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# Foreword

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This issue of the *Journal of Elasticity* features an English translation, by Lehoucq & Von Lilienfeld-Toal, of an important 1955 paper by Walter Noll, "Die Herteitung der Grundgleichungen der Thermomechanik der Kontinua aus der statistischen Mechanik." In this paper, Noll addresses and analyses the seminal paper of Irving & Kirkwood, published five years earlier, on "The Statistical Mechanical Theory of Transport Processes. IV, The Equations of Hydrodynamics." Noll gives new interpretations and provides a firm setting for ideas advanced by Irving & Kirkwood that clearly and directly relate to the basic principles of continuum mechanics. However, the original German paper of Noll seems not to have gained the attention that it deserved as the field of statistical mechanics grew both fundamentally and in applications. No doubt, this oversight is partly because the article was published in a journal devoted largely to applied analysis. Noll's contributions place emphasis on fundamental concepts and eliminate potentially confusing applications of the Dirac-delta function and the tacit neglect of far field effects that so often afflict the literature of the physical sciences. Noll exhibits an appreciation of elementary mathematics to discover physical effects, to explain physical concepts, and to draw conclusions of a physical nature.

The concrete advances upon the work of Irving & Kirkwood contained in Noll's paper are described well enough in its introduction. However, what seems underplayed is the importance of his two elementary lemmas. Together, these results provide closed-form representations for stress and heat flux. Moreover, they show how the series representations provided by Irving & Kirkwood, as well as related convergence and accuracy issues, may be avoided. Noll's paper should be of interest to researchers in physics, mechanics, atomistic/multiscale simulation, and materials science and engineering.

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By providing an English translation of Noll's paper, Lehoucq & Von Lilienfeld-Toal have provided a great service to the scientific community. Even so, the arrival of a translation is tardy. Today, atomistic and molecular theories and attendant computations are of fundamental importance in mechanics. They provide a platform for the description of material behaviour at small scales and they create a cornerstone to support the bridge to phenomenological continuum theories. The Noll translation is presented here to expose fundamental ideas of statistical mechanics that are of major importance in the modeling of small-scale behaviour and its link to macroscopic observations. In recent years there has been a rapidly increasing reliance upon and interest in multiscale methods in computation. This has accentuated the need to establish meaningful connections between atomistic and continuum descriptions of contact interactions such as stress and heat flux. In fact, a consensus among researchers regarding the basis and form of such connections is yet lacking, as a sampling [1–5] of recent papers illustrates. While the existence of contact surfacial interaction is a fundamental cornerstone hypothesis in continuum mechanics, in atomistic terms it is defined in various ways depending upon the particle interaction and momentum transfer one conceives.

The concept of contact interactions appears to go back to Cauchy, who was also the first to think about stress from an atomistic point of view. This perspective has been revived many times. The publications [6–10] are representative of the questions that have been addressed periodically, but there have been many other significant contributions, such as those of Clausius, Maxwell, Born & Huang, Irving & Kirkwood, Noll, Tsai, Hardy, and Murdoch. There is a need to unify the atomistic basis of stress if the concept, itself, is to survive as a rational fundamental element of importance in small-scale modeling. Clearly, at some reasonably small-scale, the bridge between atomistic and continuum theories needs to connect with controllable error. The contributions of Murdoch and Admal & Tadmor contained in this special issue are devoted to the concept of stress from an atomistic origin.

In recognition of Noll's contribution, the translation is accompanied by four relevant and invited papers, including one, entitled "Thoughts on the Concept of Stress," by Noll himself. Therein, Noll describes a physical system through the notion of a materially ordered set and introduces the abstraction of an interaction that may be interpreted as forces, torques, or heat transfers. He discusses the law of action and reaction in general terms. Surface and volume interactions are conceptually distinguished and representations for contact and volume interactions are obtained. For mutual volume interactions, the novel idea of a 'reaching' stress is introduced and its existence is proven. This development draws upon ideas of Noll that were described in his original improvement of the work of Irving & Kirkwood. How the reaching stress fits into constitutive theory and related thermodynamic considerations has yet to be determined. Moreover, its connection to the atomistic modeling of media exhibiting structural dependencies of physical importance is an open problem.

