Peter Cummings – A pillar in the field of statistical mechanics and molecular simulation

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We are delighted to present this special issue of *Molecular Physics* honouring Peter Cummings on the occasion of his 65th birthday. Over the course of 40 years, Peter has come to be one of the central figures in molecular theory and molecular simulation (MTMS), notable both for his prolific scholarship (including almost 50 papers in this journal alone) and for his outstanding leadership. Peter's research in MTMS has had an enormous impact on the development and application of theory and simulation, and has substantially shifted community attitudes about best practice in molecular modeling. His influence continues undiminished today as he leads the charge for better reproducibility in molecular simulation, helping to set the standards and provide the tools that will ensure that our field generates knowledge that is of the highest scientific caliber.

Peter Cummings grew up in Newcastle, one hundred miles north of Sydney on the east coast of Australia. He was the fourth second youngest of the five children of Harry Cummings, a nationally renowned life-insurance salesman, and Mary Cummings, a homemaker who raised the family. He grew up alongside his three older sisters (Meryl, Margaret, and Maureen) and younger brother (Tony). Meryl, Maureen, and Tony all became teachers, while Margaret (Maggie) became one of Australia's best-known opera singers (a soprano), a lead performer in operas staged in Sydney, including the iconic Opera House; her now-adult children, Katie and Ty Noonan are bona fide stars in the Australian music business. Peter describes his home as being infused with music—violin, piano and voice. Not surprisingly, whilst at university Peter played the guitar and sang in Newcastle rock bands, a card-carrying member of the Musician's Union!

Peter always had a strong interest in science. He "geeked out" with *Meccano* construction sets, biology and chemistry sets, and physics experiments. (At age ten, he even built a cloud chamber but the experiment failed when he could not procure a vacuum pump). In high school he bought the classic physics text by Resnick and Halliday and taught himself how to calculate moments of inertia of rigid bodies knowing only single-variable calculus. In the midst of this height of geekdom, he also loved participatory rock and roll, and the beach, where he spent as much time as possible body surfing. A goal-oriented young man, Peter would catch the bus after school each day to the inner-city beaches, or bike 3km to the ones nearest his home. On the day he turned 17, he passed his driving test, opening up the opportunity to surf in the early morning before school.

Peter was the first member of his family to attend university (his siblings attended teachers' colleges or conservatoriums of music). Inspired by his high school physics teacher, he began studies at the University of Newcastle as a physics major, but switched the next year to mathematics after having experienced the kind of letdown Feynman talks about in the introduction to the *Feynman Lectures*. The University of Newcastle Mathematics Department was an innovator in the early 1970s, offering instruction in computer programming and numerical methods, sparking Peter's love of coding which continues to this day. The University of Newcastle was also a hotbed of statistical mechanics, with people like Tony Guttmann, Clive Croxton, and Ed Smith on the faculty. Peter did an undergraduate honours year research project under the direction of Ed Smith, resulting in his first publication, and it was – of course! – published in *Molecular Physics*. He moved with Ed Smith to the University of Melbourne to complete his PhD. Melbourne was another breeding ground of statistical mechanics, counting on Colin Thompson, Tony Guttmann (who had moved a year earlier), Barry Hughes, Derek Chan, and others. After completing his PhD, Peter spent one year (1980) as a postdoc in physics at the University of Guelph in southern Ontario, yet another hub for statistical mechanics (with Chris Gray, Don Sullivan, and Peter Egelstaff in Physics, Saul Goldman in Chemistry, and Bill Smith in Mathematics). Being independently funded by an Australian government fellowship from the CSIRO, Peter was able to publish papers with all five of these researchers. This time period also marked his introduction to the interpretation of neutron scattering results, a theme that would come back later in his career.

In 1981 Peter moved to SUNY Stony Brook to work with the legendary fluid-state statistical mechanician, George Stell. In George, whose PhD was also in Mathematics (from the Courant Institute at NYU with Jerry Percus), Peter found a kindred spirit, and performed some of his most cherished work. At this time, Peter was primarily a theoretician, dabbling in simulation occasionally in order to validate theory. One of his most outstanding accomplishments from this time was his derivation of the exact asymptotic form of the site-site direct correlation function (SSDCF) defined in the site-site OZ (SSOZ) approach, more often referred to as the reference interaction site model (RISM). He demonstrated that the SSDCF had a pathological long-range behavior[1,2] even in cases where the site-site interaction was short-ranged (or of zero range, such as hard spheres). His most cited work from this period is an integral equation model for reacting species that is now known as the shielded sticky sphere (SSS) model. In a series of papers, he analytically solved models for the association reaction of like and unlike species,

including in the presence of an explicit solvent[3-5]. This series of papers is significant for two reasons: it revealed the origin of the pathologies of the SSDCF in RISM theory; and the concept of steric saturation in associating-fluid interactions became a key idea in Wertheim's work that led to the development of the statistical associating fluid theory (SAFT).

