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Solving The Longstanding Problem Of Low-Energy Nuclear Reactions At the Highest Microscopic Level - Final Report

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SOLVING THE LONG-STANDING PROBLEM OF LOW-ENERGY NUCLEAR REACTIONS AT THE HIGHEST MICROSCOPIC LEVEL

FINAL REPORT

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Background

A 2011 DOE-NP Early Career Award (ECA) under Field Work Proposal (FWP) SCW1158 supported the project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" in the five-year period from June 15, 2011 to June 14, 2016. This project, led by PI S. Quaglioni, aimed at developing a comprehensive and computationally efficient framework to arrive at a unified description of structural properties and reactions of light nuclei in terms of constituent protons and neutrons interacting through nucleon-nucleon (NN) and three-nucleon (3N) forces. Specifically, the project had three main goals: 1) arriving at the accurate predictions for fusion reactions that power stars and Earth-based fusion facilities; 2) realizing a comprehensive description of clustering and continuum effects in exotic nuclei, including light Borromean systems; and 3) achieving fundamental understanding of the role of the 3N force in nuclear reactions and nuclei at the drip line.

The ECA project provided each year $500k of funding to support S. Quaglioni (75%), one post-doc (75%), and one graduate student (18%) to be hired in the summer. Besides Quaglioni, the personnel involved in the project included:

- Post-doc Guillaume Hupin, who was supported by the ECA in the December 2011 – July 2014 period and is currently filling a post-doc position at CEA,DAM,DIF;
- Post-doc Carolina Romero-Redondo, who joined the project in the fall of 2014 and will continue to work on it until September 2016 supported by carryovers funds from the ECA; and
- Graduate student Micah D. Schuster, who was an intern within the LLNL Computation Directorate Scholar program working under Quaglioni's mentorship in support of this ECA project in the summers of 2012, 2013, and 2014 and is currently a Distinguished Post-doc at the National Center for Computational Sciences, Oak-Ridge National Laboratory.

To this date, the ECA project generated a total of 33 publications[1]–[33] (including 8 Letters, 3 Rapid Communications and a Review paper), 26 invited talks at major national and international conferences and workshops, 10 invited seminars/colloquia at national and international institutions, and 3 sets of graduate-level lectures. Quaglioni was also invited to publish a comment in *Nature*.[10] In the following we highlight the most important accomplishments. Citations in square brackets correspond to the Project Bibliography. Other cited references are reported as footnotes.

Research Accomplishments

To achieve the three main goals summarized in the *Background* section, the project started from and build upon the *ab initio* no-core shell model combined with the resonating-group method (NCSM/RGM),[i,ii] which in 2011 had emerged as a promising technique to reach a fundamental description of low-energy binary reactions between light ions. Using expansions over fully-antisymmetric 'microscopic-cluster' states made of a projectile and a target in relative motion with respect to each other, in which each of the nuclei is described within the *ab initio* NCSM, the NCSM/RGM approach had been successfully applied to a variety of binary processes[iii,iv,v] based on

[i] S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008); Phys. Rev. C **79**, 044606 (2009).
[ii] P. Navrátil and S. Quaglioni, Phys. Rev. C **83**, 044609 (2011).
[iii] P. Navrátil and S. Quaglioni, Phys. Rev. C **83**, 044609 (2011).

similarity-renormalization-group (SRG) evolved NN potentials. Two main activities carried out under this ECA project were 1) the extension of the NCSM/RGM approach to include the full range of 3N interactions (those initially present in the Hamiltonian as well as those induced by the SRG procedure);[22] and 2) the development of the formalism and codes for the treatment of three-cluster bound and continuum states required to achieve an ab initio description of Borromean systems as well as three-body breakup reactions.[23] As these two activities progressed, it became evident that to achieve the goals of this ECA project we first had to address practical limitations of the NCSM/RGM approach. Convergence at short-to-medium distances required the inclusion of numerous excited or pseudo-excited states of the target and/or projectile nucleus, unfeasible for calculations including 3N forces or describing three-cluster dynamics (which on their own posed an unprecedented computational challenge). This led to the development, in collaboration with TRIUMF, of a more efficient unified approach to nuclear bound and continuum states: the no-core shell model with continuum (NCSMC).[5],[27],[29] ECA activities concentrated in particular on the inclusion of the 3N force and treatment of three-cluster dynamics within the NCSMC. A final major activity carried out under this ECA project was the implementation and study of operator renormalization within the framework of the SRG used to 'soften' the nuclear Hamiltonian in NCSM/RGM and NCSMC calculations. Such renormalization is required, e.g., for fully consistent calculations of perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. The most significant results enabled by these activities are highlighted in the following.

Harnessing cluster excitations – The NCSMC adopts an extended model space that, in addition to continuous 'microscopic-cluster' states, encompasses also NCSM static solutions for the aggregate system. Such aggregate-system solutions introduce in the trial wave function short- and medium-range many-body correlations, significantly decreasing the need for excited states of the clusters in the NCSM/RGM sector of the basis. At the same time, the NCSM/RGM cluster states provide an effective description of the tail of the wave function, and make the theory able to handle the scattering physics of the system. As part of this ECA project, the impressive gain in the convergence rate and overall accuracy of the NCSMC versus the NCSM/RGM was demonstrated in large-scale calculations of nucleon-^{4}He scattering, as evidenced by the ^{4}He(n,n)^{4}He scattering phase shifts of Figs. 1a and 1b. The various curves represent results obtained with a chiral NN+3N Hamiltonian as a function of the number of excited states of the ^{4}He included in the calculations.

