CURRICULUM VITAE

Christopher J. Tymczak

Email: christopher.tymczak@hccs.edu

BIOGRAPHY

Dr. C. J. Tymczak is an expert in the development of new scientific codes for exploiting advanced computing resources impacting large scale computation in diverse areas such as Many-body physics, Quantum Chemistry and ab initio Molecular Dynamics. While at Texas Southern University, Dr. Tymczak spearheaded the integration of supercomputing resources into various STEM programs and was the founder and director of the Texas Southern High Performance Computing Center (TSU-HPCC). At Los Alamos National Laboratory, Dr. Tymczak was a co-developer of the FreeON code suite, a massively parallel linear scaling computational chemistry code that was under development in collaboration with Dr. Matt Challacombe (T-12) and Dr. Anders Niklasson (T-1). Dr. Tymczak was one of the first to exploit wavelet-based methods in large scale computing for understanding the electronic structure of materials for which he wrote one of the seminal papers [12]. For the last twelve years, Dr. Tymczak have been advancing the FreeON code through the exploitation of advanced data structures and machine architectures. FreeON is now recognized as one of the first quantum chemical codes with demonstrable scalable parallelism as well as linear scaling. Dr. Tymczak was the first to show the correct implementation of exact exchange in real space [21,23], he has developed multiple reduced complexity methods [19,22], and he was instrumental in the development of the first time-reversible form of Born-Oppenheimer molecular dynamic scheme that allows geometric integration of both the nuclear and electronic degrees of freedom which forms the basis for the next generation of first principles molecular dynamics [24-26]. At Texas Southern University, Dr. Tymczak has: in collaboration with Dr. Gonzalez-Szwacki, discovered a novel form of boron hydride [27]; discovered a unique molecular system for the efficient storage of hydrogen [38] in collaboration with A. R. Akbarzadeh; and in collaboration with A. M. N. Niklasson been developing a reduced complexity many-body theory for the highly accurate computation of the electronic structure [40]. In addition, Dr. Tymczak has mentored three postdoctoral scholars and five graduate students

EDUCATION

May 1995	Doctor of Philosophy in Theoretical Physics Texas A&M University, College Station, Texas
December 1989	Master's of Science in Physics Clemson University, Clemson, South Carolina
May 1987	Bachelor of Science in Physics

PAST FUNDING

- ARO-62904RTREP, PI, June 23, 2013-2017, $634,000/3years, "Many-Body Density matrix Theory: Excitations"
- NSF-CREST, Co-PI and Project Director, September 2011-2017, CREST-1137732, $5,000,000/5year, "Center for Research on Complex Networks"
- NSF-MRI, September 2011-Present, PI, MRI-1126251, $220,000/2year, "Acquisition of HPC at Texas Southern University to Expand Capabilities for Research and Training through Shared High Performance Computing
- Welch Foundation Grant, PI, September 2007-Present, J-1675, $250,000/5year,"Many-body Density Matrix Perturbation Theory"
- NIH-RCMI, Co-PI and Project Director, September 2003-August 2009, RR003045-20, $7,215,000/5years
- Texas Southern University Seed Grant Award, PI, September 2006, $15,000/1year, "Advanced Methods for large Scale and Accurate Electronics Structure Simulation"
- Los Alamos National Laboratory LDRD, Co-PI, September 2005, $300,000/1year, 20060551ER, "Simulation and Modeling of the Quantum Response", Los Alamos National Laboratory"

EXPERIENCE

Adjunct Professor: August 2019 to Present
University of St. Thomas
Houston, Texas 77339

I taught Physics 4334, "Introduction of Quantum Mechanics" for which I developed new course material to incorporate ideas of computational chemistry into this standard physics course.

Adjunct Professor: August 2017 to Present
Houston Community College
Houston, Texas 77339

I taught Physics 1401 "College Physics", Physics 2625 "University Physics I", and Physics 2626 "University Physics I". In the summer of 2017 I visited Los Alamos National Laboratory for one month in order to develop a linear scaling multi-determinant method for electronic structure calculations.

Professor August 2006-April 2017
Texas Southern University
Houston, Texas 77339

I was the Founder and director of the Texas Southern University High Performance Computer Center (NSF Grant#1126251). Instituted a Theoretical Quantum Chemistry Research group based on the FreeON program suite. I was

also the Co-author/developer of the FreeON program suite under continuing development at Los Alamos National Laboratory, and the Co-director of the CREST-NSF center on complex network. For teaching, I started the development of an advanced Computational Physics/Quantum Chemistry course at Texas Southern University.

