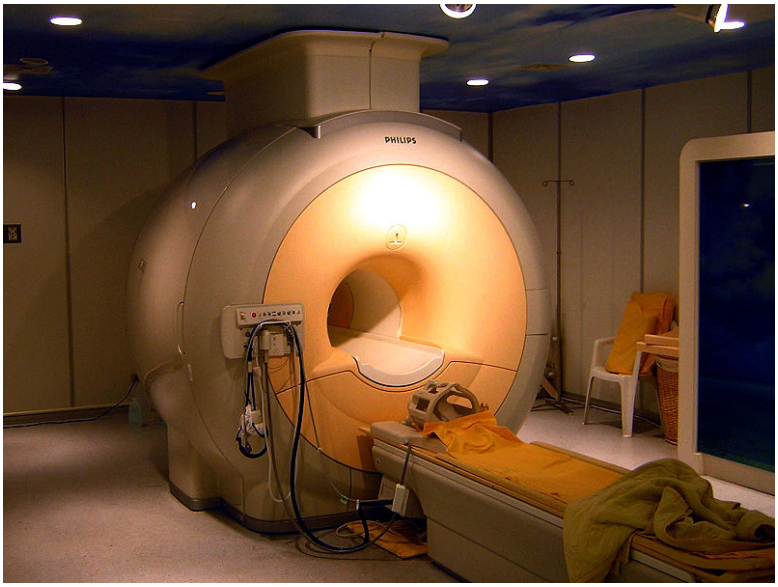
2D-FT NMRI and spectroscopy

2D-FT Nuclear magnetic resonance imaging (**2D-FT NMRI**), or **two-dimensional Fourier transform** nuclear magnetic resonance imaging (**NMRI**), is primarily a non-invasive imaging technique most commonly used in biomedical research and medical radiology to visualize structures and functions of the living systems and single cells. The physical principle[1] is essentially the same in N(MRI), nuclear magnetic resonance, FT (NMR) spectroscopy, topical NMR, or even in electron spin resonance (ESR); however, the details are significantly different at present for ESR, as only in the early days of NMR the static magnetic field was scanned for obtaining spectra, as it is still the case in many ESR spectrometers. NMRI, on the other hand, often utilizes a linear magnetic field gradient to obtain an image that combines the visualization of molecular structure and dynamics. It is this dynamic aspect of NMRI, as well as its highest sensitivity for the ^{1}H nucleus that distinguishes it very dramatically from X-ray CAT scanning that 'misses' hydrogens because of their very low X-ray scattering factor.

Chemical Shifts



Advanced 3 T clinical diagnostics and biomedical research NMR Imaging instrument.

NMR is a very useful family of techniques for chemical and biochemical research because of the chemical shift; this effect consists in a frequency shift of the nuclear magnetic resonance for specific chemical groups or atoms as a result of the partial shielding of the corresponding nuclei from the applied, static external magnetic field by the electron orbitals (or molecular orbitals) surrounding such nuclei present in the chemical groups. Thus, the higher the electron density surrounding a specific nucleus the larger the chemical shift will be. The resulting magnetic field at the nucleus is thus lower than the applied external magnetic field and the resonance frequencies observed as a result of such shielding are lower than the value that would be observed in the absence of any electronic orbital shielding. Furthermore, in order to obtain a chemical shift value independent of the strength of the applied magnetic field and allow for the direct comparison of spectra obtained at different magnetic field values, the chemical shift is defined by the ratio of the strength of the local magnetic field value at the observed (electron orbital-shielded) nucleus by the external magnetic field strength, $\mathbf{H}_{loc}/\mathbf{H}_{0}$. The first NMR observations of the chemical shift, with the correct physical chemistry interpretation, were reported for ^{19}F containing compounds in the early 1950s by Herbert S. Gutowsky and Charles P. Slichter from the University of Illinois at Urbana (USA).

A related effect in metals is called the Knight shift, which is due only to the conduction electrons. Such conduction electrons present in metals induce an "additional" local field at the nuclear site, due to the spin re-orientation of the conduction electrons in the presence of the applied (constant), external magnetic field. This is only broadly `similar' to the chemical shift in either solutions or diamagnetic solids.