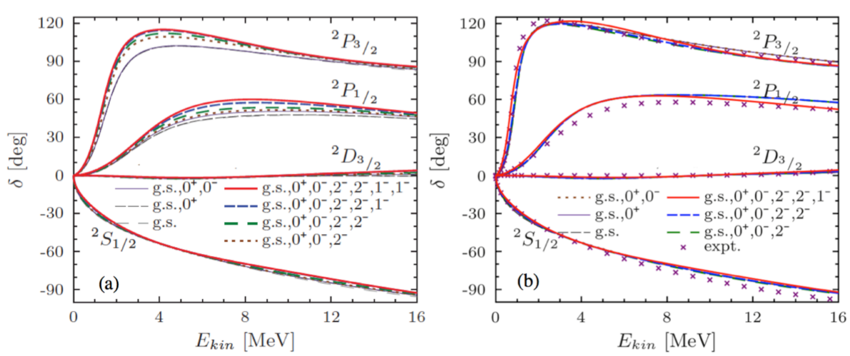

Figure 1 Scattering phase shifts for the ^{4}He(n,n)^{4}He reaction obtained using the SRG-evolved N^{3}LO NN + N^{2}LO 3N interaction with λ = 2.0 fm^{-1}, by (a) working within a n+^{4}He NCSM/RGM binary-cluster basis as in Ref. [22], and (b) further including the first eight NCSM eigenstates of ^{5}He.[5] The calculations of panel (b) are also compared to experiment (crosses).

[iv] P. Navrátil, S. Quaglioni and R. Roth, Phys. Lett. **B704**, 379 (2011).
[v] P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **108**, 042503 (2012).

While in Fig. 2a, where the adopted model space is spanned only by n+^{4}He binary-cluster states,[22] the convergence pattern is quite slow and arguably not fully complete, the calculations of Fig. 2b, further including the first eight NCSM eigenstates of ^{5}He,[5] are all but independent of the excitations of the ^{4}He nucleus and hence fully converged. This study demonstrated that the effect of cluster excitations is non negligible, even for a tightly bound target such as ^{4}He, and that the inclusion of aggregate eigenstates within the model space is an efficient (implicit) way of accounting for such an effect. Post-doc G. Hupin and PI S. Quaglioni carried out this work in collaboration with P. Navratil (TRIUMF).

Nucleon- and deuterium-nucleus scattering with chiral NN+3N forces – A major outcome of this ECA project was the development of the capability to compute nucleon and deuterium collisions on s-shell targets with chiral NN+3N interactions. The high fidelity of NCSMC calculations with chiral NN+3N interactions – particularly the excellent convergence properties and the importance of the 3N force for the description of low-energy nuclear reactions – was demonstrated for the first time in large-scale calculations of neutron[6] and proton scattering on ^{4}He.[16] In particular, we showed that the direct solution of the quantum mechanical problem using chiral NN+3N forces constitutes a predictive theory for nuclear reactions used to characterize hydrogen and helium impurities in material's surfaces (see Fig. 2).[16]

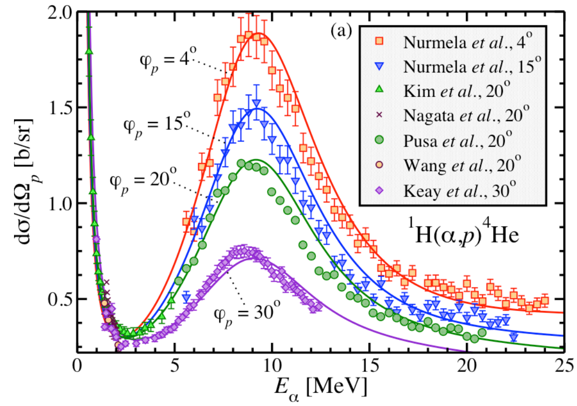

Figure 2 Calculated (solid lines) and measured (symbols) differential angular cross sections for the elastic recoil of protons by ^{4}He nuclei (or a particles) in a range of incident energies E_α and recoil angles φ_p of interest to ion-beam analyses of hydrogen impurities in various materials.

Through our collaborations with TRIUMF and TU Darmstadt, the approach was later extended to p-shell targets and applied to unravel the interplay between continuum degrees of freedom and 3N forces in shaping the low-lying spectrum of ^{9}Be[13] and, more recently, of ^{17}C[9] and ^{11}Be.[1]

Further, we completed and published in Physical Review Letters[12] the most advanced unified study of the ^{6}Li structure and d-^{4}He dynamics, using chiral NN+3N forces. The inclusion of continuum degrees of freedom was essential for a true understanding of a nucleus with low breakup threshold such as ^{6}Li, the ground state of which lies only 1.47 MeV (compared to its absolute energy of nearly 32 MeV) below the ^{4}He+d separation energy. In particular, we solved the outstanding problem of the ^{6}Li asymptotic *D*- to *S*-state ratio in the d-^{4}He configuration, the experimental determination of which was still uncertain even to its sign. Further, we achieved, for the first time, a proper treatment of the d-^{4}He elastic cross sections (see Fig. 3) using realistic NN+3N interactions, and paved the way for the future treatment of the ^{2}H(α,γ)^{6}Li process, responsible for the big-bang nucleosynthesis of ^{6}Li. More recently, through our collaboration with TRIUMF, the approach was extended to the treatment of deuteron collisions on p-

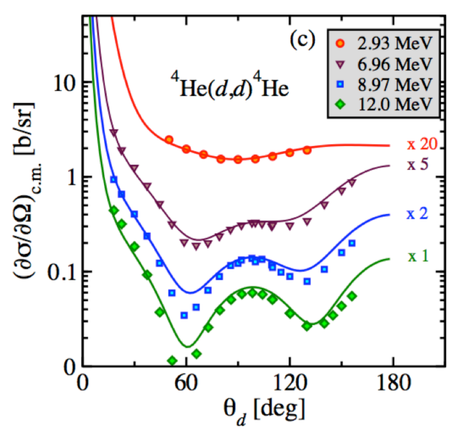

Figure 3 Predicted (lines) and measured (symbols) angular cross sections for the scattering of deuterium (d) off ^{4}He (rescaled as indicated) as a function of the scattering angle q_d at the incident energies E_d = 2.93,6.96, 8.97 MeV.

shell nuclei, though based only on NN interactions.[4] We also have preliminary results for the ^{3}H(d,n)^{4}He fusion based on chiral NN+3N forces (in preparation). Post-doc G. Hupin carried out the activities highlighted in this section with assistance from PI S. Quaglioni.

