Numerical noise due to binning in particle simulations

BLonD developers meeting
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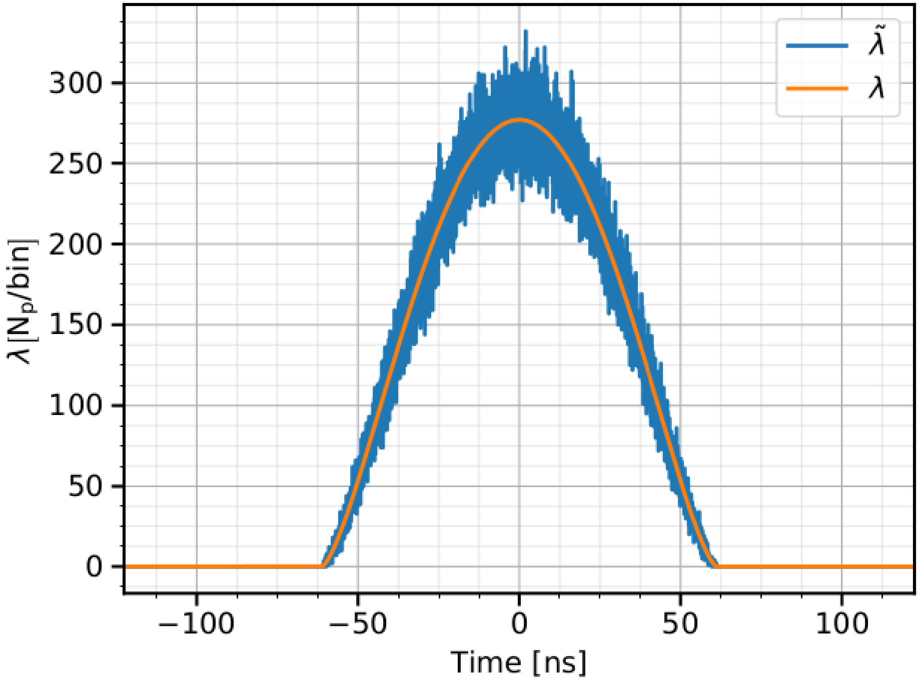
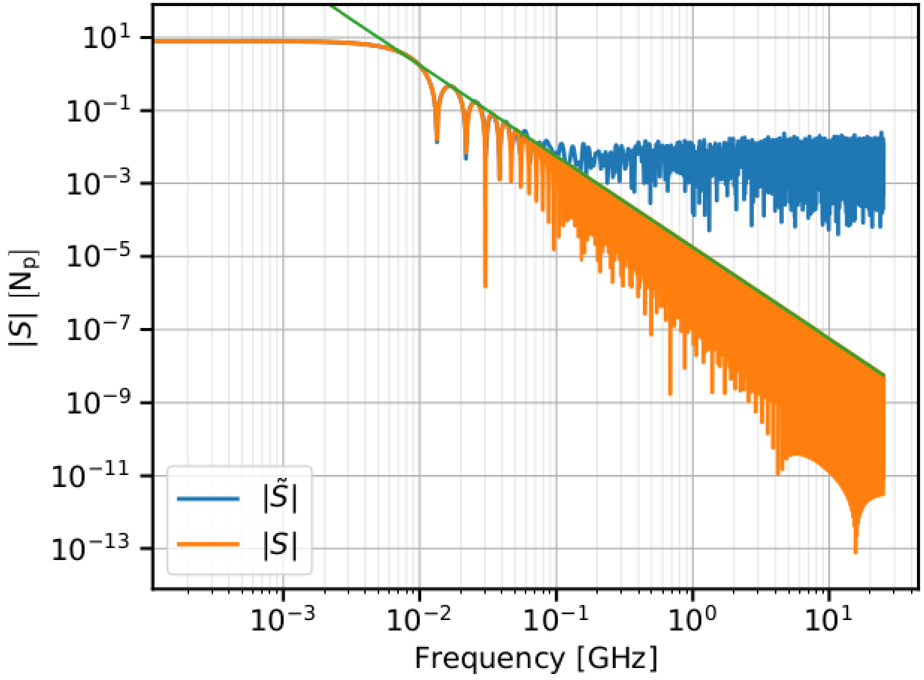
Outline

- Introduction
- Definition of the spectrum for a binomial distribution
- Definition of the noise due to binning of particles
- Expression of the signal-to-noise ratio
- Examples
- Conclusions

