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David P. Nicholls

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1 Award Details

- **DOE Award Number:** DE–SC0001549 (ER25954)
- **Recipient:** University of Illinois at Chicago
- **Project Title:** "High–Order Numerical Methods for the Simulation of Linear and Nonlinear Waves: High–Frequency Radiation and Dynamic Stability"
- **Principal Investigator:** David P. Nicholls
- **Date:** April 23, 2014
- **Period of Report:** September 2009–August 2013

2 Progress and Accomplishments

2.1 Activities

Over the past four years the Principal Investigator (PI) has worked on several projects in connection with award DE–SC0001549. Of the greatest import has been the continued supervision of five Ph.D. students (Robyn Canning, Travis McBride, Andrew Sward, Zheng Fang, and Venu Tammali). Canning and McBride defended their theses and graduated in May 2012, while Sward defended his thesis and graduated in May 2013. Both Fang and Tammali plan to defend their theses within the year and graduate in May 2015. Fang is now a very experienced graduate researcher with one paper accepted for publication and another in preparation. Tammali is nearly to the point of writing a paper and will work this summer as an intern at Argonne National Laboratory in the Mathematics and Computer Science Division under the supervision of Paul Fischer.

Canning selected a problem in the field of ideal fluid mechanics studying the evolution of interfacial waves between two incompressible, inviscid and irrotational fluids meant to model the interaction of layers of fluid in the ocean which possess different salinities. A great deal of work has been done on the numerical simulation of the classic surface water wave problem (which is a multi–fluid problem where the upper fluid is simply taken to be the vacuum), but much less has been attempted for multi–fluid configurations. While Integral Equation methods have been used for this problem, the Boundary Perturbation (BP) methods that the PI investigated in this grant had not been extended to this scenario. Canning formulated the problem, coded up a BP algorithm for two–dimensional two–fluids, completed testing and verification, and conducted several sample numerical simulations. Both her thesis and a refereed journal publication [CN12] came from this work.

McBride chose a problem in stability of surface ocean flows for his thesis. An enormous amount of work on the stability of Stokes waves (traveling waves on the surface of a two–dimensional fluid: one vertical and one horizontal) to two– and three–dimensional disturbances has been done. More recently, attention has focused on the dynamic stability of short–crested waves (genuinely two–dimensional traveling patterns on the surface of a three–dimensional ocean) to three–dimensional disturbances. While some progress has been reported, a complete study and discussion are missing and McBride helped fill this out in the case of deep water. Travis implemented an algorithm for this on a parallel computer and conducted simulations of stability of hexagonal wave patterns. Both his thesis and a refereed journal publication [MN12] came from this work.

Sward chose a problem in Mathematical Finance which was effectively unrelated to the work envisioned for this proposal. He devised and implemented a Discontinuous Galerkin algorithm to price American options on assets following a "Constant Elasticity of Variance" (CEV) process. This is an interesting and difficult free–boundary problem not unrelated to the water wave simulations mentioned above, however, the numerical techniques are quite different. Both his thesis and a submitted refereed journal publication [NS13] came from this work.

Fang selected a problem on the scattering of linear elastic waves by layered media. He began by working on extending the PI's work on Boundary Perturbation Methods for the two– and three–dimensional acoustic wave scattering problems to the elastic case. This proved to be highly nontrivial as not only are both the independent and dependent variables three dimensional, but also the coupling of the boundary conditions at the layer interfaces is quite intricate. While the analysis and implementation of this aspect took much longer than anticipated, it has resulted in a refereed journal publication [FN14]. We are now working on the inverse problem of identifying layer interface properties given prescribed inputs and far–field measurements.

Tammali is working with the PI on the simulation of scattering of electromagnetic waves by periodic layered structures in three dimensions. This involves implementing one of the PI's Boundary Perturbation algorithms for the Helmholtz equation in three dimensions, and then deriving the appropriate boundary conditions (for the vector Maxwell equations) which must be enforced at the layer interfaces. Once this is accomplished we will study how three–dimensionality affects the character of "Surface Plasmon Resonances" which have applications in many areas of engineering and science.

In addition to supervision of students, over the past four years the PI has visited many colleagues and collaborators (including F. Reitich, A. Malcolm, J. Shen, D. Ambrose) and given over 30 invited conference lectures and departmental seminars. Also, the PI has invested a great deal of time working closely with the computational science group in the Division of Mathematics and Computer Science at Argonne National Laboratory, in particular M. Min, Y. He, and P. Fischer.

