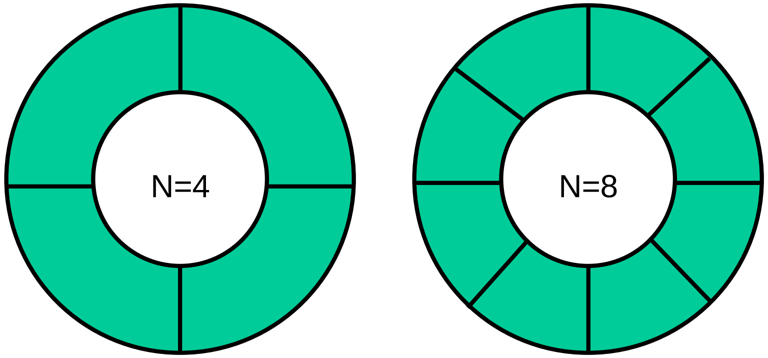
Analysis of Complex Rotation Spectra

1. Fourier and All Poles transforms
2. Maximum Entropy spectral analysis
3. Time domain analysis versus frequency domain analysis

Grouping for TF Data

A dephasing effect will reduce the asymmetry of TF data if not enough groups are used:



Dephasing factor = sin(π/N) / (π/N)

TF Groups	Dephasing Factor
16	99 %
8	98 %
4	90 %
2	64 %

i.e. 8 TF groups are sufficient for most purposes

Fourier and All-Poles Transforms

FFT (Fast Fourier Transform) is the standard way to convert from time domain to frequency domain.

FFT assumes frequency spectrum is well represented by array of evenly spaced points, which works well for spectra containing broad spectral features.

However, if the spectrum contains very narrow features, other types of frequency transform can work better.

The All-Poles (maxent) method is one such method, which makes an expansion of the data in terms of a series of sharp frequencies

See Press et al, Numerical Recipes, CUP for further details of the All-Poles transform

All transform methods assume that the data error is independent of time, which is clearly not the case for μSR data.

Data filtering (apodization) is an important step before transforming.

Apodization

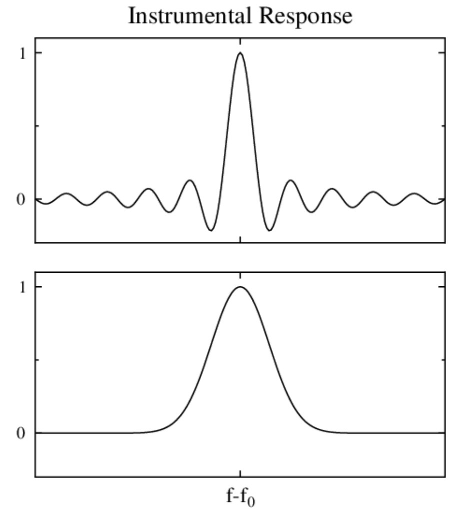
Apodization involves multiplying the time data by a smooth cutoff function (e.g. a Gaussian or exponential decay) before making the transform into frequency space

This addresses two problems:

1) Finite time window of the data (e.g. 0 to 32 μs at ISIS)

without apodization the instrument response in frequency space is a sinc function

with apodization the instrumental function becomes smooth without any troublesome lobes, however the frequency resolution is lowered



2) Decrease of signal to noise ratio at longer times

By weighting towards early time data and against long time data the S/N of the frequency spectrum is kept under control

