

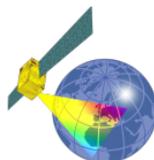
Proposal for a new parametrisation of the instrumental spectral response function in DOAS retrievals

DOAS workshop 2016, Brussels

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MAX-PLANCK-INSTITUT
FÜR CHEMIE



Satellite Remote
Sensing

Motivation

- Instrumental Spectral Response Function (ISRF) (“Slit Function”) is a key quantity in spectroscopy
- Wavelength calibration
- DOAS: cross-sections at instrument resolution
- ISRF can be measured (e.g. Hg lines, tunable laser)
- But:
 - ISRF changes with wavelength
 - ISRF **changes with time!**
- → Parametrisation required

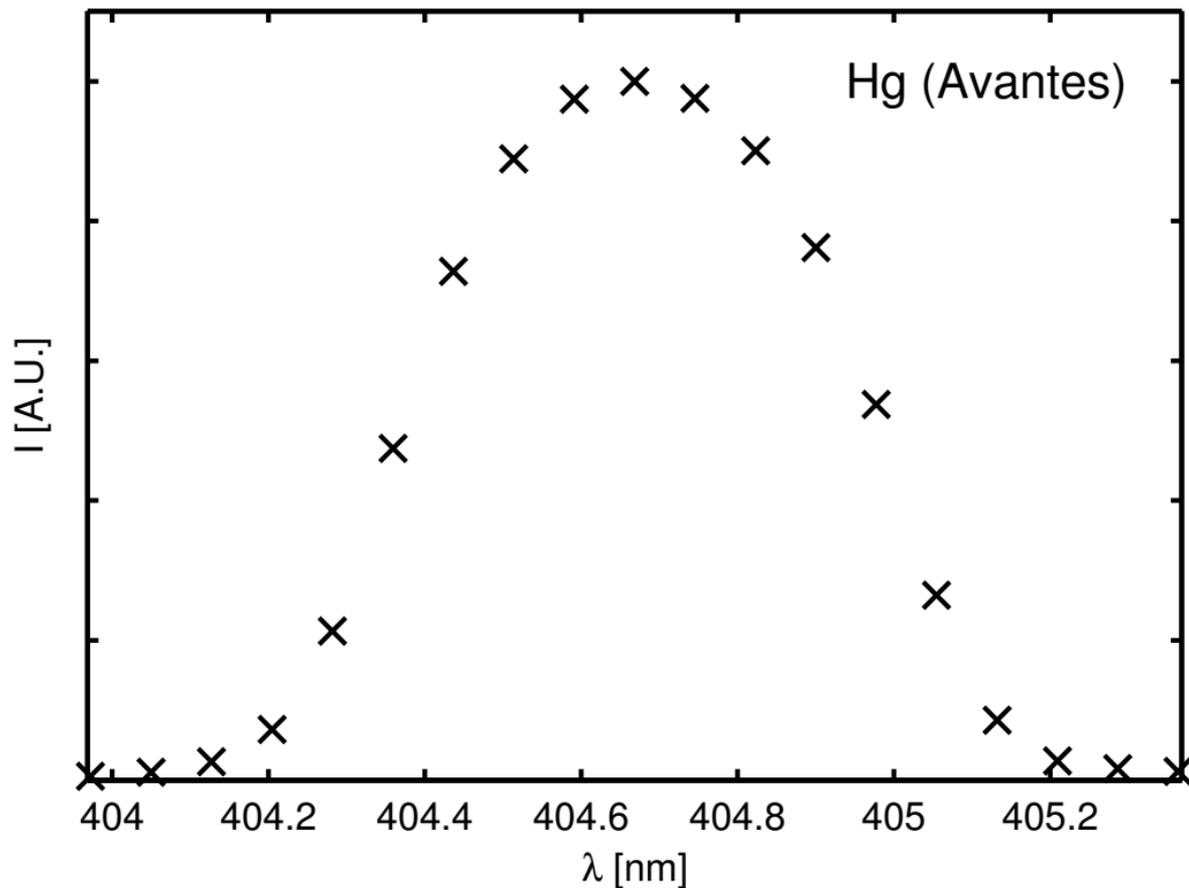
Motivation

If “true” ISRF not known (or not trusted):

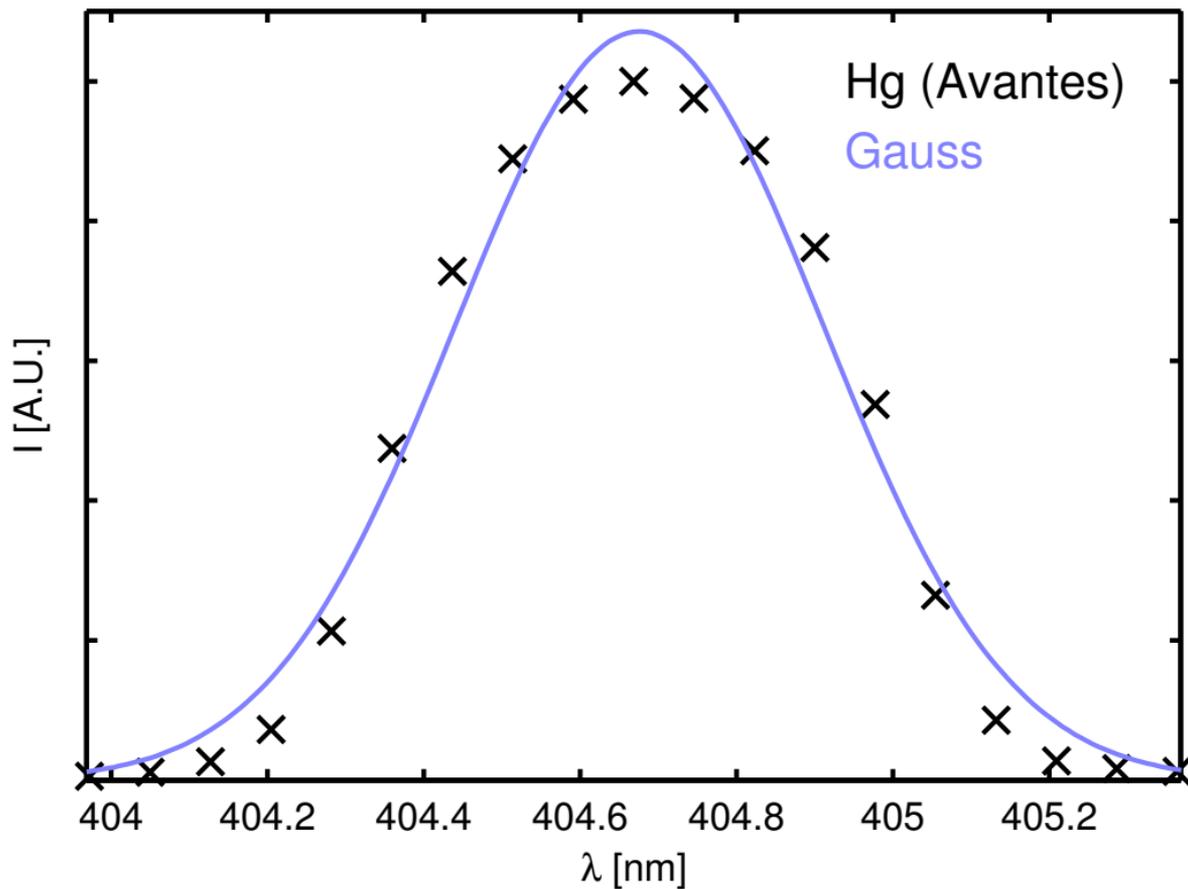
- Gained from “Kurucz-fit”
- Standard option in DOASIS, WinDOAS, Q-DOAS...
- Default: Gaussian (1 free parameter)
- Not always perfect...
- Several possible extensions
 - increase of number of fitted parameters
 - dedicated parametrisations for specific instruments

Here: proposal for a new parametrization which covers a wide range of possible shapes by few parameters

