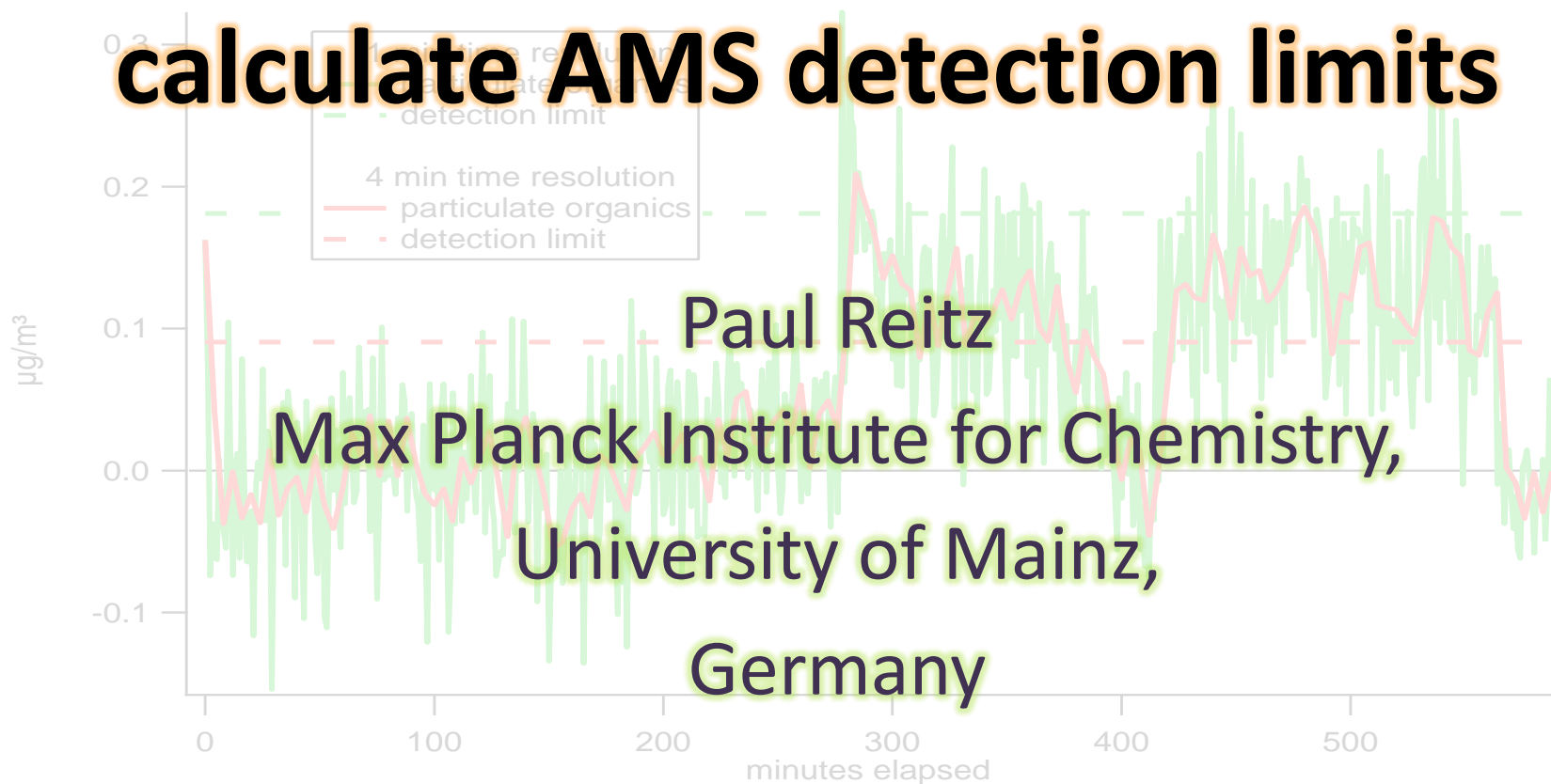


$$\sigma = \sqrt{\frac{18}{35} \frac{1}{N-5} \sum_{i=2}^{N-3} \left( F_i - \frac{2}{3} F_{i-1} + \frac{1}{6} F_{i-2} - \frac{2}{3} F_{i+1} + \frac{1}{6} F_{i+2} \right)^2}$$

# A new and easy method to calculate AMS detection limits



Paul Reitz

Max Planck Institute for Chemistry,

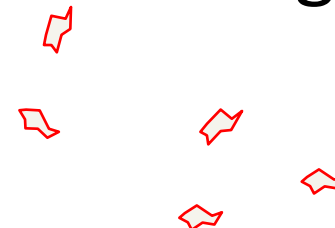
University of Mainz,

Germany

- Motivation
- Principle of work
- Test results

- Detection limits are important when measuring:

- in remote areas
- thin coatings in the lab



- Classic (e.g.: Allan et al, Bahreini et al.):  
estimation via counting statistics

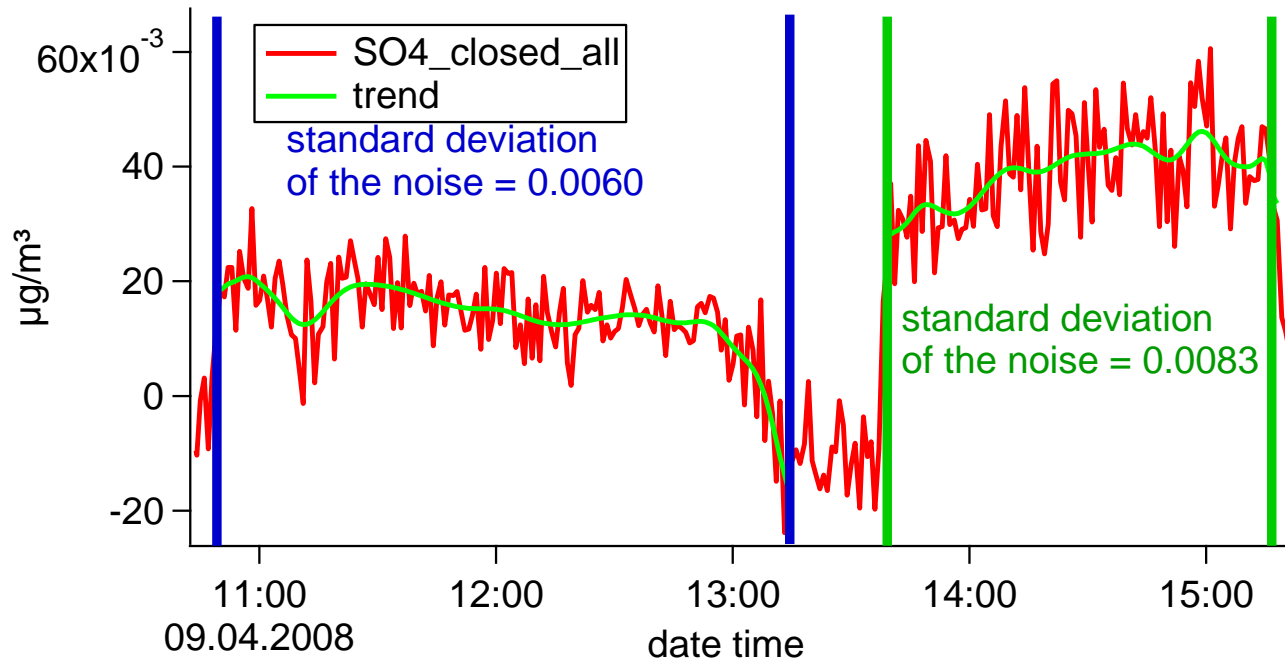
or:

3 x standard deviation of filter measurement




- New: From the noise of the closed signal during  
regular measurements (Drewnick et al. AMT 2009):

$$3 \times \sqrt{2} \times \textit{standard deviation of closed signal noise}$$

- Detection limits are dependent on instrument history  
=> detection limit during the filter period is often different from the one during a certain measurement.  
=> the new method is preferable