Noisy profile and spectrum

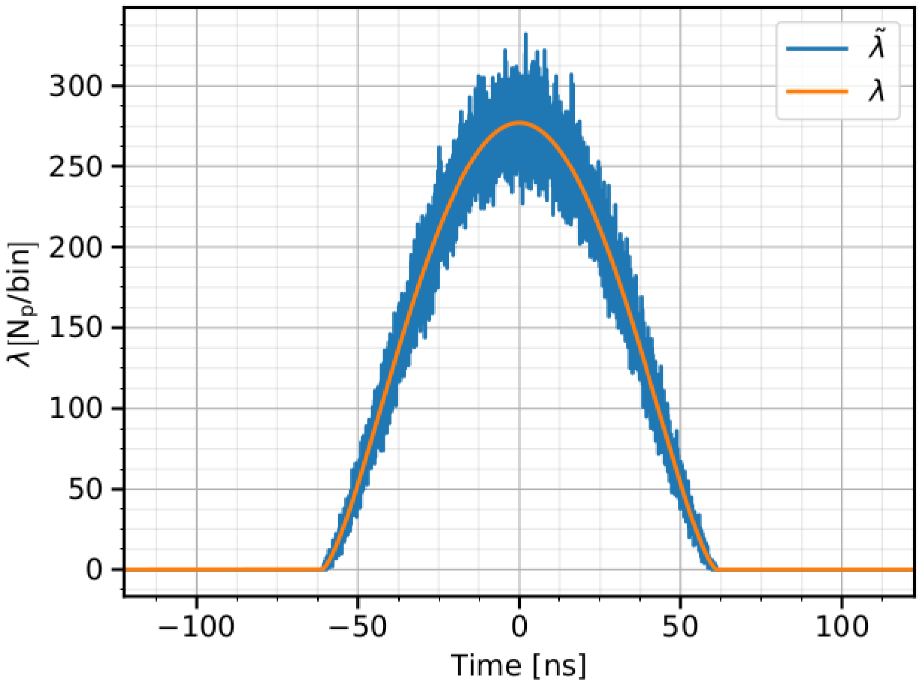


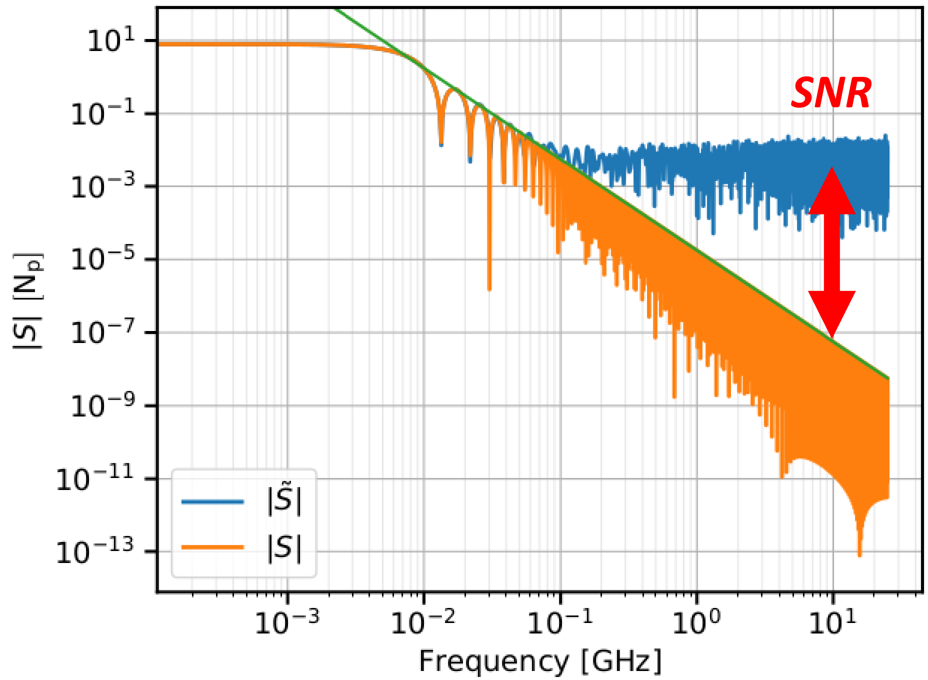


- Binning a discrete number of (macro-)particles as a histogram lead to numerical noise.

- By evaluating the spectrum of the binned profile, the noise can be seen at high frequency and can lead to issues with microwave instability study (extra blow-up damping the instability, or seed leading to early start of instability).

Noisy profile and spectrum

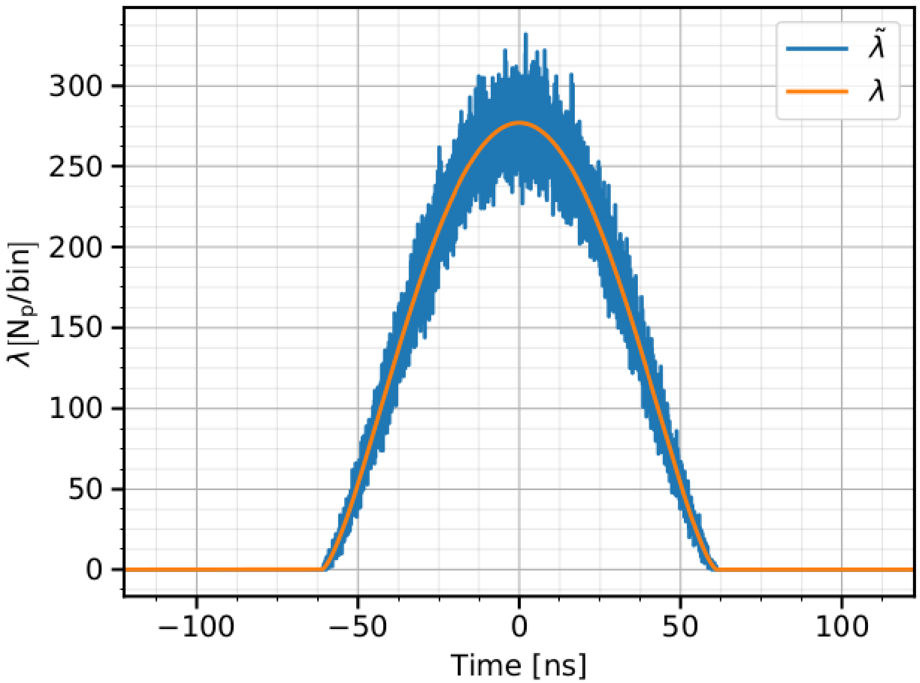


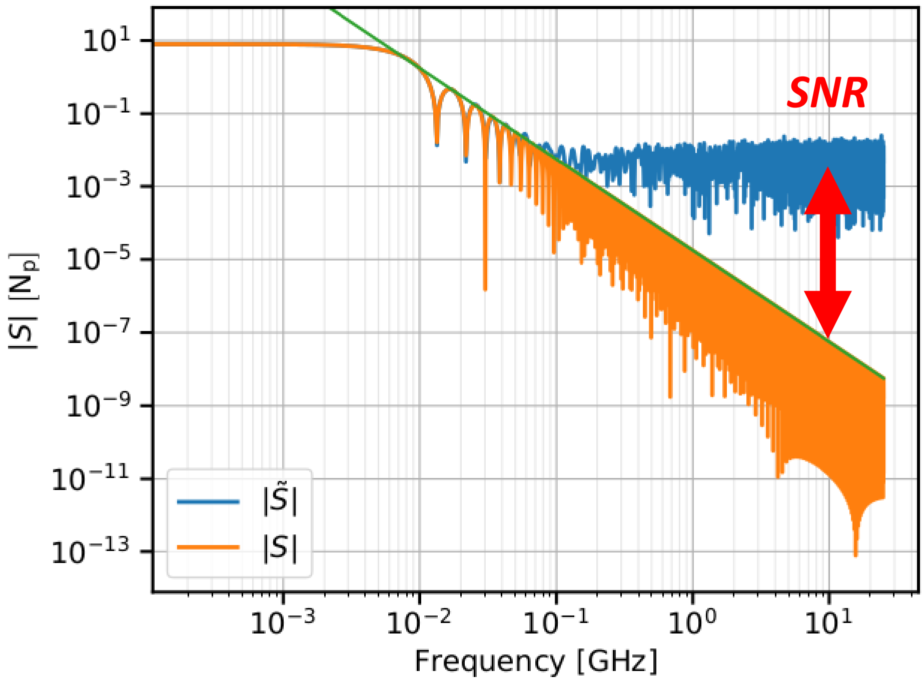


- An expression of the signal-to-noise ratio (SNR) vs. the number of macroparticles at a given frequency would help evaluate whether the simulated bunch is too noisy.