2.2 Findings

In the past four years the PI has made substantial progress on a number of projects resulting in the publication of twenty–eight (28) papers in refereed research journals. While not all of these were directly related to award DE–SC0001549, most of them were completed in some measure with the assistance of this grant. These contributions were quite diverse in nature, but the PI has attempted to categorize them in the following sections with a brief description of the findings under each heading. Papers which are submitted (but not accepted for publication) or in preparation are not included in these descriptions.

2.2.1 Layered Media and Seismic Inversion

In the early phases of award DE–SC0001549 the PI began an extremely stimulating and fruitful collaboration with A. Malcolm (Earth, Atmospheric, and Planetary Sciences at MIT) on the scattering of acoustic waves by layered media. This has resulted in five (5) publications which have been accepted for publication, and the topic remains absolutely central to the PI's current research portfolio. This work has evolved along two fronts: The forward problem and the inverse problem.

As the name suggests, the forward problem consists of setting incident acoustic radiation and computing the scattering returns by a *known* model of sediment layers. In [MN11b] the PI and Malcolm generalized Bruno & Reitich's [BR93] two–layer "Method of Variation of Boundaries" to accommodate an arbitrary number of layers. In [Nic12] the PI extended Milder's [Mil91] "Method of Operator Expansions" to doubly perturbed domains and then showed how such operators could be utilized in a surface–layer reformulation of layered media scattering. In [FN14] the PI and his Ph.D. student, Z. Fang, extended Milder's method to the Navier equations of linear elastodynamics.

The inverse problem consists of specifying incident radiation, measuring far–field quantities, and then attempting to reconstruct the *unknown* model for the sediment layers under study. For this the PI and Malcolm pursued an explicit inversion strategy for the forward equations posed at the layer interfaces [MN11a], while they followed a regularized optimization approach in [MN14] in order to ameliorate the strong ill–conditioning found in the former algorithm.

1. Fang & Nicholls, "An Operator Expansions Method for Computing Dirichlet-Neumann Operators in Linear Elastodynamics" (2014) [FN14].

2. Malcolm & Nicholls, "Operator Expansions and Constrained Quadratic Optimization for Interface Reconstruction: Impenetrable Acoustic Media," *Wave Motion*, Volume 51, 23–40, (2014) [MN14].

3. Nicholls, "Three–Dimensional Acoustic Scattering by Layered Media: A Novel Surface Formulation with Operator Expansions Implementation," *Proceedings of the Royal Society of London, A*, Volume 468, 731–758, (2012) [Nic12].

4. Malcolm & Nicholls, "A Boundary Perturbation Method for Recovering Interface Shapes in Layered Media," *Inverse Problems*, Volume 27, Number 9, (2011) [MN11a].

5. Malcolm & Nicholls, "A Field Expansions Method for Scattering by Periodic Multilayered Media," *Journal of the Acoustical Society of America*, Volume 129, Number 4, 1783–1793, (2011) [MN11b].

2.2.2 Interaction of Electromagnetic Waves with Layered Media

On the topic of the interaction of electromagnetic waves with three–dimensional, layered media, the PI has worked on a number of extensions of Boundary Perturbation Methods to the time–harmonic Maxwell equations. In particular, the PI showed how the stable and high–order "Transformed Field Expansions" approach could be extended to *families* of diffraction gratings [Nic09a], while with a graduate student, J. Orville, the PI extended these results to the full vector Maxwell equations [NO10].

In collaboration with Y. He and J. Shen, the PI has investigated the extension of "Transformed Field Expansions" for Maxwell equations to doubly layered media [HNS12] coupled to a rigorous numerical analysis produced in [NS09].

The PI has also showed how transparent, non–reflecting boundary conditions at *perturbed* boundaries can be enforced with Dirichlet–Neumann Operators (DNOs) via Boundary Perturbation Methods. In Cartesian coordinates this has been investigated by the PI in [Nic11a], while in polar coordinates T. Binford, N. Nigam, T. Warburton, and the PI displayed an implementation coupled to an *hp*–FEM algorithm in [BNNW09].