Technical Staff Member March 2000-August 2006
Los Alamos National Laboratory, Group T-14
Los Alamos, New Mexico 87545

Implemented periodic boundary conditions into the Gaussian orbital linear scaling program suite FreeON**.** Devised new density matrix projection schemes into the Gaussian orbital linear scaling program suite FreeON**.**

Postdoctoral Research March 1998-March 2000
Los Alamos National Laboratory, Group T-1
Los Alamos, New Mexico 87545

I developed a bi-orthogonal wavelet basis that is optimized for electronic structure calculation in multi-dimensions. With this basis, have developed order N codes for calculating electronic structure for condensed matter systems. Also started applying this new wavelet basis to image and video compression.

Postdoctoral Research July 1995-March 1998
CTSPS, Clark Atlanta University
Atlanta, Georgia 30082

I initiated a program to adapt wavelet techniques for use in theoretical solid-state physics. Specifically, implemented an orthogonal wavelet basis to calculate the electronic structure for condensed matter systems. I also Taught Graduate Level Quantum Physics I, Fall Semester 1998.

Research Assistant (½) and Teaching Assistant (½) 1990-May 1995
Texas A&M University
Department of Physics
College Station, Texas 77843

In collaboration with Dr. Eckhard Krotscheck, helped developed theories on the structure and excitations of inhomogeneous zero-temperature He-3 and He-4 systems. I also taught recitation & lab; Fall Semester 1991, 1992, 1993 and 1994

Research Assistant (¼) and Teaching Assistant (¾) 1988-1989
Clemson University
Department of Physics
Clemson, South Carolina, 16801

In conjunction with Dr. John Ray, studied the crystallization and melting of sodium as it was super-heated or super-cooled in a molecular dynamics study. I also taught recitation & lab; Fall 1987, Spring 1988, Fall 1988.

PROGRAMINNG LANGUAGES

Expert: Fortran 77, Fortran 95, Fortran 2018, C, C++, and Visual Basic
Moderate: Mathematica and Matlab, C#, Python, xhtml, Java, Javascript, MySQL, PHP.

PUBLICATIONS

TOP FIVE:

1 A. M. N. Niklasson, C. J. Tymczak and Matt Challacombe, *"Time-reversible Born - Oppenheimer Molecular Dynamics",* Physics Review Letters, September 22 2006, 97, no 6, p.123001. **Citations: 145**

2 A. M. N. Niklasson, C. J. Tymczak, and M. Challacombe, "*Trace Re-Setting Density Matrix Purification in O(N) Self-Consistent Field Theory*", J. Chem. Phys. May 15 2003; **118**, no.19, p.8611-8620. **Citations 110**

3 Anders M. N. Niklasson, Peter Steneteg, Anders Odell, Nicolas Bock, Matt Challacombe, C. J. Tymczak, Erik Holmström, Guishan Zheng, and Valery Weber, "*Extended Lagrangian Born–Oppenheimer molecular dynamics with dissipation*", J. Chem. Phys. **130**, 214109 (2009). **Citations: 99**

4 C. J. Tymczak and X. Q. Wang, "*Orthonormal Wavelet Bases for Quantum Molecular Dynamics"*, Phys. Rev. Let., **78,** 3654 (1997). **Citations: 81**

5 B. E. Clements, E. Krotscheck and C. J. Tymczak, "*Mutiphonon Excitations in Boson Quantum Films*.", Phys. Rev. B, **53**, 12253 (1996). **Citations: 72**

FULL LIST

1 C. J. Tymczak and John R. Ray, "*Asymmetric Crystallization and Melting Kinetics in Sodium.",* Phys. Rev. Let. **64**, 1278 (1990).

2 C. J. Tymczak and John R. Ray, "*Interface response function for a model of sodium: a molecular dynamics study*", J. Chem. Phys., **92** 7520 (1990).

3 Krotscheck and C. J. Tymczak, "*Dynamic Structure Function of Quantum Liquid Films.*" Phys. Rev. B**, 45**, 217 (1992).

4 B. E. Clements, J. L. Epstein, E. Krotscheck, M. Saarela, and C. J. Tymczak, *"Dynamics of helium films"*, J. Low Temp. Phys., **89**, 585 (1992).