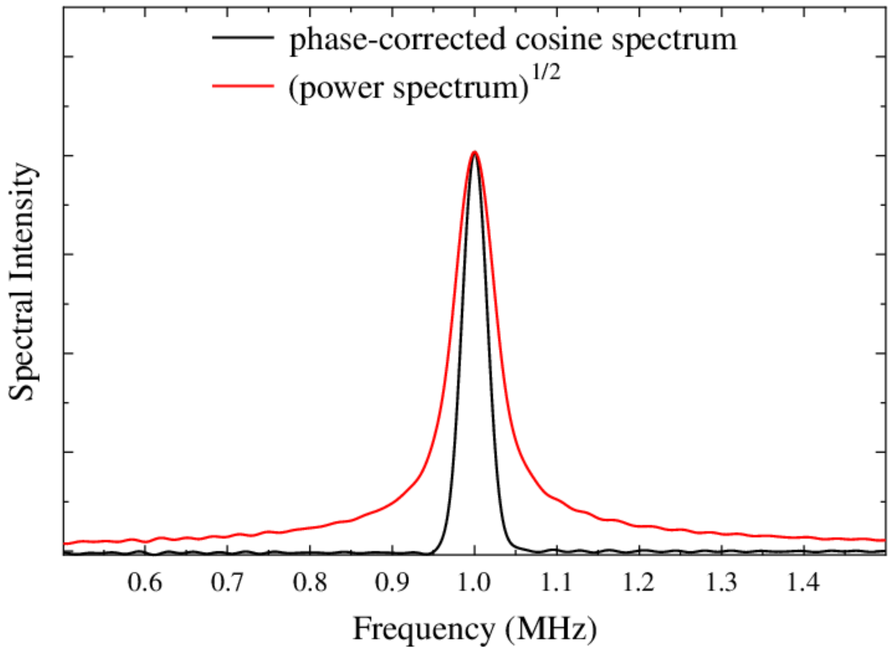
For narrow spectra one can turn off the apodization and directly model the instrumental function in frequency space

Combining Groups: Power Spectra versus Phase-Corrected Cosine Spectra

<u>Spectral intensity from power spectra</u>

Advantages:
simplicity
copes with different t_0 for different components

Disadvantages:
broadened spectral tails
non-linear processing distorts errors



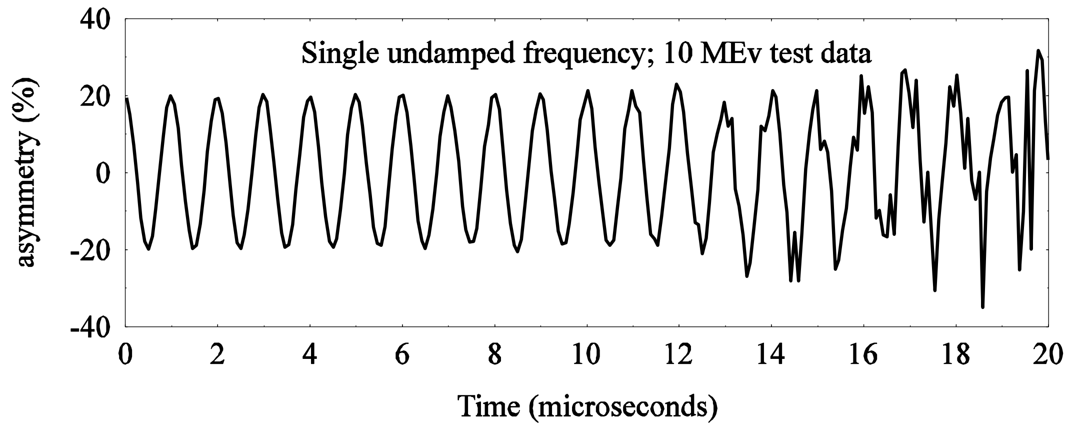
<u>Spectral intensity from phase-corrected spectra</u>

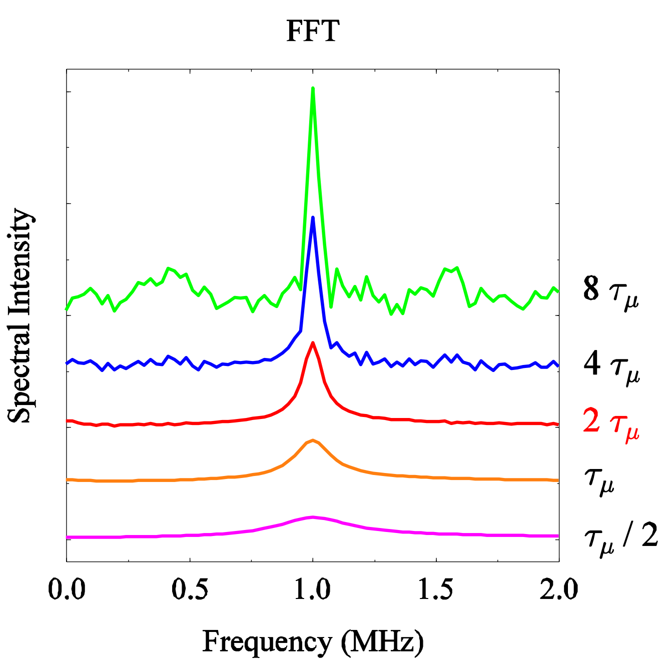
Advantages:
no extra broadening or tails
linear process