- This evaluation can also be done with the real number of particles.

Smooth profile and spectrum

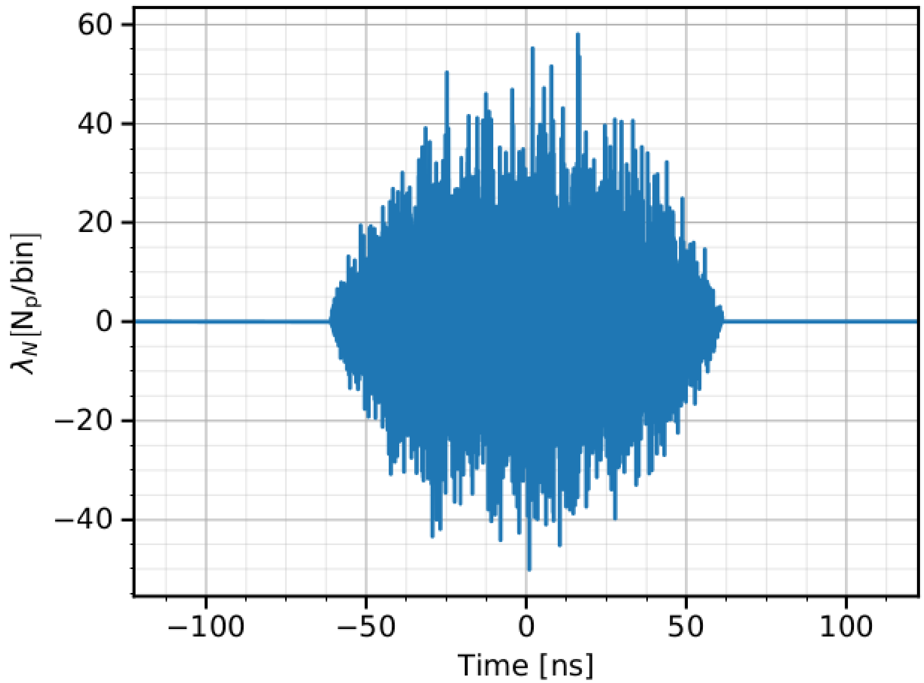


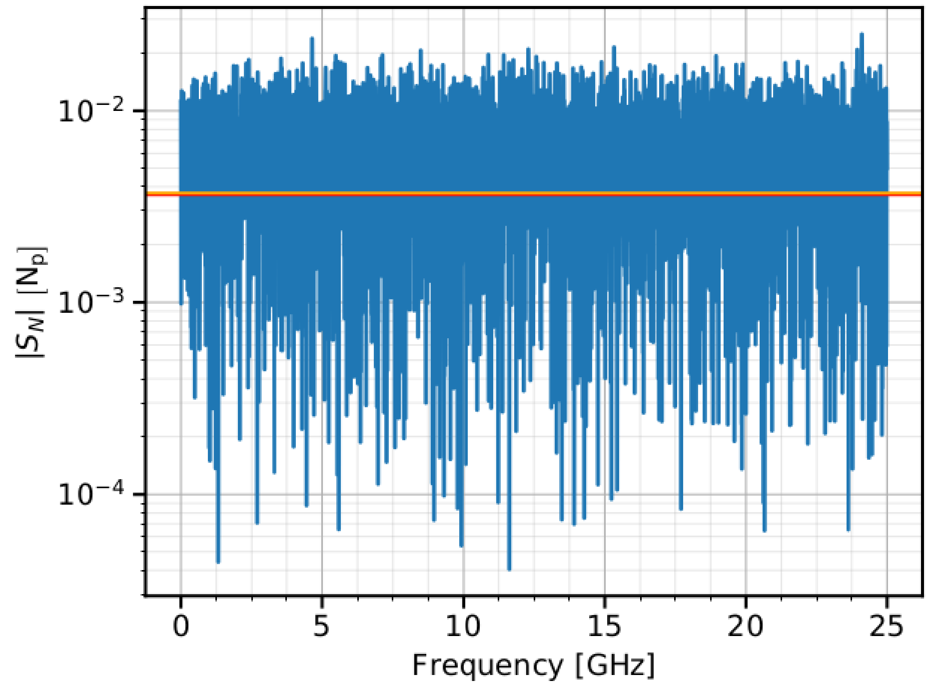


$$\lambda\left[t\right] = N_p\lambda_0\left[1-4\left(\frac{t}{\tau_l}\right)^2\right]^{\mu}$$

$$S\left[f\right] \sim \frac{2N_p}{\sqrt{\pi}N_b}\frac{1}{\left(\sigma_l f\right)^{\mu+1}}F\left(\mu\right)$$

Noisy profile and spectrum





$$\tilde{\lambda}\left[t\right] = \lambda\left[t\right] + \lambda_N\left[t\right]$$

$$\lambda_N\left[t\right] \sim \sqrt{\lambda\left[t\right]} \times \mathcal{N}_{[0,1]}$$

$\downarrow$

w

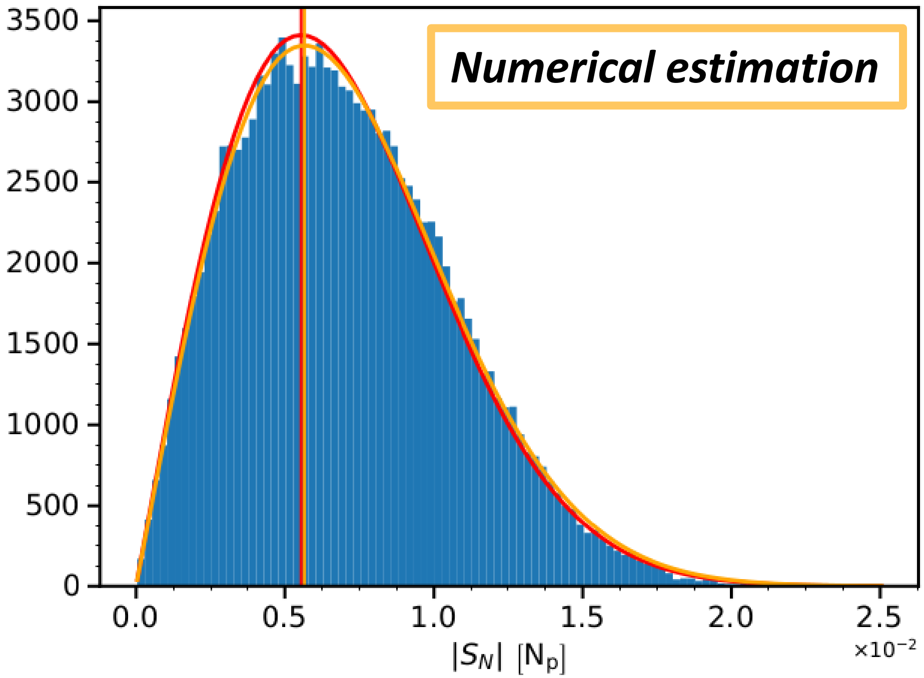
Weighted white noise

$$\mathrm{Re}\left(S_N\right), \mathrm{Im}\left(S_N\right) \sim \sigma_N \times \mathcal{N}_{[0,1]}$$

$$\boxed{\sigma_N = \sqrt{\frac{\sum^{N_b} w^2}{2}\frac{2}{N_b}} = \frac{\sqrt{2N_p}}{N_b}}$$

