WESTERN SYDNEY
UNIVERSITY

Nanoscale Organisation
and Dynamics Group

NANOSCALE RESEARCH NEWSLETTER

ISSUE 11 – JUNE 2020

Dr Scott A. Willis

Facility Manager

The BMRF in Brief

Access to the BMRF remains closed at this time because of the COVID-19 event. HDR users of the facility have been provided with a sample submission request form to complete and email the facility manager. There is the possibility to have some limited experiments completed by the facility manager or NIF fellow (with facility manager approval) as users are not permitted to enter the facility areas (NMR facility, Preparation room, FFC room and MicroCT room) at this time. If you require further information during the COVID-19 closure, please contact the facility manager.

What's new in NIF

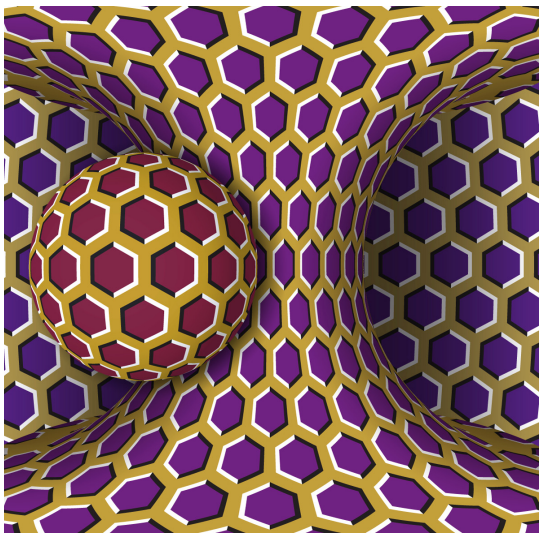
Due to the COVID-19 pandemic and consequent restrictions on laboratory facilities, both at WSU and at other institutions wishing to access our facilities, there has been reduced NIF scanning this year. Many other NIF nodes have been similarly affected.

Continued on page 4

Dr Tim Stait-Gardner

NIF Facility Fellow

9th (biennial) Western Sydney University & Inaugural Asian Symposium on NMR, MRI & Diffusion



Watch this space

and save the date

3rd December 2020

SPECIAL POINTS OF INTEREST

BMRF Application Highlight - Honey

Dr Scott A. Willis

MicroCT, MRI and NMR of the BMRF was used for a compassion of store-bought chunk-honey (e.g., Figure 1) by Dr Scott A. Willis. These results were presented at the 12th Australian and New Zealand Society for Magnetic Resonance (ANZMAG) Conference in 2019. Two batches of the same product were compared and being a chunk-honey sample, this enabled comparison of the jar honey to the unharvested honey trapped in the capped honeycomb cells (i.e., four honeys present).

Figure 1 - Photograph of chunk-honey product

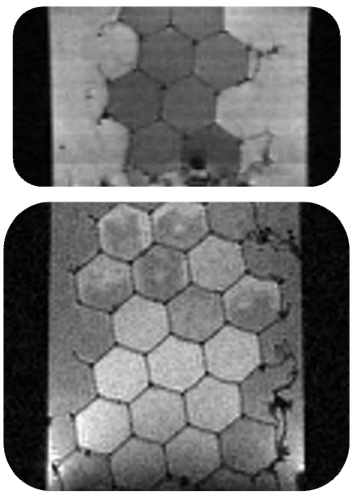


Figure 2 - Example of processed MR images (14.1 T Bruker Avance IIIHD) acquired at 300 um voxels, 3 ms echo time, 3.5 s repetition time. These images are of the honeycomb (capped honeycomb cells) piece from Jar 1 (upper) or Jar 2 (lower) submerged in honey from the Jar it was in. Some cells have broken caps and mixing can be seen (e.g., Jar 2).

Experiments performed included imaging, spectroscopy and relaxation analysis. There was a notable difference between the honey samples (from the jar and the honeycomb cells when extracted) in terms of colour and apparent viscosity but also immediately in the MR images (Figure 2 and Figure 4). MRI provided contrast for cell walls, trapped air bubbles and the different honeys present (i.e., honey surrounding the honeycomb from the jar and honey in the capped honeycomb cells). MicroCT only provided contrast for the cell walls and air bubbles (and pipette bulb at the top of the image), i.e., the electron densities of the honeys were not sufficiently different for contrast (e.g., Figure 3 and Figure 4).

Figure 3 -Example of a processed MicroCT image (PerkingElmer Quantum GX) from Jar 1 acquired at 9um voxels, processed to 90 um voxels, 14 min exposure @ 90 kV/88 uA.

WHAT DO BEES DO WITH THEIR HONEY?

THEY CELL IT!

