A Science Gateway for Atomic and Molecular Physics

B. I. SCHNEIDER, National Institute of Standards and Technology, K. BARTSCHAT, K. R. HAMILTON, O. ZATSARINNY, Drake University, I. BRAY, Curtin University, A. SCRINZI, Ludwig-Maximilians Universität, F. MARTIN, J. GONZALEZ-VAZQUEZ, Universidad Autonoma de Madrid, J. TENNYSON, University College London, J. D. GORFINKIEL, The Open University, S. PAMIDIGHANTAM, Indiana University and the eXtreme Science and Engineering Discovery Environment (XSEDE). — We describe the creation of a new Atomic and Molecular Physics science gateway [1,2]. It is designed to bring together members of the AMP community to work collectively on making their codes publicly available and easy to use. A project such as this requires the developers to work on issues of portability, documentation, ease of input, as well as ensuring that the codes run on a variety of architectures. We present an outline of our efforts to build the gateway, the current status as discussed in a recent workshop held at NIST on Dec 11-13, 2019, and our long-range plans to further extend the functionality of the gateway. [1] https://ampgateway.org/ [2] https://arxiv.org/abs/2001.02286

1Supported by MolSSI, NSF, NIST, and XSEDE.