Numerical estimation

Noise spectrum in amplitude



$$|S_N| = \sqrt{\mathrm{Re}\left(S_N\right)^2 + \mathrm{Im}\left(S_N\right)^2}$$

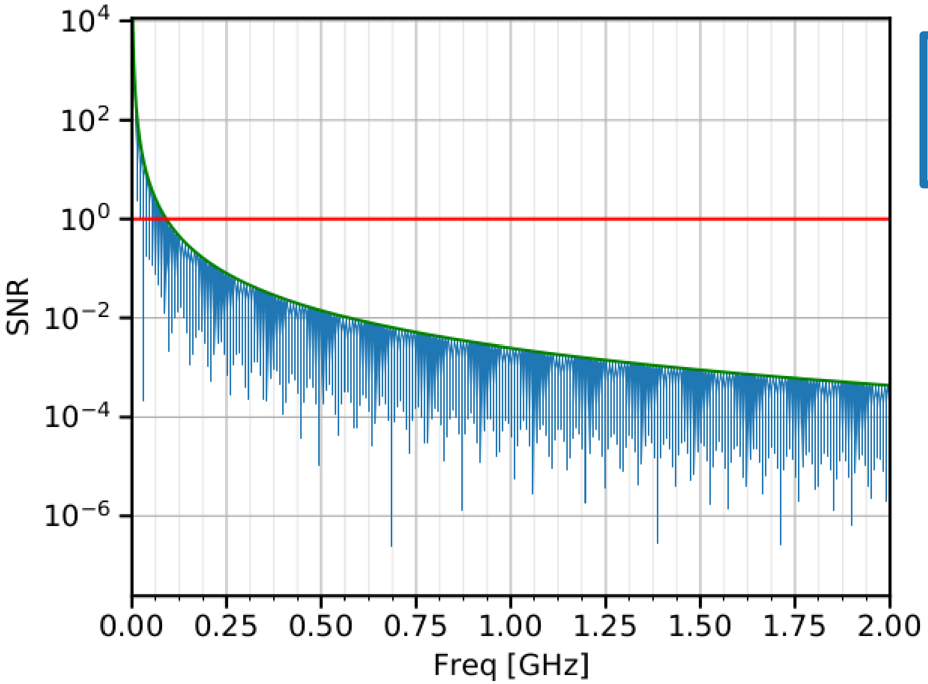
$$\mathcal{R}_{\sigma_N^2}\left(|S_N|\right) = \frac{|S_N|}{\sigma_N^2}\exp\left(\frac{-\left|S_N\right|^2}{2\sigma_N^2}\right)$$

$$\boxed{\mu_{\mathcal{R}} = \sqrt{\frac{\pi}{2}}\sigma_N = \frac{\sqrt{\pi N_p}}{N_b}}$$

$$\sigma_{\mathcal{R}} = \sqrt{\frac{4-\pi}{2}}\sigma_N = \frac{\sqrt{(4-\pi)\,N_p}}{N_b}$$

- We are interested in the amplitude of the noise spectrum.
- The real and imaginary parts are independent random variables, the combination follows a Rayleigh distribution.
- We get μ_R, the mean amplitude of noise spectrum, **independent from frequency.**

Signal-to-noise ratio vs. frequency



$$\mathrm{SNR}[f] = \frac{S[f]}{\mu_{\mathcal{R}}} = 2\sqrt{\frac{N_p}{\pi}}\frac{\Gamma(\alpha+1)}{(\pi\tau_l f/2)^{\alpha}}J_{\alpha}(\pi\tau_l f)$$

$$\mathrm{SNR}[f] \approx \frac{2}{\pi}\frac{\sqrt{N_p}}{(\sigma_l f)^{\mu'+1}}F(\mu')$$

- The SNR is evaluated by comparing the noise mean amplitude with the smooth spectrum.
- A simple scaling law can be obtained by using the asymptotic form of the Bessel function, and using the truncated binomial distribution to avoid SNR to diverge.
- The frequency at which noise starts to become dominant is obtained when SNR<1.

Remarks (1)

$$\mathrm{SNR}\left[f\right] \approx \frac{2}{\pi} \frac{\sqrt{N_p}}{\left(\sigma_l f\right)^{\mu'+1}} F\left(\mu'\right)$$

- The noise at a given frequency weakly depends on the bin size! Increasing the resolution does not bring more noise at a given frequency, it brings more noise from higher sampling frequencies.

- The SNR for a parabolic profile scales as $\sqrt{N_p}/(\sigma_l f)^2$. Doubling the bunch length or the frequency of interest requires $\underline{\times \mathbf{16}}$ in the number of particles to keep SNR constant.

- The SNR scales strongly with frequency. Simulations with low frequency impedance sources (coupled-bunch instability) are less affected than with high frequency ones (microwave instability).

Remarks (2)

$$\mathrm{SNR}\left[f\right] \approx \frac{2}{\pi} \frac{\sqrt{N_p}}{\left(\sigma_l f\right)^{\mu'+1}} F\left(\mu'\right)$$

- Diverging impedance sources like space charge (constant $\mathrm{Im}Z/f$) will introduce large noise at high frequency if the resolution in time is too small.

- The SNR scales strongly with μ'. An interpretation is that more particles are needed to have a good enough representation of the tails so that their contribution to intensity effects is not dominated by noise.

Criterion for the number of macroparticles

$$\mathrm{SNR}\left[f\right] \approx \frac{2}{\pi} \frac{\sqrt{N_p}}{\left(\sigma_l f\right)^{\mu'+1}} F\left(\mu'\right)$$

$$\boxed{N_m > \left(\frac{\pi}{2} \frac{\left(\sigma_l f\right)^{\mu'+1}}{F\left(\mu'\right)} \right)^2}$$

with $N_m \leq N_p$, and μ' computed from N_p

- A simple criterion to select the number of macroparticles N_m is to find $\mathrm{SNR}(N_m) = 1$ for fixed distribution parameters and frequency of interest.

