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The National Grid Service (NGS) aims to provide coherent electronic access for UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location.

You can find further information about the NGS on its website at www.ngs.ac.uk. The website contains a wide range of documentation including technical details, software listings, user case studies and online tutorials for self-guided learning.

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The NGS produces a quarterly newsletter containing a large variety of news about the NGS including user case studies, NGS site news, application updates and conference reports. The latest edition of NGS News can be found on our website in the Outreach section or join our mailing list to receive an announcement when the latest edition is released.

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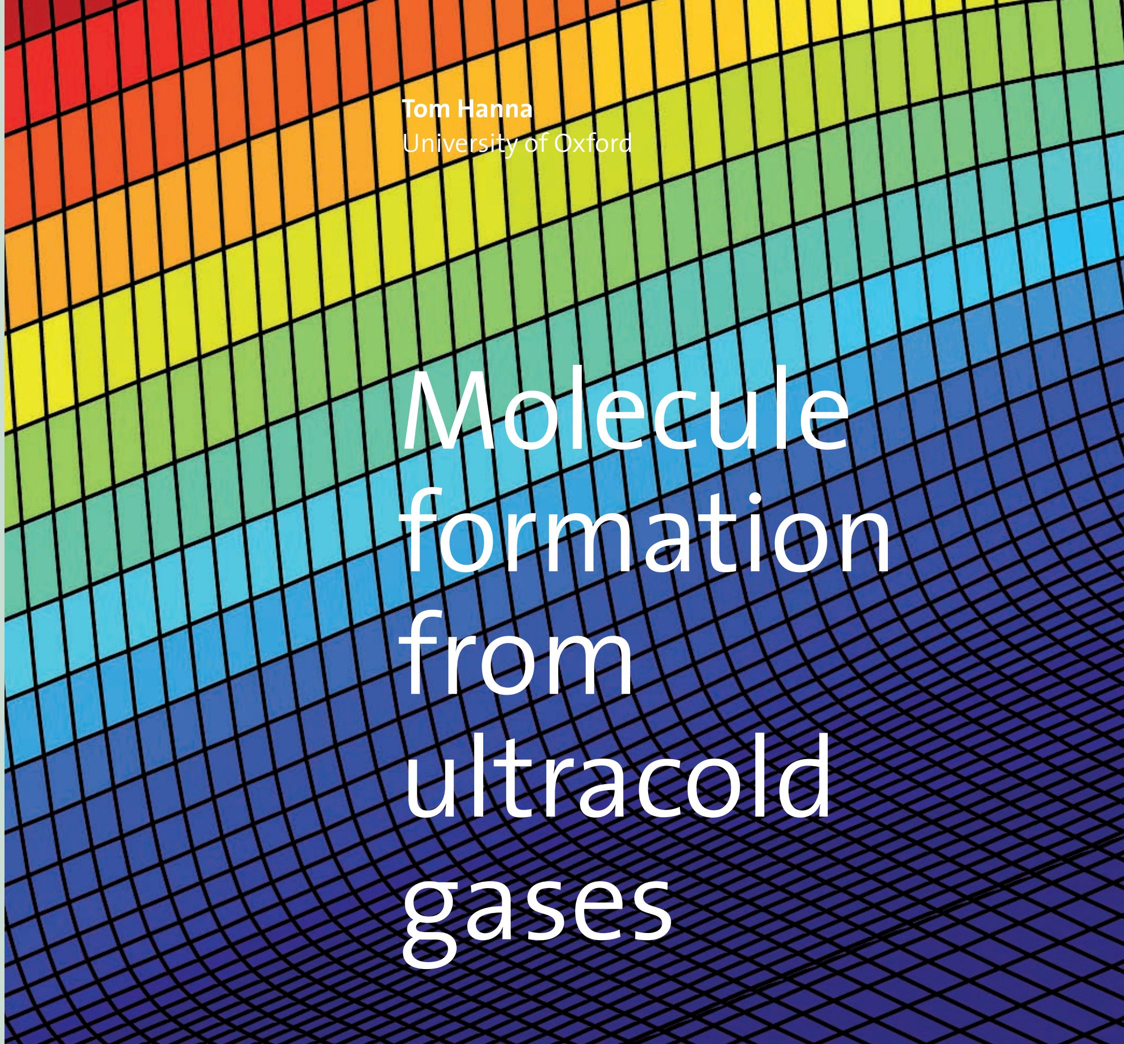