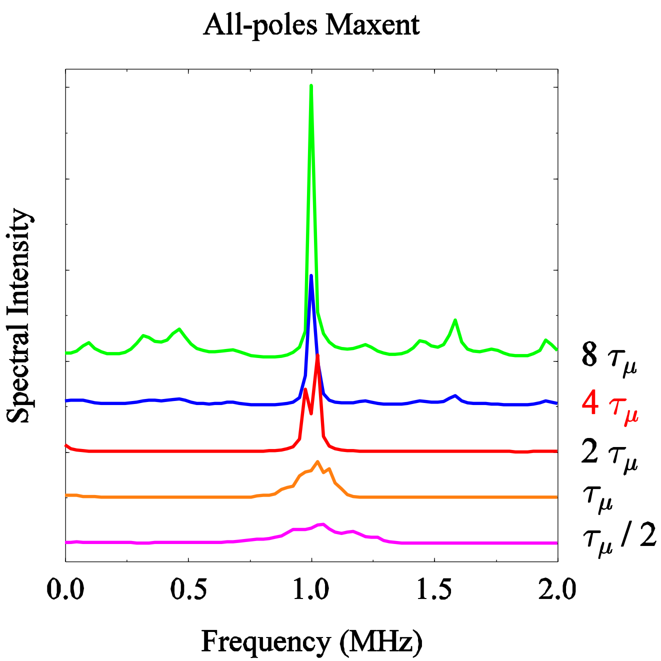
Disadvantages:
phase estimation step needed
problem if t_0 varies across spectrum