- This criterion is however derived only from a stationary distribution, SNR for perturbations (instabilities) would need some further derivations.

Examples (SPS, 1)

Bunch	Particles N_p $\times 10^{11}$ (/bunch)	Length $4\sigma_l$ (ns)	Exponent μ	Effective exponent μ'	Macroparticles N_m (/bunch)
Injection	1.2	3.0	1.5	≈ 1.5	960 k
Extraction	1.2	1.65	2.0	≈ 2.0	265 k

- The number of macroparticles to use for microwave instability studies (with vacuum flanges at 1.4 GHz) was obtained empirically in the SPS (500k-1M macroparticles per bunch).

- The obtained number of macroparticles from the criterion is comparable to the one obtained empirically.

Examples (SPS, 2)

Bunch	Particles N_p $\times 10^{11}$ (/bunch)	Length $4\sigma_l$ (ns)	Exponent μ	Effective exponent μ'	Macroparticles N_m (/bunch)
Injection	1.2	3.0	1.5	≈ 1.5	960 k
Extraction	1.2	1.65	2.0	≈ 2.0	265 k
Long bunches	2.5	25.0	1.0	≈ 1.0	39 B

- The high frequency impedance sources in the SPS were measured by injecting long bunches with RF off.
- In simulations, reproducing the measured results depended greatly on the initial distribution and the number of macroparticles. Measurements were better reproduced by taking PS bunch profiles instead of smooth starting conditions.
- The criterion indicates that to have a good enough SNR starting from a smooth profile, extremely large number of macroparticles should have been used.

Examples (PS, 1)

Bunch	Particles N_p $\times 10^8$ (/bunch)	Length $4\sigma_l$ (ns)	Exponent μ	Effective exponent μ'	Macroparticles N_m (/bunch)
Parabolic	5	10.0	1.0	≈ 1.0	672 k
Gaussian	5	10.0	∞	$\mu'_{\max} \approx 16.1$	N_p

- Microwave instability in the PS was observed with the ion beam at transition crossing.
- The bunch is very short and due to the attenuation of the cables, the measured bunch profile looks more Gaussian than it is.
- According to the criterion, using a Gaussian bunch instead of a parabolic bunch requires an extremely high number of macroparticles. A good correction of the bunch profile is needed.

Examples (PS, 2)

Bunch	Particles N_p $\times 10^{11}$ (/bunch)	Length $4\sigma_l$ (ns)	Exponent μ	Effective exponent μ'	Macroparticles N_m (/bunch)
Transition	4x1.2	20.0	1.0	≈ 1.0	11 M
Flat top	4x1.2	50.0	1.0	≈ 1.0	420 M
Before rotation	1.2	12.0	1.5	≈ 1.5	31 M
After rotation	1.2	4.0	1.5	≈ 1.5	126 k

- The variation in bunch length of the LHC beam in the PS is large (almost 2 orders of magnitude from the longest to the shortest bunch along the ramp).
- The number of macroparticles to use for a simulation (e.g. end-to-end) will depend on what is the maximum bunch length in that time frame.
- The number of macroparticles required according to the criterion is large and requires to use large scale facilities and optimization with MPI.

Conclusions

- The numerical noise due to binning of particles was evaluated by comparing the spectrum from a smooth binomial profile to the noise of a weighted white noise.
- An expression of the scaling of the noise with the distribution type, bunch length, number of particles, resolution in time, frequency of interest was obtained.
- The scaling of the signal-to-noise ratio was used to give a simplified criterion to evaluate the number of macroparticles to use in a tracking simulation.
- This criterion compared to known studies in PS/SPS gave reasonable results with respect to empirical estimations.

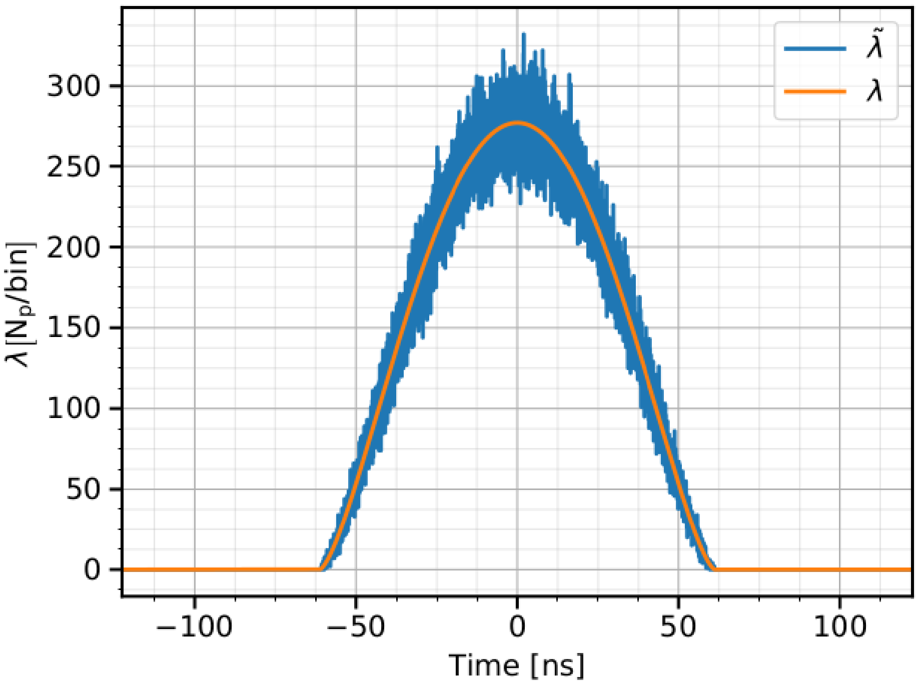
Further ideas

- Evaluate the signal-to-noise ratio for multibunch spectrum and for a perturbation of known amplitude.

- Improve the representation of tails by treating two different sets of macroparticles with different weights.
  - One distribution to represent the core bunch with a parabolic distribution and a second to represent the tails only.