Eventually it became time to secure a permanent position, but Australia, unfortunately, had essentially no open academic positions. Encouraged and supported by several chemical engineers who were familiar with his integral equation work (Keith Gubbins then of Cornell, Eduardo Glandt from the University of Pennsylvania, Carol Hall then at Princeton, and John O'Connnell then at the University of Florida), Peter applied for faculty positions in chemical engineering. Despite the odds, he was offered two faculty positions, and began his faculty career in 1991 as a tenure-track assistant professor at the University of Virginia. Peter found that the chemical engineering field was, in many ways, an applied mathematician's dream discipline, and so, building on his expertise in MTMS and applied mathematics, he expanded his research interests into areas such as process design and bioengineering. He became a regular contributor to the annual Mid-Atlantic Thermodynamics and Statistical Mechanics symposium, an informal gathering of the "early adopters" of molecular simulation in chemical engineering in that part of the U.S. It was there that one of us (D.K.), then a graduate student at Penn, made Peter's acquaintance, a relationship that developed into a lifelong friendship.

In 1994 Peter was lured to a joint position as Distinguished Professor and Distinguished Scientist, respectively, at the University of Tennessee-Knoxville and Oak Ridge National Laboratory (ORNL). Peter continued at ORNL for 20 years, eventually serving for six years as chief scientist of the ORNL Center for Nanophase Materials Sciences (CNMS). Prior to this, he was the founding director of the Nanomaterials Theory Institute, the theory program within the CNMS, one of the five principal investigators who wrote the successful $62M proposal to establish the CNMS. A legacy of Peter's involvement in the founding and early leadership of the CNMS is that its theory group is one of the largest and strongest in the country. During this period (in 2002), Peter moved his university affiliation from Tennessee-Knoxville to Vanderbilt University (making for quite a commute between Nashville and Oak Ridge!). He is now full time at Vanderbilt, where he is the John R. Hall Professor in Chemical and Biomolecular Engineering, and Associate Dean for Research in the School of Engineering.

Although Peter's early simulations were mainly conducted in an effort to test the accuracy of molecular theories, this changed in the 90s. Frustrated with the limited number of simple systems that could be modeled with analytic theory, he came to value molecular simulation as a route by which one could model real systems relevant to chemical engineering. Inspired by a conversation with John Prausnitz, who challenged Peter to understand the role of polar forces in transport properties, he turned to non-equilibrium molecular dynamics (NEMD) and began a decade's-long fascination with transport properties. Peter developed new non-equilibrium methods to predict rheological properties of bulk fluids (e.g., the NEMD algorithm calculating non-linear diffusivity in systems under shear[6]) and nanoconfined fluids[7,8], including lubricants, polymer melts, and solutions. This work culminated in new capabilities for the design of

molecules for advanced lubrication applications. One of his early and influential review articles in the field[9] focused attention on chemical engineering applications of these methods.

Peter is one of a handful of computational scientists who are transforming molecular-level simulation from being primarily a way to validate theory or explain experimental findings to a discovery tool that can function as an equal partner with experiment. This trend was heralded by his 1991 predictions of the structure of supercritical water[10]. Subsequent neutron scattering (NS) experiments contradicting his results were reported in Nature in 1993, questioned by Peter and others, and ultimately found to be incorrect, prompting improvements in NS analysis and ushering in a new view of the value of molecular simulation. Other examples: his 2008 JACS paper reported the discovery of an energy release mechanism in gold nanowires undergoing elongation and rupture[11]; his 2006 Cell paper predicted the key role of the microenvironment in tumorigenesis, showing how tumor-level complexity emerges from cell-cell and cell-environment interactions[12]; his 2011 JPC Letters paper predicted the dependence of capacitance on electrode pore size[13], and his 2012 JCTC paper predicted the impact of electrode curvature on capacitance[14].

Peter is world-renowned for his molecular simulations of water and aqueous solutions, in bulk[10], nanoconfined[7], and at interfaces[15], revealing remarkable insights into their structure and properties. In 2005, his group developed one of the most broadly accurate molecular model for water to date[16]. He is an international leader in computational nanoscience, making seminal contributions to, for example, understanding phase transitions in nanoconfined fluids[8], the sliding behavior of carbon nanotubes[17], rupture of gold nanowires[11], electrical double layers in supercapacitors[13], and the properties of nanostructured composite materials[18].

Peter has applied his background in mathematics, statistical mechanics, and computational simulation to the emergence of complexity in other areas of chemical engineering besides molecular thermodynamics. For example, he pioneered the use of simulated annealing for chemical process design and optimization (which became a standard tool in industry), discovering new paradigms for heat exchanger network design[19], batch process design[20], and separations sequencing. He has been a pioneer of cellular-level approaches to computational modeling of the collective behavior of cells in chemotaxis[21,22] and tumor growth[12,23].