5 B. E. Clements, H. Forbert, E. Krotscheck, H. J. Lauter, and C. J. Tymczak, "*Dynamics of Quantum Films.*", Physica B; Feb. 1994; **194-196**, p.659-60.

6 B. E. Clements, H. Forbert, E. Krotscheck, H. J. Lauter, M. Saarela, and C. J. Tymczak, "*Dynamics of Boson Quantum Films.*", Phys. Rev. B, **50,** 6958 (1994).

7 B. E. Clements, H. Godfrin, H. J. Lauter, M. Leiderer, E. Krotscheck, and C. J. Tymczak, "*Theoretical Analysis of Neutron Scattering Spectra of Helium-4 Films on Graphite.*", Low Temp. Phys., (rapid communications), **102**, 1 (1996).

8 B. E. Clements, E. Krotscheck and C. J. Tymczak, "*Mutiphonon Excitations in Boson Quantum Films*.", Phys. Rev. B, **53**, 12253 (1996).

9 B. E. Clements, H. Godfrin, E. Krotscheck, H. J. Lauter, M. Leiderer, V. Passiouk, and C. J. Tymczak, "*Excitations in a thin liquid Helium-4 film from inelastic neutron scattering",* Phys. Rev. B, **53**, 12242 (1996).

10 B. E. Clements, E. Krotscheck, and C. J. Tymczak, "*Thermal properties of Helium-4 surfaces and interfaces*", Low Temp. Phys., **107,** 387 (1997).

11 Krotscheck and C. J. Tymczak*, "Excitations in Two-Dimensional and Three-Dimensional Quantum Fluids."*, Vol. 257 of NATO Advanced Study Institute, Series B: Physics, edited by A. F. G. Wyatt and H. J. Lauter (Plenum, New York, 1997) p. 257.

12 C. J. Tymczak and X. Q. Wang, "*Orthonormal Wavelet Bases for Quantum Molecular Dynamics"*, Phys. Rev. Let., **78,** 3654 (1997).

13 C. J. Tymczak, G. S. Japordize, C. R. Handy, X. Q. Wang, "*A New Perspective on Inner Product Quantization"*, Phys. Rev. Lett, **80,** 3673 (1998).

14 C. J. Tymczak, G. S. Japordize, C. R. Handy, X. Q. Wang, "*Iterative solutions to quantum-mechanical problems"*, Phys. Rev. A, **58,** 2708 (1998).

15 C. R. Handy, D. Khan, Xiao-Qian Wang, C. J. Tymczak "*Multi-scale reference function analysis of the PT symmetry breaking solutions for the* P^2+iX^3+iaX *Hamiltonian*", J. Phys. A. **34**(2001) pp 5593-5602.

16 C. J. Tymczak, Anders Niklasson and Heinrich Roder, "*Separable and Non-separable Multi-wavelets in Multi-dimensions*", J. Comp. Phys., **175**, 363-397 (2002).

17 A. M. N. Niklasson, C. J. Tymczak, and H. Roder, "*A multi-resolution density matrix approach to electronic structure calculations*", Phys. Rev. B., **66**, p. 155120 (2002).

18 C. R. Handy, C. J. Tymczak and A. Z. Msenane, *"Regge poles and residues for singular scattering potentials", Phys*. Rev. A, Nov. 2002**, 66**(5), p.050701-701.

19 A. M. N. Niklasson, C. J. Tymczak, and M. Challacombe, "*Trace Re-Setting Density Matrix Purification in O(N) Self-Consistent Field Theory*", J. Chem. Phys. May 15 2003; **118**, no.19, p.8611-8620.

20 C. K. Gan, C. J. Tymczak and Matt Challacombe, "*Linear scaling computation of the Fock matrix. VI. Parallel computation of the Coulomb matrix*", Journal of Chemical Physics; October 8 2004, **121**, no.14, p.6608-6614

21 C. J. Tymczak, V. Weber, E. Swegler and Matt Challacombe, "*Linear scaling computation of the Fock matrix VII. Periodic boundaries, exact exchange and the Minimum Image Condition",* Journal of Chemical Physics, March 22 2005, **122**, no.12, p.124105-1-6

22 C. J. Tymczak and Matt Challacombe, *"Linear scaling computation of the Fock matrix. VIII. Periodic density functional theory at the Gamma point"*, Journal of Chemical Physics, April 22 2005, **122**, no.13, p.1-9

23 V. Weber, C. J. Tymczak and Matt Challacombe, "*Energy gradients with respect to atomic positions and cell parameters for the Kohn-sham density-functional theory at the Gamma point.",* Journal of Chemical Physics, June 14 2006, **124**, no.22, p.224107-1-7.