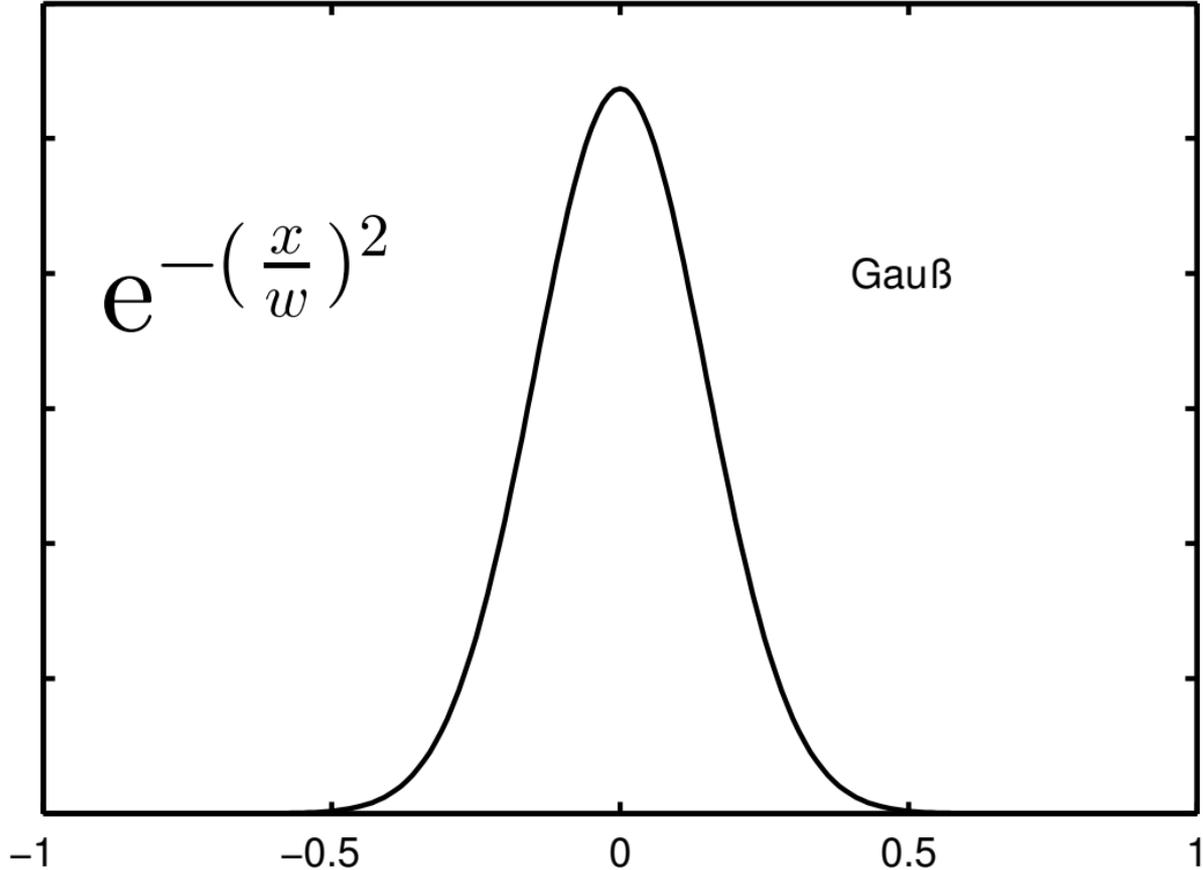
An example:



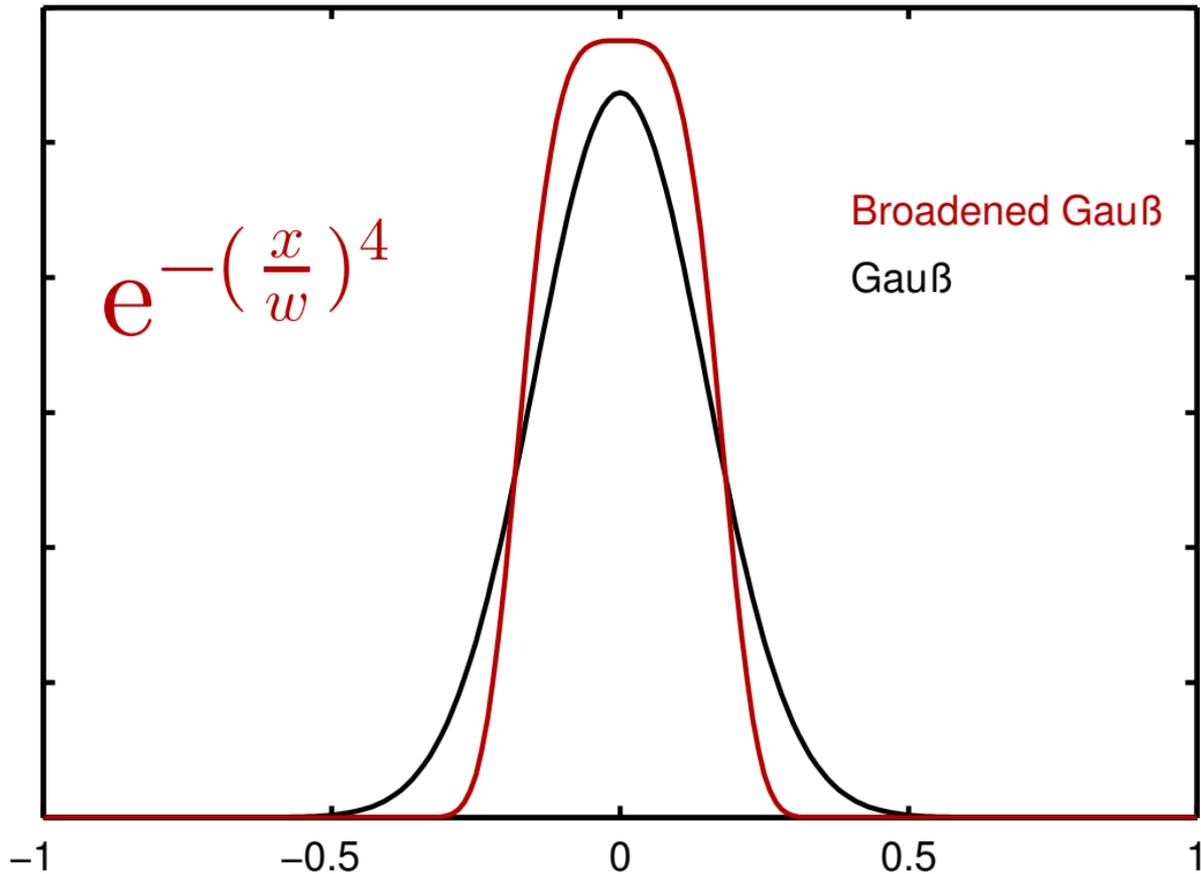
An example:



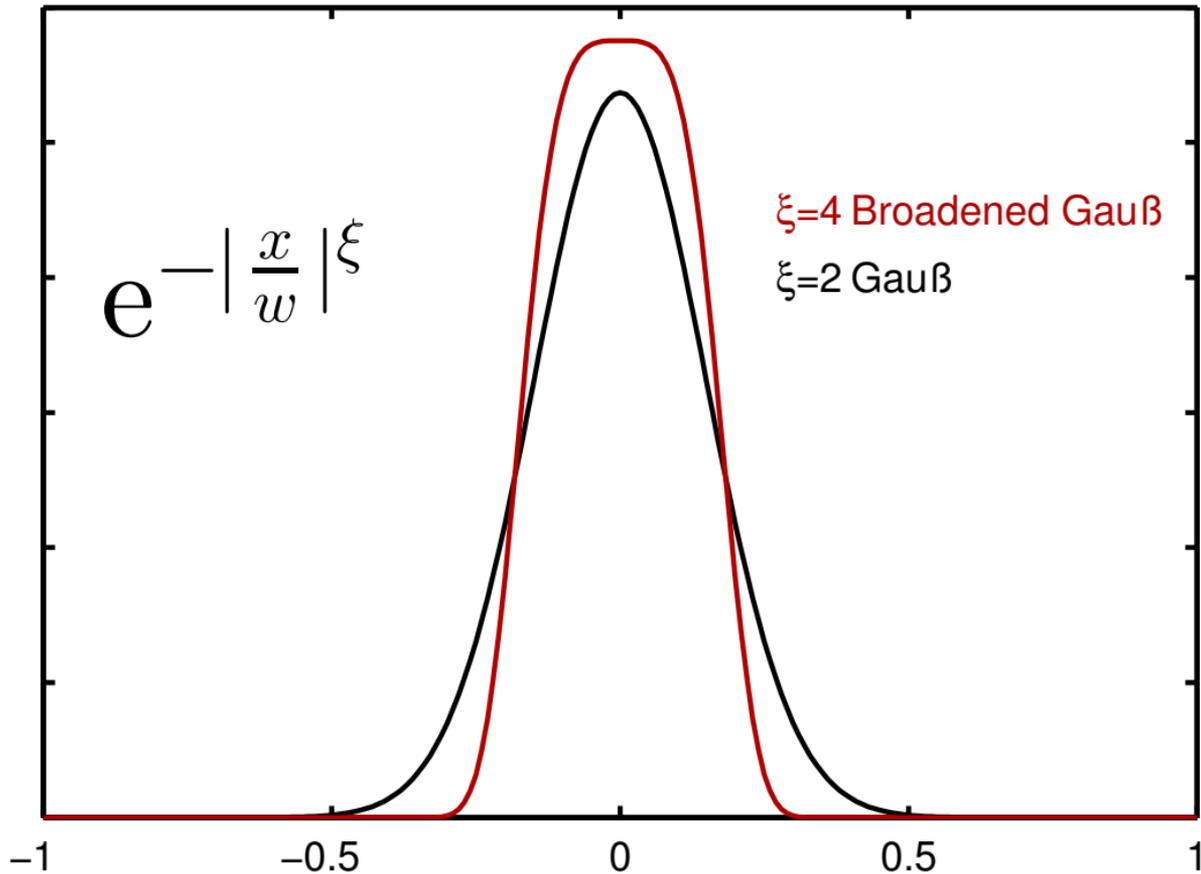
ISRF parameterization



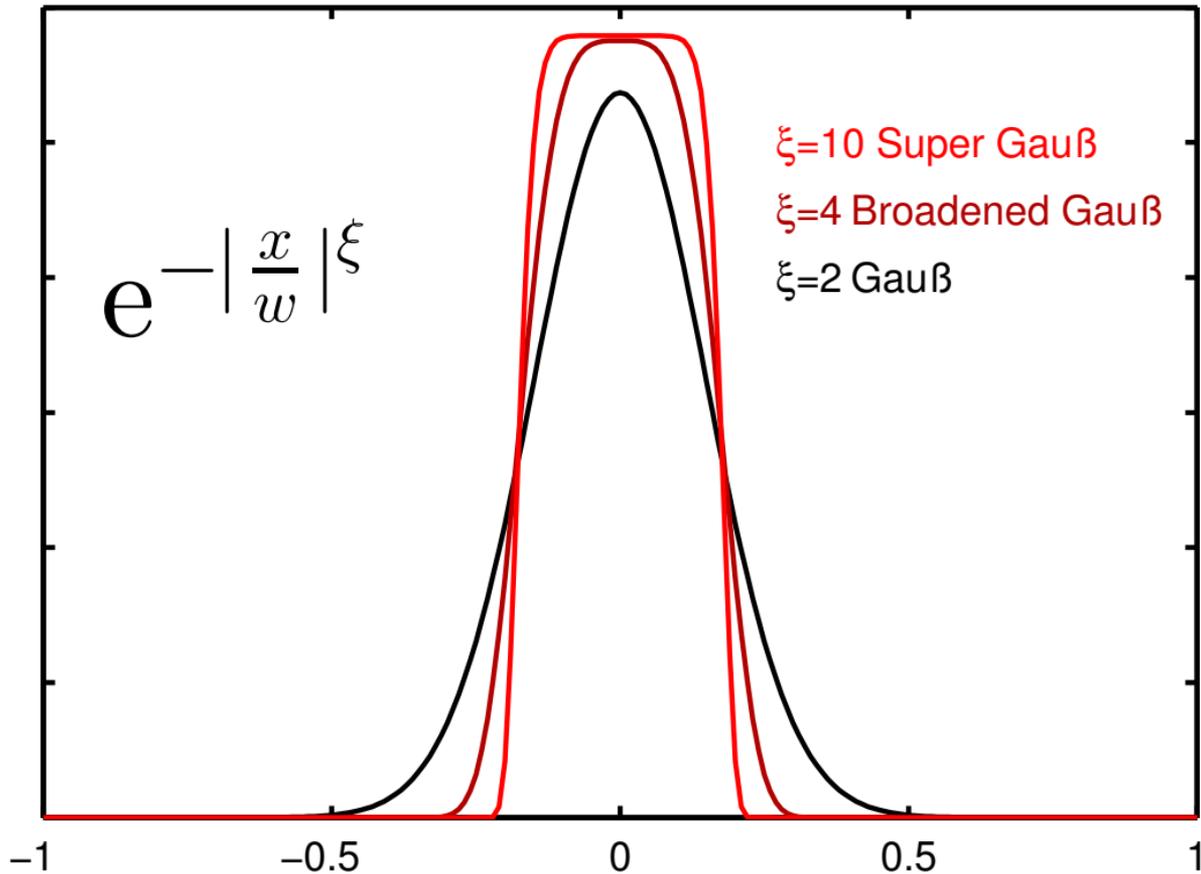
ISRF parameterization



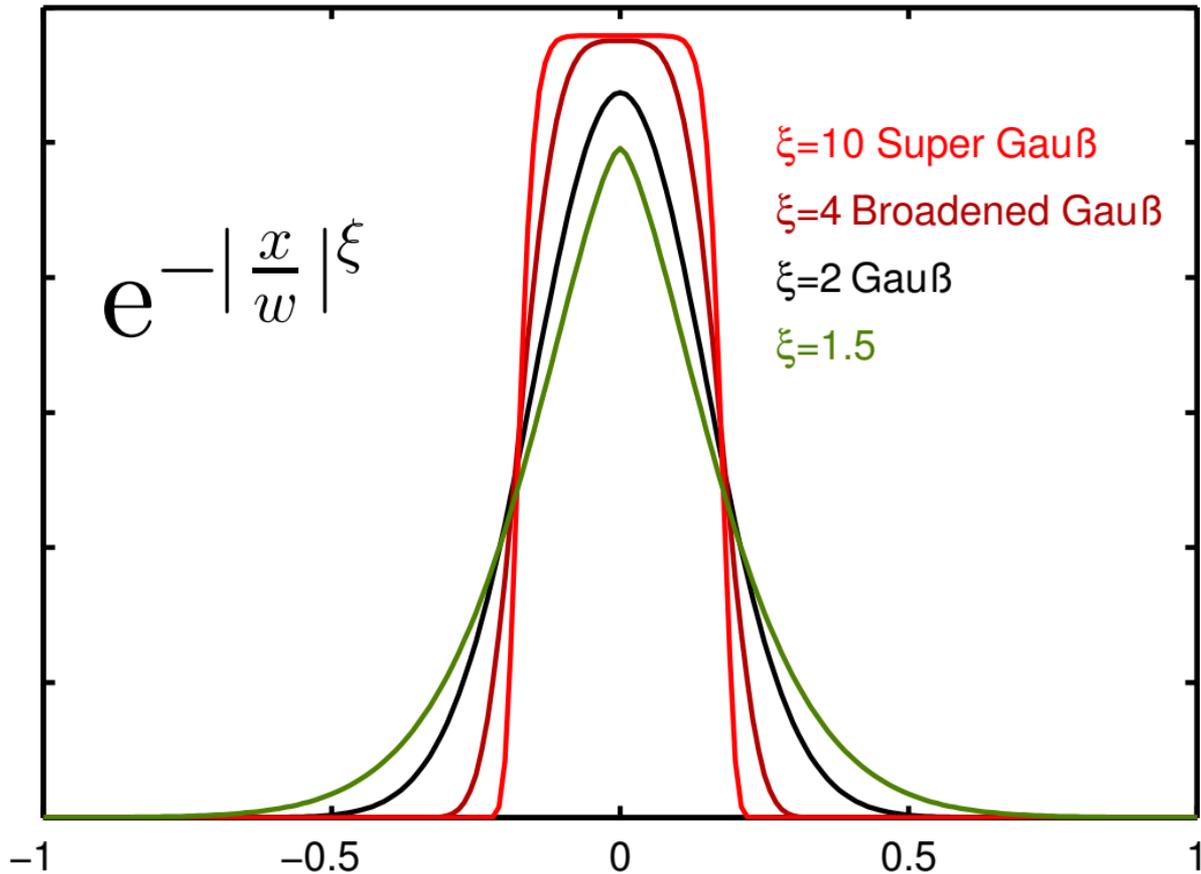
ISRF parameterization



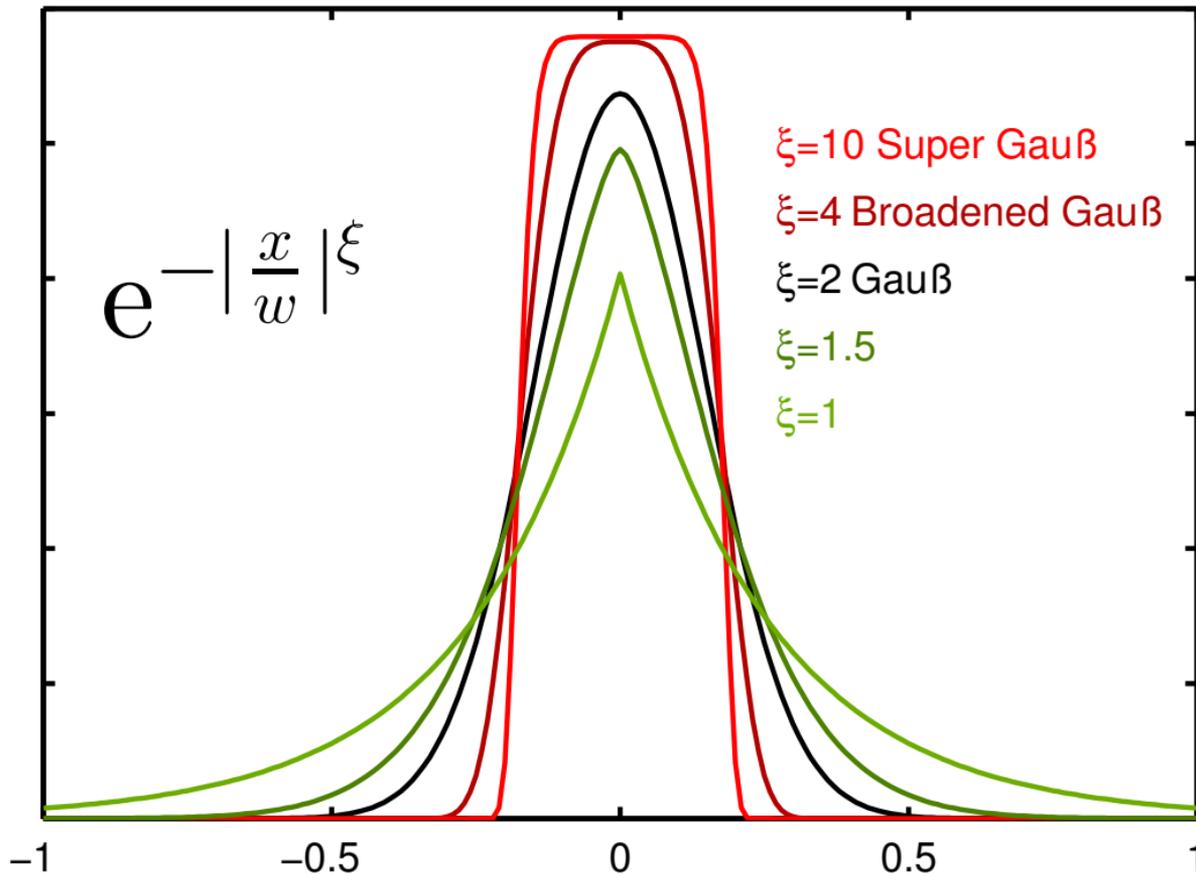
ISRF parameterization



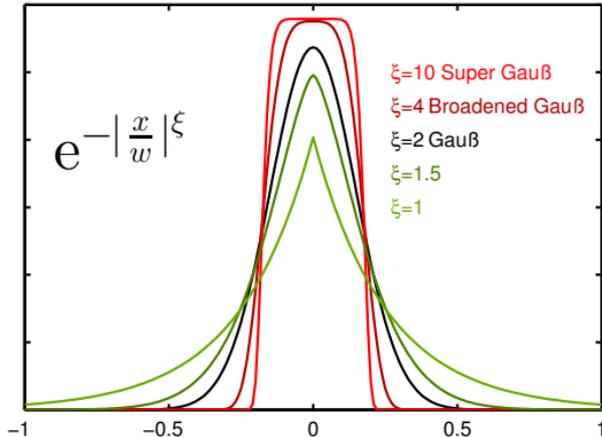
ISRF parameterization