Fourier and All-Poles Transforms

Optimal filtering time constant for a single undamped test frequency

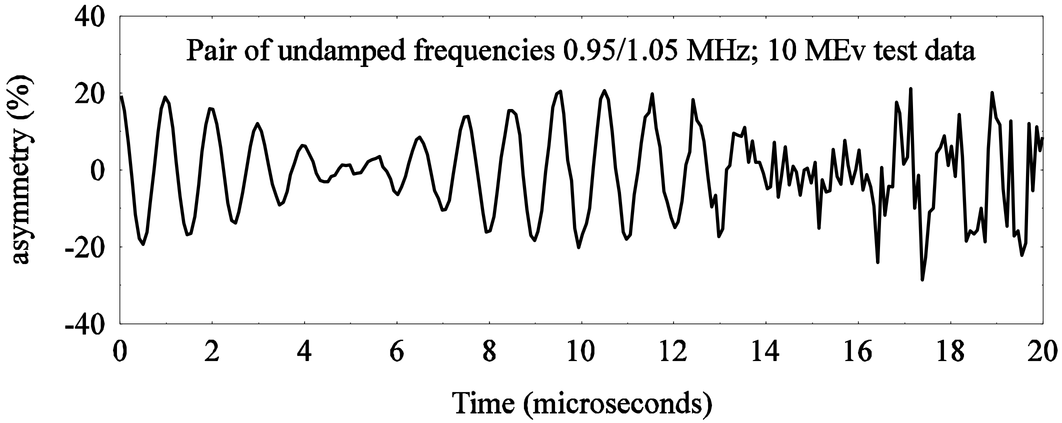


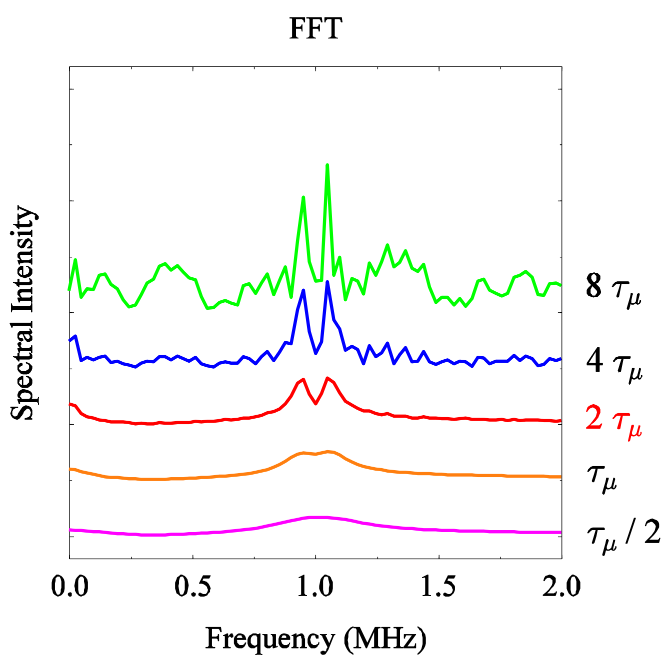


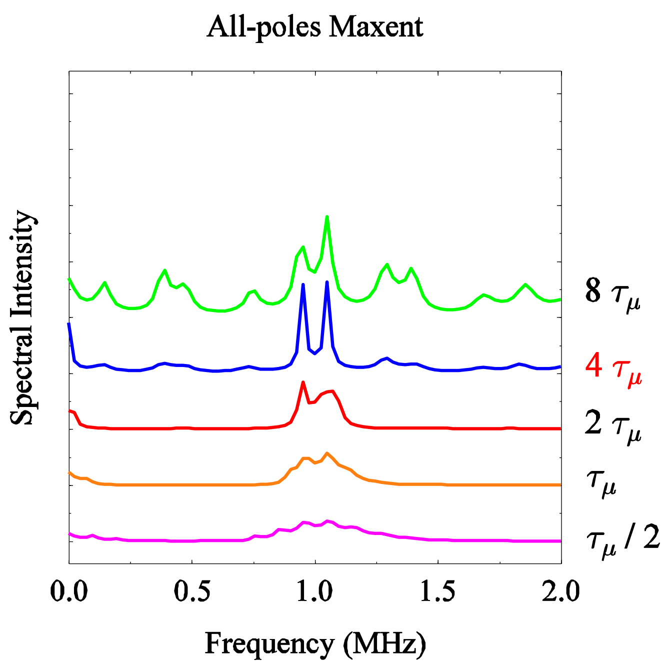


Fourier and All-Poles Transforms

A close pair of undamped test frequencies







The Maximum Entropy Method

Avoids the noise problem and need for filtering; takes data errors fully into account

Iterative procedure for constructing the frequency spectrum with the minimum structure (i.e. maximum entropy) that is consistent with the measured data

Entropy here is determined from the frequency spectrum p_k

$$S = -\sum_k \frac{p_k}{b} \log \frac{p_k}{b}$$

The procedure involves maximising $S - \lambda \chi^2$, where λ is a Lagrange multiplier

a key point is that the model spectrum is being transformed rather than the data

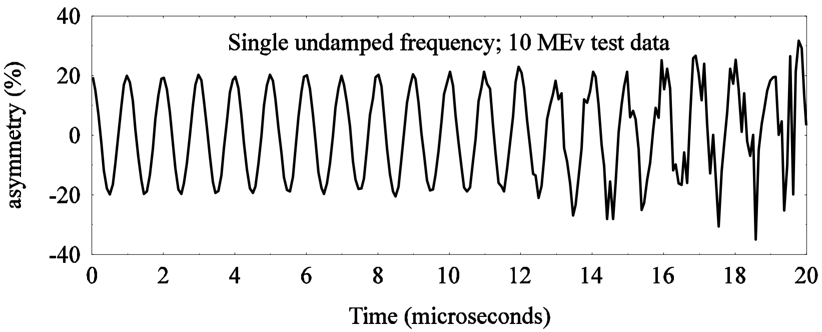
See Rainford and Daniell, Hyperfine Interactions 87, 1129 (1994)
for a detailed discussion of using Maximum Entropy in μSR

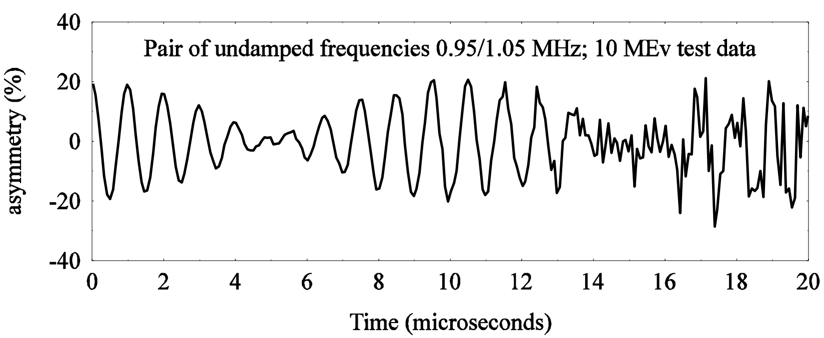
for a general reference see:

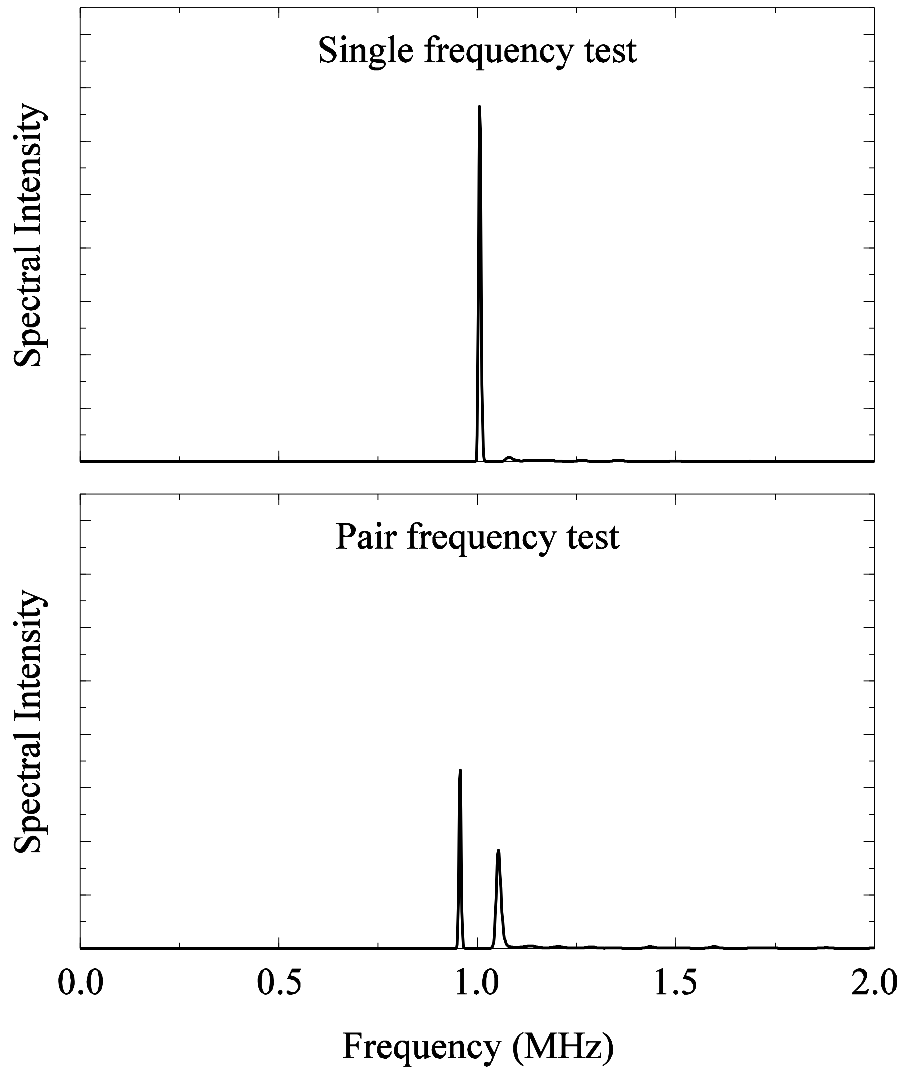
'Maximum Entropy in Action', Buck and Macaulay, OUP (1991)

