Laudation for Prof. Dr. Christoph Ortner

by Prof. Dr. Endre Süli

It is befitting to write this laudation on the tenth anniversary of the death of John Todd (May 16, 1911 – June 21, 2007), a British mathematician and a pioneering figure in the field of Numerical Analysis, who made notable contributions to several branches of mathematics and had an important role after the end of World War II in securing the survival of the MFO.

The work of the MFO's 2017 John Todd Award winner, Christoph Ortner, based at the University of Warwick (UK), focuses on deep and difficult questions that arise in the numerical approximation of mathematical models in Materials Science and Solid Mechanics. Ortner completed his doctoral studies at the University of Oxford in 2006. He then became a Postdoctoral Research Assistant in the EPSRC-funded five-year Critical Mass Programme *New Frontiers in the Mathematics of Solids*, whose aim was to strengthen the interactions between Applied Analysis, Materials Science and Engineering Solid Mechanics. In 2007 Ortner was appointed to a prestigious RCUK Academic Fellowship in *Solid Mechanics and the Mathematics of Solids* in the Mathematical Institute at Oxford in association with Merton College. In 2011 he became Associate Professor at the University of Warwick, where he quickly rose to the rank of Professor. He is the recipient of a Philip Leverhulme Prize and the 2015 Whitehead Prize of the London Mathematical Society.

Much of Ortner's current research emerged from his doctoral project, which had several aspects, the most prominent of which was concerned with atomistic models in materials science, and more specifically the mathematical analysis of the quasicontinuum (QC) method: a difficult and mathematically poorly understood, yet practically relevant, subject. Ortner has, over the last decade, made outstanding contributions to the numerical analysis of quasicontinuum methods and is widely considered to be a world-leading specialist in this field.

The quasicontinuum method is a coarse-graining technique for reducing the complexity of atomistic simulations in a static and quasistatic setting. In his doctoral thesis Ortner gave a complete analysis of the quasicontinuum method in one space dimension, including both a-priori and a-posteriori bounds on the approximation error between the quasicontinuum solution and the full atomistic solution, and provided a careful argument how these results could be extended to several space dimensions. By considering atomistic models with Lennard–Jones type long-range interactions, he proved the existence, the local uniqueness and the stability, with respect to the discrete $\mathrm{W}^{1,\infty}$-norm, of elastic and fractured atomistic solutions, which then enabled him to establish the existence of a quasicontinuum approximation satisfying an optimal a-priori error bound. He also proved that, for a stable QC solution with a sufficiently small residual, which is computed in a discrete Sobolev-type norm, there exists an exact solution of the atomistic model problem for which an a-posteriori error estimate holds. He then derived practically computable bounds on the residual and on the inf-sup constants, which measure the stability of the QC solution. Finally, by supplementing the QC method with a proximal point optimization method with local-error control, he proved that the parameters can be adjusted so that at each step of the optimization algorithm there exists

an exact solution to a related atomistic problem whose distance to the numerical solution is smaller than a pre-set tolerance.

Ortner has also made an original contribution to the Gamma-convergence of Galerkin finite element approximations of nonconvex variational problems. Another excellent piece of work has been his proof that if the residual of a stable numerical solution is sufficiently small, then there exists a nearby exact solution for which an a-posteriori error estimate holds. This result demonstrates that it is not necessary to assume the existence of exact solutions in the a-posteriori error analysis of numerical approximations of nonlinear equations. He pursued the analysis at a general level, in a Banach space setting, and the practical implications of this important theoretical work were shown through numerical simulations. Possible applications include an improved a-posteriori error analysis for nonlinear equations but also a numerical investigation of the existence of solutions to nonlinear partial differential equations where insufficient analytical knowledge is available about the solution.

Ortner's current research falls into three general areas: Atomistic-Continuum Hybrid Numerical Methods, Numerical Approximation of Variational Problems in Fracture Mechanics, and Numerical Analysis of Partial Differential Equations. The primary focus of his current research is the analysis of quasicontinuum methods. In a recent collaboration with Mitchell Luskin (University of Minnesota in Minneapolis) he developed a careful stability analysis of a large class of quasicontinuum methods. This research provides clearer understanding of how well quasicontinuum methods are able to predict nucleation, stability, and motion of defects. Many difficult questions, particularly for complex lattices (more than one species of atoms), are still open and one of Ortner's research objectives is to investigate these. In a related collaboration with Luskin and Dobson, Ortner carried out, what is, the first rigorous analysis of the force-based quasicontinuum method. They showed that the operator resulting from the force-based quasicontinuum method is not coercive, nor is it stable in the most commonly used function spaces. This mathematical result has important practical repercussions in engineering computations. Much of this work is summarized in the 112-page survey paper with Luskin published in Acta Numerica in 2013.