24 A. M. N. Niklasson, C. J. Tymczak and Matt Challacombe, *"Time-reversible Born - Oppenheimer Molecular Dynamics",* Physics Review Letters, September 22 2006, 97, no 6, p.123001

25 A. M. N. Niklasson, C. J. Tymczak and Matt Challacombe, "*Time-reversible ab initio Molecular Dynamics*", J. Chem. Phys. **126**, 144103 (2007)

26 Anders M. N. Niklasson, Peter Steneteg, Anders Odell, Nicolas Bock, Matt Challacombe, C. J. Tymczak, Erik Holmström, Guishan Zheng, and Valery Weber, "*Extended Lagrangian Born–Oppenheimer molecular dynamics with dissipation*", J. Chem. Phys. **130**, 214109 (2009)

27 Nevill Gonzales-Szwacki, Valery Weber and C. J. Tymczak, "*Aromatic Borozene*", Nanoscale Research Letters, Volume 4, Number 9, September, 2009

28 Anders M. N. Niklasson, Matt Challacobe, C. J. Tymczak and Karoly Nemeth, "*Trace correcting density matrix extrapolation in self-consistant geometry optimization*", J. Chem Phys, **132**, 124104 (2010)

29 N. Gonzalez Szwacki and C. J. Tymczak, " *The symmetry of the boron buckyball and a related boron* ", Chemical Physics Letters, 494 (2010) 80–83

30 N. Gonzalez Szwacki, V. Weber and C. J. Tymczak, "*$B_{12}H_n$ and $B_{12}F_n$: Planar vs Icosahedral Structures* ", Nanoscale Research letters, 2012, 7:236

31 M. F. Khan, D. Vrinceanu, K. Chilakamarri and C. J. Tymczak. "*Minority Student Involvement in High Performance Computing activities at Texas Southern University*", Article No. 63, ACM New York, NY, USA ISDN: 978-1-4503-1602-6

32 Mohammad Hoque, Md. Rezaul Raju, C. J. Tymczak, Kiran Chilakamarri and Daniel Vrinceanu, "*Parallel Sparse Matrix-Matrix Multiplication: A Scalable Solution with 1-D Decomposition*", IEEE HPCC Conference, Zhangjiajie China.

33 Kiran B. Chilakamarri, M. F. Khan, C. E. Larson, C. J. Tymczak, "*Self Similar Graphs*", arXiv:1310.2268

34 Jonathan Jerke and C.J. Tymczak, "*Universal Lattice Basis*"**,** arXiv:1309.0166

35 Jonathan Jerke, Y. Lee and C.J. Tymczak "*Solving One-Electron Systems in a Novel Gaussian-Sinc Mixed Basis Set" arXiv:1405.5073, 2014*

36 BM Prince, TR Cundari, CJ Tymczak "*DFT Study of the Reaction of a Two-Coordinate Iron (II) Dialkyl Complex with Molecular Oxygen*", J. Phys. Chem. A, 2014, 118 (46), pp 11056–11061

37 Jonathan Jerke, Y. Lee and C.J. Tymczak, "*A Novel Gaussian-Sinc mixed Basis Set for Electronic Structure Calculations",* J. Chem. Phys. **143**, 064108 (2015); http://dx.doi.org/10.1063/1.4928577

38 Mohammad Hoque, Md. Rezaul Raju, C. J. Tymczak, Kiran Chilakamarri and Daniel Vrinceanu, "*Parallel Sparse Matrix-Matrix Multiplication: A Scalable Solution with 1-D Decomposition*", IJCSE 11 (4), 391-401 (2015)

39 A. R. Akbarzadeh, D. Vrinceanu and C. J. Tymczak*, "Metalloboranes from first-principles calculations; a candidate to high-density hydrogen storage*", arXiv:1512.02128 (2016)

In Preparation

40 C. J. Tymczak and A. M. N. Nikalsson, "*Multi-determinant non-orthogonal Hartree-Fock*", in preparation.

41 C. J. Tymczak, "*An Introduction to Quantum Chemistry For Physicists*", 1st Edition, in preparation.

CONFERENCES

Attended and Presented, IEEE HPCC 2013, Zhangjiajie, China, November 14th, 2013, accepted paper