1. He, Nicholls, & Shen, "An Efficient and Stable Spectral Method for Electromagnetic Scattering from a Layered Periodic Structure," *Journal of Computational Physics*, Volume 231, Number 8, 3007–3022, (2012) [HNS12].

2. Nicholls, "Efficient Enforcement of Far–Field Boundary Conditions in the Transformed Field Expansions Method," *Journal of Computational Physics*, Volume 230, Number 22, 8290–8303, (2011) [Nic11a].

3. Nicholls & Orville, "A Boundary Perturbation Method for Vector Electromagnetic Scattering from Families of Doubly Periodic Gratings," *Journal of Scientific Computing*, Volume 45, Number 1, 471–486, (2010) [NO10].

4. Nicholls & Shen, "A Rigorous Numerical Analysis of the Transformed Field Expansion Method," *SIAM Journal on Numerical Analysis*, Volume 47, Number 4, 2708–2734 (2009) [NS09].

5. Binford, Nicholls, Nigam, & Warburton, "Exact Non–Reflecting Boundary Conditions on Perturbed Domains and *hp*–Finite Elements," *Journal of Scientific Computing*, Volume 39, Number 2, 265–292 (2009) [BNNW09].

6. Nicholls, "A Rapid Boundary Perturbation Algorithm for Scattering by Families of Rough Surfaces," *Journal of Computational Physics*, Volume 228, Number 9, 3405–3420 (2009) [Nic09a].

2.2.3 Stability of Surface Water Waves

In a continuing collaboration with B. Akers (a former post–doc of the PI at UIC) we have studied both the effects of surface tension on the shape and properties of traveling water waves [AN10], and also methods to simulate the dynamic stability of traveling water waves in the presence of resonance. Regarding the latter, the author's original BP method for simulating the spectrum of the water wave operator specifically excluded instances of resonance [Nic09b, FN10, Nic11b]. The resonance in question involves configurations where at least one eigenvalue of the trivial traveling water wave (i.e., "flat water") is of multiplicity higher than one. With Akers the PI has expanded the BP approach to account for the higher dimensional null space associated to these eigenvalues [AN12b]. Results for finite depth [AN14] and non–zero surface tension [AN12a] have also come out.

Finally, the PI has completed a thorough evaluation of his conjecture connecting singularities of his BP approach to numerical simulation of the spectrum of the linearized water wave operator (about a Stokes wave) and dynamic stability of these waves [Nic09b, Nic11b]. The comparison was made to a direct numerical simulation of the spectrum of the linearized operator and showed the valuable predictive behavior of the new method at a greatly reduced cost [MN12]. While the conjecture was deemed largely accurate for deep water waves, significant differences in the prediction of onset of instability were detected in the shallow–water regime.

1. Akers & Nicholls, "The Spectrum of Finite Depth Water Waves," *European Journal of Mechanics B/Fluids* (2014) [AN14].
2. Akers & Nicholls, "Spectral Stability of Deep Two–Dimensional Gravity–Capillary Water Waves," *Studies in Applied Mathematics*, Volume 130, 81–107, (2012) [AN12a].
3. McBride & Nicholls, "On Stability of Generalized Short–Crested Water Waves," *Physica D*, Volume 241, 1406–1416, (2012) [MN12].
4. Akers & Nicholls, "Spectral Stability of Deep Two–Dimensional Gravity Water Waves: Repeated Eigenvalues," *SIAM Journal on Applied Mathematics*, Volume 72, Number 2, 689–711, (2012) [AN12b].
5. Nicholls, "Spectral Stability of Traveling Water Waves: Eigenvalue Collision, Singularities, and Direct Numerical Simulation," *Physica D*, Volume 240, Issues 4-5, 376–381, (2011) [Nic11b].
6. Akers & Nicholls, "Traveling Waves in Deep Water with Gravity and Surface Tension," *SIAM Journal on Applied Mathematics*, Volume 70, Number 7, 2373–2389, (2010) [AN10].
7. Fazioli & Nicholls, "Stable Computation of Variations of Dirichlet–Neumann Operators," *Journal of Computational Physics*, Volume 229, Number 3, 906–920 (2010) [FN10].
8. Nicholls, "Spectral Data for Traveling Water Waves: Singularities and Stability," *Journal of Fluid Mechanics*, Volume 624, 339–360 (2009) [Nic09b].

