

PERCH NMR Software

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Classical Spectral Analysis

Observed Spectrum

1. Order Analysis
Not Exact!



V_A, V_B, V_C
 J_{AB}, J_{AC}, J_{BC}

Calculated Spectrum

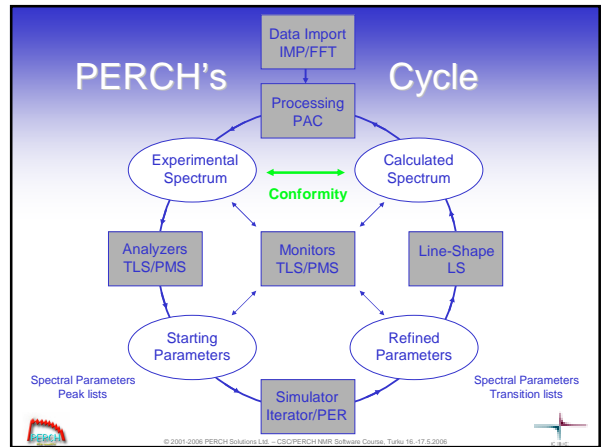
Exact!

V_A, V_B, V_C
 J_{AB}, J_{AC}, J_{BC}

Calculation






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PERCH Shell

Status Bar ≡ Short Info

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PERCH Syntax

- Control Commands
- Display Controls (Zooming)
- PERCH Files & Naming Convention




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Interface

The screenshot shows the PERCH software interface with several key components labeled:

- Frequency Cursors:** Two vertical red lines on the spectrum plot.
- Scaling Buttons:** A set of buttons on the right side of the plot area.
- Spectrum Window:** The main plot area showing the spectrum.
- Function Buttons:** A row of buttons at the bottom of the interface.
- Input Prompt:** A small box at the bottom right where a value '1' is entered.

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Control Commands

- Button (or short cut)
- Number followed by ENTER $5\downarrow$ or $5,6\downarrow$
- Number followed by short cut $5w$
- SHIFT, CTRL and ALT keys +...

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Display Controls (Zooming)

- Using the mouse pointer (frequency cursors/zoom box)
- Entering frequencies
- Using short cuts (buttons)
- (Using the cursor keys)

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PERCH Files & Naming Convention

- Same directory
- Same name, different extension
- No long file names - 8.3 DOS-format.
- No sharing
- Copying only in special cases

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PERCH Files

NAME.TXT	contains the original digital spectrum or FID. This file also may have a user-defined name.
NAME.FID	contains the imported FID in the PERCH format. BINARY
NAME.NF	contains spectral information and the current state of the analysis. ASCII
NAME.OBS	contains the imported spectrum in the PERCH format. BINARY
NAME.DAT	contains the peak-top-frequencies and assignments for PERCHit. ASCII
NAME.PMS	contains the trial spectral parameters for PERCHit. ASCII
NAME.PAR	contains control parameter read by PER (call PER PAR), command prompt only. ASCII
NAME.SAV	contains the last iterated spectral parameters. The iteration is continued from these values using the option 1 in PERCHit (or with PER SAV). ASCII
NAME.OUT	contains the calculated frequencies produced by PER. BINARY
NAME.CAL	contains the computed digital spectrum. BINARY
NAME.VEC	contains the eigenvectors. BINARY (NEW : previous VECTORS)
NAME.TOP	contains the result of the deconvolution. ASCII
NAME.XYI	A TLS-fit stored under TLS (i = 1...99). ASCII
ITOBSCAL	contains observed IT-spectrum from PER with option 34 (i = 1...99). BINARY
ITCALICAL	contains calculated IT-spectrum from PER with option 35 (i = 1...99). BINARY

The following files are created and used by the PERCH Shell (WPERCH.EXE) only:

NAME.DOC	contains the collected documents of the PERCH programs. ASCII
NAME.HIS	contains history information concerning the document files. ASCII
NAME.ZIP	contains all the files of the case in compressed form. The file is formed by the File/Close Case menu under the PERCH Shell. Use the File/Open Case menu under the shell.

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PERCH Output

- Text Output (Parameters, Protocols) Text Editor (Notepad)
- Spectra via Print Module as Metafile

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Flow of Analysis

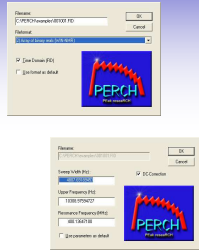
- Sample preparation
- Acquisition
- Processing
- Analysis
- Interpretation