Extra slides

“Smooth” profile definition



$$\boxed{\lambda\left[t\right] = N_p \lambda_0 \left[1 - 4\left(\frac{t}{\tau_l}\right)^2\right]^{\mu}}$$

N particles

Full bunch length

“Tails” exponent

$$\sigma_l = \frac{\tau_l}{2\sqrt{3+2\mu}}$$

RMS bunch length

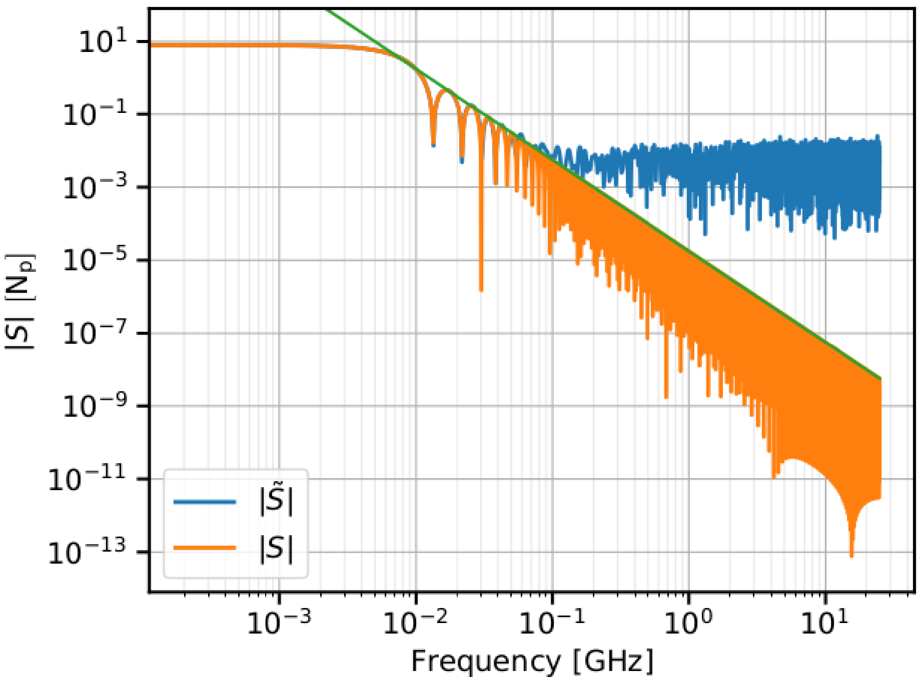
Bin size

$$\lambda_0 = \frac{2\Gamma\left(\mu + 3/2\right)}{\tau_l\sqrt{\pi}\Gamma\left(1+\mu\right)}\Delta t$$

- Taking an example smooth profile λ with $\sigma_l = 100$ ns.

- The usage of the rms bunch length is preferred over the full bunch length as a Gaussian profile is obtained for $\mu \rightarrow \infty$, with $\tau_l \rightarrow \infty$, for a given σ_l

“Smooth” spectrum definition



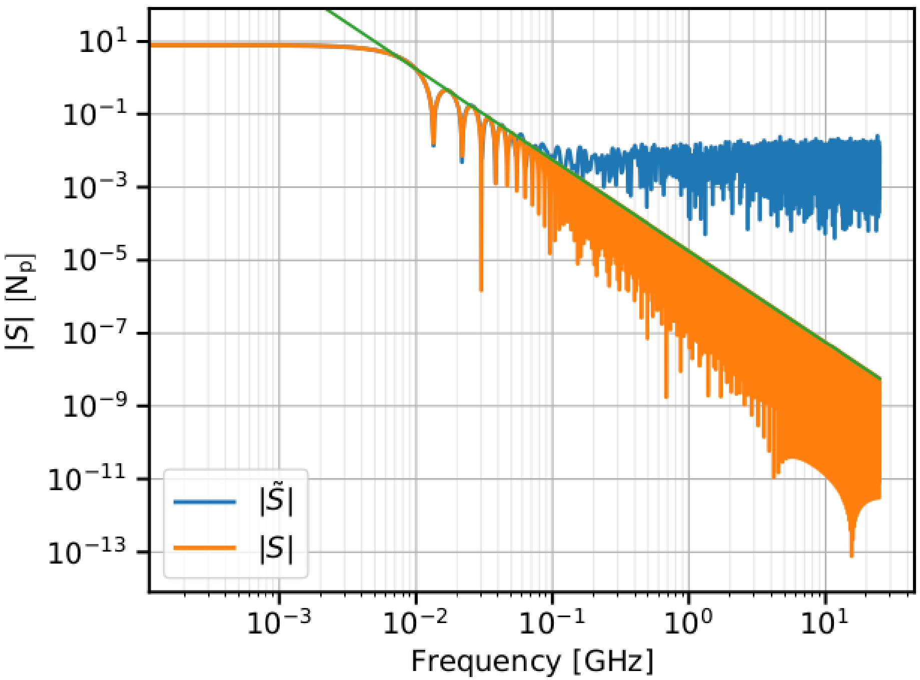
$$\boxed{S\left[f\right] = \frac{2N_p}{N_b}\frac{\Gamma\left(\alpha+1\right)}{\left(\pi\tau_l f/2\right)^{\alpha}} J_\alpha\left(\pi\tau_l f\right)}$$

N bins

$$\alpha = \mu + \frac{1}{2}$$

- Computing the corresponding spectrum with a Fourier Transform (normalization factor from the Discrete Fourier Transform)
- A binomial spectrum has lobes coming from the Bessel Function J_α.

"Smooth" spectrum definition

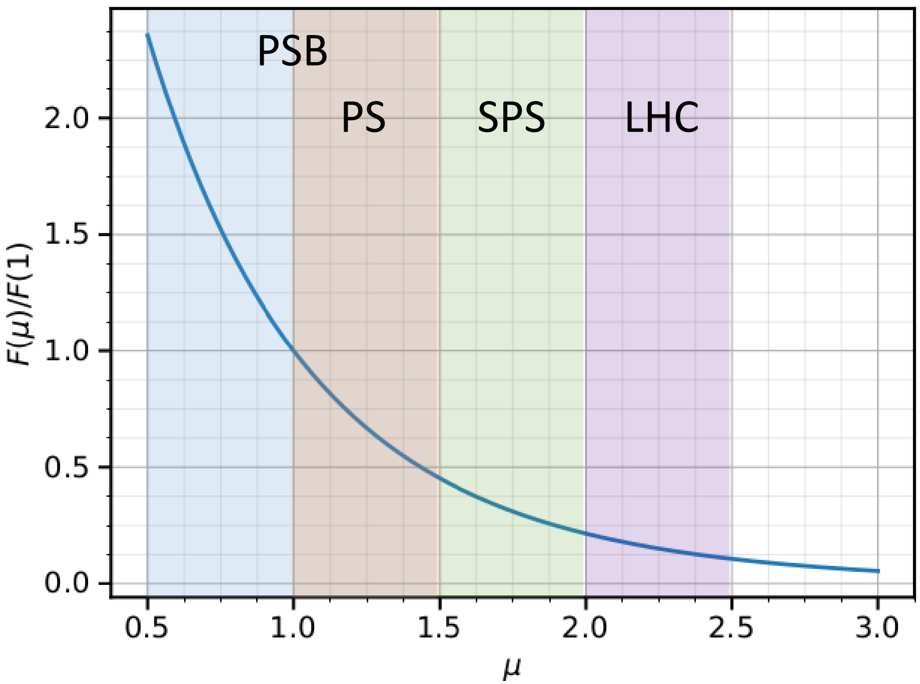


$$\boxed{S[f] \sim \frac{2N_p}{\sqrt{\pi}N_b}\frac{1}{(\sigma_l f)^{\mu+1}}F(\mu)}$$