ISRF parameterization

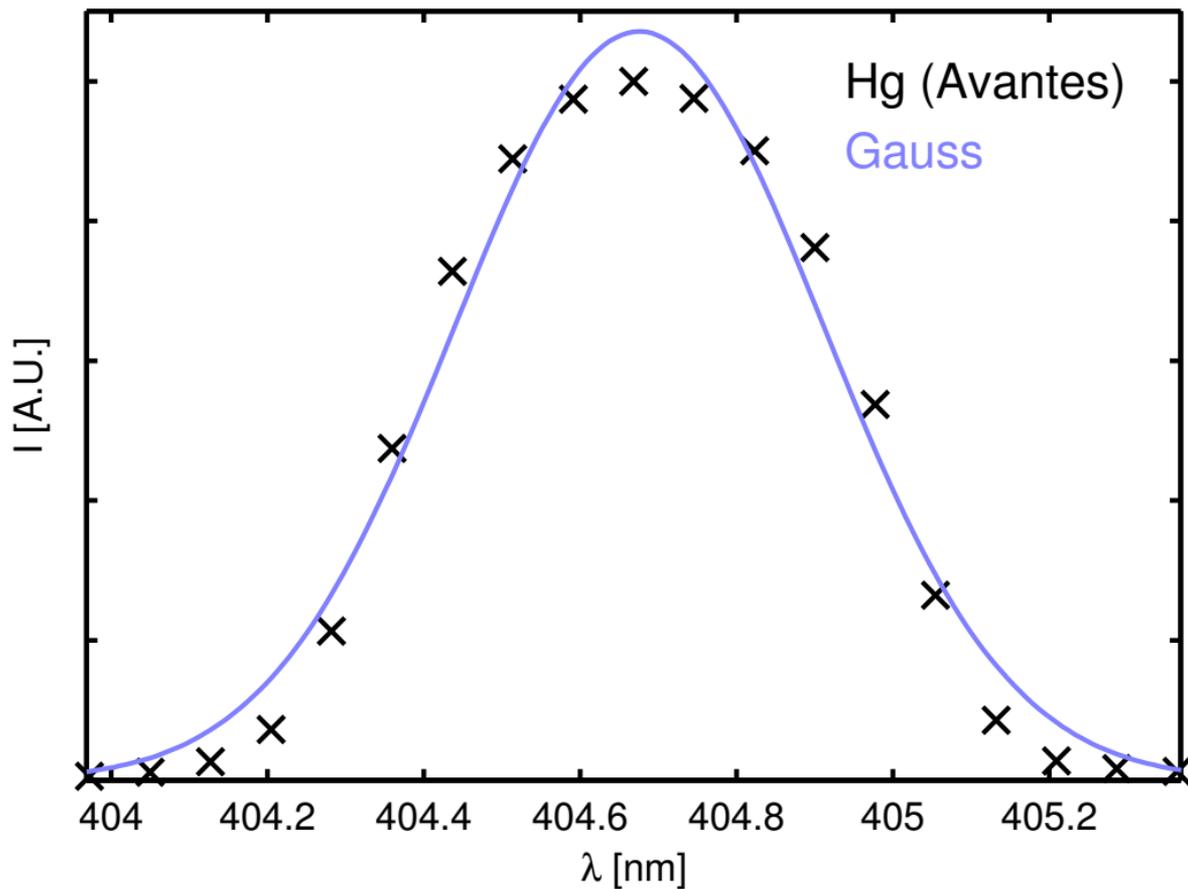


The “Super Gaussian”

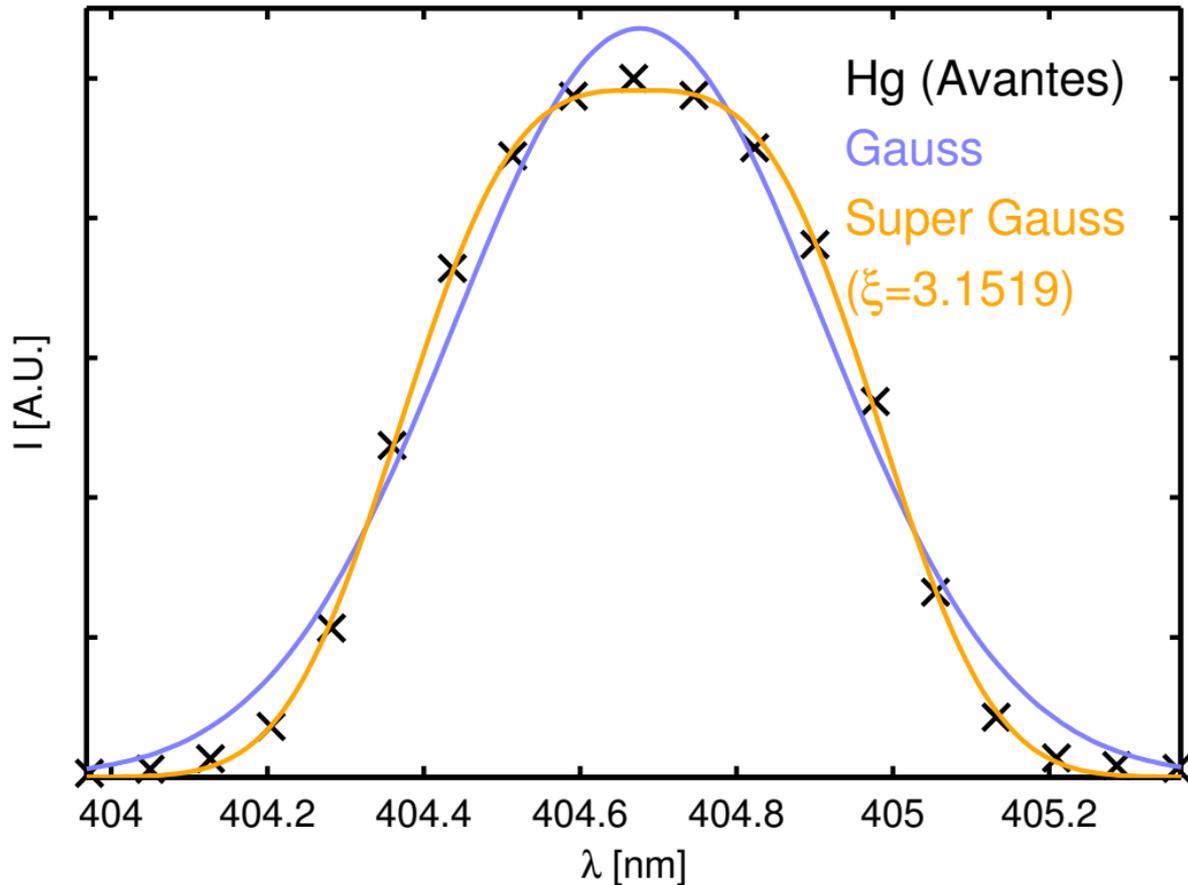


- Used in laser physics to describe beam cross-section
- w determines width; $\text{FWHM}=2(\ln 2 \times w)^{1/\xi}$
- ξ determines *shape*
- Wide range of ISRF shapes can be parametrised by 2 parameters only!