Two-dimensional Fourier transform imaging and spectroscopy

2D-FT analysis is a very powerful method for both NMRI and two-dimensional nuclear magnetic resonance spectroscopy (2D-FT NMRS)[2] that allows the three-dimensional reconstruction of polymer and biopolymer structures at atomic resolution[3] for molecular weights (Mw) of dissolved biopolymers in aqueous solutions (for example) up to about 50,000 MW. For larger biopolymers or polymers, more complex methods have been developed to obtain limited structural resolution needed for partial 3D-reconstructions of higher molecular structures, e.g. for up 900,000 MW or even oriented microcrystals in aqueous suspensions or single crystals; such methods have also been reported for *in vivo* 2D-FT NMR spectroscopic studies of algae, bacteria, yeast and certain mammalian cells, including human ones.

2D-FT Definition

A *2D-FT, or two-dimensional Fourier transform*, transforms a function of two temporal variables into a function of two frequency variables. In MRS the frequencies relate to the resonant frequency offsets caused by chemical shift or J-coupling. In MRI a resonance frequency offset is introduced as a function of position; the frequency variables in the Fourier transformed time-data correspond to spatial location in the final image.[4]

Example

A 2D Fourier transformation and phase correction is applied to a set of 2D NMR (FID) signals: $\mathbf{s}(t_1,t_2)$ yielding a real 2D-FT NMR `spectrum' (collection of 1D FT-NMR spectra) represented by a matrix **S** whose elements are

$$\mathbf{S}\ (\nu_1, \nu_2) = \mathbf{Re} \int \int \cos(\nu_1 t_1) \exp^{(-i\nu_2 t_2)}\ s(t_1, t_2) dt_1 dt_2$$

where ν_1 and ν_2 denote the discrete indirect double-quantum and single-quantum(detection) axes, respectively, in the 2D NMR experiments. Next, the *covariance matrix* is calculated in the frequency domain according to the following equation

$$\mathbf{C}\ (\nu_2', \nu_2) = S^T S = \sum_{\nu^1} [S(\nu_1, \nu_2') S(\nu_1, \nu_2)],$$

with ν_2, ν_2' taking all possible single-quantum frequency values and with the summation carried out over all discrete, double quantum frequencies ν_1.

Brief explanation of NMRI diagnostic uses in Pathology

As an example, a diseased tissue such as a malignant tumor, can be detected by 2D-FT NMRI because the hydrogen nuclei of molecules in different tissues return to their equilibrium spin state at different relaxation rates, and also because of the manner in which a malignant tumor spreads and grows rapidly along the blood vessels adjacent to the tumor, also inducing further vascularization to occur. By changing the pulse delays in the RF pulse sequence employed, and/or the RF pulse sequence itself, one may obtain a `relaxation—based contrast', or contrast enhancement between different types of body tissue, such as normal vs. diseased tissue cells for example.

See also

- Nuclear magnetic resonance (NMR)
- Edward Mills Purcell
- Felix Bloch
- Medical imaging
- Paul C. Lauterbur
- Magnetic resonance microscopy
- Peter Mansfield
- Computed tomography (CT)
- Solid-state NMR
- Knight shift
- John Hasbrouck Van Vleck
- Chemical shift
- Herbert S. Gutowsky
- John S. Waugh
- Charles Pence Slichter
- Protein nuclear magnetic resonance spectroscopy
- Kurt Wüthrich
- Nuclear Overhauser effect
- Fourier transform spectroscopy(FTS)
- Jean Jeneer
- Richard R. Ernst
- FT-NIRS (NIR)
- Magnetic resonance elastography
- Relaxation
- Earth's field NMR (EFNMR)
- Robinson oscillator

