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Is the microscopic stress computed from molecular simulations in mechanical equilibrium? ALEJANDRO TORRES-SNCHEZ, Universitat Politcnica de Catalunya, JUAN M. VANEGAS, Sandia National Laboratories, MARINO ARROYO, Universitat Politcnica de Catalunya — The microscopic stress field connects atomistic simulations with the mechanics of materials at the nano-scale through statistical mechanics. However, its definition remains ambiguous. In a recent work [1,2] we showed that this is not only a theoretical problem, but rather that it greatly affects local stress calculations from molecular simulations. We find that popular definitions of the local stress, which are continuously being employed to understand the mechanics of various systems at the nanoscale, violate the continuum statements of mechanical equilibrium. We exemplify these facts in local stress calculations of defective graphene, lipid bilayers, and fibrous proteins. Furthermore, we propose [1,3] a new physical and sound definition of the microscopic stress that satisfies the continuum equations of balance, irrespective of the many-body nature of the inter-atomic potential. Thus, our proposal provides an unambiguous link between discrete-particle models and continuum mechanics at the nanoscale. [1] Torres-Sanchez, A; Vanegas, J. M.; Arroyo, M.; Phys. Rev. Lett. 114, 258102 (2015). [2] Vanegas, J. M.; Torres-Sanchez, A; Arroyo, M.; J. Chem. Theor. Comput., 10 (2), 691702 (2014). [3] Torres-Sanchez, A; Vanegas, J. M.; Arroyo, M.; Submitted to J. Mech. Phys. Solid

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