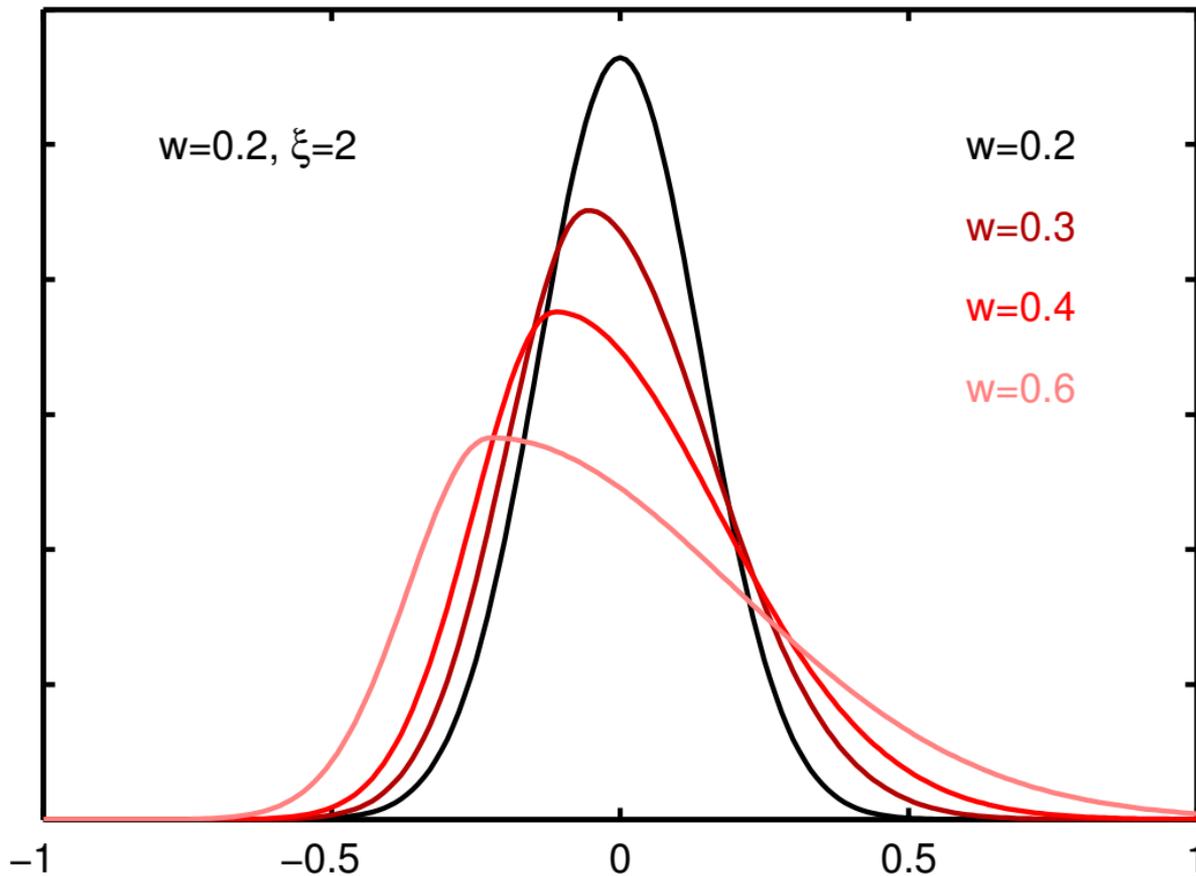
An example:



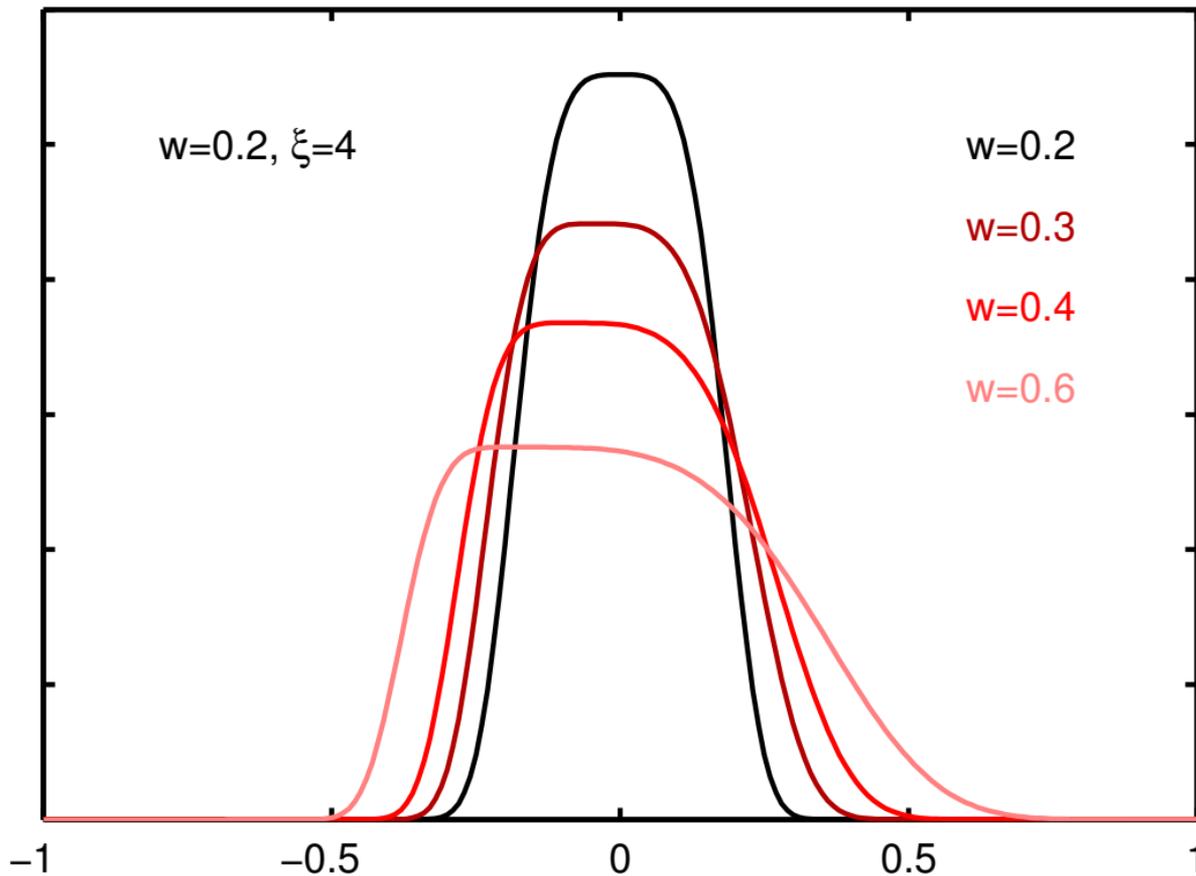
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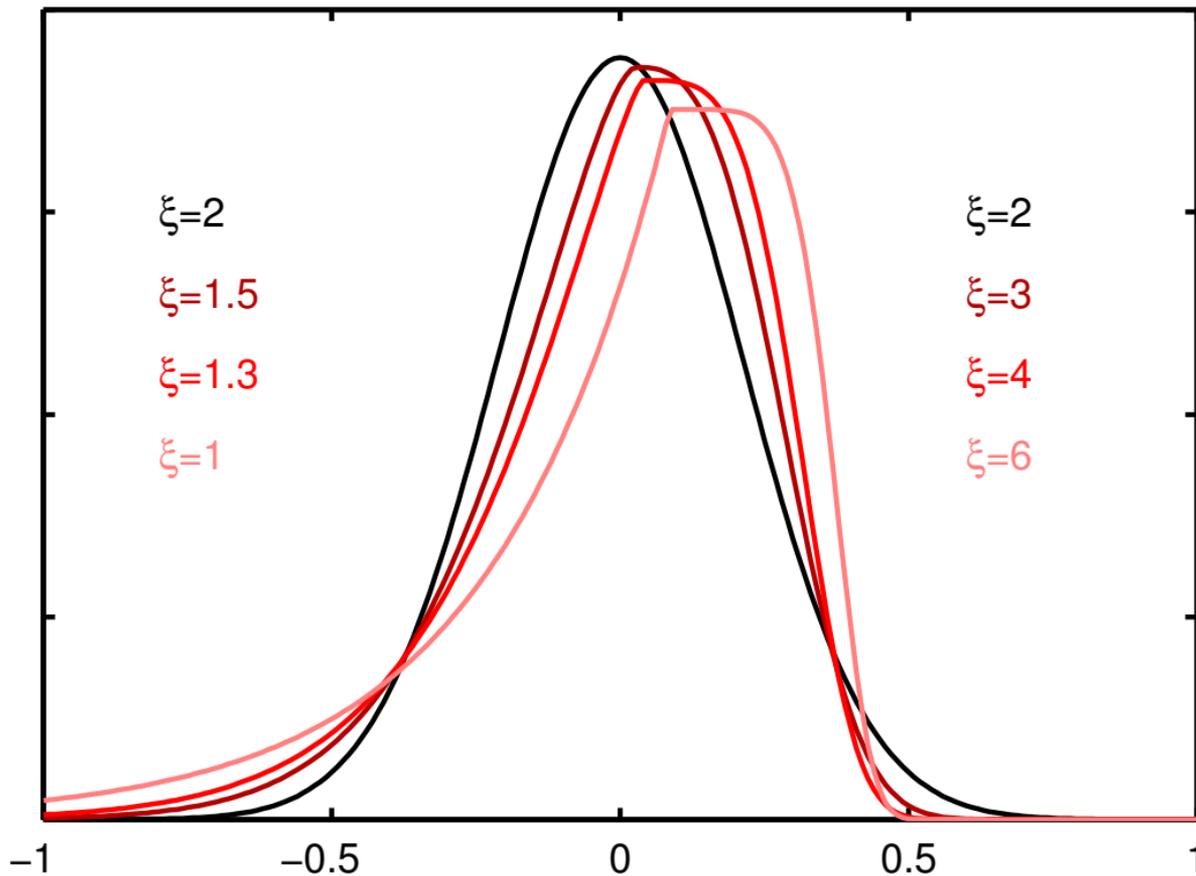
Asymmetric ISRF: 3 parameters (fixed ξ)