Ab initio description of three-cluster dynamics – A rigorous description of nuclei for which the lowest threshold for particle decay is of the three-body nature, such as ^{6}He or ^{11}Li, requires the treatment of three clusters in the continuum of energy. The same is true of nuclear reactions characterized by three-body final states, such as the ^{3}He(^{3}He,2*p*)^{4}He solar rate or the ^{3}H(^{3}H, 2*n*)^{4}He process used in diagnostics of modern fusion experiments, or the ^{4}He(2n,γ)^{6}He reaction (one of the mechanism by which stars can overcome the instability of the five- and eight-nucleon systems and create heavier nuclei). We achieved the *ab initio* treatment of three mutually interacting nuclear clusters, based on softened (SRG-evolved) chiral NN interactions. Specifically, at first PI Quaglioni in collaboration with TRIUMF, developed the NCSM/RGM formalism and codes to describe systems of two separate nucleons in relative motion with respect to a core,[23] and published in Physical Review Letters[18] the first investigation of the low-lying spectrum of the ^{6}He nucleus within an *ab initio* framework that encompasses the ^{4}He+n+n three-cluster dynamics of its lowest particle-emission channel (see Fig. 4). Post-doc C. Romero-Redondo, with assistance from PI Quaglioni, then completed the development of the full NCSMC approach for core+n+n dynamics and accomplished the most advanced unified description of the structure (including matter and point-proton root-mean-square radii) and low-lying continuum of the ^{6}He nucleus, by simultaneously addressing six-body correlations and ^{4}He+n+n dynamics.[1] In particular, we solved the long-standing problem of simultaneously reconciling *ab initio* theory with the observed small binding and extended mass and charge radii of ^{6}He. This work has been submitted to Physical Review Letters.

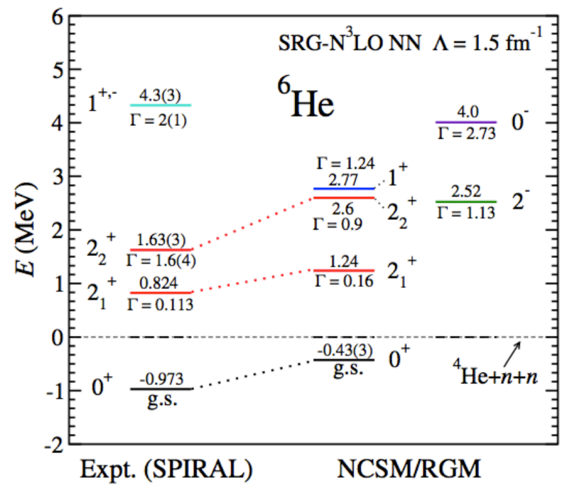

Figure 4 Low-lying energy spectrum for the ^{6}He nucleus obtained within the NCSM/RGM compared to the levels measured at the SPIRAL facility (GANIL), including the newly observed second 2^+ state. Also shown are predicted negative-parity resonances, not observed.

Ab initio description of ^{3}H/^{3}He-nucleus collisions – The ^{3}He(α,γ)^{7}Be radiative capture is one of the most poorly known steps in the entire nucleosynthetic chain leading to ^{8}B, which in turn is the dominant source of the high-energy solar neutrinos (through beta-decay to ^{8}Be) detected in terrestrial experiments. In a collaboration involving TRIUMF, LLNL, Hokkaido U., and CEA,DAM,DIF, we have extended the NCSMC formalism and codes to describe challenging ^{3}He/^{3}H-nucleus collisions, and completed large-scale calculations of the ^{3}He(α,γ)^{7}Be solar fusion

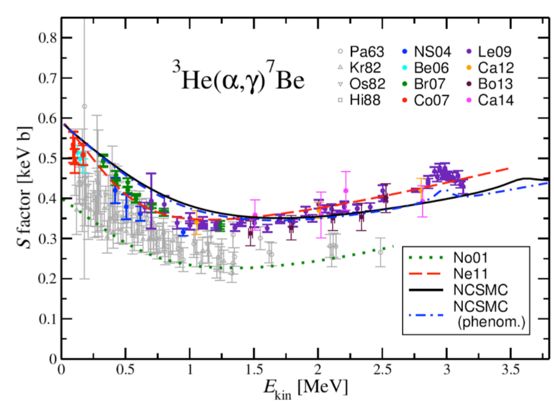

Figure 5 Astrophysical S-factor for ^{3}He(α,γ)^{7}Be radiative capture (NCSMC) compared to experiment and earlier calculations. A quantitative description requires accounting for 3N-force effects.

(see Fig. 5) and mirror ^{3}H(α,γ)^{7}Li reactions based on SRG-evolved chiral NN potentials. These calculations, published in Physics Letters B[3], set the stage for the future accurate prediction, based on chiral NN+3N forces, of these reactions crucial to understanding the neutrino signature of our sun.

