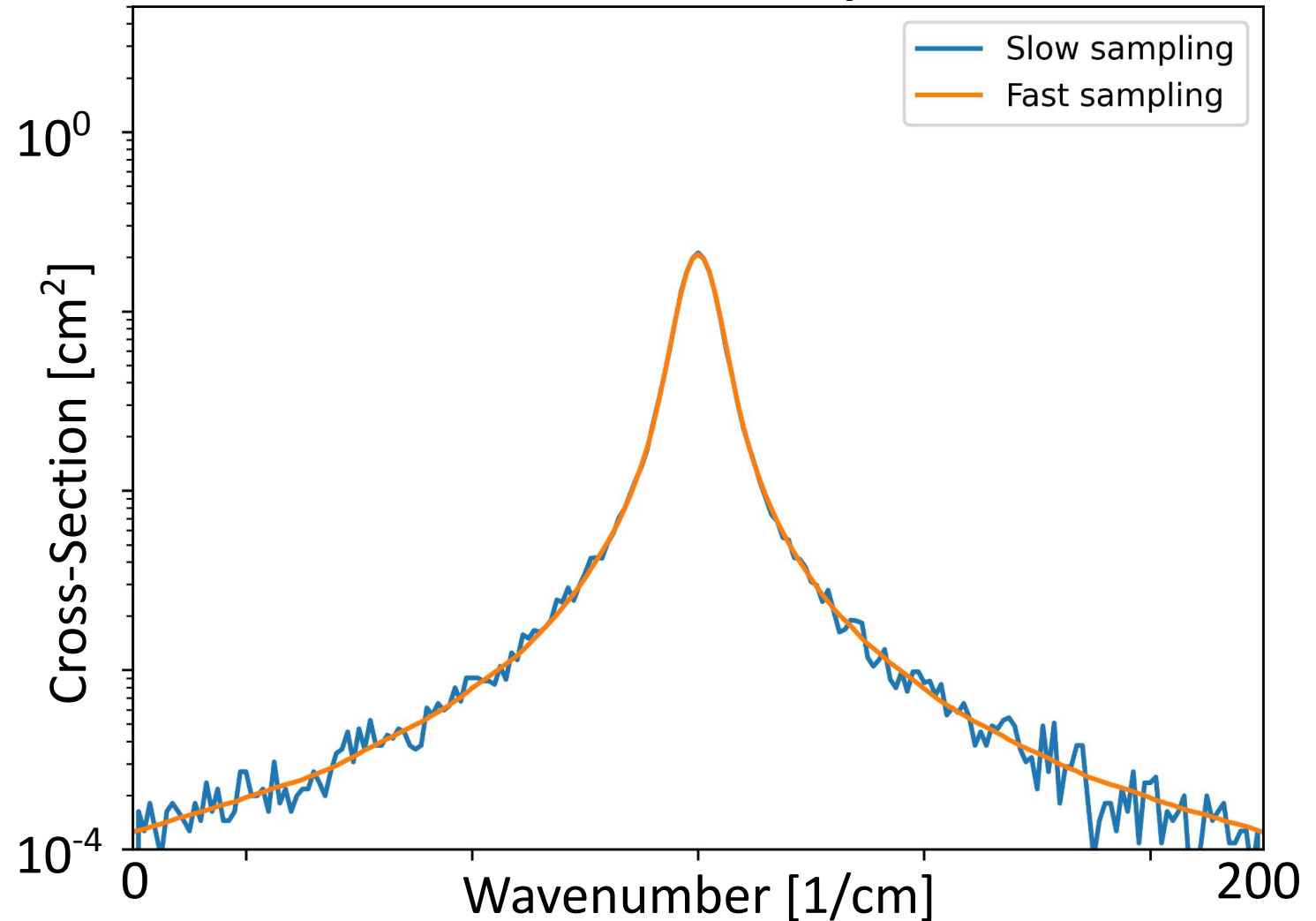
# Sampling the Voigt Profile Faster (Min, 2017)



110 529 samples

Speedup:

- Spread the sample
- Weight by the width



# Sampling Profiles is Faster

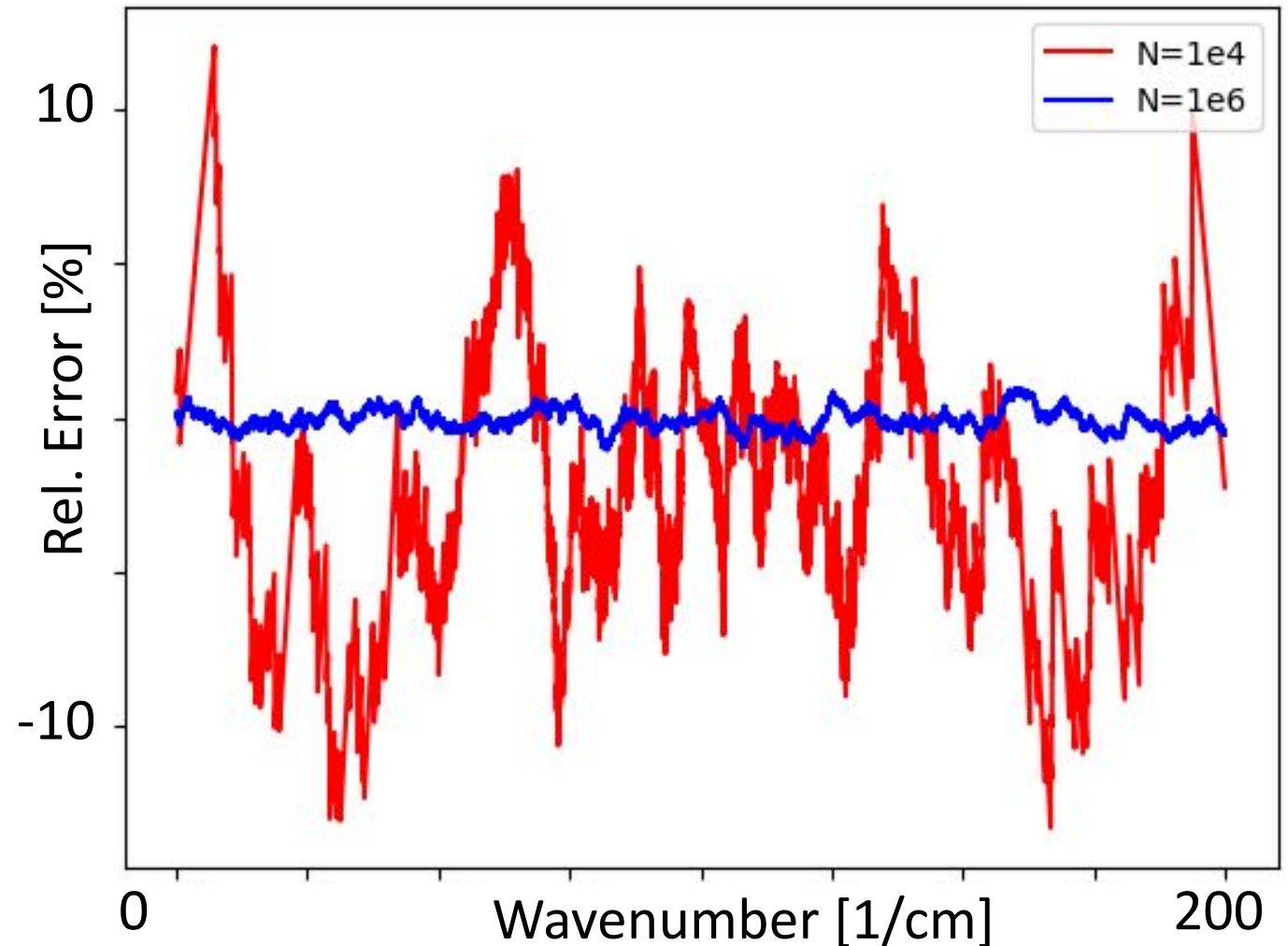


Sampled vs. Calculated Profile

- Line dependent calculation time
- Number of samples is function of

$S, \gamma, R, \varrho$

- $S$ : Line strength
- $\gamma$ : Lorentz width
- $R$ : Resolution
- $\varrho$ : Line density





# Sampling Profiles is Faster - Speedup

- With this method: Up to  $10^5$  lines/s
- Bottleneck: Normalizing the profiles
- Speedup  $\rightarrow$  new in my work: Use pre-normalized samples  $\rightarrow$  up to  $4 \times 10^6$  lines/s
- Sampling weak lines as continuum lines