Data Transfer

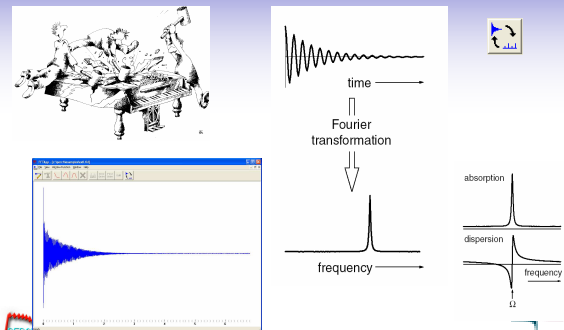
- File Transfer Protocol (FTP)
- Network File System (NFS)
- Vendor specific solutions
Bruker (Bruknet, NMRLink etc.)
- Serial port (antique)

Import

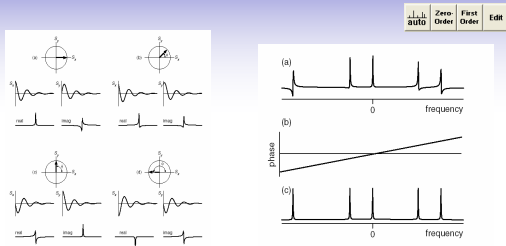
- Bruker (WIN-NMR, Aspect 3000, UXNMR, XWIN-NMR)
- Varian (16/32 bit binary)
- Jeol (binary data for GX)
- Chemagnetics (32 bit binary)
- General Electrics (32 bit binary)
- G.E. Nicolet (20 bit binary), only spectra
- JCAMP-DX (PAC form)
- LYBRICS binary
- SMIS, raw-data, ASCII
- NUTS binary
- Siemens ACR-NEMA
- Philips SUNspec1 Sun floats
- Columns of ASCII data
- Custom format for binary data
(16/24/32 bit, header size, bit swap, value skip)



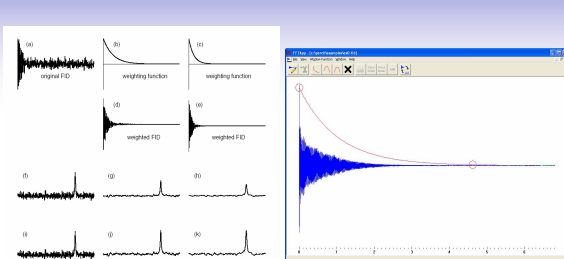
Fourier Transformation



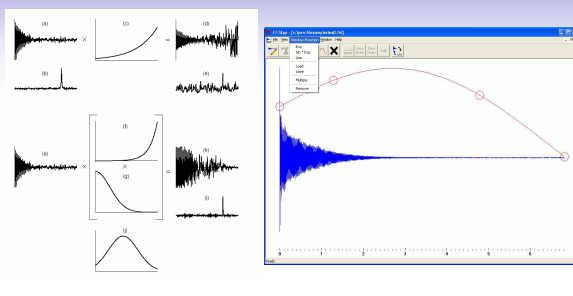
Phase Correction



Sensitivity Enhancement



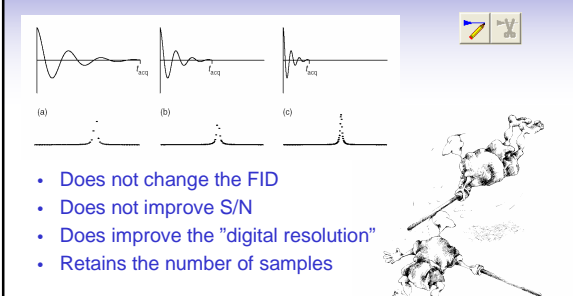
Resolution Enhancement



The slide illustrates resolution enhancement techniques. On the left, a series of plots shows the effect of increasing the resolution factor (from 1 to 10) on a peak. The central plot shows a software interface for resolution enhancement, with a peak selected and a resolution factor of 10.0. The resulting spectrum shows a significantly narrower and taller peak compared to the original.

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Zero - Filling



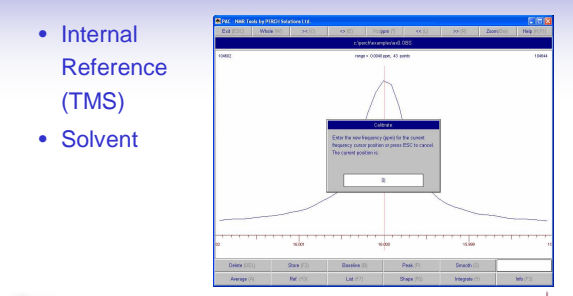
The slide illustrates zero-filling. It shows three plots: (a) the original spectrum, (b) the spectrum with zero-filling, and (c) the resulting spectrum with a higher digital resolution. The zero-filled spectrum shows a smoother appearance and more defined peaks. A software interface shows a peak selected for zero-filling.