Operator evolution for ab initio nuclear theory – Success in the *ab initio* description of light-nucleus reactions with the NCSMC approach has been made possible in part by the development of modern effective interaction theory, where the size of the model space required for an accurate solution of the many-body problem is substantially reduced by means of unitary transformations of the nuclear Hamiltonian. In particular, in our calculations we use similarity-renormalization group or SRG evolved two- and three-body forces. However, caution has to be taken when these interactions are used to describe, e.g., perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. Indeed, for a fully consistent calculation the same unitary transformation applied to the Hamiltonian should be applied to any external operator. As for the Hamiltonian, this generates induced many-body terms.

We implemented the renormalization of external scalar operators up to the three-body level in the framework of the SRG and studied for the first time the behavior of such renormalized three-body operators in systems with more than three nucleons, thus assessing the importance of higher-body terms. Our large-scale NCSM calculations of ^{4}He radii and total dipole strength (see Fig. 6) provided a quantitative answer to the long-sought question of how operators other than the Hamiltonian have to be treated in the context of the SRG approach.[17] Later, we generalized this work by developing the capability to evolve, and embed in finite nuclei, nonscalar operators such as, e.g., the electric dipole. This allowed us a first assessment of the consistency of the SRG approach for the description of continuum observables, specifically the ^{4}He photoabsorption cross section and electric-dipole polarizability.[11] In particular, we showed that the dependence of the ^{4}He photoabsorption cross section on the SRG resolution scale is significant and becomes three times smaller when the dipole operator is evolved up to the 2-body level. This and the previous work were the result of research conducted, in collaboration with Sand Diego State University and TRIUMF, by (then) graduate student M. Schuster under the supervision of Quaglioni over three consecutive summer internships at LLNL.

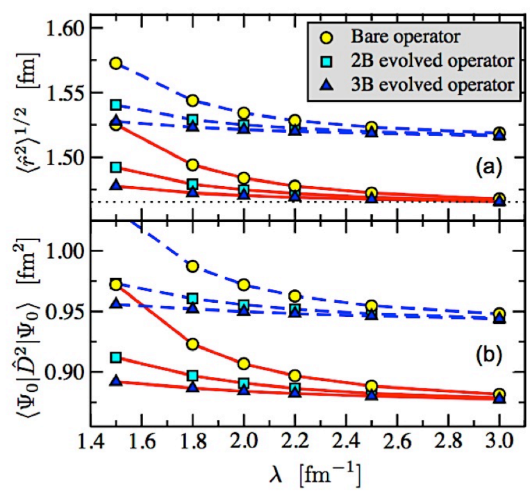

Figure 6 Calculated (a) RMS radius and (b) total dipole strength of ^{4}He as a function of SRG evolution parameter, λ. Shown are results obtained with (red solid line) and without (blue dashed line) 3N force, and with three levels of operator evolution: bare operator (circles), operator evolved in the two-body space (squares), and operator evolved in the three-body space (triangles). The dotted line is the RMS radius with bare Hamiltonian and bare operator.

Opportunities for Training and Professional Development

This ECA contributed to the training of the following four young researchers in the in the use of ab initio approaches combined with high-performance computing to accurately describe light-nucleus structure and reaction properties.

Post-doc G. Hupin – Dr. G. Hupin was hired into the ECA project in December 2012 fresh after his Doctorate Degree in Physics from the University of Caen – GANIL in 2011 for studies and research on the "Functional approach of pairing in nuclei". Upon joining the project, Dr. Hupin acquired new expertise in ab initio nuclear theory and high-performance computing techniques, eventually taking leadership of one of the main activities of this ECA: the description of nucleon- and deuterium-nucleus scattering with chiral NN+3N forces. In particular, he led the publication of three major articles[12][16][22] (one of which a Letter), and contributed to two more.[13][18] Dr. Hupin left LLNL in August 2014, but continued to collaborate with the ECA effort and contribute to its publications. He is currently continuing his postdoctoral training in nuclear theory at the French laboratory CEA/DAM Ile De France, Bruyères-le-Châtel, Arpajon Cedex.

Post-doc C. Romero-Redondo – Dr. C. Romero-Redondo was hired into the project in September 2014 after a first postdoctoral appointment at TRIUMF, Canada, during which she had started to collaborate with the PI on the development of the NCSM/RGM framework to describe the dynamical interactions of three nuclear fragments. Her experience and skills in the area of structure and reactions in three-body systems, acquired during her Ph.D. studies at the Complutense University in Madrid, greatly complemented and enhanced the ECA project. At the Same time, Dr. Romeor-Redondo acquired new expertise in ab initio nuclear theory and high-performance computing techniques. Once at LLNL, Dr. Romeor-Redondo took leadership of the development of the NCSMC formalism for the description of three-cluster dynamics. Including the period in which she was an external collaborator, Dr. Redondo led the publication of two Letters[2][18] and contributed two one Review[5] and one regular article.[23] She is currently finishing her second year of post-doc at LLNL, were she will continue to work until September 2016 supported by carryovers funds from this ECA.

Graduate Student M. D. Schuster – Dr. Schuster, was an intern within the LLNL Computation Directorate Scholar program working under Quaglioni's mentorship in support of this ECA project in the summers of 2012, 2013, and 2014. At the time he was a graduate student at Claremont Graduate University and Sand Diego State University, supervised by Prof. Calvin W. Johnson. While he had a strong background in computational science, at LLNL Dr. Schuster acquired experties in ab initio nuclear theory and carried out one of the major acytivities of this ECA: the implementation and study of operator renormalization within the framework of the SRG method. A large portion of Dr. Schuster Ph.D. thesis stemmed from the research he conducted under the ECA, which also yielded the publication of two journal articles.[11][17] Additionally, each of the three summers he participated in the LLNL Laboratory-wide Student Poster Symposia and received a special recognitions award for the Physics and Life Science Directorate. Dr. Schuster graduated in the summer of 2015 and is currently a Distinguished Post-doc at the National Center for Computational Sciences, Oak-Ridge National Laboratory, where he continues to support nuclear theory research.

