Understanding, collaborating and educating

The collaborative efforts of **Professors Jerry P Draayer**, **Kristina D Launey** and **Tomas Dytrych** have been focused on providing unprecedented information concerning nuclear structure. Here, they discuss their work along with the opportunities it provides for answering problems posed in astrophysics, neutrino physics and energy-related applied physics



Could you introduce your studies on atomic nuclei?

Atomic nuclei are ruled by intriguing physics. They are the 'condensed matter' of nuclear material. However, how the strong force bonds protons and neutrons into a plethora of nuclei is still not well understood, and presents a foremost challenge.

We study nuclear structure and reactions from first principles. This means that the interaction between the constituent protons and neutrons is realistic (no parameters to tweak), typically tied to underlying quark/gluon considerations, and hence powers our nuclear simulations with predictive capability.

In what ways does your research benefit your students and postdocs?

Our postdocs, graduate and undergraduate students acquire skills and knowledge in both advanced nuclear theory and working with supercomputers. This makes them highly competitive not only within the field, but also in other areas, including condensed-matter and high-energy physics, or even industry, which often share the computational and theoretical methods we train our students in.

Over the years, our students and postdocs have advanced their careers in national labs and universities, as well as the banking and insurance industries. The undergraduates in our group are also provided with the unique chance to work with our collaborators.

Have you been involved in any partnerships that have helped your studies in ways you did not expect?

Our approach, the symmetry-adapted no-core shell model (SA-NCSM), was developed under a five-year US National Science Foundation (NSF)-sponsored award 'Collaborative Research: Taming the scale explosion in nuclear structure calculations' in partnership with Iowa State University and the Ohio State University, and with help from the Czech Technical University in Prague.

The multidisciplinary team consisted of nuclear and mathematical physicists together with computer scientists, including Professor James Vary of Iowa State University, who together with Dr Petr Navrátil (TRIUMF) and Professor Bruce Barrett (University of Arizona) developed the *ab initio* NCSM. Another partnership that has proved invaluable has been the ongoing work with Professors David Rowe (University of Toronto) and George Rosensteel (Tulane University), who were the first to point to the approximate symplectic symmetry in nuclei. We are also excited about research opportunities, opened by our collaboration with Dr Anna Hayes (Los Alamos National Lab), related to studies of interest to neutrino physics and the National Ignition Facility (NIF), which has recently achieved first fusion energy tests.

How do you approach finding funding for your work?

Our primary support comes from NSF, especially through multidisciplinary programmes, such as those encouraging synergy research in physics, mathematics and/or computer science. Our nuclear theory research is a great match for such programmes, as it combines large-scale simulations, handling massive datasets and extracting essential information from these, as well as group theoretical and statistical mathematics.

Another important initiative we have participated in is the US Department of Energy's Experimental Program to Stimulate Competitive Research (EPSCoR) that encourages partnerships between universities and national labs. In addition, our investigations depend on the use of supercomputer resources, so we seek access to high-performance computing facilities around North America.

What is your opinion on programmes such as the NSF-supported Research Experience for Undergraduates (REU)?

REU is a great initiative. It provides a unique opportunity for undergraduate students to be trained in frontier research and gain hands-on experience. In the case of our research, undergraduates also learn to work with supercomputers and parallel programming environments at an early stage in their career.

Addressing the puzzle of the Hoyle state started as the REU project of Ali Dreyfuss, who published her pilot findings in the leading *Physics Letters B* journal. Following this, Ali joined our group as a graduate student and was well prepared to start working right away on advanced nuclear theory research. Another graduate student in our group, Robert Baker, joined Louisiana State University (LSU) after positive feedback from a friend who had participated in LSU's REU programme.

REU is also quite efficient at helping students choose a research area that best matches their interests. We have always encouraged our REU students to learn more about other fields of physics and to discuss the REU projects with their peers.

Do you organise meetings to promote nuclear theory?

Almost every year, our group hosts a small workshop on *ab initio* nuclear structure and reactions. These meetings typically aim to bring together our collaborators; although in the past, they have occasionally been expanded to 20-80 physicists and computer scientists, including undergraduate and graduate students.