$$F(\mu) = \frac{\Gamma\left(\mu + \frac{3}{2}\right)}{\pi^{\mu+1}(3+2\mu)^{\frac{\mu+1}{2}}}$$

- The zeros of J_α will be an issue for an expression of the SNR scaling law.
- We look at the high frequency part, we can use the asymptotic form to get the amplitude of the lobes only.
- The $F(\mu)$ function is a form factor

Spectrum form factor at high freq.



$$F(\mu) = \frac{\Gamma\left(\mu + \frac{3}{2}\right)}{\pi^{\mu+1}\left(3 + 2\mu\right)^{\frac{\mu+1}{2}}}$$

- The form factor $F(\mu)$ is also an issue for SNR scaling law as $F(\mu \to \infty) \to 0$.

- How can we get an expression for Gaussian profiles?

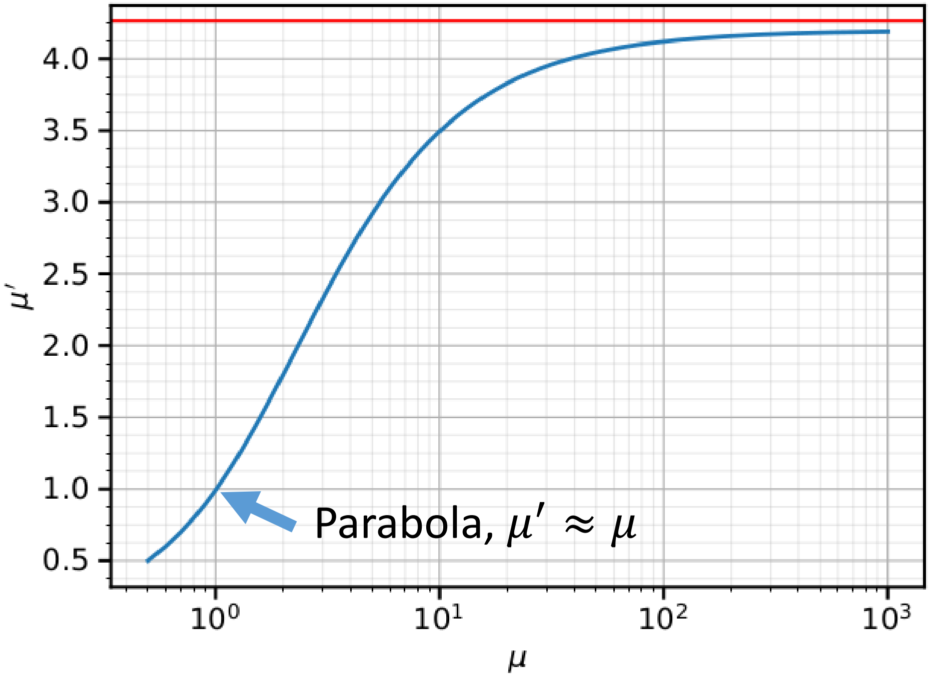
Gaussian profile with discrete N_p

$$\tau_l' = \tau_l \sqrt{1 - \left(\frac{1}{N_p \lambda_0}\right)^{\frac{1}{\mu}}}$$

$$\sigma_l' = \frac{\tau_l'}{2\sqrt{3 + 2\mu'}} \approx \sigma_l$$

- A profile cannot have infinite tails for a discrete profile and can be truncated when $\lambda(\tau_l) < 1$ (or at the limit of the RF bucket).
- This condition can be used for a fixed number of particles and bin size to get the truncated bunch full bunch length τ_l.
- We can also assume that the rms bunch length for the truncated bunch stays the same.

Spectrum form factor at high freq.



$$\mu' = \frac{(3+2\mu)\left[1-\left(\frac{1}{N_p\lambda_0}\right)^{\frac{1}{\mu}}\right]-3}{2}$$

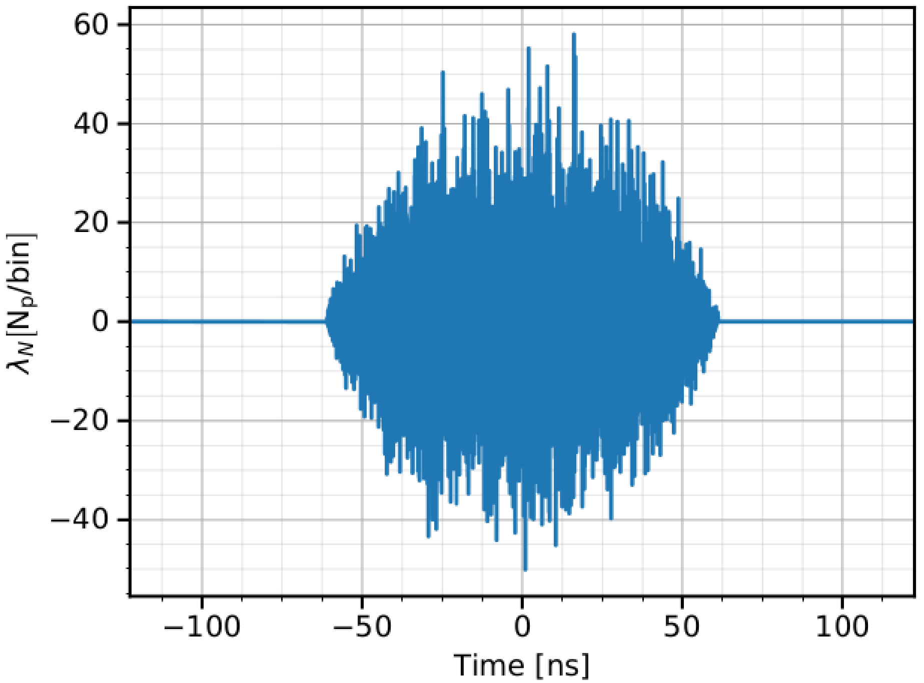
$$\boxed{\mu'_{\max} = \lim_{\mu\to\infty}\mu' = \frac{2\ln\left(\frac{N_p\Delta t}{\sigma_l}\right)+\ln\left(\frac{1}{2\pi}\right)-3}{2}}$$

- For a fixed rms bunch length and truncated full bunch length, the effective tails exponent μ' can be obtained.