Visiting Graduate Student J. Dohet-Eraly – In 2012 the ECA (under the Academic Coperation Program) supported a one-month-long visit of Dr. Dohet-Eraly, who at the time was a Ph.D. student at the Université Libre de Bruxelles and F.R.S.-FNRS research fellow. During the visit, he became acquainted with the NCSM/RGM formalism. Immediately after his graduation, Jérémy was hired at TRIUMF, Canada, to work on the fromalism for the calculation of radiative processes within the NCSM/RGM and NCSMC approaches, an activity partly carried out in collaboration with this ECA. Dr. Dohet-Eraly left TRIUMF in the summer of 2016 and is now continuing his post-doctoral training in nuclear theory at the INFN, Pisa.

Outreach Activities

In January 2014, S. Quaglioni was one of the speakers at the 2014 Conference for Undergraduate Women in Physics, held at UC Berkeley (http://cuwip.physics.berkeley.edu/speakers.html), where she shared personal experiences in her path to becoming a nuclear physicist, and talked one-on-one with students during the Physics EXPO. In addition, in July 2015 Quaglioni delivered graduate-level lectures, including a homework session, at the TRIUMF Summer Institute School on "Theory for exploring experiments in light and medium-mass nuclei" (http://tsi.triumf.ca/2015/contact.html).

Scientific Community Engagement

Over the course of (and with support from) this ECA, PI Quaglioni engaged in a growing number of activities within the nuclear theory community. In 2012, she co-organized the ECT* workshop "Electro-Weak Probes: from Low-Energy Nuclear Physics to Astrophysics". She served on the FRIB Theory User Group Executive Committee (2012-2015), and in 2015 delivered the nuclear theory plenary talk at the 2015 Low-Energy Community Meeting. Quaglioni was a member of Institute for Nuclear Theory (INT) National Advisory Committee from the summer of 2013 to the summer of 2016, and in 2014-2015 served on the INT Director Search committee. Quaglioni further served on two DOE-NP, ASCR Panels: "Exascale Requirements Review for Nuclear Physics" (2016), and "Large Scale Computing and Storage Requirements for Nuclear Physics" (2014). During the ECA period, she also served as Nuclear Theory Panelist for the National Science Foundation, and as Technical Reviewer for the DOE Office of Science (Nuclear Theory), including the Early Career Research Program. Finally, she took part to a number of Scientific Advisory Committees for International Conferences: Direct Reactions with Exotic Beams (December 2014 – present); Few-Body Problems in Physics (December 2013 – present); Nuclear Theory in the Supercomputing Era 2014 and 2016.

High-Performance Computing Resources

Research conducted under this ECA project was the basis for securing a significant amount of computing time on Livermore supercomputers through a proposal review process, known as `Institutional Computational Grand Challenge'. Quaglioni's Grand Challenge Project "From nucleons, to nuclei, to nuclear reactions" was awarded Tier II for the first four Years and Tier I in the last Year of the ECA, respectively. Since the beginning, over 0.5 Billion LLNL high-performance computing cycles were dedicated to this ECA project, 330 Millions of which in the past year alone. Our collaborators freely utilized about half of the cycles.

Dissemination

Refereed Publications

[1] *Can ab initio theory explain the phenomenon of parity inversion in ^{11}Be?*, A. Calci, P. Navrátil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, submitted to Physical Review Letters, arXiv:1608.03318.

[2] *How many-body correlations and α-clustering shape ^{6}He*, C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, submitted to Physical Review Letters, arXiv.1606.00066.

[3] *$^{3}He(\alpha,\gamma)^{7}Be$ and $^{3}H(\alpha,\gamma)^{7}Li$ astrophysical S factors from the no-core shell model with continuum*, J. Dohet-Eraly, P. Navrátil, S. Quaglioni, W. Horiuchi, and F. Raimondi, Physics Letters B **757,** 430 (2016).

[4] *Deuteron-induced nucleon transfer reactions within an ab initio framework: first application to p-shell nuclei*, F. Raimondi, G. Hupin, P. Navrátil, and S. Quaglioni, Physical Review C **93**, 054606 (2016).

[5] *Unified ab initio approaches to nuclear structure and reactions*, P. Navrátil, S. Quaglioni, G. Hupin, C. Romero Redondo, and A. Calci, Physica Scripta **91** 053002 (2016).

[6] *Ab initio calculations of reactions with light nuclei*, S. Quaglioni, G. Hupin, A. Calci, P. Navrátil, and R. Roth, EPJ Web Conferences **113**, 01005 (2016).

[7] *Advances in the ab initio description of three-cluster systems*, C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, EPJ Web Conferences **113**, 03004 (2016).

[8] *Towards an ab initio description of light-nuclei radiative captures*, J. Dohet-Eraly, P. Navrátil, S. Quaglioni, W. Horiuchi and G. Hupin, EPJ Web Conferences **113**, 06002 (2016).

[9] *Life-time measurements of C-17 excited states and three-body and continuum effcets*, D. Smalley et al., Physical Review C **92**, 064314 (2015).

[10] *Nuclear Physics: Close encounters of the alpha kind*, S. Quaglioni, Nature **528**, 42 (2015).

[11] *Operator evolution for ab initio electric dipole transitions of ^{4}He*, M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, Physical Review C **92**, 014320 (2015).