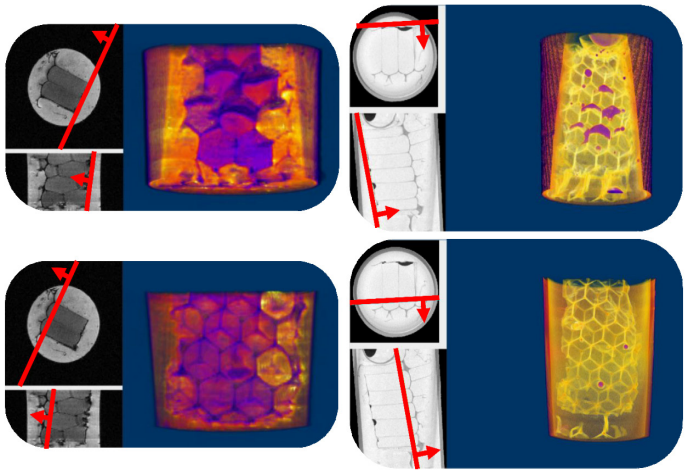


Figure 4 Figure 4 – Rendered volumes (partial transparency; using ImageJ – Volume Viewer 2.0) of the MR (left) and MicroCT (right) images for the sample from Jar 1 (honeycomb submerged in jar honey). Different rendered 'depths' are shown as indicated on the 2D insets by the red line and arrows. The trihedral bases of the honeycomb cells can be seen giving the (isometric) cube illusion.

Spectroscopy of the dilute honeys and spectroscopy and relaxation of the undilute samples also showed differences (Figure 5 and

Figure 6). Spectra of the dilute and undilute honey samples showed a difference in the water content for each honey (somewhat could be expected from the colour/ viscosity). The spectra of the dilute samples also showed differences in the minor components (compare the zoomed regions in Figure 5).

Unique relaxation analysis (T_1 and T_2 relaxation vs Chemical shift) was performed for the undiluted honey samples. The difference in the water content was visible in the spectra and relaxation results for the undilute honey samples. Relaxation in each batch showed a different trend for the honey from the jar and honey from the honeycomb cells (i.e., already noted qualitatively in the MR images). Relaxation analysis for the undilute honeys was done at two field strengths (9.4 T and 14.1 T). An example of the relaxation analysis for one of the samples at 14.1 T is shown in Figure 6.

Although differences could be expected due to honey being a natural product (and comparison of the Jar honey to the Honeycomb honey effectively compares honey from a bulk batch to honey in a few cells), the experiments here highlight some (and only some) of the tools available in the BMRF. Contact the facility manager for more information.

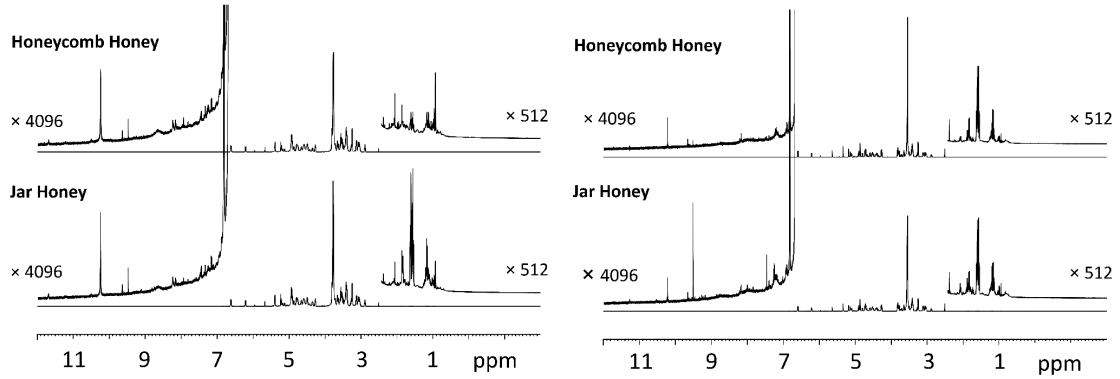


Figure 5 – Example ^{1}H NMR spectroscopy (14.1 T Bruker Avance IIIHD) of dilute honey samples from Jar 1 (left) and Jar 2 (right). Comparison of the honey from the jar and honeycomb for each Jar shows differences in the minor components and water content (i.e., Jar to Jar and Jar to Honeycomb). NB: while similar concentrations was used for the jar and honeycomb honey in each the concentration was different for samples from Jar 1 and Jar 2 in the spectra shown here. Spectra were also acquired (not shown) for a jar honey sample from Jar 2 at a similar concentration as Jar 1 – the main difference from concentration was the position and width of the water signal at ~3.6 – 3.8 ppm, i.e., minor components were similar appearance and position.