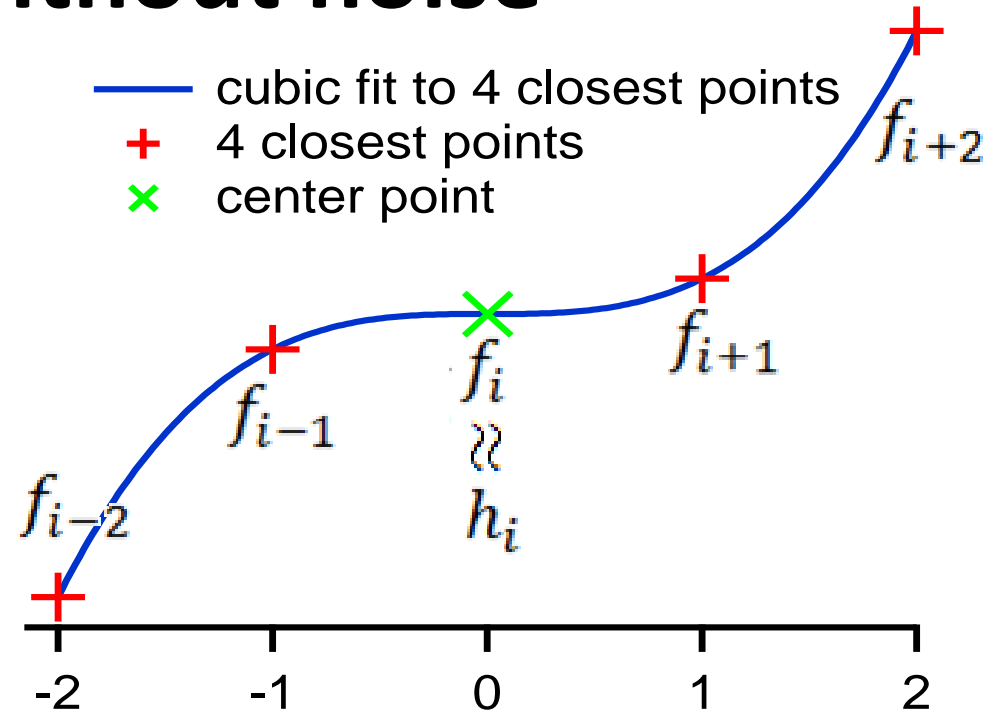


Problem: long scale variations in closed signal  
=> Standard deviation cannot be calculated directly

- Requirements:
  - Noise varies on a much shorter time scale than the closed signal without noise 
  - Closed signal is reasonably smooth 
  - Time series has equidistant time steps 
- Step 1: Combine adjacent points to an expression which is only constituted of the noise.
- Step 2: Combine these terms to an expression that is proportional to the standard deviation of the noise.

## Ideal case without noise

- cubic fit to 4 closest points
- + 4 closest points
- x center point



$f_i$ : Ideal closed signal

Interpolated point

$$h_i = \frac{2}{3}f_{i-1} - \frac{1}{6}f_{i-2} + \frac{2}{3}f_{i+1} - \frac{1}{6}f_{i+2}$$

$$f_i - h_i \approx 0$$

## Realistic case with noise

**Real closed  
signal**

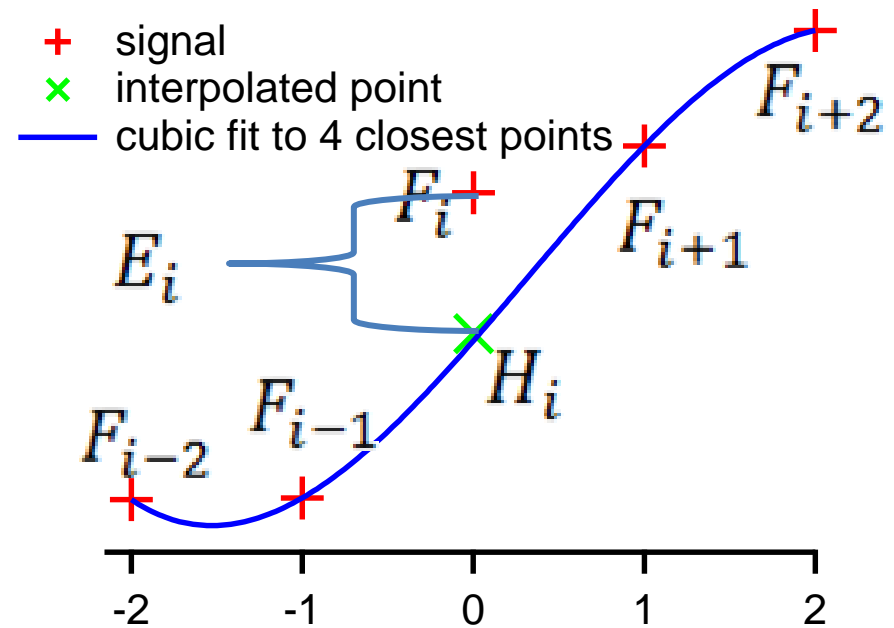
**noise**

$$F_i = f_i + \varepsilon_i$$

$$E_i = F_i - H_i$$

$$E_i \approx \varepsilon_i - \frac{2}{3}\varepsilon_{i-1} + \frac{1}{6}\varepsilon_{i-2} - \frac{2}{3}\varepsilon_{i+1} + \frac{1}{6}\varepsilon_{i+2}$$

$E_i$  depends only on the noise



Standard deviation:

$$\sigma = \sqrt{\frac{1}{n-1} \sum_{i=0}^{n-1} \varepsilon_i^2}$$

Similar sum with  $E_i^2$ :

$$R := \sqrt{\frac{1}{(N-4)-1} \sum_{i=2}^{N-3} E_i^2}$$

After some calculation:

$$R \approx \sqrt{\frac{35}{18}} \sigma$$

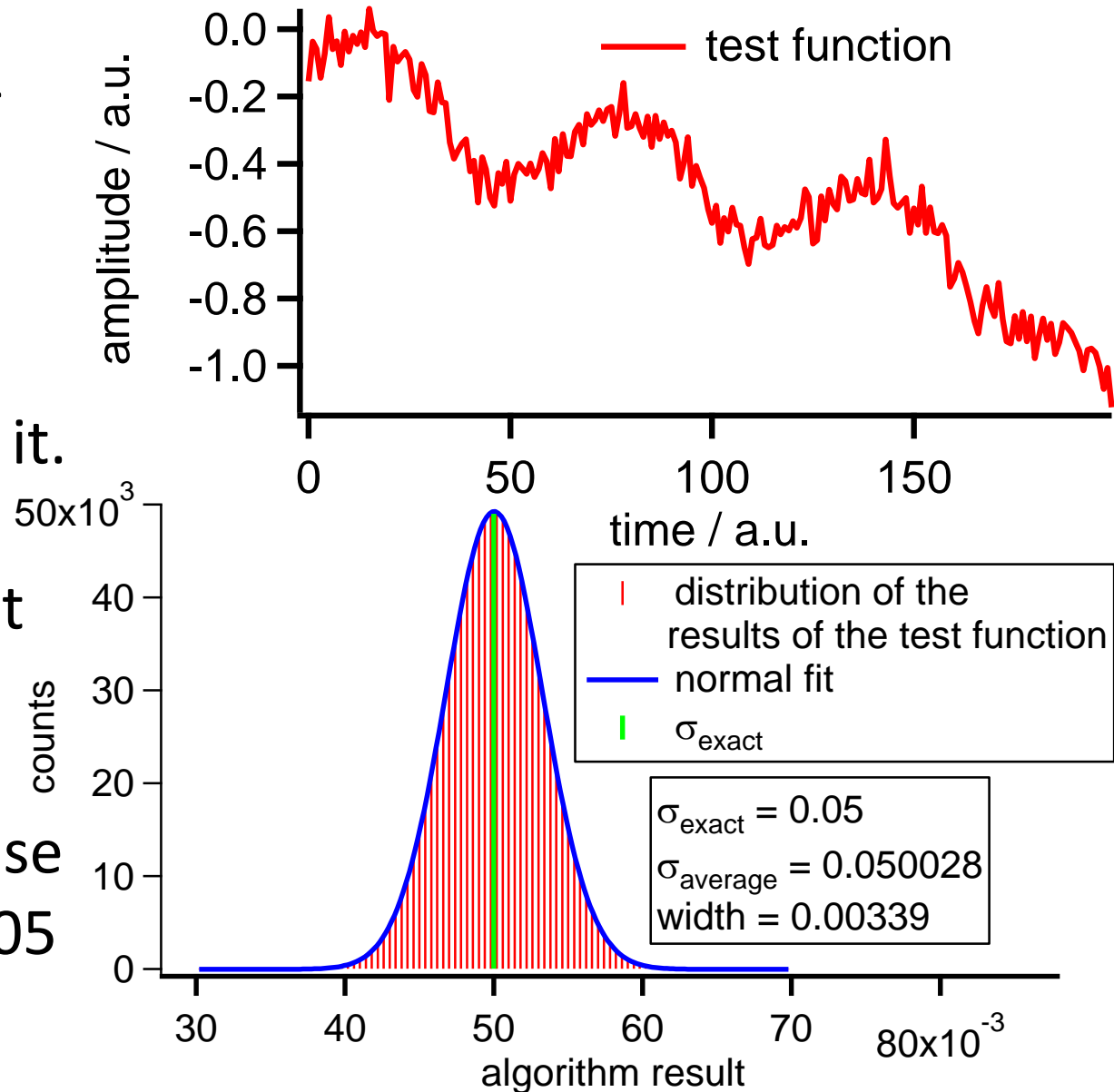


*After replacing  $E_i$  in  $R$ ,  
inserting  $F_i$  and  $H_i$  in  $E_i$   
and inserting  $F_i$  in  $H_i$ ,  
we finally get the standard deviation  
as a function of the measured values  $F_i$*

$$\sigma = \sqrt{\frac{18}{35} \frac{1}{N-5} \sum_{i=2}^{N-3} \left( F_i - \frac{2}{3} F_{i-1} + \frac{1}{6} F_{i-2} - \frac{2}{3} F_{i+1} + \frac{1}{6} F_{i+2} \right)^2}$$

Test:  
Add random noise of known standard deviation (0.05) on different signals and use the algorithm on it.

Result of 100,000 test runs:  
Same signal wave  
100,000 different noise waves with sdev = 0.05



- With this new algorithm now it is possible to get experimental detection limits during regular measurement:
  - With sufficient precision (if period has more than 50 points)
  - Without losing measurement time for filter periods
  - Without falsification of the detection limit due to changed background during filter measurement

**Igor procedure will be available!**

**Paper with detailed description in preparation for  
Atmospheric Measurement Techniques**