In the paper, "On Molecular Modelling and Continuum Concepts," Murdoch concentrates on spacetime atomistic averaging. It is shown how spatial averaging using a weighting function procedure leads to a local balance of linear momentum with several possible candidate stress fields. Physically distinguished weighting functions are introduced. In addition, a cellular localization procedure is described and in this case it is shown how an interaction stress tensor field enters the resulting global balance. These approaches give rise to a Cauchy stress that involves distinct interaction and thermokinetic contributions. The physical interpretation of various candidate interaction stress tensors is discussed. In this context, the overall aim of Murdoch's work is to draw attention to certain methods of linking continuum fields and concepts to the process of scale-dependent molecular averaging. In the end, a molecular context for handling configurational forces—one which involves temporal averaging and material systems whose content changes with time—is proposed.

The paper of Admal & Tadmor, "A Unified Interpretation of Stress in Molecular Systems," takes up the various existing microscopic definitions of the Cauchy stress tensor. Here the ambition is to establish a unifying framework in which all of these molecular surfacial interactions can be derived and the connections between them made evident. Developments in this paper draw upon the non-equilibrium statistical mechanics of Irving & Kirkwood and Noll, together with spatial averaging techniques. Extensions of the early work of Irving & Kirkwood to include multibody potentials and a generalization of the lemmas of Noll to include non-straight bonds are incorporated. Connections to the direct spatial averaging approach of Murdoch and Hardy are exposed and the troublesome sources of non-uniqueness of the stress tensor are identified. Finally, numerical experiments based on molecular dynamics and lattice statics are reported. These contrast the various definitions of stress, including convergence questions related to the size of the domain over which spatial averaging is performed.

It is natural to wonder about the connection between works focused on the microscopic foundation of stress and more kinematically-focused works, such as those of Ericksen, Pitteri, and Zanzotto, which emphasize the utility of and explore the validity of the Cauchy–Born rule. Podio-Guidugli's paper, "On (Andersen–)Parrinello–Rahman Molecular Dynamics, the Related Metadynamics, and the Use of the Cauchy–Born Rule," discusses scale bridging between molecular dynamics and continuum mechanics for Parrinello–Rahman molecular dynamics. The metadynamics that is employed to explore the energy landscape of a crystalline substance along paths connecting local minima, and the use of the Cauchy–Born rule in implementing this search, are of special concern in Podio-Guidugli's work.

## References


1. Subramaniyan, A.K., Su, C.T.: Continuum interpretation of virial stress in molecular simulations. Int. J. Solids Struct. **45**, 4340–4346 (2008)
2. Webb, E.B. III, Zimmerman, J.A., Seel, S.C.: Reconsideration of continuum thermomechanical quantities in atomic scale simulations. Math. Mech. Solids **13**, 221–266 (2008)
3. Murdoch, A.I.: A critique of atomistic definitions of the stress tensor. J. Elast. **88**, 113–140 (2007)
4. Zhou, M.: A new look at the atomic level virial stress: on continuum-molecular system equivalence. Proc. R. Soc. A, Math. Phys. Eng. Sci. **459**, 2347–2392 (2003)
5. Zimmerman, J.A., Webb, E.B. III, Hoyt, J.J., Jones, R.E., Klein, P.A., Bammann, D.J.: Calculation of stress in atomistic simulation. Model. Simul. Mat. Sci. Eng. **12**, S319–S332 (2004)
6. Slater, J.C.: The virial and molecular structure. J. Chem. Phys. **1**, 687–691 (1933)
7. McLellan, A.G.: Virial theorem generalized. Am. J. Phys. **42**, 239–243 (1974)
8. Nielsen, O.H., Martin, R.W.: First-principles calculation of stress. Phys. Rev. Lett. **50**, 697–700 (1983)
9. Filippetti, A., Fiorentini, V.: Theory and applications of the stress density. Phys. Rev. B **61**, 8433–8442 (2000)
10. Morante, S., Rossi, G.C., Testa, M.: The stress tensor of a molecular system: An exercise in statistical mechanics. J. Chem. Phys. **125**, 034101 (2006)