Curriculum Vitae of Donald J. Kouri

Birthdate: July 25, 1938

1. Education

Ph.D. in Physical Chemistry, University of Wisconsin, 1965 M.S. in Chemistry, University of Wisconsin, 1962

B.A. in Chemistry, Math, and Physics, Oklahoma Baptist University, 1960

2. Professional Experience

A. Employment

Director, University of Houston (UH) Institute for Digital Informatics and Analysis, 2002 to present

UH, Cullen Distinguished Professor, Chemistry, Mathematics, and Physics, 1996 to present

UH, Distinguished University Professor, Chemistry and Physics, 1988–96

UH, Professor, Departments of Chemistry and Physics, 1973–88

UH, Associate Professor, Department of Chemistry, 1971–73

UH, Assistant Professor, Department of Chemistry, 1967–71

Consultant, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, 1981 to present

Fellow of Institute for Advanced Studies, Hebrew University of Jerusalem, 1978–79

Visiting Scientist, Max Planck Institut fur Stromungsforschung, 1973–74

Institute Fellow, Weizmann Institute for Science, Department of Chemical Physics, 1973 (spring)

Visiting Lecturer, Department of Chemistry, University of Illinois at Urbana. 1972 (fall)

Visiting Scientist, TCI, University of Wisconsin, Madison, Wisconsin, 1971 (summer)

Scientific Programming Specialist, Lockheed Electronics Company, 1969–70 (summers)

Midwestern University, Assistant Professor, Department of Chemistry, 1966–67

Postdoctoral Fellow, Joint Institute for Laboratory Astrophysics, 1965–66

B. Special Honors

UH Research Excellence Award, 1998 Sigma Xi Faculty Research Excellence Award, 1995

Special Creativity Award, National Science Foundation, 1992–94

U.S. Senior Scientist Summer Fellowship, A. von Humboldt Foundation, Germany, 1985

Esther Farfel Award, University of Houston, 1982

ACS Southeastern Texas Section Award, 1981

J. S. Guggenheim Foundation Fellowship, 1978-79

Fellow of the Institute for Advanced Studies, Hebrew University of Jerusalem, 1978–79

Alfred P. Sloan Foundation Fellow, 1972-74

Outstanding Alumni Achievement Award, Oklahoma Baptist University, 1975

Humboldt Award of the Alexander von Humboldt Foundation, 1973-74

Fellow of the Weizmann Institute, 1973

Fellow of the American Physical Society (elected 1974)

Fellow, New York Academy of Sciences

Who's Who in America

Who's Who in the South and Southwest

Outstanding Young Men of America, 1970

Fellow of Wisconsin Graduate School, 1964-65

K. K. Knapp Fellow, University of Wisconsin, 1964-65

C. Professional Memberships and Honor Societies

American Chemical Society

American Physical Society

IEEE

American Association of Physics Teachers

Phi Eta Sigma

Omicron Delta Kappa

American Society of Composers, Authors, and Publishers

D. Other Professional Service

Dr. Kouri is often asked to serve as an external evaluator for promotion and tenure decisions at other universities. He also referees numerous grant proposals for the National Science Foundation (in Chemical Physics, Thermodynamics and Structure, Theoretical Physics, and Atomic and Molecular Physics), Department of Energy, Army Research Office—Durham, U.S.—Israel Binational Science Foundation, Petroleum Research Fund, and Research Corporation. In November, 1992, he served as a member of the panel reviewing currently funded research programs in molecular dynamics for the DOE. In January, 1999, he served on the site-visit panel of NSERC of Canada for the evaluation of proposed new computing facilities. He is curently a member of the Science Advisory Board in Chemistry for the U.S.—Israel Binational Science Foundation.

Dr. Kouri is on the editorial boards of Theoretical Chemistry Accounts, Computer Physics Communications, Journal of Theoretical and Computational Chemistry, and Journal of Computational Methods in Sciences and Engineering and also referees many journal articles for the Journal of Chemical Physics, Journal of Physics B (London), Nuclear Physics A, The Journal of Physical Chemistry A/B, Physical Review A (General Physics), Physical Review C: Nuclear Physics, Physical Review Letters, Chemical Physics Letters, Chemical Physics, Journal of Mathematical Physics, Computational Physics, and Computer Physics Communications.

E. Research Topics

- 1. j_z -conserving coupled states approximation for molecular scattering (with P. McGuire)
- 2. Factorization of general scattering amplitudes, phenomenological and ordinary cross-sections within the IOS approximation (with R. Goldflam and S. Green)
- 3. Correct J_z CCS-theory of general relaxation processes such as line shapes, NMR spin-lattice relaxation, etc. (with R. Goldflam)
- 4. 1-labeled IOS approximation for reactive scattering (with V. Khare and M. Baer)
- 5. Importance of l-labeling in the coupled states approach to molecular collisions (with Y. Shimoni)