- Does not change the FID
- Does not improve S/N
- Does improve the "digital resolution"
- Retains the number of samples

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Calibration

- Internal Reference (TMS)
- Solvent

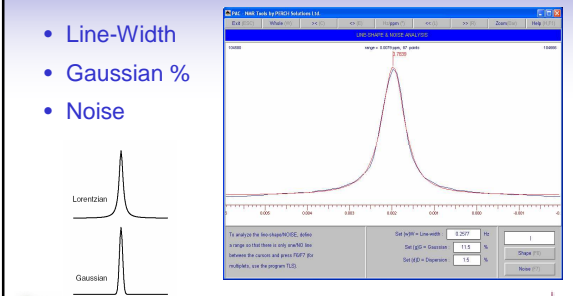


The slide shows a software interface for calibration. A peak is selected, and a dialog box prompts for the reference peak position in ppm. The interface includes a list of peaks and a search function.

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Line - Shape Analysis

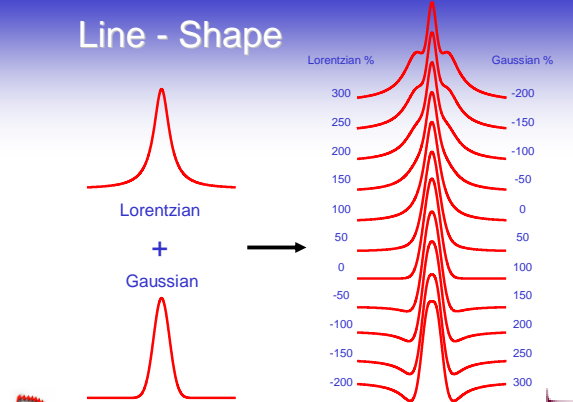
- Line-Width
- Gaussian %
- Noise



The slide shows a software interface for line shape analysis. A peak is selected, and the interface displays the Lorentzian and Gaussian components. The Lorentzian component is shown as a narrow peak, and the Gaussian component is shown as a broader peak. The resulting fit is shown as a smooth curve.

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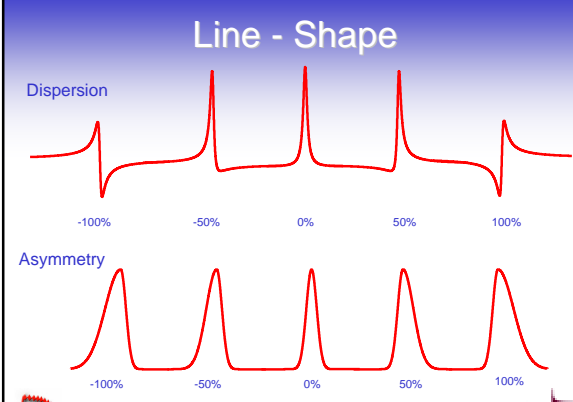
Line - Shape



The slide illustrates the combination of Lorentzian and Gaussian line shapes. On the left, a Lorentzian peak and a Gaussian peak are shown, with a plus sign between them. An arrow points to a series of plots showing the resulting line shape for different percentages of Lorentzian and Gaussian components. The Lorentzian percentage ranges from 300% to -200% in increments of 50%, and the Gaussian percentage ranges from -200% to 300% in increments of 50%.

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Line - Shape

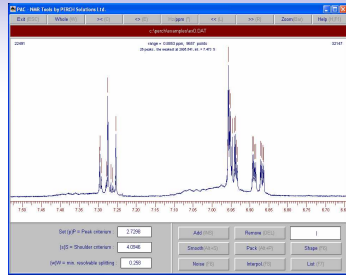


The slide illustrates the effect of dispersion and asymmetry on line shape. The top row shows the effect of dispersion, with plots for -100%, -50%, 0%, 50%, and 100%. The bottom row shows the effect of asymmetry, with plots for -100%, -50%, 0%, 50%, and 100%.

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Peak - Picking

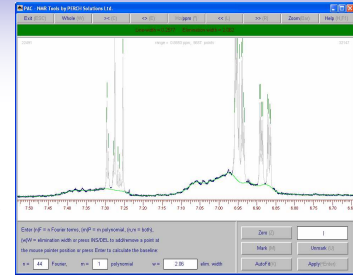
- Automatic
- Manual
- Interpolation
- Smoothing
- Packing



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Base - Line Correction

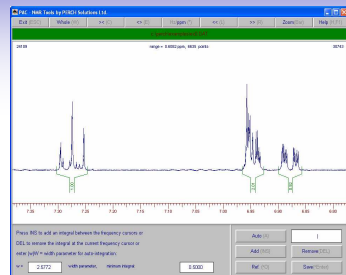
- Fourier
- Polynomial
- Elimination
- Width
- Mark/Unmark



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Integration

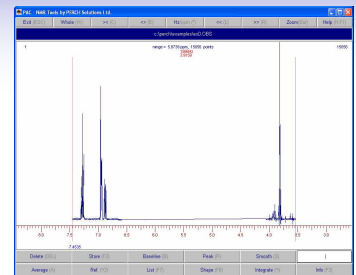
- Automatic
- Manual
- Width Parameter
- Minimum Integral



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Spectrum Editing

- Removing Parts
- Smoothing
- Averaging



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