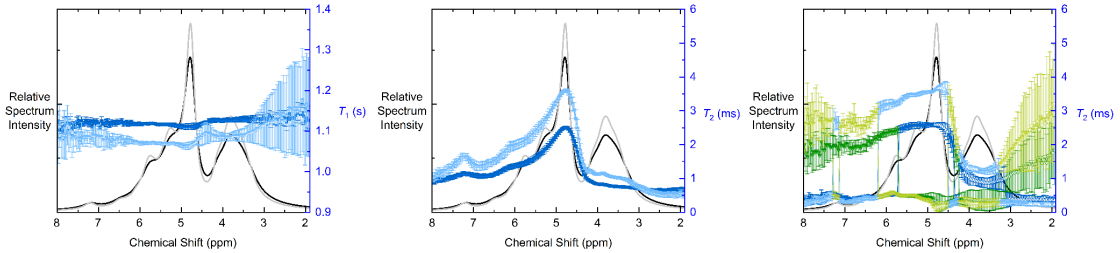


*Figure 6 – T_1 and T_2 relaxation vs Chemical shift and ^{1}H NMR spectra for the undiluted honey samples at 14.1 T from Jar 2. Four fitting functions were considered to determine the best fits and those shown here are Relaxation/Analysis: T_1 /monoexponential with offset (left); T_2 /monoexponential (middle); T_2/ biexponential (right). Shown in Dark Blue are the results from monoexponential $T_{1,2}$ analysis for the Jar Honey or the major component T_2 from biexponential analysis for the Jar Honey, Light Blue are the results from monoexponential $T_{1,2}$ analysis for the Honeycomb Honey or the major component T_2 from biexponential analysis for the Honeycomb Honey, Dark Green is the minor component T_2 from biexponential analysis for the Jar Honey and Olive Green is the minor component T_2 from biexponential analysis for the Honeycomb Honey. Behind the relaxation data are the ^{1}H NMR spectra for the undiluted honey samples: **Jar Honey - Honeycomb Honey -** (the chemical shift is referenced so water is at 4.79 ppm).*

A LITTLE BIT OF TRIVIA

The component shapes that make up the honeycomb cells are parallelohedra [1] (e.g., hexagonal prism and the rhombic dodecahedron like cell bases) but the combined shape is not strictly a Parallelohedron.

The complete shape of the honeycomb cells are possibly best described by the space-filling polyhedra formed by cutting a long trapezo-rhombic dodecahedron in half (i.e., to make two honeycomb cells).

The 'why and how' bees make honeycomb cells like this is the subject of much discussion [2].

[1] P. Engel, Cryst. Res. Technol. 2015, 50, 929-943.

[2] a) L. F. Tóth, Bull. Am. Math. Soc. 1964, 70, 468-481; b) F. Nazzi, Sci. Rep. 2016, 6, 28341.

NCRIS
National Research Infrastructure for Australia
An Australian Government Initiative

Dr Tim Stait-Gardner

NIF Facility Fellow

National Imaging Facility

NIF News Continued

Prior to shutdown, work was started on a project with UNSW, partly funded by NIH, extending previous work on prostate core imaging. Initial diffusion tensor datasets were acquired using the Bruker 500 MHz scanner to plan the protocol for future work using perfused prostate cores. The planned scanning will require tailor-made equipment for in-bore perfusion of the prostate core.

Planned scanning for the research foundation, Spine Labs (Kogarah NSW, spinelabs.org), on the effects of smoking (and bushfire smoke) on spine health had to be delayed due to the pandemic. We have used the delay to plan further experiments and apply for funding from the NHMRC.

With the Ingham Institute we are extending on previous work [1] on rectal cancer MRI biomarker discovery to include many other gastrointestinal (GI) cancers and plan a significant ramp-up of scanning with the aims of: (i) characterising the heterogeneity of tumours ex vivo at the ultra-high field strengths available in the BMRF (11.7 T and 14.1 T) as well as at clinical field strengths; (ii) creating the link between ultra-high field and clinical field strength using AI methods such as deep learning super resolution and (iii) translating these ex vivo MRI findings to in vivo clinical MRI from patients with GI tumours. An NHMRC Ideas grant has been submitted for this project with CIs and AIs from across Australia (Ingham Institute, UNSW, University of Queensland) and New Zealand (University of Auckland).

Each of the specimens will be scanned in 3D at high field and at clinical field strength and sliced for histopathology. It is thus important that an efficient means of co-registration be developed. We have designed a fiducial vial that fits securely into the 30 mm micro 2.5 imaging insert (see Figures 1 and 2). The specimen is embedded in gel within the specially designed vial, which enables easy comparison between datasets obtained on different instruments and with the histopathology. The sample holder was designed using CAD and sent to the WSU 3D Printing Hub just prior to the widespread shutdown due to the pandemic. Printing and testing of the specimen holder is planned to take place in the second half of 2020.