- The effective μ' represents the fact that the bunch cannot have infinite tails is bounded and can be used in $F(\mu')$ from now on for SNR calculations.

- NB: this can also be used as bound for fitting with binomial!

Noise profile



$$\tilde{\lambda}[t] = \lambda[t] + \lambda_N[t]$$

$$\lambda_N[t] \sim \underbrace{\sqrt{\lambda[t]} \times \mathcal{N}_{[0,1]}}_{w}$$

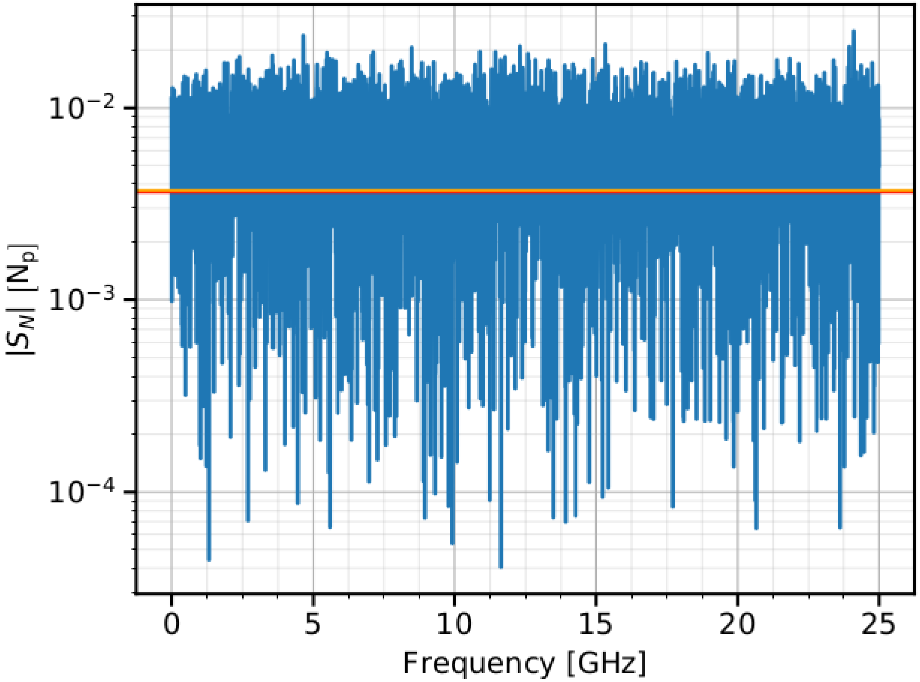
Weighted white noise

- The profile is decomposed as a sum of the smooth profile and a noise contribution

- The noise follows a Poisson law at each bin, with the variance at each bin being equal to the particles in that bin.

- Since the number of particles is large, the Poisson law converges to a Gaussian law.

Noise spectrum



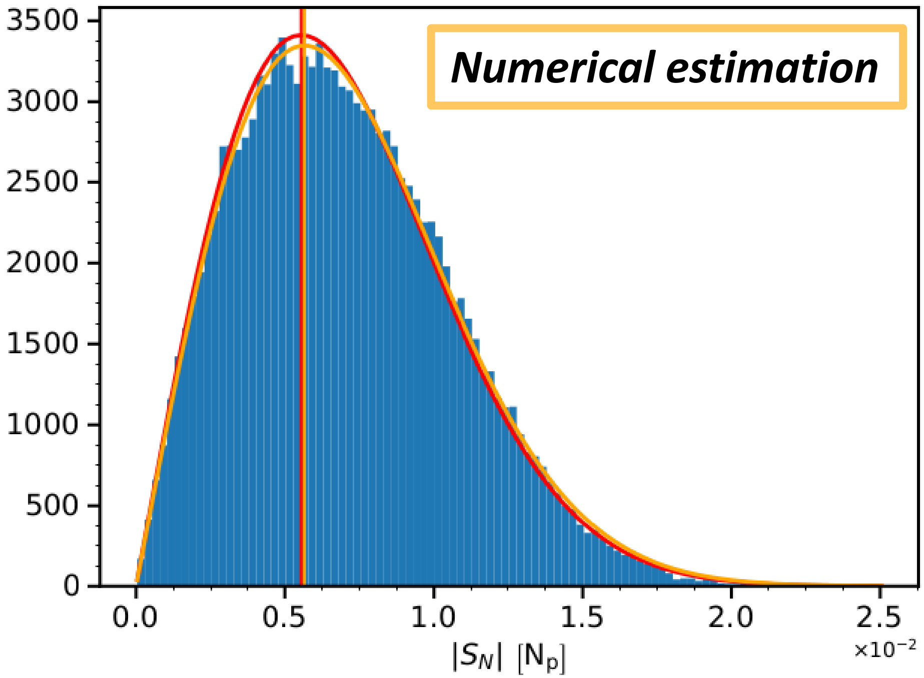
$$\mathrm{Re}\left(S_N\right), \mathrm{Im}\left(S_N\right) \sim \sigma_N \times \mathcal{N}_{[0,1]}$$

$$\boxed{\sigma_N = \sqrt{\frac{\sum^{N_b} w^2}{2} \frac{2}{N_b}} = \frac{\sqrt{2N_p}}{N_b}}$$

Numerical estimation

- The spectrum of a weighted white noise is a white noise in the real and imaginary part, independent from frequency.
- The standard deviation of the noise σ_N indicates that to have constant **noise** amplitude (independent of the smooth distribution), doubling the resolution in time already requires $\times\ 4$ is N_p.

Noise spectrum in amplitude



$$|S_N| = \sqrt{\mathrm{Re}(S_N)^2 + \mathrm{Im}(S_N)^2}$$

$$\mathcal{R}_{\sigma_N^2}(|S_N|) = \frac{|S_N|}{\sigma_N^2}\exp\left(\frac{-|S_N|^2}{2\sigma_N^2}\right)$$

$$\boxed{\mu_{\mathcal{R}} = \sqrt{\frac{\pi}{2}}\sigma_N = \frac{\sqrt{\pi N_p}}{N_b}}$$

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