Further Reading

- Antoine Abragam. 1968. *Principles of Nuclear Magnetic Resonance.*, 895 pp., Cambridge University Press: Cambridge, UK.
- Charles P. Slichter.1996. *Principles of Magnetic Resonance.* Springer: Berlin and New York, Third Edition., 651pp. ISBN 0-387-50157-6.
- Kurt Wüthrich. 1986, *NMR of Proteins and Nucleic Acids*., J. Wiley and Sons: New York, Chichester, Brisbane, Toronto, Singapore. (Nobel Laureate in 2002 for 2D-FT NMR Studies of Structure and Function of Biological Macromolecules [5]
- Protein structure determination in solution by NMR spectroscopy [6] Kurt Wüthrich. J Biol Chem. 1990 December 25;265(36):22059-62
- Richard R. Ernst. 1992. Nuclear Magnetic Resonance Fourier Transform (2D-FT) Spectroscopy. Nobel Lecture [7], on December 9, 1992.
- Peter Mansfield. 2003.Nobel Laureate in Physiology and Medicine for (2D and 3D) MRI [8]
- D. Benett. 2007. PhD Thesis. Worcester Polytechnic Institute. PDF of 2D-FT Imaging Applications to NMRI in Medical Research. [9] Worcester Polytechnic Institute. (Includes many 2D-FT NMR images of human brains.)
- Paul Lauterbur. 2003.Nobel Laureate in Physiology and Medicine for (2D and 3D) MRI. [10]
- Jean Jeener. 1971. Two-dimensional Fourier Transform NMR, presented at an Ampere International Summer School, Basko Polje, unpublished. A verbatim quote follows from Richard R. Ernst's Nobel Laureate Lecture delivered on December 2, 1992, "A new approach to measure two-dimensional (2D) spectra." has been proposed by Jean Jeener at an Ampere Summer School in Basko Polje, Yugoslavia, 1971 (Jean Jeneer,1971)). He suggested a 2D Fourier transform experiment consisting of two $\pi/2$ pulses with a variable time t_1 between the pulses and the time variable t_2 measuring the time elapsed after the second pulse as shown in Fig. 6 that expands the principles of Fig. 1. Measuring the response $s(t_1,t_2)$ of the two-pulse sequence and Fourier-transformation with respect to both time variables produces a two-dimensional spectrum $S(O_1,O_2)$ of the desired form. This two-pulse experiment by Jean Jeener is the forefather of a whole class of $2D$ experiments that can also easily be expanded to multidimensional spectroscopy.
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External links

- Cardiac Infarct or "heart attack" Imaged in Real Time by 2D-FT NMRI [13]
- Interactive Flash Animation on MRI [14] - *Online Magnetic Resonance Imaging physics and technique course*
- Herbert S. Gutowsky
- Jiri Jonas and Charles P. Slichter: NMR Memoires at [[NAS [15]] about Herbert Sander Gutowsky; NAS = National Academy of Sciences, USA,]
- 3D Animation Movie about MRI Exam [16]
- International Society for Magnetic Resonance in Medicine [17]
- Danger of objects flying into the scanner [18]

Related Wikipedia websites

- Medical imaging
- Computed tomography
- Magnetic resonance microscopy
- Fourier transform spectroscopy
- FT-NIRS
- Chemical imaging
- Magnetic resonance elastography
- Nuclear magnetic resonance (NMR)
- Chemical shift
- Relaxation
- Robinson oscillator
- Earth's field NMR (EFNMR)
- Rabi cycle

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[1] Abragam, Antoine (1968). *Principles of Nuclear Magnetic Resonance*. Cambridge, UK: Cambridge University Press. ISBN 019852014X.

[2] Ernst, Richard R. (9 December 1992). Nobel Lecture "Nuclear Magnetic Resonance Fourier Transform (2D-FT) Spectroscopy" (http://nobelprize.org/nobel_prizes/chemistry/laureates/1991/ernst-lecture.pdf). Nodel Foundation. Nobel Lecture. Retrieved 29 November 2009.

[3] http://en.wikipedia.org/wiki/Nuclear_magnetic_resonance#Nuclear_spin_and_magnets Kurt Wüthrich in 1982-1986 : 2D-FT NMR of solutions

[4] Slichter, Charles P. (1996). *Principles of Magnetic Resonance, Third Edition*. Berlin and New York: Springer. ISBN 0-387-50157-6.

[5] http://nobelprize.org/nobel_prizes/chemistry/laureates/2002/wutrich-lecture.pdf

[6] http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=2266107&query_hl=33&itool=pubmed_docsum

[7] http://nobelprize.org/nobel_prizes/chemistry/laureates/1991/ernst-lecture.pdf

[8] http://nobelprize.org/nobel_prizes/medicine/laureates/2003/mansfield-lecture.html

[9] http://www.wpi.edu/Pubs/ETD/Available/etd-081707-080430/unrestricted/dbennett.pdf

[10] http://nobelprize.org/nobel_prizes/medicine/laureates/2003/lauterbur-lecture.html

[11] http://www.pubmedcentral.nih.gov/articlerender.fcgi?tool=pmcentrez&artid=1568902

[12] http://www.pnas.org/cgi/pmidlookup?view=long&pmid=9990066

[13] http://www.mr-tip.com/exam_gifs/cardiac_infarct_short_axis_cine_6.gif

[14] http://www.e-mri.org

[15] http://books.nap.edu/html/biomems/hgutowsky.pdf

[16] http://www.patiencys.com/MRI/

[17] http://www.ismrm.org

[18] http://www.simplyphysics.com/flying_objects.html

[19] http://planetphysics.org/encyclopedia/2DFTImaging.html

[20] http://planetphysics.org/

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