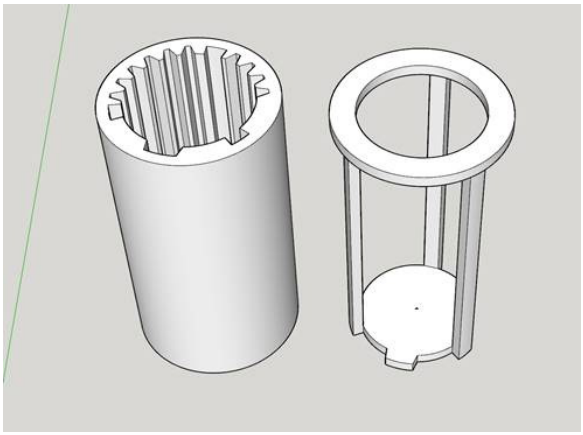
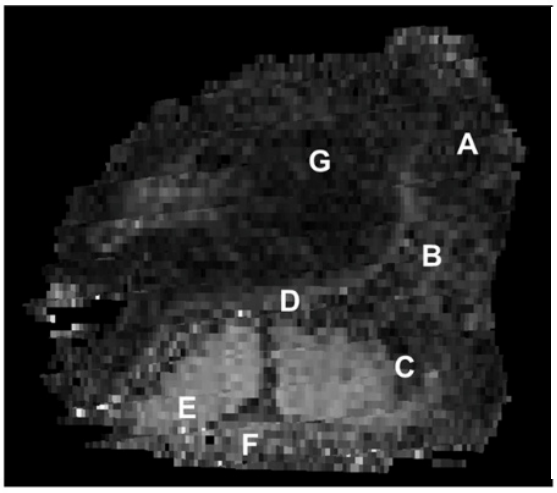


Figure 1. The prototype fiducial specimen vial enabling easy co-registration between MRI scans and histopathology.

Another long-term project is with Prof. Masaya Ishikawa, a world expert in freezing injury in plants, from Tokyo University. Normal clinical MRIs are only capable of conducting imaging at ambient temperature. The research grade 11.7 and 14.1 T MRIs at the WSU node are special as they are able to conduct imaging over as wide temperature range (i.e., ~253 – 353 K) greatly increasing the potential of these machines for studying agricultural and industrial problems. Nevertheless, undesirable temperature gradients of a few degrees at moderate sub-zero temperatures (~269 K) are a barrier to achieving precise quantitative results. Due to these temperature control problems with the micro 2.5 imaging probe, we have designed a new temperature regulation system, again using CAD, which is to be 3D printed at the

WHAT DO YOU GET WHEN YOU CROSS A SNOWMAN WITH A VAMPIRE?

FROSTBITE!



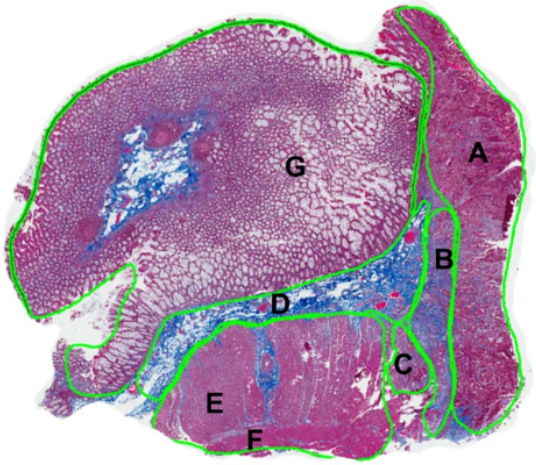


Figure 2 Example of the comparisons needed between MR images and histopathology. On the left is a fractional anisotropy image generated from a 3D MRI dataset acquired at WSU; on the right is the same slice as later analysed using histopathology. (A) cancer (B) desmoplasia (C) cancer invasion into muscularis propria (D) fibrous tissue (E) muscularis propria inner circular layer (F) muscularis propria outer circular layer and (G) mucosa. This image is adapted from [1]. Many such comparisons are needed for this project. The newly designed fiducial vial will largely automate the process of co-registration.

WSU 3D Printing Hub and which is planned undergo testing in the second half of 2020. If successful, this will enable us to conduct accurate and precise (to within 0.5 K) freezing experiments on small specimens less than 8 mm diameter.

Both the novel fiducial vial and the temperature regulation system will greatly increase the imaging ability of the WSU node of the National Imaging Facility, extending the range of capabilities and specialty projects.