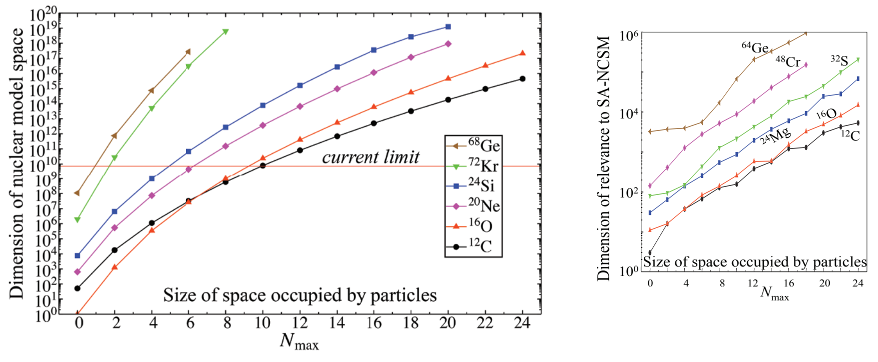
Fuel of the **cosmos**

The field of nuclear physics is deeply connected to a vast array of astrophysical phenomena. Through the development of novel theoretical and computational strategies, many intricate and enigmatic physical processes are now beginning to be unravelled by a team from the Department of Physics and Astronomy at **Louisiana State University**

THE FOUR BASIC forces in nature are the strong, weak, gravity and electromagnetic forces. As the strongest and having the shortest range of these forces, the strong force acts to hold subatomic particles of the nucleus together. However, the intricacies and consequences of the strong force in nuclei are currently unknown, and thus better understanding the principles of strongly interacting particles forms an area of intense research, as Professors Jerry P Draayer, Kristina D Launey and Tomas Dytrych from Louisiana State University's Department of Physics and Astronomy elaborate: "At this energy regime, quarks are bound by gluons into 'molecules' of protons and neutrons, which, in turn, make up the nuclei responsible for the cosmos' 'fireworks'. But exactly how the strong force shapes these nuclei remains a mystery".

AB INITIO INSIGHTS

Through multidisciplinary collaboration and alongside undergraduate and graduate students, Draayer and his team hope to build upon existing knowledge and models of the strong force. His group has developed a novel methodology for *ab initio*, or first principles, modelling. This *ab initio* approach is called the symmetry-adapted no-core shell model (SA-NCSM) – a model of nuclear structure based upon the many-body theory from first principles, which means that it treats each atomic nucleus as a system of many constituent particles that interact with one another via realistic interactions derived from the underlying physics, including quark and gluon considerations.



Explosive growth of the nuclear model space (the red line shows the current limit on best-in-class supercomputers) (**left**) and tamed in the SA-NCSM (**right**).

Modelling the nucleus as such a system is a computationally intense task and faces the difficulty of accounting for emergent phenomena. As such, *ab initio* models that describe atomic nuclei have generally been limited only to light nuclei in simply structured states.

The SA-NCSM takes advantage of novel nuclear approximate symmetries that dominate atomic nuclei, and uses them to reduce the number of possible proton and neutron configurations to only the physically relevant. This decreases the computational challenge faced when modelling atomic nuclei from first principles, as Draayer, Launey and Dytrych explain: "Our approach utilises a new, physically relevant basis or set of 'coordinates'. Working with the 'right' coordinates makes a significant difference: we see this all the time in physics – calculations become simpler and solutions can become feasible".

UNMASKING FEATURES INSIDE NUCLEI

Using this methodology, together with state-of-the-art computer resources, Draayer and colleagues are now building realistic nuclear models from the ground up, which means that the method can be used to predict as well as describe what has been observed experimentally.

The novel approach has allowed the team to learn more about atomic nuclei, by unmasking a basic physical feature of the structure of nuclei, which is usually not observed in conventional *ab initio* studies, as Draayer, Launey and Dytrych further elaborate: "We observed, from first principles, the emergence of simple orderly patterns that favour strong deformation and low intrinsic spin in low-lying nuclear states".

NEW HORIZONS WITH THE SA-NCSM

Further demonstrating the power of their methodology, the team has described several intermediate-sized nuclei – selected isotopes of neon, magnesium and silicon – which are far more complex than the next best *ab initio* methodology can model, and have calculated nuclear structure observables and a wealth of data that can be used for the study of nuclear reactions; for example, the group has studied astrophysical proton-capture reactions.

The work is particularly exciting because it opens up a previously inaccessible region of the periodic

INTELLIGENCE

NUCLEI-FUELED COSMOS IN A SUPERCOMPUTING ERA

OBJECTIVES

To provide nuclear structure information of unprecedented quality and scope that can be used to gain further understanding of fundamental symmetries in nature that are lost in massive datasets, and on extracting essential information from these for astrophysics (eg. nucleosynthesis and stellar processes), neutrino physics and energy-related applied physics problems.

