Four New Contributions to the Local Stress Tensor in Molecular Models of Matter J. MATTHEW MANSELL, North Carolina State University — There exists considerable controversy regarding the local stress tensor and pressure tensor fields in molecular models of matter. While most researchers agree that these fields are not uniquely defined, they have nonetheless gained attention in recent years as a result of evidence that they may be uniquely defined, and may explain a wide range of anomalous phenomena. I briefly describe the current methods of calculating these fields, and the evidence for and against the existence of a unique definition of each field. I then present four new contributions to the topic. The first is the description of an error in a key dataset which had supported the existence of unique definitions. The second is a generalization of the current definitions in systems of a certain symmetry, arising from the recognition of an unjustified constraint. The third is a new method to rapidly obtain the pressure field according to any acceptable definition from the many-body density. The fourth consists of possible additional constraints on the definition of these fields, arising from relationships with the analogous fields in macroscopic, continuum models. It is hoped that these ideas will motivate increased discussion, and hasten the resolution of the current controversy.

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