[1] Pham, T., Stait-Gardner, T., Lee, C. S., Barton, M. B., Graham, P. L., Liney, G., Wong, K., Price, W. S., 2019, Correlation of ultra-high field MRI with histopathology for evaluation of rectal cancer heterogeneity, Scientific Reports, 9(1), 9311

Library Presentation

The Library gave a very informative talk to our Laboratory group on the 6th June and led a discussion about the pros and cons of using 'Open Access' Journals which covered:

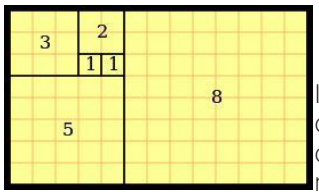
- The changing nature of the publishing industry
    - What are the benefits of Open Access (OA)
    - OA policy / funder mandates: WSU, ARC and NHMRC
- Routes of publishing (Conventional; Green (OA); Gold (OA))
- Avoiding predatory publishers (Reputation; Solicitation; Red Flags)
- Evaluating journals (Best Fit Vs Highest Impact Metrics; Journal comparision links)
- Locating OA journals
- Q&A

Further support for researchers is available from WSU Library

- Ria Hamblett (Research Engagement Coordinator, Outreach) - R.Hamblett@westernsydney.edu.au
- Karen Sheehy (Science Librarian) - K.Sheehy@westernsydney.edu.au

I ASKED THE LIBRARIAN IF THEY HAD A BOOK ABOUT PAVLOV'S DOG AND SCHRODINGER'S CAT.

THEY SAID IT RANG A BELL BUT WEREN'T SURE IF IT WAS THERE OR NOT!



Fibonacci Sequence & Design

In mathematics, the Fibonacci numbers, commonly denoted by Fn form a sequence, called the Fibonacci sequence, such that each number is the sum of the two preceding ones.

1+1=2; 2+1=3; 3+2=5; 5+3=8; 8+5=13

Simply put the Fibonacci Sequence is a series of numbers with the pattern of each number being the sum of the previous two. So starting at zero the sequence would be as follows:

0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144...

The sequence could go on indefinitely but as you notice it is a pretty simple principle and seems more fixed in mathematics than in design. But the sequence actually relates closely to design in a number of key ways.

In the first place the sequence is very close to the Golden Ratio. The Golden Ratio is a design concept that if followed, creates visually appealing proportions in art, architecture and design.

Secondly the sequence is commonly seen in nature. This pattern and sequence is found in branching of trees, flowering artichokes and the arrangement of leaves on a stem. These apparently, random patterns which appear in nature also have a strong aesthetic appearance.

Precise and effective space management can make the difference between an average design and an amazing one. Every aspect of your design or publication layout, requires you to make decisions on the use of space, everything from the width and height of various sections to the space between a heading and the paragraph of text below it. This can extend further by considering the proportions of the inclusions i.e.., the size of the header compared to the body of text; the figure dimensions in comparison to the page. These proportions make or break the balance, emphasis and flow of a design.

Many designers pick size and spacing arbitrarily or based on "instinct." A 20 px margin and a 400 px tall header look reasonably good and many designers can get away with this eyeball approach but even though these sizing choices may look good to your eye, your brain is trying to find harmony in the relationships. If that agreement doesn't exist it will always feel unpolished.


1


2


3


5


8

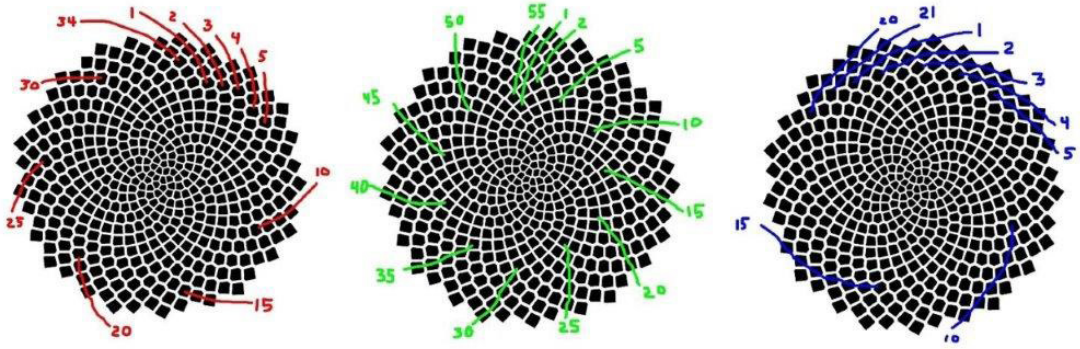

13


21


34

Whether we realize it or not, our brains are constantly looking for order and understanding in the world around us.

Fibonacci Spirals in Sunflowers



The Fibonacci Sequence is one method of bringing a sizing and spacing system into your designs. It's basis is proven aesthetically in appeal in design, in architecture and in nature.