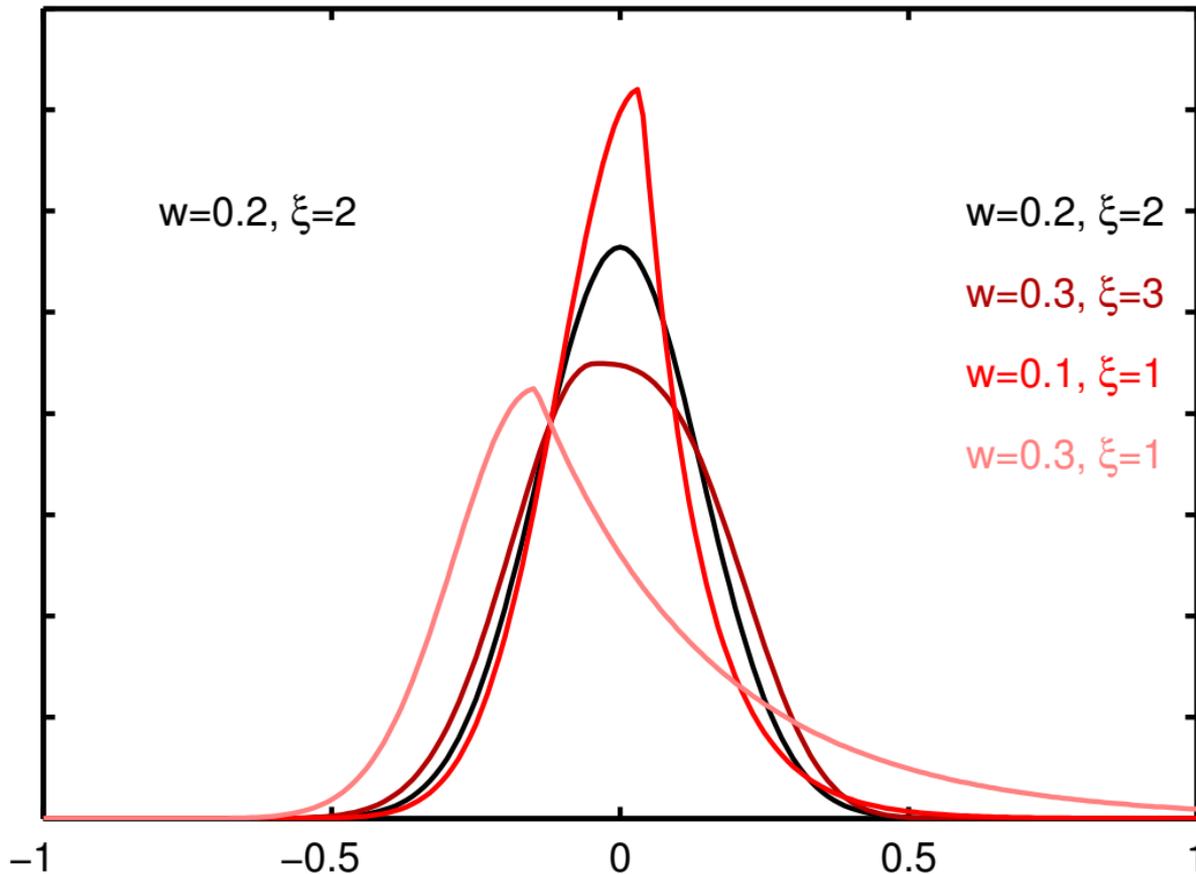
Asymmetric ISRF: 3 parameters (fixed ξ)



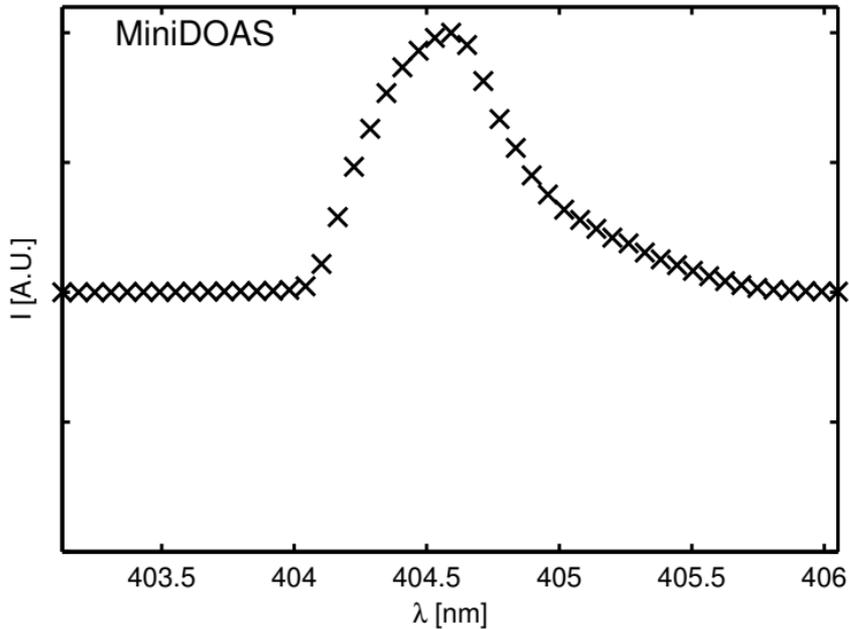
Asymmetric ISRF: 3 parameters (fixed w)