[12] *Unified description of ^{6}Li structure and deuterium-^{4}He dynamics with chiral two- and three-nucleon forces*, G. Hupin, S. Quaglioni, and P. Navrátil, Physical Review Letters **114**, 212502 (2015).

[13] *Continuum and three-nucleon force effects on ^{9}Be energy levels*, J. Langhammer, P. Navrátil, S. Quaglioni, G. Hupin, A. Calci, and R. Roth, Physical Review C **91**, 021301(R) (2015).

[14] *Toward a Fundamental Understanding of Nuclear Reactions and Exotic Nuclei*, S. Quaglioni, G. Hupin, J. Langhammer, C. Romero-Redondo, M. D. Schuster, C. W. Johnson, P. Navrátil, and R. Roth, JPS Conference Proceedings **6**, 010022 (2015).

[15] *Microscopic Study of α+N Bremsstrahlung from Effective and Realistic Inter-nucleon Interactions*, J. Dohet-Eraly, S. Quaglioni, P. Navrátil, and G. Hupin, JPS Conference Proceedings **6**, 010022 030086 (2015).

[16] *Predictive Theory for Elastic Scattering and Recoil of Protons from ^{4}He*, G. Hupin, S. Quaglioni, and P. Navrátil, Physical Review C **90**, 061601(R) (2014).

[17] *Operator evolution for ab initio theory of light nuclei*, M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, Physical Review C **90**, 011301(R) (2014).

[18] *^{4}He+n+n continuum within an ab initio framework*, C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, Physical Review Letters **113**, 032503 (2014).

[19] *Progress on Light-Ion Fusion Reactions with Three-Nucleon Forces*, G. Hupin, S. Quaglioni, J. Langhammer, P. Navrátil, A. Calci, R. Roth, Few-Body Systems **55,** 1013 (2014).

[20] *Ab initio NCSM/RGM for three-body cluster systems and application to ^{4}He+n+n*, C. Romero-Redondo, P. Navrátil, S. Quaglioni, and G. Hupin, Few-Body Syst. **55,** 927 (2014).

[21] *Precision measurement of the electromagnetic dipole strengths in ^{11}Be*, E. Kwan et al., Physics Letters B **732**, 210 (2014).

[22] *Ab initio many-body calculations of nucleon-^{4}He scattering with three-nucleon forces*, G. Hupin, J. Langhammer, P. Navrátil, S.Quaglioni, A. Calci, and R. Roth, Physical Review C **88,** 054622 (2013).

[23] *Three-cluster dynamics within an ab initio framework*, S. Quaglioni, C. Romero-Redondo and P. Navrátil, Physical Review C **88**, 034320 (2013).

[24] *T-T neutron spectrum from inertial confinement implosions*, A. D. Bacher et al., Few-Body Systems **54**, 1599 (2013).

[25] *No-core shell model analysis of Light nuclei*, S. Quaglioni, P. Navrátil, G. Hupin et al., Few-Body Systems **54**, 877 (2013).

[26] *Computational Nuclear Quantum Many-Body Problem: The UNEDF Project*, S. Bogner, A. Bulgac, J.A. Carlson, J. Engel, G. Fann, R.J. Furnstahl, S. Gandolfi, G. Hagen, M. Horoi, W.W. Johnson, M. Kortelainen, E. Lusk, P. Maris, H.A. Nam, P. Navratil, W. Nazarewicz, E.G. Ng, G.P.A. Nobre, E. Ormand, T. Papenbrock, J. Pei, S.C. Pieper, S. Quaglioni, K.J. Roche, J. Sarich, N Schunck, M. Sosonkina, J. Terasaki, I.J. Thompson, J.P. Vary, S.M. Wild, Computer Physics Communications **184**, 2235 (2013).

[27] *Unified ab initio approach to bound and unbound states: no-core shell model with continuum and its application to ^{7}He*, S. Baroni, P. Navrátil and S. Quaglioni, Physical Review C **87**, 034326 (2013).

[28] *Ab initio calculations in three-body cluster systems*, C. Romero-Redondo, P. Navrátil, and S. Quaglioni, AIP Conference Proceedings **1541**, 156 (2013).

[29] *Ab initio description of the exotic ^{7}He nucleus*, S. Baroni, P. Navrátil and S. Quaglioni, Physical Review Letters **110**, 022505 (2013).

[30] *From nucleons to nuclei to fusion reactions*, S. Quaglioni, P. Navrátil, R. Roth, and W. Horiuchi, Journal of Physics: Conference Series **402**, 012037 (2012).

[31] *Ab initio calculations of light-ion reactions*, P. Navrátil, S. Quaglioni, R. Roth, and W. Horiuchi, Progress of Theoretical Physics Supplement **196**, **117** (2012).

[32] *Ab initio calculations of light-ion fusion reactions*, G. Hupin, S. Quaglioni and P. Navrátil, AIP Conference Proceedings **1491**, 387 (2012).

[33] *Measurements of the T(t,2n)^{4}He neutron spectrum at low reactant energies from inertial confinement implosions*, D. T. Casey et al., Physical Review Letters **109**, 025003 (2012).