- $S$ : Line strength
- $\gamma$ : Lorentz width
- $R$ : Resolution
- $w$ : Weight
- $\nu_{\text{eff}}$ : Effective wavenumber
- $\Delta\nu_{\text{press}}$ : Lorentz sample shift

Min, 2017

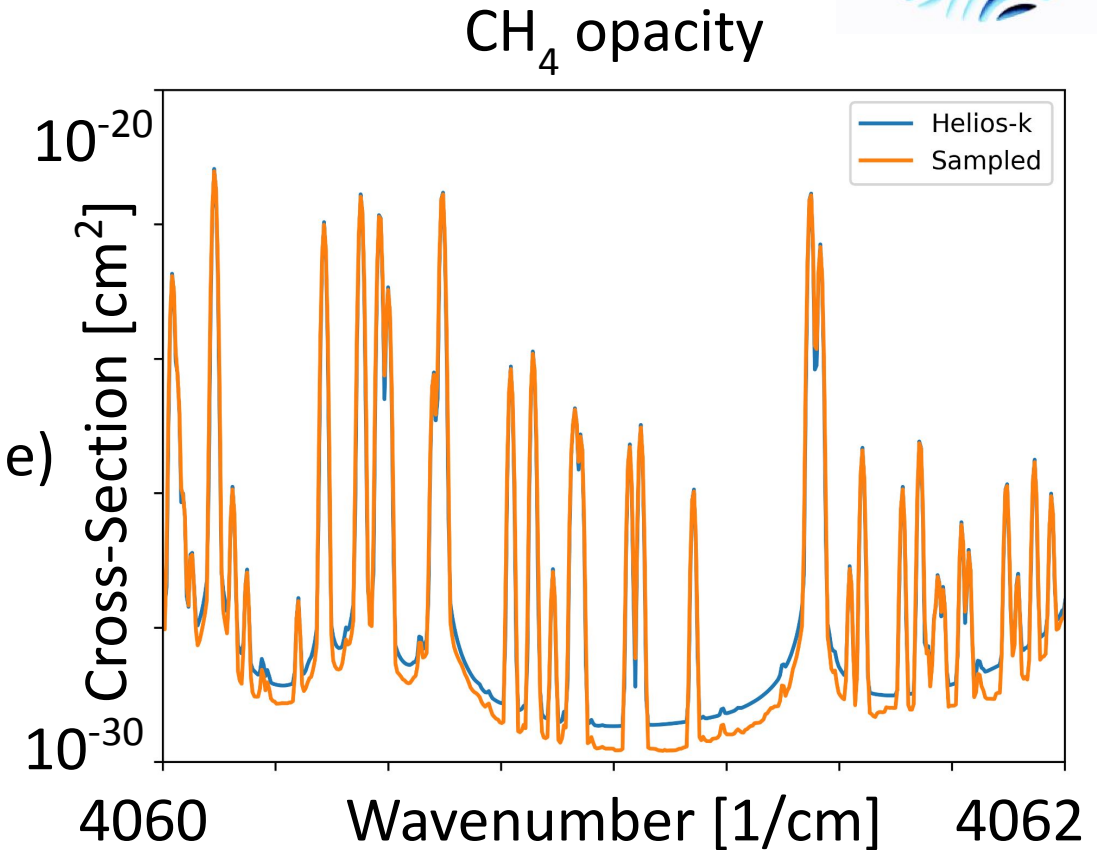
$$w = \frac{\Delta\nu_{\text{press}}^2}{\Delta\nu_{\text{press}}^2 + \gamma^2} \frac{2S}{N_{\text{samples}}} \frac{R}{\nu_{\text{eff}}}$$

# Thin Lines are a Problem



- CH<sub>4</sub> Exomol, 80K, 10<sup>-6</sup> bar
- Unlikely to sample in the wings
- More samples per line -> slow
- Fix: Straight forward profile calculation (own code)
  - $\Delta\nu_{\text{press}}$ : Lorentz sample shift
  - $\gamma$ : Lorentz width
  - $\gamma_{\text{random}}$ : Lorentz sample