If you look at the Fibonacci Sequence and consider them as possible section, margin and font sizing it should be clear that it can structure your entire design. The smaller range of the sequence (8, 13, 21, 34, 55) are perfect to decide margins, line heights and font sizes and the higher range of the sequences (144, 233, 377, 610, 987) could easily be used to decide column widths and other section dimensions. Using the Fibonacci sequence to set the font size for paragraph and heading text and the margins between them will create rhythm and visual harmony, as well as a balanced and aesthetically design.

Reprinted from article by Ross Johnson, 2010

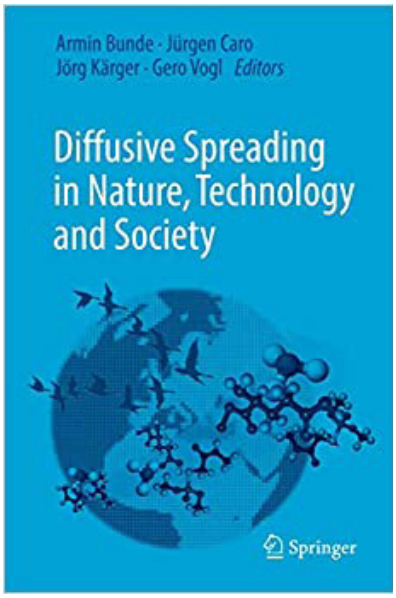
Fibonacci Sequence Examples

1. Fibonacci retracement; Fibonacci retracement is a method of technical analysis which uses the Fibonacci sequence to determine at what point the price of a financial asset will stop and reverse in the opposite direction. Stock traders frequently take a cue from Fibonacci retracement to predict future share prices.

2. Fibonacci numbers can be found in several biological settings; Apart from drone bees, Fibonacci sequence can be found in other places in nature like branching in trees, arrangement of leaves on a stem, the fruitlets of a pineapple, the flowering of artichoke, an uncurling fern and the arrangement of a pine cone. Also on many plants, the number of petals is a Fibonacci number. Many plants including buttercups have 5 petals; lilies and iris have 3 petals; some delphiniums have 8; corn marigolds have 13 petals; some asters have 21 whereas daisies can be found with 34, 55 or even 89 petals.

Diffusive Spreading in Nature,Technology and Society

Awarded the Literature Prize of the Fonds der Chemischen Industrie (2019).



This book deals with randomly moving objects and their spreading. The objects considered are particles like atoms and molecules, but also living beings such as humans, animals, plants, bacteria and even abstract entities like ideas, rumors, information, innovations and linguistic features. The book explores and communicates the laws behind these movements and reports about astonishing similarities and very specific features typical of the given object under considerations. Leading scientists in disciplines as diverse as archaeology, epidemics, linguistics and sociology, in collaboration with their colleagues from engineering, natural sciences and mathematics, introduce the phenomena of spreading as relevant for their fields. An introductory chapter on "Spreading Fundamentals" provides a common basis for all these considerations, with a minimum of mathematics, selected and presented for enjoying rather than frustrating the reader.

Invited Chapter; Scott A. Willis, Timothy Stait-Gardner, Amninder Virk, Reika Masuda, Mikhail Zubkov, Gang Zheng, William S. Price. (2018) NMR Versatility. In Diffusive Spreading in Nature, Technology and Society Chapter 12. pp. 233-260 (A. Bunde, J. Caro, J. Kärger, G. Vogl Eds.) Springer. ISBN 978-3-319-67798-9.

24 Books now in the RSC Series on NMR

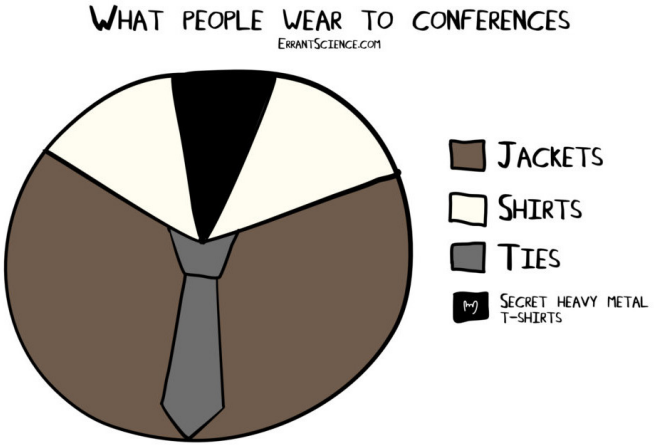
Focusing on novel aspects of method and instrumentation development, applications in emerging fields and new techniques and technologies, this Series documents the important advances being made in this field. The books provide comprehensive introductions to the relevant theory to facilitate greater understanding and to encourage wider usage of NMR techniques, making them ideal for students, researchers and practising analytical scientists, as well as manufacturers with an interest in the instrumentation. Series DOI: 10.1039/2044-2548