Invited Talks (Conferences, Workshop, Meetings)

1) Recent progress and future perspectives in the theory of direct reactions and exotic nuclei, S. Quaglioni, (keynote theory talk) 2016 Conference on Direct Reactions with Exotic Beams (DREB2016), Halifax, Canada, July 11-15, 2016.
2) *Ab initio no-core shell model with continuum for three-cluster dynamics*, C. Romero-Redondo, Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, BC, Canada, February 23-26, 2016.
3) *Frontiers of (Low-Energy) Nuclear Theory*, S. Quaglioni, (plenary talk) 2015 Low-Energy Community Meeting, Michigan State University, East Lansing, Mi, Aug 21-22, 2015.
4) *Ab initio calculations of reactions with light nuclei*, S. Quaglioni (plenary talk) 21st International Conference on Few-Body Problems in Physics, Chicago, Illinois, May 18-22, 2015.
5) *Ab Initio Nuclear Theory at LLNL*, S. Quaglioni, Stewardship Science Academic Alliance (SSAA) Meeting, LLNL, March 17, 2015.
6) *Unified structure and interactions of light nuclei*, S. Quaglioni, Institute for Nuclear Theory, Workshop "Reactions and Structure of Exotic Nuclei", Seattle, WA, March 12, 2015.
7) *Bound and continuum properties of A = 6 nuclei*, C. Romero-Redondo, Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, BC, Canada, February 17-20, 2015.
8) *Ab initio calculations of light-nucleus reactions and three-nucleon forces*, S. Quaglioni, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
9) *Toward a fundamental understanding of nuclear reactions and exotic nuclei*, S. Quaglioni, (plenary talk) Nuclear Structure 2014 (NS2014), Vancouver BC, July 21-25, 2014.
10) *Ab initio theory including the continuum*, S. Quaglioni, ECT* Workshop: Resonances and non-hermitian quantum mechanics in nuclear and atomic physics, ECT*, Trento, Italy, June 23-27, 2014.
11) *Toward a fundamental understanding of nuclear reactions and exotic nuclei*, S. Quaglioni, (plenary talk) Advances in Radioactive Isotope Science 2014 (ARIS2014), Tokyo, Japan, June 1-6, 2014
12) *Present and Future Computing Requirements for Ab Initio Calculations of Nuclear Reactions and Light Exotic Nuclei*, S. Quaglioni, Large Scale Computing and Storage Requirements for Nuclear Physics (NP): Target 2017, Bethesda, MD, April 29-30, 2014
13) *Three-cluster dynamics within an ab initio framework*, S. Quaglioni, Institute for Nuclear Theory, Program "Universality in Few-Body Systems", Seattle, WA, March 26, 2014;

14) *Ab initio nuclear theory including the continuum*, S. Quaglioni, TRIUMF Theory Workshop "Nuclear Structure and Reactions: Experimental and Ab Initio Theoretical Perspectives", TRIUMF, Vancouver, BC, Canada, February 18 - 21, 2014
15) *Toward a Fundamental Understanding of Nuclear Fusion*, S. Quaglioni, Joint Meeting of the Science & Technology Committee of the Lawrence Livermore National Security/Los Alamos National Security Board of Governors, Livermore, CA, January 28, 2014.
16) *From nucleons, to nuclei, to fusion reactions*, S. Quaglioni, (plenary talk) West Coast Conference for Undergraduate Women in Physics – 2014, UC Berkeley, January 19, 2014.
17) *Five- and six-nucleon scattering from QCD-based interaction,* G. Hupin, TRIUMF Theory Workshop "Nuclear Structure and Reactions: Experimental and Ab Initio Theoretical Perspectives", TRIUMF, Vancouver, BC, Canada, February 18 - 21, 2014.
18) *Recent progress towards ab initio calculations of light-nuclei reactions*, G. Hupin, EMMI program on "Halo Physics at the Neutron Drip Line", GSI Darmstadt, Germany, February 3 – 14, 2014.
19) *Ab-Initio Light-Ion Reactions with Chiral Two- and Three-Body Interactions*, by G. Hupin, TRIUMF Theory Workshop "Progress in Ab Initio Techniques in Nuclear Physics", TRIUMF, Vancouver, BC, Canada, February 21 - 23, 2013.
20) *Towards a realistic description of low-energy fusion reactions for astrophysics: applications to n-^{4}He and d-^{4}He scattering*, by G. Hupin, International Workshop XLI on Gross Properties of Nuclei and Nuclear Excitations: "Astrophysics and Nuclear Structure", Hirshegg, Kleinwalsertal, Austria, January 29, 2013.
21) *Some recent development in the description of light-nuclei reactions within the NCSM/RGM approach*, by G. Hupin, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24, 2012.
22) *Ab initio calculations of light-ion fusion reactions*, by S. Quaglioni, INT-12-3 Workshop "Structure of Light Nuclei", Seattle, WA, October 11, 2012.
23) *Towards realistic calculations of light-ion fusion reactions*, by G. Hupin, INT-12-3 "Light nuclei from first principles", Seattle, WA, October 2012.
24) *No-core shell model analysis of light nuclei*, (plenary talk) by S. Quaglioni, 20th International Conference on Few-Body Problems in Physics (FB20), Fukuoka, Japan, August 20 – 25, 2012.
25) *Recent developments in the NCSM/RGM treatment of light-ion reactions*, by S. Quaglioni, Argonne Theory Institute Workshop "Facing up to contemporary challenges in light nuclei", ANL, Illinoi, July 30 – August 3, 2012.
26) *From nucleons to nuclei to fusion reactions*, by S. Quaglioni, Conference on Computational Physics 2011 (CCP2011), Gatlinburg, Tennessee, October 30 - November 3, 2011.

Invited Seminars, Colloquia

27) *Can we build a predictive theory of thermonuclear reactions and exotic nuclei?*, by S. Quaglioni, Washington University, Saint Louis, Mo, Apr 22, 2016.
28) *How many-body correlations and α-clustering shape ^{6}He*, by C. Romero Redondo, (seminar) TRIUMF, Vancouver, Canada, Feb 17, 2016.