Tom Hanna
University of Oxford

Molecule formation from ultracold gases

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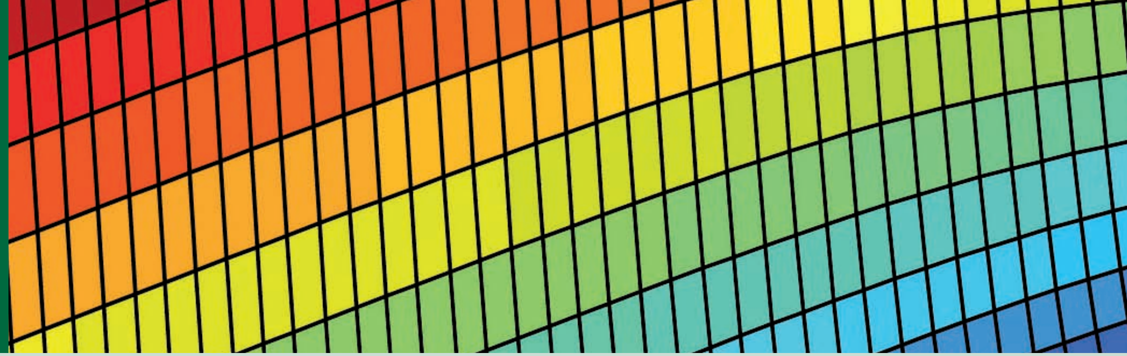


Name: **Tom Hanna**

Institution: University of Oxford

Research: **Molecule formation from ultracold gases**

In 2001 the Nobel prize was won by three physicists in the US for their observation of Bose-Einstein condensates.

This extreme state of matter was first predicted in 1924 by Satyendra Nath Bose and Albert Einstein, but wasn't observed until 1995.

A Bose-Einstein condensate is a weird state of matter where at sufficiently low temperatures all the particles converge in the lowest energy state. A material in such a state will have many unusual properties, showing quantum effects on macroscopic scales.

The large time lag between prediction and observation of a Bose-Einstein condensate was due to the difficulties of cooling a gas down to the low temperatures required. Ultracold atomic gases have temperatures less than 1μK above absolute zero. The advance of laser-based techniques in the 1980s opened the way for super-cooling of alkali atom gases.

The collisions between atoms in an ultracold atomic gas can be precisely controlled using lasers as well as magnetic and electric fields. These collisions are well understood. This allows the study of a wide range of fundamental problems within physics.

Tom Hanna has spent the last three years at the University of Oxford studying the dynamics of ultracold gases. In particular he's focused on the problem of molecule formation at such low temperatures.

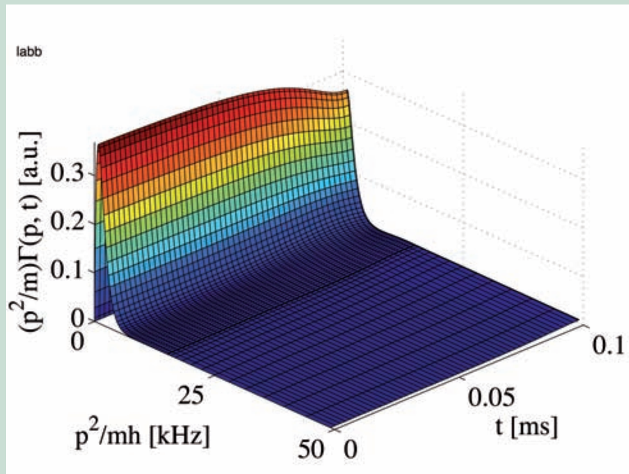
Tom has written programs to solve a non-Markovian Boltzmann-like equation (NMBE) for the dynamics of ultracold gases. He has applied this to the formation of molecules from cold gases using the variation of a magnetic field. His approach includes the exact time-variation of the interactions, and realistically models the evolution of the atomic gas.

Large computations are required to model this process for a realistic set of parameters. This has only been made practical through the use of the NGS.

The kernel of the NMBE is parallelisable. Calculation of the kernel used to take 2 months on a single computer. Accessing resources through the NGS with up to 100 processors at a time has reduced the time taken to less than two days.

Using the kernel for dynamics requires 40 hours of processor time. Tom uses OpenMP to speed up this computation. He's reduced the computation time to a single afternoon.

"The NGS has made a huge difference to my research" Tom explains. "I've been able to calculate the kernel for a realistic ramp, and do 15 dynamical simulations. It's shown the method works and so I am working on extending it. It's one of those problems you couldn't think about doing without access to a cluster!"



The evolution of the one-body density matrix given by the non-Markovian Boltzmann equation, giving the distribution of atomic kinetic energy as the system evolves