The Maximum Entropy Method

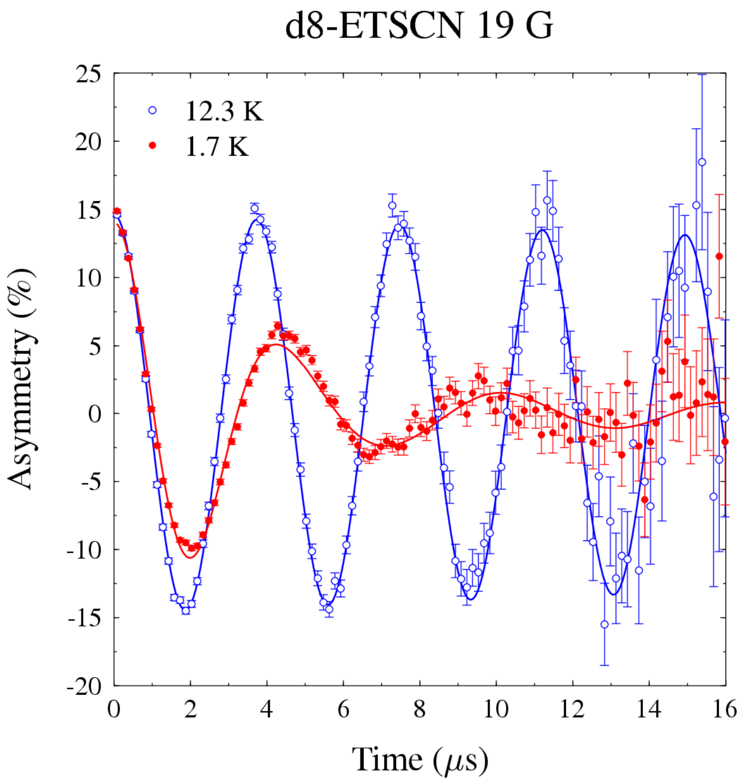
Demonstration of MaxEnt using the test data used for the transforms



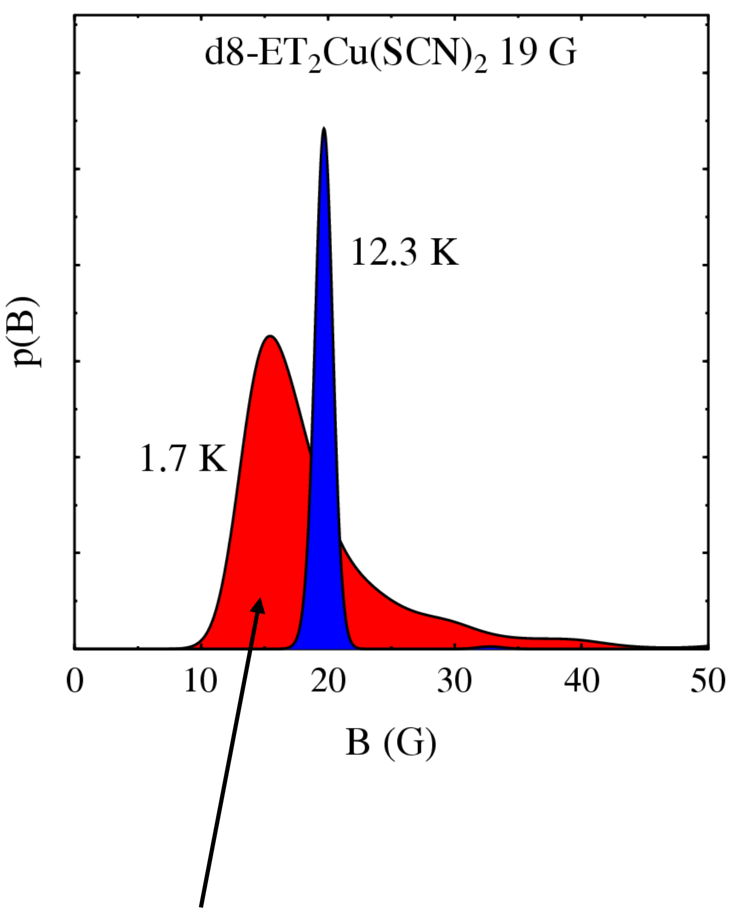




Organic Superconductor Example



Maximum Entropy Spectra



Characteristic field distribution
due to vortex lattice

Time Domain Analysis versus Frequency Domain Analysis

Single Frequency

	Freq (MHz)	Width (MHz)
Test Data	1.0000	0.000
Time domain fit	0.9998(1)	0.001(1)
Maximum Entropy	1.006	0.003

Pair of Frequencies

	Freq (MHz)		Width (MHz)	
Test Data	0.9500,	1.0500	0.000,	0.000
Time domain fit	0.9493(1)	1.0499(3)	0.003(3)	0.004(3)
Maximum Entropy	0.956	1.054	0.002	0.005

Time Domain Analysis versus Frequency Domain Analysis

Transforms are good for determining a qualitative picture of data:

FFT best for spectra containing relatively broad features

All-poles transform best for spectra composed of sharp features

Iterative Maximum Entropy Method gives an ‘unbiased’ view of the data

but Time Domain Fitting gives best ultimate accuracy, provided the correct model is being used.

CONCLUSION

A combination of Frequency Domain and Time Domain analysis usually works best in practice