29) *Can we build a predictive theory of thermonuclear reactions and exotic nuclei?*, by S. Quaglioni, Nuclear Seminars of the National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Mi., Nov 18, 2015.
30) *Continuum and three-nucleon forces in light nuclei*, by S. Quaglioni, ANL Physics Division Seminar, ANL, March 23, 2015.
31) *Toward a Realistic Description of Light-ion Fusion Reactions for Astrophysics*, by G. Hupin, IHPC/CNRS, Strasbourg, France, September 17, 2013.
32) *Toward Realistic Description of Low-energy Fusion of Light Ions for Astrophysics*, by G. Hupin, (seminar) University of Notre Dame, Notre Dame, Indiana, April 8, 2013.
33) *Light-element fusion reactions from first principles*, by S. Quaglioni, (colloquium) MIT, Laboratory for Nuclear Science, Nuclear and Particle Physics Colloquium, Boston, MA, November 26, 2012.
34) *Ab initio calculations of light-ion fusion reactions*, by S. Quaglioni, ISOLDE seminar, CERN, Switzerland, July 11, 2012.
35) *Ab initio calculations of light-ion fusion reactions*, by S. Quaglioni, JLab Theory Seminars, JLab, Virginia, May 21st, 2012.
36) *Ab Initio Theory Of Light-Ion Reactions*, by S. Quaglioni, California State University of Sacramento, Sacramento, CA, February 16, 2011.

Invited Lectures

37) *Ab initio many-body theory of nuclear reactions*, by S. Quaglioni, 2015 TRIUMF Summer Institute, Vancouver BC, Canada, July 13-24, 2015.
38) *Lectures on Ab Initio Methods for Nuclear Physics*, by S. Quaglioni, ISOLDE group, CERN, Switzerland, July 9 - 10, 2012.
39) *No-Core Shell Model and Resonating-Group Method*, by S. Quaglioni, Third UiO-MSU-ORNL-UT School on Topics in Nuclear Physics: The computational quantum many-body problem, ORNL, Tennessee, January 23-27, 2012.

Contributed Talks

40) *Ab initio NCSMC for three-cluster systems and application to ^{6}He*, By C. Romero-Redondo, 2015 Fall Meeting of the APS Division of Nuclear Physics, Santa Fe, New Mexico, October 2015.
41) *Advances in the ab initio description of nuclear three-cluster systems*, by C. Romero Redondo, 21st International Conference on Few-Body Problems in Physics (FB21), Chicago, Illinois, May 2015.
42) *Ab Initio NCSM/RGM for Three-Cluster Structure Systems*, by C. Romero-Redondo, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
43) *Operator evolution for ab initio theory of light nuclei*, by M. D. Schuster, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
44) *Progress on Light-Ion Fusion Reactions with Three-Nucleon Forces*, by G. Hupin, 22nd European conference on few-body problems in physics, Cracow, Poland, September 9 -13, 2013.
45) *Toward realistic calculations of light-ion fusion reactions*, By G. Hupin, Canadian Association of Physics Congress, Montreal, Canada, May 27 – 31, 2013.

46) *Ab initio many-body calculations of the ^{4}He photoabsorption cross section*, by M. Schuster, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24 - 27, 2012.
47) *Three-nucleon interactions in light-ion reactions*, by G. Hupin, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24 - 27, 2012.
48) *Ab initio calculations of light-ion fusion reactions*, by G. Hupin, Nuclear Structure and Dynamics II, Opatija, Crotia, July 9 – 13, 2012.

Participants

Project Personnel

- S. Quaglioni, PI
- G. Hupin, Post-doc, December 2011 – July 2014
- C. Romero-Redondo, Post-doc, September 2014 – present
- M. Schuster, Graduate Student, May-August 2012, 2013, and 2014

External Visitors

- Dr. Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL for one week, supported from her home institution, on December 5 - 9, 2011.
- Ph.D. student J. Dohet-Eraly (Université Libre de Bruxelles) visited Dr. Quaglioni at LLNL for a month, from April 16 to May 15, 2012. He was supported by this DOE/SC/NP project in the form of a perdiem.
- Dr. Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL for two weeks, supported from her home institution, from the 22 of October to the 2nd of November 2012.
- Dr. Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL, supported from her home institution, from the 9 to the 19 of December 2013.
- Prof. Christian Forssen (Chalmers University of Technology) visited S. Quaglioni and the LLNL Nuclear Data and Theory Group on June 11-12, 2015.
- Dr. Jeremy Dohet-Eraly (TRIUMF) visited Dr. Quaglioni and the LLNL Nuclear Data and Theory Group, supported in part from this project, on June 15-26, 2015.
- Prof. Tom Luu (Forschungszentrum Jülich) visited Dr. Quaglioni and the LLNL Nuclear Data and Theory Group, supported in part from this project, on July 29 – August 8, 2016.

Collaborators (who contributed to, but were not funded by this grant)

- A. Calci (TRIUMF)
- J. Dohet-Eraly (INFN, Pisa)
- C. W. Johnson (San Diego State University)
- J. Langhammer (Technishe Universität Darmstadt)
- P. Navrátil (TRIUMF)
- F. Raimondi (University of Surrey)
- R. Roth (Technishe Universität Darmstadt)
- W. Horiuchi (Hokkaido University)

Additional Information

To ensure a third full year of support for Post-doc C. Romero-Redondo, in Year 5 of the ECA PI Quaglioni roughly reduced in half her ECA effort and Dr. Romero-Redondo was supported for about 40% of her time by LLNL funds. This led to $200k of ECA carryover funds, which will entirely be used to support Post-doc C. Romero-Redondo until September 2017. Besides completing and publishing ongoing work, during this time Dr. Romero-Redondo will apply recently developed NCSMC formalism and codes for the description of three-cluster dynamics to study the low-lying spectrum of three-cluster systems and develop the necessary formalism and codes to compute the $^{6}He(\gamma,2n)^{4}He$ photodissotiation.