- 6. Noniterative solution of close coupling integral equations for scattering and bound states (with W. N. Sams)
- 7. Coupled arrangement channel T-operator equations, integral equations for reactive amplitude density, and L²-methods for calculating the generalized reactive amplitude density using the channel permuting coupling scheme (with M. Baer and F. S. Levin)
- 8. Rigorous derivation of quantum Boltzmann equation for reactive fluid mixtures (with D. K. Hoffman and J. Evans)
- 9. Exact factorization relations for inelastic and reactive scattering (with L. H. Beard and D. K. Hoffman)
- 10. Detailed explication of the optimum form of the CS approximation for gas-phase molecular collisions and demonstration of propensity for j_z-conservation in the apse frame (with D. K. Hoffman and V. Khare)
- 11. L²-method for solving the permutatively coupled reactive amplitude density integral equations for collinear reactive scattering with smooth potential surfaces (with Y. Shima and M. Baer)
- 12. Close coupling wavepacket method for solving molecular scattering problems (with R. C. Mowrey and Y. Sun)
- 13. L²-amplitude density approach to solving the Miller–Micha–Fock coupling scheme arrangement channel quantum mechanics equations for 3-dimensional reactive scattering; application to asymmetric 3-D reactive scattering (with Z.-H. Zhang, K. Haug, Y. Shima, D. Schwenke, and D. G. Truhlar)
- 14. Algebraic variational L²-amplitude density approach to solving the Fock coupling scheme ACQM equations for 3-D reactive scattering; application to asymmetric 3-D reactive scattering (with Y. Sun, Z.-H. Zhang, D. Schwenke, K. Haug, M. Zhao, and D. G. Truhlar)
- 15. Converged 3-D reactive scattering cross sections for D + H₂ \rightarrow HD + H and H + H₂ \rightarrow H₂ + H at high collision energies (with M. Zhao, D. W. Schwenke, and D. G. Truhlar)
- 16. Time dependent wavepacket treatment of 3-D quantum reactive scattering using complex absorbing potentials to decouple arrangements and reduce grid sizes; evaluation of numerically exact S-matrices; computation of converged total reactive cross sections in 3-D for the $F + H_2 \rightarrow HF + H$ reaction (with R. S. Judson, D. Neuhauser, and M. Baer)
- 17. Converged state-resolved 3-D reactive scattering cross sections for $D + H_2$ from 1.4 to 2.2 eV total energy computed by wavepacket methods (with D. Neuhauser and R. S. Judson)
- 18. Distributed approximating functional (DAF) theory, approximation of multi-variate functions and derivatives from discrete input (with D. K. Hoffman)
- 19. DAF-propagation of wavepackets; DAF-path integration (with D. K. Hoffman)
- 20. Time-independent wavepacket Schrodinger and Lipp-mann-Schwinger equations, TIW-versions of variational principles (with M. Arnold, D. K. Hoffman, Y. Huang, and W. Zhu)
- 21. Orthogonal polynomial representation of Green's functions, spectral density operators, lifetime operators (with D. K. Hoffman and Y. Huang)

- 22. Faber polynomial representation of operator-valued functions, including general, non-Hermitian operators (with Y. Huang and D. K. Hoffman)
- 23. Diagonalization of operators by polynomial expansions of the spectral density operator; evaluation of resonances in scattering(with Wei Zhu and D. K. Hoffman)
- 24. Filter diagonalization of matrices using particular subspace basis vectors (with Y. Huang, G. A. Parker, and D. K. Hoffman)
- 25. Stable, accurate DAF-based solutions of various nonlinear partial differential equations (Klein-Gordon, Sine-Gordon, nonlinear Schrödinger, Kuramoto-Sivashinsky in polar coordinates, Fokker-Planck, Burgers' equation for Reynolds number up to 10⁵, Navier-Stokes equation for 2-dimensional, nonperiodic flow in a cavity) (with G. W. Wei, D. S. Zhang, G. H. Gunaratne, and D. K. Hoffman)
- 26. Noninterpolative DAF-based methods for data padding, periodic extension and noise filtering for multidimensional systems, images, etc. (with D. K. Hoffman, M. Arnold, G. H. Gunaratne, and D. S. Zhang)
- 27. Interpolative-DAF based methods for signal processing, imaging, denoising, etc. using both wavelet and nonwavelet methods (with G. W. Wei, Zhuoer Shi, and D. K. Hoffman)
- 28. Evaluating a new "disorder" parameter, using DAFs, for various experimental pattern data; characterization of experimental patterns (with D. S. Zhang, G. H. Gunaratne, and D. K. Hoffman)
- 29. Divide-and-conquer, time-independent wave packet approaches to reactive scattering and photodissociation; applications to 3-D reactions (with S. C. Althorpe, J. Z. H. Zhang, and D. K. Hoffman)
- 30. DAF-Wavelet solution methods for solving quantum dynamics equations: applications to 3-D reactive scattering (with S. C. Althorpe, G. W. Wei, D. S. Zhang, and D. K. Hoffman)
- 31. Dual DAF-propagation method for inverting spectroscopic data, periodic padding of spectroscopic data, DAF-denoising of spectroscopic data (with D. K. Hoffman, E. Pollak, S.-Y. Lee, and D. S. Zhang)
- 32. DAF-wavelet multiresolution analyses for various signal processing problems, including denoising and enhancement of digital mammograms, MRIs, etc. (with Zhuoer Shi, D. K. Hoffman, D. S. Zhang, H. Zhang, and H. Wang)
- 33. DAF—Neural Network approaches to pattern recognition, denoising and enhancement of EKGs and EMGs, and multidimensional surface fitting (with Zhuoer Shi, D. S. Zhang, and D. K. Hoffman)
- 34. Generalized Gaussians and new minimum uncertainty solutions of Heisenberg's uncertainty principle (with D. K. Hoffman)
- 35. Absolutely convergent inverse scattering series for acoustic scattering, based on a new Volterra-transform of the Lippmann-Schwinger equation (with A. Vijay and D. K. Hoffman)
- 36. U.S. Patent: DAF Sparkle Image Enhancement (with Z. Shi, D. K. Hoffman, G. W. Wei, and H. X. Wang)