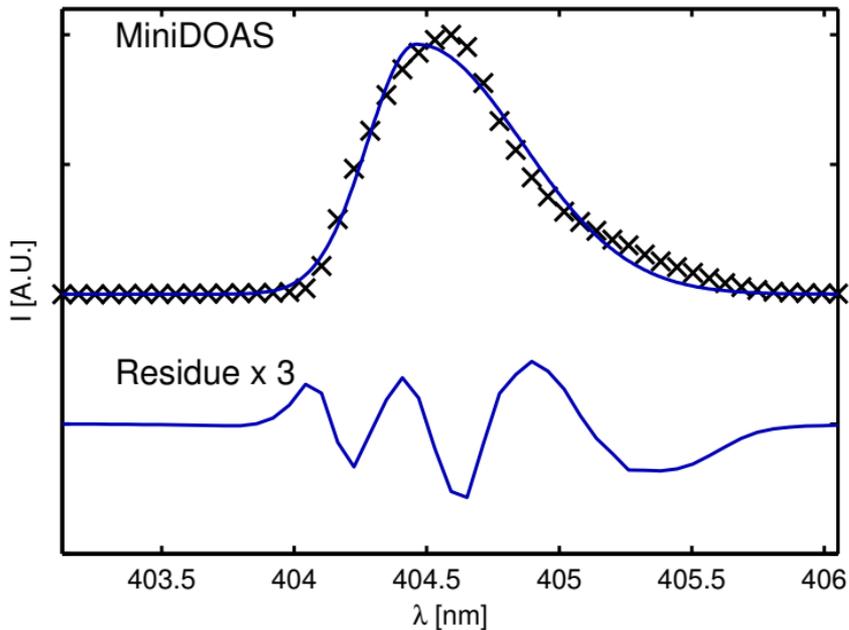
Asymmetric ISRF: 4 parameters



Asymmetric ISRF: Example 1

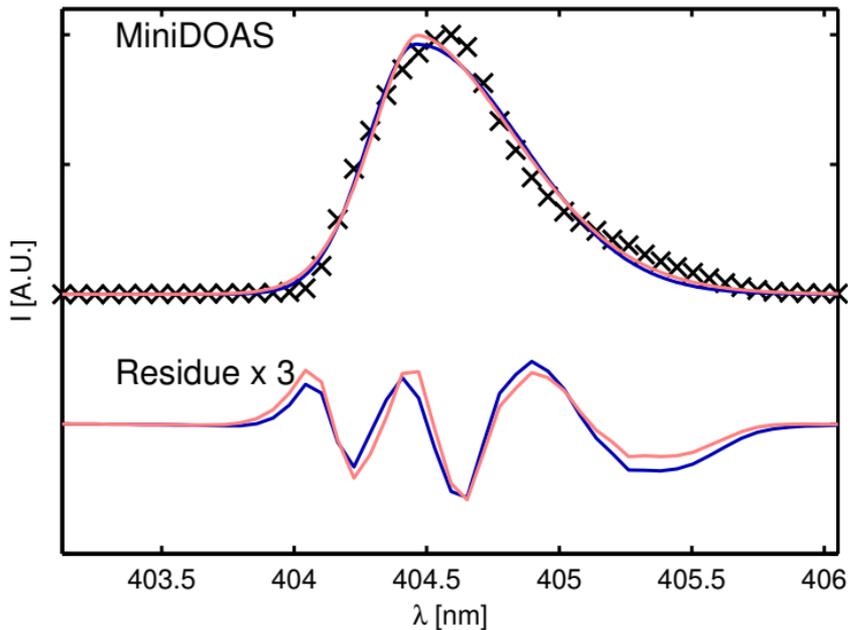


Asymmetric ISRF: Example 1



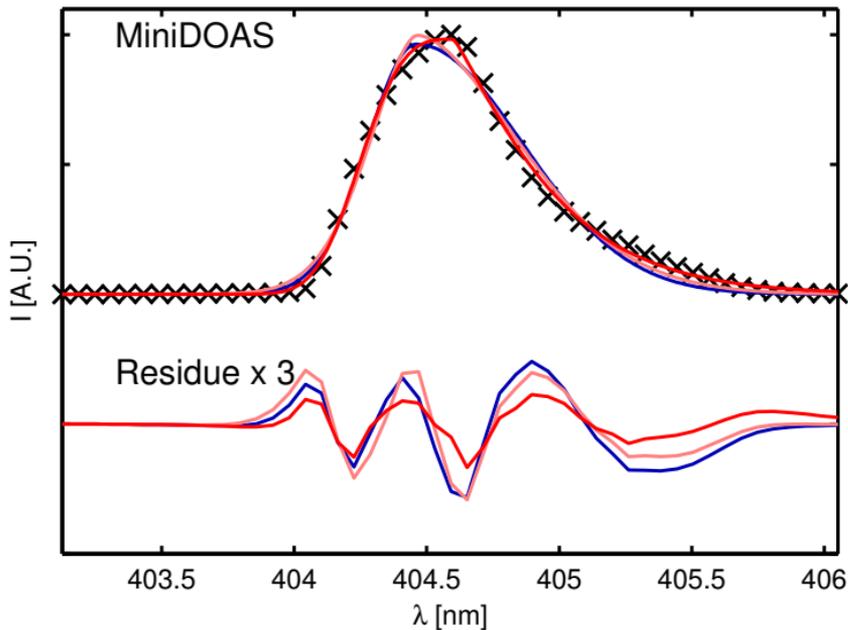
- Gaussian
- Asym. Gauss
- Super Gauss
- Asym. Super Gauss (w)
- Asym. Super Gauss (ξ)
- Asym. Super Gaussian

Asymmetric ISRF: Example 1



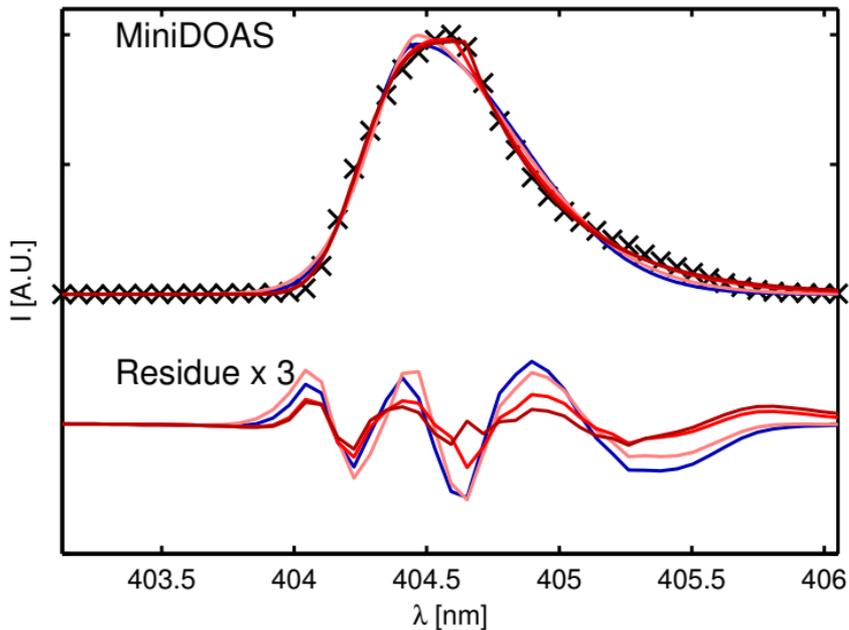
- Gaussian
- Asym. Gauss
- Super Gauss
- Asym. Super Gauss (w)
- Asym. Super Gauss (ξ)
- Asym. Super Gaussian

Asymmetric ISRF: Example 1



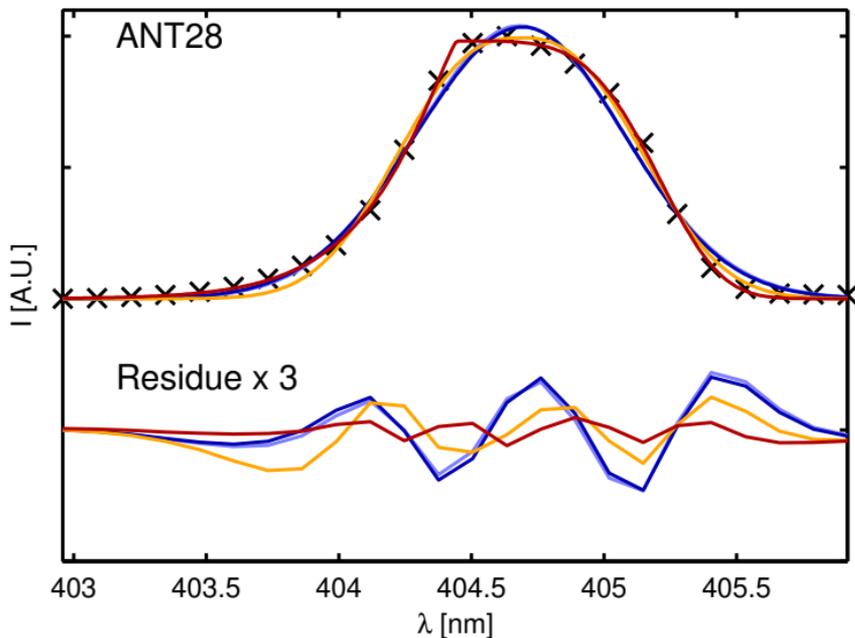
- Gaussian
- Asym. Gauss
- Super Gauss
- Asym. Super Gauss (w)
- Asym. Super Gauss (ξ)
- Asym. Super Gaussian

Asymmetric ISRF: Example 1



- Gaussian
- Asym. Gauss
- Super Gauss
- Asym. Super Gauss (w)
- Asym. Super Gauss (ξ)
- Asym. Super Gaussian

Asymmetric ISRF: Example 2



- Gaussian
- Asym. Gauss
- Super Gauss
- Asym. Super Gauss (w)
- Asym. Super Gauss (ξ)
- Asym. Super Gaussian

So far:

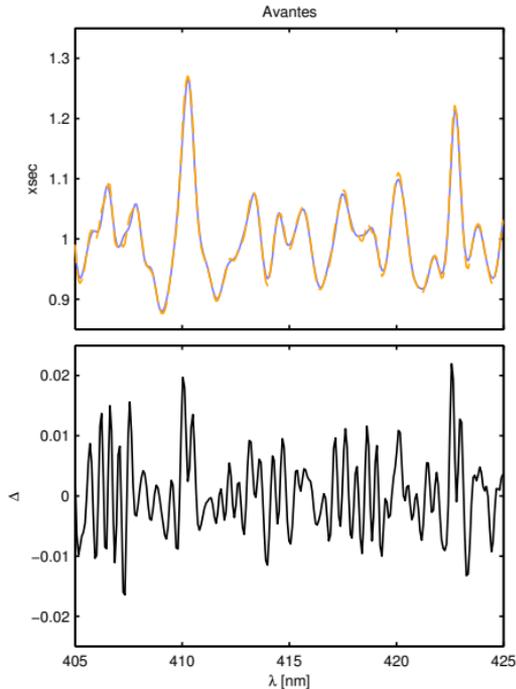
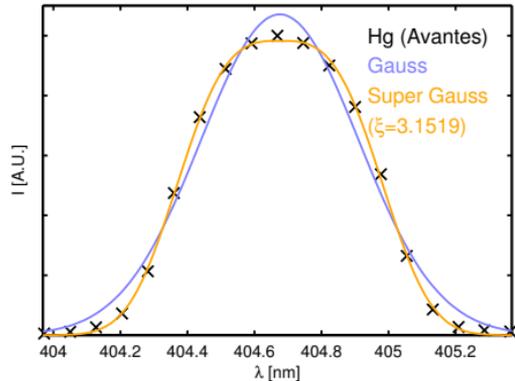
- Wide range of ISRF shapes can be parameterized by only 2-4 parameters!
- Significant improvement compared to Gauss

So what?