Another significant contribution is Ortner's work with Florian Theil (*Justification of the Cauchy–Born approximation of elastodynamics.* Arch. Ration. Mech. Anal. 207 (2013) no. 3, 1025–1073.). The main contribution of this article is a rigorous approximation error analysis of the Cauchy–Born wave equation in atomistic models. A convergence result is formulated for a general class of many-body interactions in an infinite lattice, which only requires the assumptions that the reference lattice is a stable Bravais lattice and that the interaction strength decays sufficiently fast.

Ortner's paper *Analysis of blended atomistic/continuum hybrid methods* (Numer. Math. 134 (2016), no. 2, 275–326.), with Li, Shapeev and Van Koten, provides detailed and careful numerical analysis of two prototypical atomistic-to-continuum coupling methods of blending type: the energy-based and the force-based quasi-continuum methods in two and three dimensions, for finite-range many-body interactions, and in the presence of lattice defects. The paper considers point defects and dislocations. The two main ingredients in the analysis are new force and energy consistency error estimates; and a new technique for proving energy norm stability of atomistic-continuum couplings that requires only the assumption that the exact atomistic solution is a stable equilibrium.

The paper *Analysis of boundary conditions for crystal defect atomistic simulations* (Arch. Ration. Mech. Anal. 222 (2016), no. 3, 1217–1268.), with Ehrlacher and Shapeev, is concerned with numerical simulations of crystal defects. Such simulations are necessarily

restricted to finite computational domains, supplying artificial boundary conditions that emulate the effect of embedding the defect in an effectively infinite crystalline environment. This work develops a rigorous framework within which the accuracy of different types of boundary conditions can be precisely assessed. The paper formulates the equilibration of crystal defects as a variational problem in a discrete energy space and establishes qualitatively sharp regularity estimates for the associated minimisers. Using this foundation the paper then presents rigorous error estimates for: (i) a truncation method (corresponding to the imposition of Dirichlet boundary conditions on the boundary of the, finite, computational domain); (ii) periodic boundary conditions, (iii) boundary conditions from linear elasticity, and (iv) boundary conditions from nonlinear elasticity. The theoretical results are assessed through detailed numerical experiments, which confirm the sharpness of the numerical analysis.

Ortner's work *Atomistic/continuum blending with ghost force correction* (SIAM J. Sci. Comput. 38 (2016), no. 1, A346–A375.), co-authored with Zhang, combines the ideas of atomistic/continuum energy blending and ghost-force correction to obtain an energy-based atomistic/continuum coupling scheme which exhibits, for a range of benchmark problems, the same convergence rates as optimal force-based coupling schemes. The paper presents the construction of this new scheme, including numerical results exploring the accuracy of the proposed scheme in comparison with established schemes, as well as a rigorous error analysis for an instructive special case.

Ortner's 2017 paper *QM/MM methods for crystalline defects. Part 2: Consistent energy and force-mixing* (Multiscale Model. Simul. 15 (2017), no. 1, 184–214.) with Chen, develops and analyzes QM/MM (quantum/classical) hybrid methods for crystalline defects within the context of the tight-binding model. QM/MM methods employ accurate quantum mechanical (QM) models only in regions of interest (which are, typically, regions of material defects) and switch to computationally cheaper interatomic potential molecular mechanics (MM) models to describe the crystalline bulk. The paper proposes new energy-based and force-based QM/MM methods, building on two principles: (i) locality of the QM model; and (ii) constructing the MM model as an explicit and controllable approximation of the QM model. This approach enables rigorous quantification of convergence rates in terms of the size of the QM region, which represents a significant contribution to the field.

Another important paper published this year is Ortner's work with Nazar *Locality of the Thomas–Fermi–von Weizsäcker equations* (Arch. Ration. Mech. Anal., 224(3), 2017.). The paper establishes a pointwise stability estimate for the TFW model, which demonstrates that a local perturbation of a nuclear arrangement results also in a local response in the electron density and electrostatic potential. The proof adapts the arguments for existence and uniqueness of solutions to the TFW equations in the thermodynamic limit by Catto, Le Bris and Lions. To demonstrate the utility of this combined locality and stability result several consequences are derived, including an exponential convergence rate for the thermodynamic limit, the partition of the total energy into exponentially localized site energies (and consequently, exponential locality of forces), and generalized and strengthened results on the charge neutrality of local defects.

Ortner's work in the field of Numerical Analysis demonstrates impressive mathematical breadth and depth, — very much in the spirit of the MFO's John Todd Award. Christoph Ortner has identified a practically significant, highly nontrivial, and mathematically uncharted field of research, and has made imaginative, important and lasting contributions to it. He is most certainly one of the top specialists in the world in his generation working on the numerical analysis of problems in materials science and solid mechanics.