Are we there yet?

Some problems I never managed to solve

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An overview

One common theme in my work was sitting in the three-way intersection of mathematics, computer science and various application areas:

- mathematical analysis identifies new computational techniques;
- new computational techniques open up enhanced ability to explore the science.

The other very important aspect of my CSIRO work was the close link between measurement and modelling: GASLAB and GUESSLAB

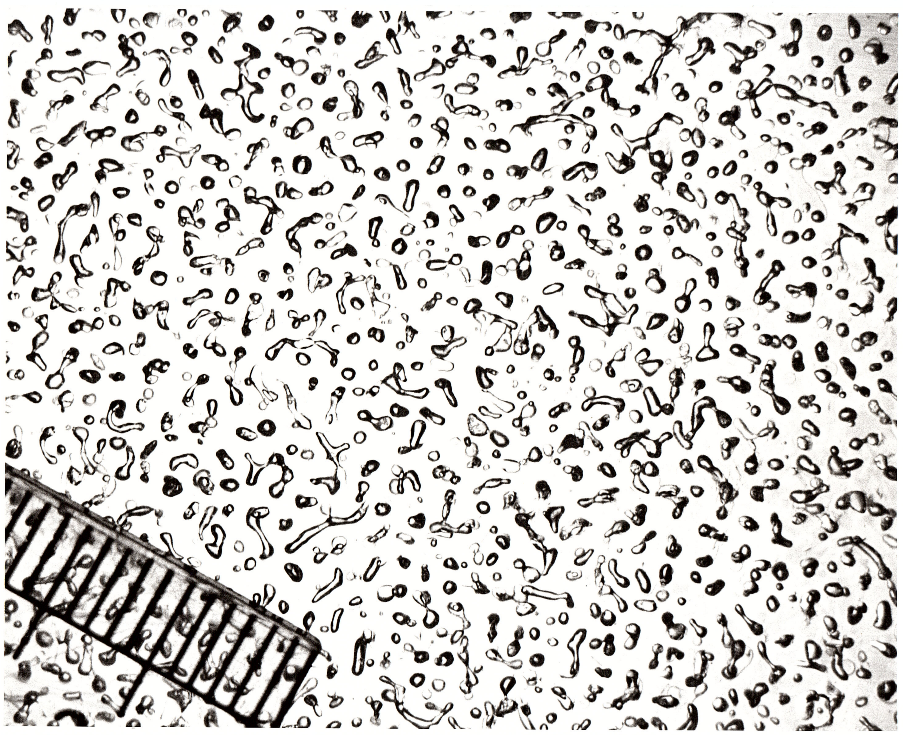
Summary

This talk looks at some things that I haven't solved:

- Do the statistics of percolation give additional insights into bubble trapping in ice?
- Can my solution of the triplet order parameter be extended to give a solution for the honeycomb lattice magnetisation?
- Is there a higher-order generalisation of Pickard Random Fields that gives insight into corner-transfer matrix series expansions?
- How does one move into non-linear inversions of trace gases?
- Are Pickard Random Fields (with $q > 2$) useful as prior models for spatial inversions?

Bubbles in polar ice

Air bubbles trapped in polar ice give a record of past atmospheric composition.
When I started at CSIRO, the pre-industrial CO_2 concentration was unknown.



Percolation

- The percolation model from lattice statistics describes the statistics of connectivity in randomly connected networks.
- Variability of trapped bubble volume near close-off suggests critical fluctuations from percolation (Enting, *Nature*).
- Simulations can explore properties.
- Actually, the age distribution of trapped gas is defined by diffusion, and not by percolation properties (Trudinger PhD etc)

Percolation - any more to say?

Can percolataion model say more about bubble trapping?

- Diffusivity appears to go to zero before total close-off. Is this just a reflection of 'conductivity' $K \sim (p - p_{\text{c}})^{-2}$ (approx)?
- Are there universal amplitude ratios for percolation that give more information about bubble trapping?
- Can percolation modelling (simulation) improve description of surface effects?

Triplet order parameter

For spins ± 1, a honeycomb lattice spin x, surrounded by triangular lattice spins a, b, c with probabilities $\mathrm{Pr}(+++)$, $\mathrm{Pr}(---)$, and 3 orientations each of $\mathrm{Pr}(++-)$ and $\mathrm{Pr}(+--)$. Relative weightings of like and unlike bonds on hc lattice are 1 and $z = \exp(-2J_{\mathrm{hc}}/k_{\mathrm{B}}T)$.