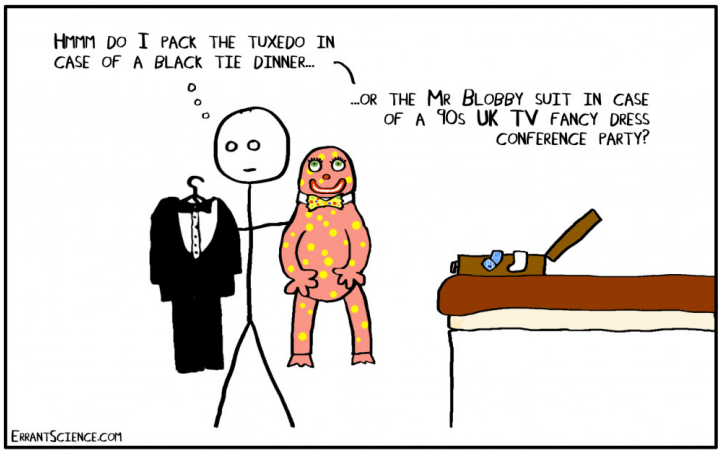
Editor in Chief: William S. Price (Western Sydney University, Australia)

Series Editors: Bruce Balcom (The University of New Brunswick, Canada), Istvan Furo (KTH Royal Institute of Technology, Sweden), Maili Liu (Chinese Academy of Sciences, China), Masatsune Kainosho (Tokyo Metropolitan University, Japan), Kavita Dorai (IISER, India), Danuta Kruk (University of Warmia and Mazury in Olsztyn, Poland)

- 2011 - Contemporary Compute-Assisted Approaches to Molecular Structure Elucidation
- 2013 - New Applications of NMR in Drug Discovery and Development
- 2014 - Advances in Biological Solid-State NMR: Proteins and Membrane Active Peptides
- 2015 - Hyperpolarized Xenon-129 Magnetic Resonance: Concept s, Production, Techniques and Applications
- 2015 - Mobile NMR and MRI: Developments and Applications
- 2016 - Gas Phase NMR
- 2016 - Magnetic Resonance Technology: Hardware and System Component Design
- 2016 - Biophysics and Biochemistry of Cartilage by NMR and MRI
- 2016 - Diffusion NMR of Confined Systems: Fluid Transport in Porous Solids and Heterogeneous Materials
- 2017 - NMR in Glycoscience and Glyctechnology
- 2017 - Fast NMR Data Acquisition: Beyond the Fourier Transform
- 2017 - Cross Relaxation and Cross Correlation Parameters in NMR: Molecular Approaches
- 2017 - Contrast Agents for MRI: Experimental Methods
- 2018 - NMR-base Metabolomics
- 2018 - Modern Methods in Solid-state NMR: A Practitioner's Guide
- 2018 - Paramagnetism in Experimental Biomolecular NMR
- 2018 - Optimizing NMR Methods for structure elucidation: Characterizing Natural Products and Other Organic Compounds
- 2018 - Field-cycling NMR Relaxometry: Instrumentation, Model Theories and Applications
- 2018 - Hybrid MR-PET Imaging: Systems, Methods and Applications
- 2019 - NMR Methods for Characterization of Synthetic and Natural Polymers
- 2019 - In-cell NMR Spectroscopy: From Molecular Sciences to Cell Biology
- 2020 - Long-lived Nuclear Spin Order: Theory and Applications
- Coming Soon - NMR and MRI of Gels
- Coming Soon - Advanced Diffusion Encoding Methods in MRI

Puzzle Page





PACKING FOR CONFERENCES IS ALWAYS SO TRICKY

A PHD DISSERTATION IS A PAPER OF THE PROFESSOR WRITTEN UNDER AGGRAVATING CIRCUMSTANCES. - ADOLF HURWITZ

DID YOU KNOW THEY WON'T BE MAKING YARDSTICKS ANY LONGER?

WHAT DO YOU DO WITH A SICK CHEMIST?

A: IF YOU CAN'T HELIUM, AND YOU CAN'T CURIUM, THEN YOU MIGHT AS WELL BARIUM.

Brain Teasers

1. Mary's mum has four children. The first child is called April. The second May. The third June. What is the name of the fourth child?