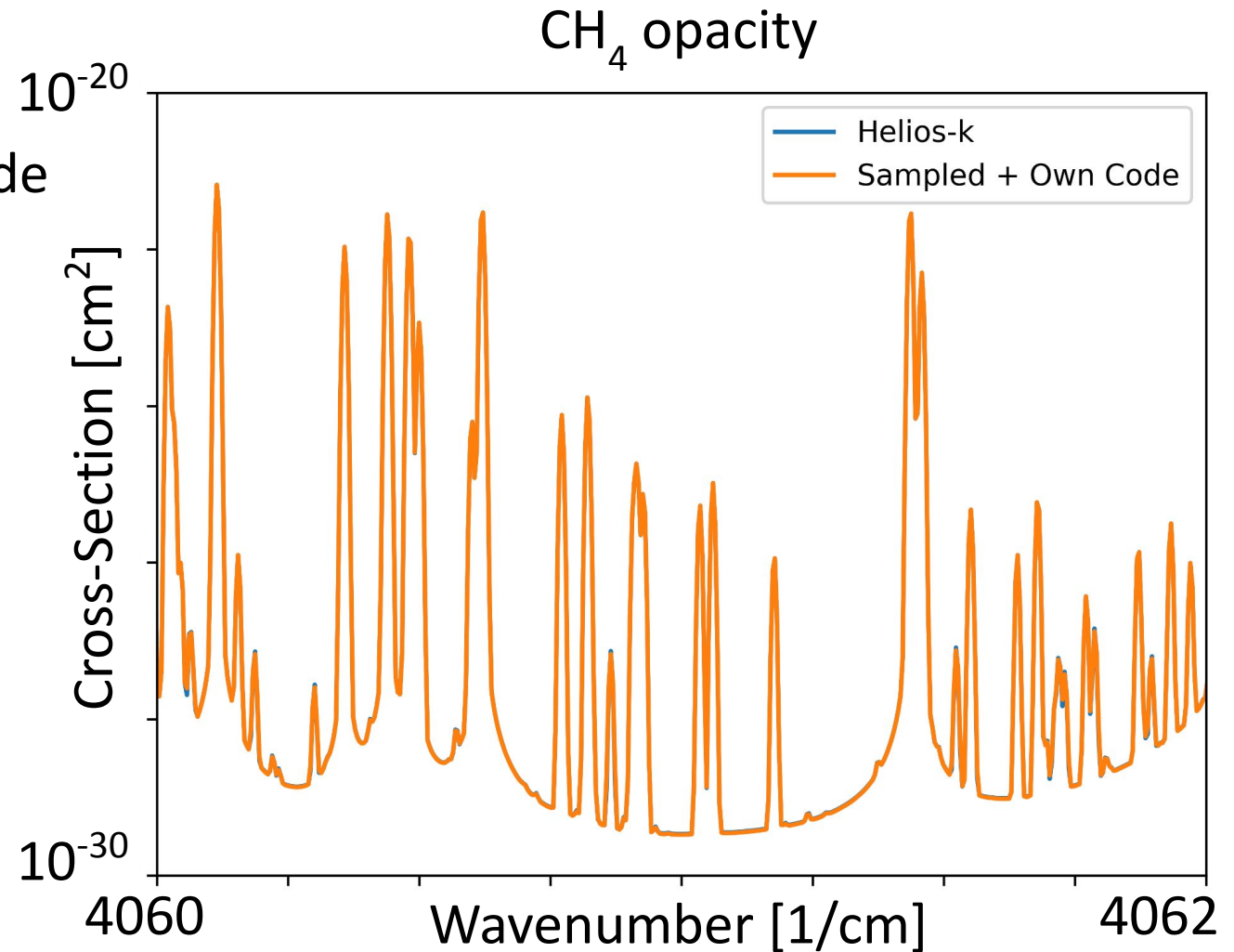
$$\Delta\nu_{\text{press}} = \gamma(p, T) \cdot \gamma_{\text{random}}$$





# Using Own Code for Strongest Lines

- CH<sub>4</sub> Exomol, 80K, 10<sup>-6</sup> bar
- Calculating strongest lines with own code
- Own code: Mollière+ 2015 method
- Speedup: Coarse grid and interpolation



# RACER



- Python package to calculate opacities
- Line profile calculation by sampling method (Min, 2017)
- Very strong lines by own code (using Humlicek algorithm)
- Fast calculation ( $4 \times 10^6$  lines/s) even for huge line lists

Happy to get any input for additional features!! 🎉

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