Peter's outstanding contributions to MTMS have been recognized with many awards, including the John M. Prausnitz Award in Applied Chemical Thermodynamics (for significant and lasting contributions to the field of applied chemical thermodynamics) in 2013; the Yeram S. Touloukian Medal of the American Society of Mechanical Engineers in 2012; the Founders Award of the American Institute of Chemical Engineers (AIChE) in 2010; the Vanderbilt University Chancellor's Award for Research in 2007; the AIChE Nanoscale Science and Engineering Forum (NSEF) Award in 2007; and the Alpha Chi Sigma Award from the AIChE in 1998. Peter is also a Fellow of the AIChE, the American Association for the Advancement of Science, and the American Physical Society.

In addition to his research accomplishments, Peter has led the mainstreaming of molecular modeling and simulation in chemical engineering, and in the wider scientific enterprise. Recognizing Peter's leadership in computational molecular engineering and science, Peter was invited in 1996 by the non-profit Computer Aids for Chemical Engineering (CAChE) educational foundation to establish a molecular modeling task force (MMTF) in order to expand CAChE's activities beyond process simulation and control. In this role, Peter established the Foundations of Molecular Modeling and Simulation (FOMMS) conference series in 2000, which has been held every three years (the 8th FOMMS is now scheduled for 2021). He has been a member of the board of trustees of CAChE for over 20 years and is a past President. Many of the MMTF members were subsequently elected to the CAChE board of trustees and some also served as presidents of CAChE (Phil Westmoreland, Dave Kofke, Ed Maginn, and Joe Golab). MTMS has become one of the core activities of CAChE. Peter was a key Member of the Formation Committee for the Computational Molecular Science and Engineering Forum (CoMSEF, Area 21) of the AIChE in 2000 and CoMSEF Chair in 2002-2004. He was also a Member of the Formation Committee for the NSEF (Area 22) of the AIChE in 2003-3004. It is no surprise that the AIChE honored Peter with the Founder's Award in 2010. Most recently his impact on MTMS was recognized with the FOMMS Medal in 2018.

Nationally, Peter has served as an advocate for MTMS and computational nanoscience as a member of: the Department of Energy Basic Energy Sciences Advisory Committee 2003-2012; the National Science Foundation Engineering Directorate Advisory Committee 2012-15; the National Science Foundation Advisory Committee on Cyberinfrastructure 2012-15; and as Panelist (2007-2008) and Strategic Directions Workshop Chair (2009) of the multi-agency international comparative assessment of Simulation-Based Engineering and Science (one of the key activities directly leading to the Materials Genome Initiative).

Peter still keeps in touch with the *31 M.S. students and 38 Ph.D. students* that he has mentored as well as the *33 post-doctoral research* associates and 30+ undergraduates who have worked with him. This is in addition to countless young faculty he has mentored (including several of the authors of this piece) as he emerged as a worldwide leader in MTMS. His impact in helping young researchers find their way in the field, while making them feel welcome as colleagues, is immeasurable (some even refer to him as "my Gubbins", a tribute to the role that Keith Gubbins played in mentoring Peter's generation). Closely related is Peter's longstanding advocacy for diversity in MTMS, where he has been quick to call out failures to include traditionally underrepresented groups in positions of significance, such as the slate of plenary speakers at a conference, or on a decision-making board (in this and other ways, Peter often serves as a conscience for the profession). Indeed, Peter has friends the world over, which is not unexpected given his outgoing personality, caring manner, and superb sense of humor.

Peter is as active as ever, mentoring new graduate students and postdocs and serving his university and profession in various service and leadership roles. One of his current passions is the development and deployment of MoSDeF, the Molecular Simulation Design Framework (mosdef.org). MoSDeF holds the promise of enabling molecular simulations that are transferable, reproducible, usable by others, and extensible (i.e., TRUE). Peter still has a strong

interest in music (living in Nashville is certainly a plus!), and has been known to sing and play guitar, even in public. (He and Carol Hall's family performed at the banquet of the PPEPPD 2010 conference). At home, Peter is raising two young children (Erin and Thomas, who are already exhibiting musical inclinations) with his wife and sometime co-author Clare McCabe (also on the faculty at Vanderbilt). He also takes extreme pride in his two adult children, Agatha (an elementary school teacher in New York City) and Calvin (a graduate student at the University of Chattanooga) from his first marriage, both of whom, in the family tradition, are very musical.

In summary, Peter Cummings has been a constantly innovating scientific force in molecular theory and molecular simulation for more than four decades. Simultaneously he has played a leading role in articulating the value of molecular modeling and simulation within our profession and across the broader scientific enterprise. He continues to support our community as an exemplary pillar and engine for the future success of our area. Together with the Editors and Advisory Board of *Molecular Physics* it gives us immense pleasure to recognize all these contributions, and certainly more to come, with this special issue of the journal.

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