PHD STUDENTS

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KEY COLLABORATORS

Professor James Vary; **Research Associate Professor Pieter Maris**, Iowa State University • **Professor David Rowe**, University of Toronto • **Professor George Rosensteel**, Tulane University • **Dr Anna Hayes**, Los Alamos National Laboratory • **Professor Ümit Çatalyürek**, The Ohio State University • **Professor Masha Sosonkina**, Old Dominion University • **Assistant Professor Tomáš Oberhuber**; **Daniel Langr** (PhD student), Czech Technical University, Prague, Czech Republic

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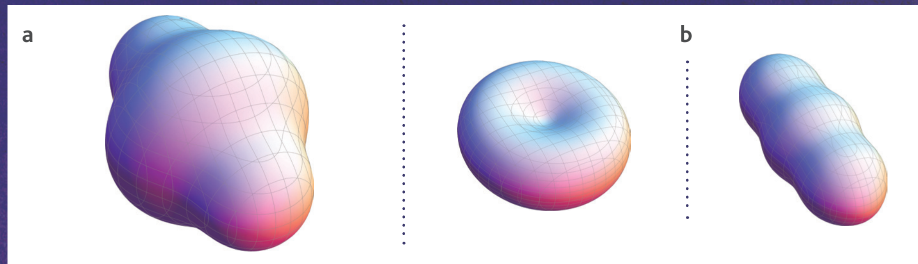
JERRY P DRAAYER is Roy P Daniels Professor of Physics; KRISTINA D LAUNEY and TOMAS DYTRYCH are Research Assistant Professors in the Department of Physics and Astronomy at LSU. Draayer is also LSU Distinguished Research Master and President of the Southeastern Universities Research Association. Draayer has authored approximately 450 published articles, about 100 of those with Launey and Dytrych, and received NSF and DOE awards totalling over $25 million. Their research focuses on nuclear structure and reactions from first principles.



(**a**) Density profile of the 20 particles in the ground state of neon from first principles (previously inaccessible by *ab initio* approaches); (**b**) nucleus of carbon-12 in the ground state from first principles (left) and in the Hoyle state from a fully microscopic no-core shell-model framework (right). The Hoyle state shows a clear alpha-particle clustering, distinct from the oblate shape of the ground state.

table for study and prediction. The intermediate mass region – from oxygen to argon – can now be investigated in a way previously impossible. This region is especially relevant in astrophysics, with many stellar processes involving these elements, such as X-ray burst nucleosynthesis and neon-sodium and magnesium-almunium stellar cycles. In addition, since many nuclear masses, energy spectra and reaction rates for such astrophysical phenomena are currently unavailable, there is a huge demand for predictive modelling to discover what experiments currently cannot achieve by themselves.

ELECTRON AND NEUTRINO SCATTERING

In an interesting study in collaboration with Los Alamos National Laboratory, the team investigated lithium-6 and carbon-12 isotopes in the context of electron and neutrino scattering, using wavefunctions calculated with the SA-NCSM. The approach was capable of reproducing both the low- and higher-momentum dependence of the charge density for these wavefunctions, forming the basis of future studies which will consider neutrino scattering from several nuclei, specifically carbon, oxygen and the intermediate-sized argon. These elements are the main components of neutrino detectors and are used in high-profile experiments including MiniBooNE, T2K and DUSEL. "Due to the complexity of the problem, up to now the intrinsic structure of the ingredient nuclei has been partially or totally neglected, resulting in large uncertainties in data analysis," outline Draayer, Launey and Dytrych. "We aim to help improve these uncertainties, as well as maybe even contribute toward shaping future neutrino experimental facilities."

CLARIFYING THE HOYLE STATE

Pursued by PhD student Alison Dreyfuss, a complementary investigation has tackled the mystery of the Hoyle state – a problem that has remained unsolved for the past 60 years. The Hoyle state is an excited resonant state of carbon-12, postulated to exist by English astronomer Sir Fred Hoyle in 1954, and is also a key step in the nucleosynthesis of heavier elements and in carbon production in asymptotic giant branch stars (evolving low- to medium-

Nuclear theory group at LSU.
Left: PhD students Baker and Dreyfuss

mass stars). This resonant state of carbon-12 arises via triple alpha processes, whereby three helium nuclei fuse to form carbon. It is experimentally very difficult to study but, using the symmetry-guided approach, Dreyfuss provided an explanation of the formation of cluster substructures within carbon-12 with no *a priori* cluster assumptions.

The work opens up a previously inaccessible region of the periodic table for study and prediction

"States in carbon-12 such as the challenging Hoyle state and its rotations have hitherto precluded a fully microscopic NCSM treatment," Draayer, Launey and Dytrych explain. This work is a major step toward understanding how the triple alpha process proceeds and forms the Hoyle state. The consequences of such a finding are far-reaching; the triple alpha process is an important factor in supernovae simulations and stellar evolution models, while also facilitating the prediction of X-ray bursts.

FUTURE INVESTIGATIONS

One of the most striking aspects of this novel research is the extensive impact that it has had, both expected and unexpected. Future research is geared towards understanding how protons and neutrons form complex stable or unstable isotopes and influence nuclear reactions, along with modelling neutrinoless double beta decay, as Draayer, Launey and Dytrych expand upon: "This will allow the type of neutrino and possibly its mass to be extracted from planned experiments".