- Impact on cross-sections
- Parametrising *changes* of ISRF

Impact on cross-sections: Ring

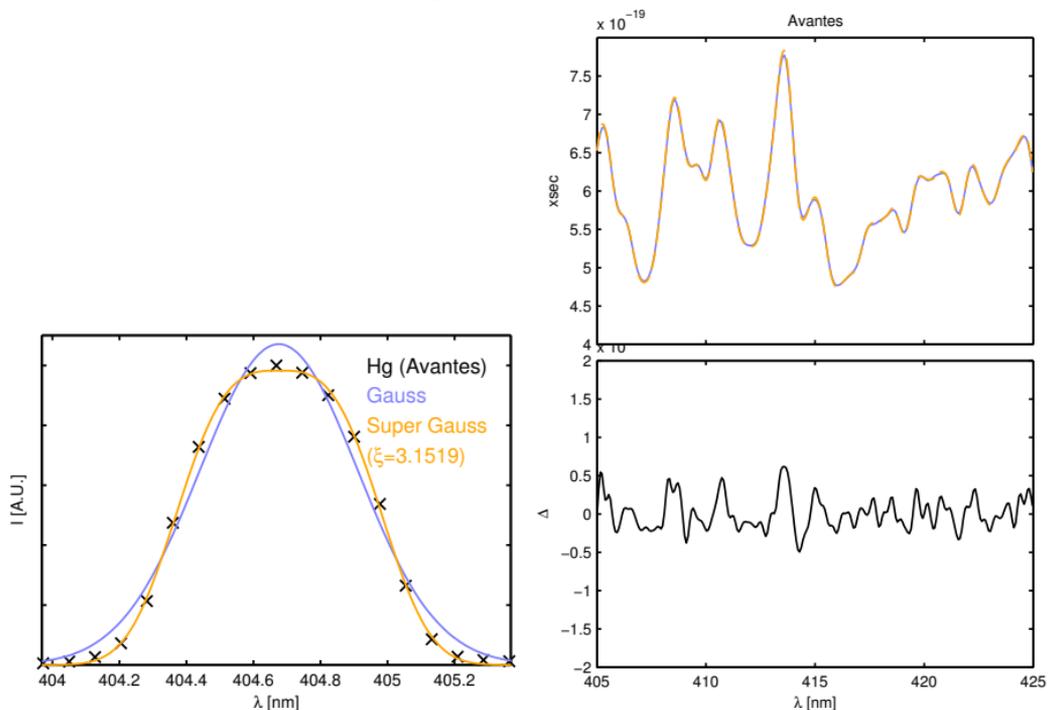
(if calculated from hi-res solar ref)



→ Effect of Super Gauss vs. Gauss: $\approx 10\%$

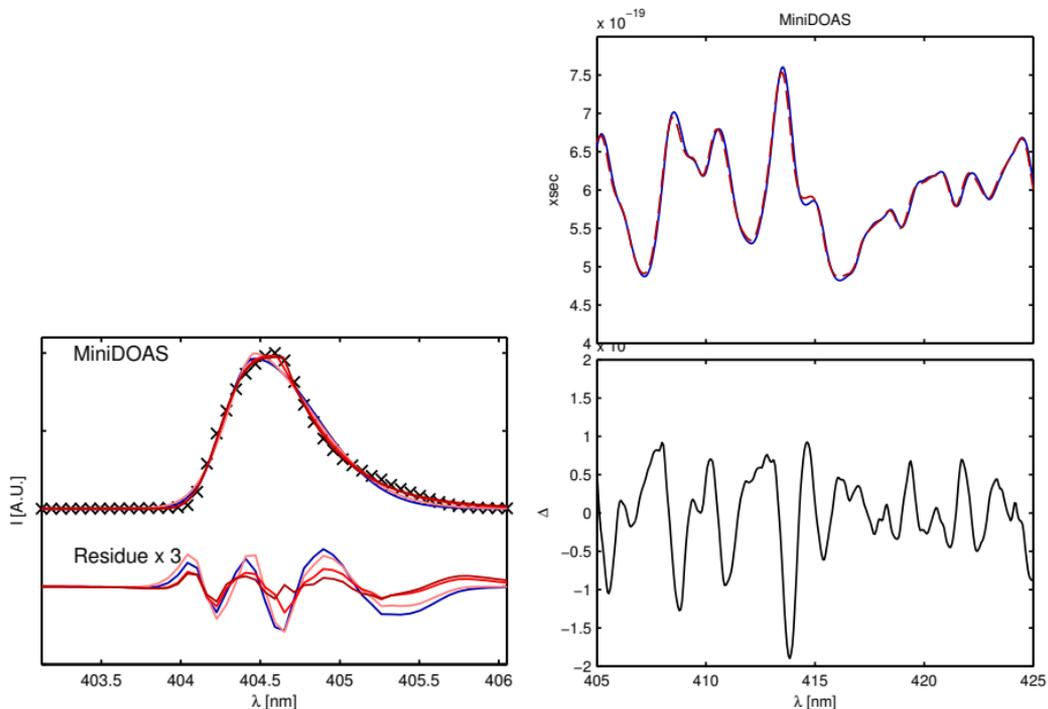
Impact on cross-sections: NO₂

(hi-freq structures, high OD)



Impact on cross-sections: NO₂

(hi-freq structures, high OD)



Impact on cross-sections: NO₂

- Effect of Super Gauss vs. Gauss: $\approx 5 - 10\%$
- For NO₂ SCD of 10^{17} molec/cm² (e.g. MAX-DOAS):
Residual structures of up to 3‰!
→ affects CHOCHO!

Parametrising changes of the ISRF

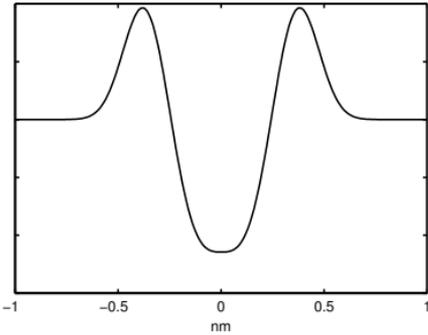
- ISRF changes with wavelength and time
- S_{cal} : ISRF at a given time/wavelength
- S : ISRF at different time/wavelength
- Assumptions: $\Delta S := S - S_{\text{cal}}$ is small
and can be expressed by change in ISRF parameters
→ Taylor expansion: $S \approx S_{\text{cal}} + \Delta p \times \frac{\partial S_{\text{cal}}}{\partial p}$
 p : ISRF parameter (e.g. w and ξ)

Effect on I and OD

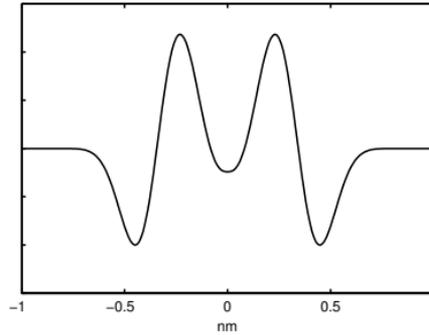
- $S \approx S_{\text{cal}} + \Delta p \times \frac{\partial S_{\text{cal}}}{\partial p}$
- $I = S \otimes I_{\text{hires}}$
 $= S_{\text{cal}} \otimes I_{\text{hires}} + \Delta p \times \frac{\partial S_{\text{cal}}}{\partial p} \otimes I_{\text{hires}}$
 $= I_{\text{cal}} + \Delta p \times f(\lambda)$
- $\ln I \approx \ln I_{\text{cal}} + \Delta p \times \frac{f(\lambda)}{I}$
→ change in I and OD can be linearized w.r.t. change in p

Effect on I and OD

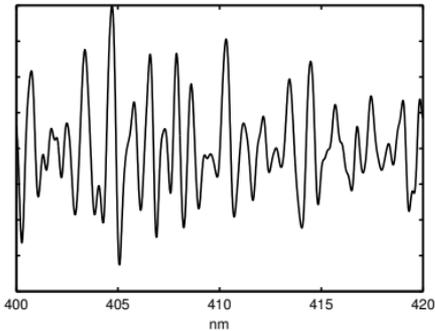
$$\frac{\partial S_{\text{cal}}}{\partial w}$$



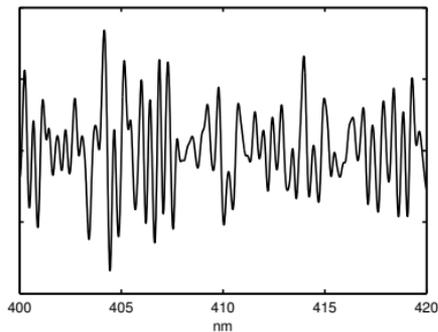
$$\frac{\partial S_{\text{cal}}}{\partial \xi}$$



$$\frac{\partial S_{\text{cal}}}{\partial w} \otimes I_{\text{hires}}$$



$$\frac{\partial S_{\text{cal}}}{\partial \xi} \otimes I_{\text{hires}}$$



Effect on I and OD

- $S \approx S_{\text{cal}} + \Delta p \times \frac{\partial S_{\text{cal}}}{\partial p}$
- $I = S \otimes I_{\text{hires}}$
 $= S_{\text{cal}} \otimes I_{\text{hires}} + \Delta p \times \frac{\partial S_{\text{cal}}}{\partial p} \otimes I_{\text{hires}}$
 $= I_{\text{cal}} + \Delta p \times f(\lambda)$
- $\ln I \approx \ln I_{\text{cal}} + \Delta p \times \frac{f(\lambda)}{I}$
→ change in I and OD can be linearized w.r.t. change in p

Application I: improved Kurucz-fit

- Fit the mean ISRF over the complete fit window
- Account for wavelength dependency by including the term $\frac{\partial S_{\text{cal}}}{\partial p} \otimes I_{\text{hires}} \times \text{Pol}(\lambda - \lambda_0)$ in the fit
- Polynomial coefficients represent the wavelength dependency of the ISRF parameters

Application II: improved trace gas fit

- Account for possible changes of S over time by including the Pseudo-Absorbers $\frac{\partial S_{\text{cal}}/\partial p \otimes I_{\text{hires}}}{I}$
- Fit coefficients represent Δp , i.e. the change of ISRF parameters
- In case of Super Gauss:
 $\Delta w \rightarrow$ change of width,
 $\Delta \xi \rightarrow$ change of shape

Conclusions

- The “Super Gaussian” is a powerful parametrisation of the ISRF, covering wide range of shapes with few parameters
 - Should be included in DOASIS and Q-DOAS
- A good parametrisation of ISRF also allows to parametrise and linearise the effects of ISRF changes