2. Six foxes catch six hens in six minutes. How many foxes will be needed to catch sixty hens in sixty minutes?

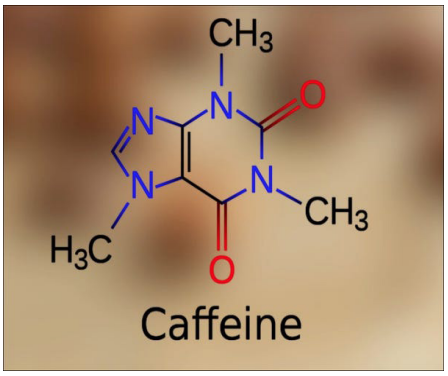
3. A bat and ball cost $1.10. The bat costs one dollar more than the ball. How much does the ball cost?

4. I have 28 grey and 8 black socks in my sock drawer. If it is completely dark and I cannot see the colour of the socks that I am picking, how many socks do I need to take from the drawer to be sure that I have at least one pair of socks that are the same colour?

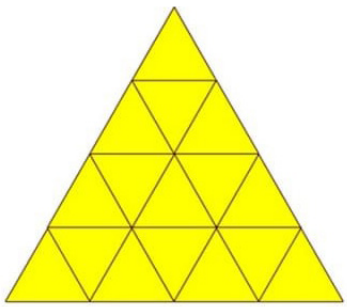
5. What can travel around the world while staying in a corner?

6. During which month do people sleep the least?

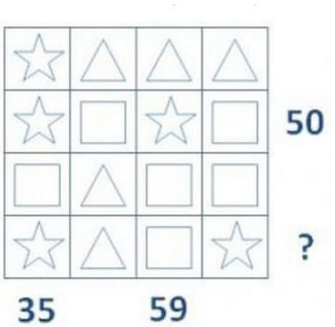
7. Forward I am heavy, but backward I am not. What am I?



8. How many triangles are there? 17, 32, 26 or 27?



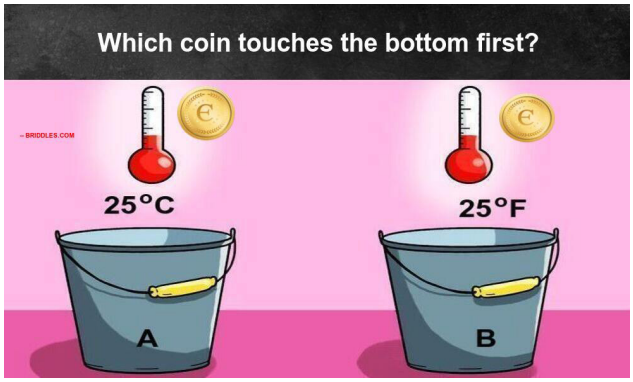
9. What number should replace the question mark? 44, 46 or 52?



10. As shown, there are two buckets of water.

- Bucket A, the temperature of the water is at 25 degrees C.
- Bucket B, the temperature of the water is at 25 degrees F.

If you drop a coin into each bucket from the same height and they hit the water at exactly the same time. Which coin touches the bottom first?



ANSWERS

1. Mary
2. 6
3. 5c
4. 3
5. A stamp
6. February (there are fewer nights in February).
7. Forward I am ton, backwards I am not.
8. 27
9. 44
10. The coin in the 1st bucket. At 25 degrees C water is liquid, while at 25 degrees F it turns into ice.

NANOSCALE ORGANISATION AND DYNAMICS

Professor William S. Price
Group Leader
- Medical Physics, MRI, NMR and diffusion

Professor Janice Aldrich-Wright
Associate Dean of Research School of Science
- Potent in-vivo cytotoxic agents

Distinguished Professor Annemarie Hennessy AM
Dean of Medicine
- Preeclampsia

Assoc. Prof. Gary Dennis
Deputy Dean School of Science
- Polymer and surface chemistry

Dr Tim Stait-Gardner
National Imaging Facility Fellow
- MRI and quantum physics

Dr Allan Torres
Research Instrumentalist
Senior Lecturer
- NMR and MRI

Dr Gang Zheng
Lecturer
- NMR pulse sequence development

Dr Scott Willis
BMRF Manager & Researcher
- NMR and MRI diffusion measurements

Dr Abhishek Gupta
Post Doctoral Fellow
- MRI contrast agent development and NMR relaxation

WE WOULD LIKE TO APOLOGIZE FOR NOT ADDING MORE JOKES...

BUT WE ONLY UPDATE THEM....

PERIODICALLY!

Group Meetings

PROFESSOR WILLIAM PRICE'S LAB GROUP

Meet every Friday at
09:30 am by ZOOM

If you wish to attend please email
to r.grey@westernsydney.edu.au

PROFESSOR JANICE ALDRICH-WRIGHT'S LAB GROUP

Contact information
02 4620 3336
nano@westernsydney.edu.au

Western Sydney University
Locked Bag 1797
Penrith NSW 2751 Australia

WESTERNSYDNEY.EDU.AU/NANOSCALE/NANOSCALE_ORGANISATION_AND_DYNAMICS