Presented: "Parallel Sparse Matrix-Matrix Multiplication: A Scalable Solution with 1-D Algorithm"

Invited Talk: Southwest Regional ACS Meeting – Baton Rouge, LA
November 4-6, 2012

Presented: "Boron, the Carbon Mimic"

Attended and Presented, APS March Meeting, Dallas Texas, March 23rd, 2011

Presented: "Many Body Density Matrix Theory"

Organizer: South West Theoretical Chemistry Conference, October 24th, 2009

Invited Talk: University of Houston Department of Physics, October 6th, 2009

Presented: "Linear Scaling Quantum Chemistry"

Attend APS March Meeting, New Orleans LA, March 2008

Attend and Presented XXIII Southwest Theoretical Chemistry Conference, Texas A&M, College Station

Presented: "*Many-Body density Matrix Perturbation Theory"*

Invited Talk: Texas A & M Department of Physics. April 25th, 2007

Presented: "*Many-Body density Matrix Perturbation Theory"*

Attend and Presented at the Texas section of APS-in College Station

Presented: "*Many-Body density Matrix Perturbation Theory"*

Invited Talk: University of Houston Department of Chemistry, October 16, 2006

Presented: "*Time Reversible Linear Scaling Quantum Molecular Dynamics"*

Attend and Presented XXII Southwest Theoretical Chemistry Conference, Austin, Texas

Presented: "*Time Reversible Linear Scaling Quantum Molecular Dynamics"*

Attend and Presented at the Texas section of APS-in Arlington

Presented: "*Time Reversible Linear scaling ab initio Molecular Dynamics"*

Invited Talk at the UCSB conference on Metal Oxides

Presented: "*Linear Scaling Hybrid HF/DFT Theory for Metal Oxides: Development and Application of the Minimum Image Criterion Hartree-Fock Theory"*

Invited Talk at the European Science Foundation Workshop on Molecular Dynamics Fundamentals and Recent Developments in Paris, France.

Presented: "*Linear scaling ab initio Molecular Dynamics"*

Attended and presented at the 2003 APS March meeting in Austin, Texas.

Presented: "*An Exact Bounded Error Estimate for Multipoles*".

Invited Talk at the 2002 American Conference on Theoretical Chemistry in Seven Springs, Pennsylvania.

Presented: "*Linear scaling computation of the Fock matrix VI. Gaussian orbital methods for simulation of periodic systems".*

Invited Talk at the 2001 ACS meeting in Santa Barbara, California.

Presented: "*Linear scaling computation of the Fock matrix VI. Gaussian orbital methods for simulation of periodic systems".*

Attended and presented at the 1999 APS March meeting in Atlanta, Georgia.

Presentation: ”*Separable and Non-separable Multi-wavelets in Multi-dimensions”*.

Attended and presented at the Wavelet Workshop *"Wavelets and Applications in Physics and Astro-physics"* at ITAMP at Harvard University in October 1998.

Presentation: "*Separable and Non-separable Multi-wavelets in Multi-dimensions*".

Attended and presented at the 1997 APS March meeting in St. Louis, Missouri.

Presentation: “*Orthonormal Wavelet Bases for Quantum Molecular Dynamics"*.

Attended the 1996 APS March meeting in San Jose, California.

Attended the "*Symposium on Quantum Fluids and Solids"* at Pennsylvania State University in 1992.

Attended the "*Many-Body IV Workshop"* in 1990 at Minneapolis, Minnesota.

REFERENCES

Dr. A. M. Niklasson
Los Alamos National Laboratory
Group T-1, MS B221
Los Alamos, New Mexico
Phone: (505) 667-0269
E-mail: anders.niklasson@gmail.com

Daniel Vrinceanu
Associate Professor
Department of Physics
Texas Southern University
Phone: (713) 313-4482
E-mail: vrinceanud@tsu.edu

Dr. Rasoul Saneifard
Professor,
Vice President for Academics and Faculty Affairs
Department of Electrical Engineering
Texas Southern University
Phone: (832) 335-2153
E-mail: Rasoul.Saneifard@tsu.edu

Donald Kouri
Cullen Distinguished Professor
Department of Physics
University of Houston
Phone: (713) 743-3245
E-mail: kouri@central.uh.edu