$< x >= M =$

$$\frac{1-z^3}{1+z^3}[\mathrm{Pr}(+++)-\mathrm{Pr}(---)]+3\frac{z-z^2}{z+z^2}[\mathrm{Pr}(++-)-\mathrm{Pr}(+--)]$$

The 3-site expectation on the triangular lattice is

$$M_3 = [\mathrm{Pr}(+++)-\mathrm{Pr}(---)]-3[\mathrm{Pr}(++-)-\mathrm{Pr}(+--)]$$

and the expectation of $< a+b+c >$ is

$$3M = 3[\mathrm{Pr}(+++)-\mathrm{Pr}(---)]+3[\mathrm{Pr}(++-)-\mathrm{Pr}(+--)]$$

whence $$M_3 = \frac{1-3z+3z^2-5z^3}{(1-z)^3}M$$

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Triangular Ising Magnetisation?

Is there an easy derivation of differential equation for honeycomb-triangular lattice Ising magnetisation?

Given $M =< \sigma_0 >$,

then $\frac{d}{du}M = \sum_{\mathrm{bonds}:ij} < \sigma_i \sigma_j \sigma_0 >$

So if one has an expression for the sum $\sum_{ij} < \sigma_i \sigma_j \sigma_0 >$ over three-site correlations as a multiple of M then one has the differential equation of the form

$$\frac{d}{du}M = g(u)\, M$$

From the known solution of M, we know $g(u)$ is a simple rational function. Is there an easy way of finding it?

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Pickard Random Fields

These models arose mainly from merging initiallly independent research lines, all in Canberra circa 1976–7.

- Richard Welberry (R.S.Chem) modelling x-ray diffraction of mixed disordered crystals;
- Tony Verhagen (CSIRO Maths and Stats) looking at 2-D Ising models that had 1-D statistics
- David Pickard (Stats, ANU) who generalised Verhagen's work
- Ian Enting (R.S.Phys.S) who expressed Welberry's cases as Ising models at disorder points.
- Rodney Baxter (R.S.Phys.S) who identified these cases as lowest order of corner-transfer-matrix approximations.

Markov chain property

$$
\begin{array}{ccccccc}
 & & | & & | & & \\
- & & a & — & b & — & \\
 & & | & & | & & \\
- & & c & — & d & — & \\
 & & | & & | & &
\end{array}
$$

Model specified by Pr$(d|a, b, c)$, describes one-way (crystal) growth in lower right direction.

For some cases (Welberry) there are simple solutions for correlations.

Models can be put in Ising (GRF/MRF) form and this can show ‘hidden’ symmetry (Enting).

Some cases have simple correlations structure $< \sigma_{0,0}\sigma_{m,n} >= \alpha^m \beta^m$ in 2 or 4 quadrants (Pickard).

Structure corresponds to lowest order of variational approx based on corner transfer matrices (Baxter).

Higher order Pickard fields?

- Along a line, a PRF is Markov chain:
  $\Pr(\sigma_{n+1}|\sigma_1 \dots \sigma_n) = \Pr(\sigma_{n+1}|\sigma_n)$
- Can one define a 2-D field with dependency along a line:
  $\Pr(\sigma_{n+1}|\sigma_1 \dots \sigma_n) = \Pr(\sigma_{n+1}|\sigma_n, \sigma_{n-1})$
- If so, can this be related to higher-order CTM?
- and if so, does this help us work with either PRF or CTM?

Inversions

Classic Jackson paper: *Interpretation of inaccurate, insufficient and inconsistent data* (In Geophys. J. Roy. Astron. Soc., 1972)

Inverse problems as:

- Model calibration
- Deconvolution of ice-core data
- Interpretation of spatial distribution of CO_2 in terms of sources and sinks.

Beyond Linear Least Squares?

- Linear least squares (as in Bayesian synthesis inversion) is pretty much past its use-by date.
- The so-called adjoint techniques can provide a way into non-linear estimation.
- In spite of TransCom, the quantification of transport model error is a wide-open problem.

Example: multi-tracer inversion

- Ratio method assumes no information from atmospheric transport model
- Green function approach assumes perfect atmospheric transport model
- It is almost certain that neither of these cases gives optimal estimates
- the challenge is to find a combination.

Example from Enting: *Inverse Problems in Atmospheric Constituent Transport* (CUP, 2002).

Higher order PRF?

Are Pickard Random Fields (with more than two states per site) useful as prior models for spatial inversions?

This is just speculation. The PRF Markov chain property makes these field mathematically tractable (unlike Markov random fields).

The significant point is that Pickard's expressions for consistency on the matrices are not restricted to binary variables.

Of course, if there is a generalisation to higher-spatial order (cf CTM discussion) then this might be able to be combined with going beyond binary variables.

Concluding remarks

It has been quite satisfying to swing between tightly-defined mathematical problems and the open-ended study of the carbon cycle.

And, summarising Leo Kadanoff: there may be no such thing as ‘complex systems science’ but there is a lot of good science to be done in looking at complex systems’

Co-authors

Tony Guttmann - most papers

Roger Francey – most highly-cited papers

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