2.2.4 Well–Posedness and Numerical Simulation of Surface Water Waves

One strand of the PI's research more distantly related to the objectives of this grant concerns the modeling of nonlinear waves (particularly arising in free–surface fluid mechanics) and the rigorous analysis of these model equations.

In particular, in collaboration with D. Ambrose and J. Bona, the PI has investigated water wave models with weak dissipation. In [ABN12] they showed how the addition of this dissipation generates a quite standard well–posedness theory, while in [ABN14] they showed the surprising result that low–order, Hamiltonian models of water waves may be *ill–posed* which was not the intuition of the water waves community.

The PI has also conducted numerical simulations of water wave models with a number of junior researchers. In particular, with this weakly viscous model, the PI and his Ph.D. student, M. Kakleas, have produced [KN10]. With a weakly dispersive model the PI and J. Gorsky have published [GN09], while for a two–fluid model the PI and another graduate student, R. Canning, have completed [CN12].

1. Ambrose, Bona, & Nicholls, "On Ill–Posedness of Truncated Series Models for Water Waves," *Proceedings of the Royal Society of London, A* (2014) [ABN14].

2. R. Canning and D. P. Nicholls, "Numerical Simulation of a Weakly Nonlinear Model for Internal Waves," *Communications in Computational Physics*, Volume 12, Number 5, 1461–1481, (2012) [CN12].

3. Ambrose, Bona, & Nicholls, "Well–Posedness of a Model for Water Waves with Viscosity," *Discrete and Continuous Dynamical Systems, Series B*, Volume 17, Number 4, 1113–1137, (2012) [ABN12].

4. Kakleas & Nicholls, "Numerical Simulation of a Weakly Nonlinear Model for Water Waves with Viscosity," *Journal of Scientific Computing*, Volume 42, Number 2, 274–290 (2010) [KN10].

5. Gorsky & Nicholls, "A Small Dispersion Limit to the Camassa–Holm Equation: A Numerical Study," *Mathematics and Computers in Simulation*, Volume 80, Number 1, 120–130 (2009) [GN09].

2.2.5 Other

Of course some of the work completed by the PI during the timeframe of this grant is not terribly closely related to the central goals. In collaboration with D. Mogul and A. Fine, the PI has worked on a project involving signal processing of brain signals resulting from artificially induced seizures in laboratory animals [SFG+13, FNM10].

In [HN10] the PI and B. Hu investigated the subtle analytical properties of Dirichlet–Neumann Operators in the context of solutions to Laplace's equations. We were able to show that, provided one works in an appropriately weak function class, that interfaces of quite severe roughness could be accommodated in the "Transformed Field Expansions" framework. Finally, in [NT09] the PI and his Ph.D. student, M. Taber, studied the possibility of bathymetry detection from surface water wave information. While not related directly to the goals of this grant, it did lead to the formulation of the seismic inversion scheme of the PI and Malcolm [MN11a].

1. Sobayo, Fine, Gunnar, Kazlauskas, Nicholls, & Mogul, "Synchrony Dynamics across Brain Structures in Limbic Epilepsy Vary Between Initiation and Termination Phases of Seizures," *IEEE Transactions on Biomedical Engineering*, Volume 60, Number 3, 821–829, (2013) [SFG+13].

2. Hu & Nicholls, "The Domain of Analyticity of Dirichlet–Neumann Operators," *Proceedings of the Royal Society of Edinburgh A*, Volume 140, Number 2, 367–389, (2010) [HN10].

3. Fine, Nicholls, & Mogul, "Assessing Instantaneous Synchrony of Nonlinear, Nonstationary Oscillators in the Brain," *Journal of Neuroscience Methods*, Volume 186, Number 1, 42–51 (2010) [FNM10].

4. Nicholls & Taber, "Detection of Ocean Bathymetry from Surface Wave Measurements," *European Journal of Mechanics B/Fluids*, Volume 28, Number 2, 224–233 (2009) [NT09].

3 Unexpended Funds

The grant was completely spent out.

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[HN10] Bei Hu and David P. Nicholls. The domain of analyticity of Dirichlet–Neumann operators. *Proceedings of the Royal Society of Edinburgh A*, 140(2):367–389, 2010.

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[MN11b] Alison Malcolm and David P. Nicholls. A field expansions method for scattering by periodic multilayered media. *Journal of the Acoustical Society of America*, 129(4):1783–1793, 2011.

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