Michael S. Murillo

Professor, CMSE; Department of Chemical Engineering and Materials Science
murillom@msu.edu | 517.432.0196 | 428 S. Shaw Lane, Room 1508C

BIO SKETCH

Michael Murillo is Professor of the Department of Computational Mathematics, Science and Engineering; and a professor in the Department of Chemical Engineering and Materials Science at Michigan State University.

Dr. Murillo is a Fellow of the APS. He is on the editorial board for High Energy-Density Physics. He has published more than 100 papers and has presented invited talks around the globe.

From 1995–1997, he was a Director's Fellow in the Theoretical Division at Los Alamos National Laboratory, where his research was focused on dense plasma physics and molecular dynamics techniques. In 1997 he became a Technical Staff Member at Los Alamos where he served in several roles, included a Project Leader in the Advanced Scientific Computing Program and the Team Leader for High Energy-Density Physics. In 1997 he was a Long-Term Visitor at Harvard's Institute for Theoretical for Atomic and Molecular Physics, and in 2006 he was a Visiting Scholar in the Department of Physics at Berkeley. As of 2016, he is with the Department of Computational Mathematics, Science and Engineering and Chemical Engineering and Material Science.

Dr. Murillo received his BSEE as an Excel Scholar at the University of New Mexico and his Ph.D. in physics at Rice University in 1995.

RESEARCH INTERESTS

Computational epidemiology of influenza; dynamic density functional theories; molecular dynamics methods, including multiscale; shock physics; transport physics; kinetic theory; agent-based modeling; plasma physics

GROUP MEMBERS

MSU COLLABORATORS: A. Christlieb, J. Verboncouer.
POSTDOC: Abdu Diaw. PH.D. STUDENT: Gautham Dharuman.
UNDERGRADUATE: Eric Comings.

CURRENT RESEARCH FOCUS

Accurately describing the many-body behaviors of interacting systems from the "bottom up" is the main focus of our group. We develop and employ a wide variety of methods, including kinetic models, molecular dynamics, and agent-based modeling.

1. Molecular dynamics methods. While the vast majority of plasmas in the universe and the laboratory are well described with relatively simple kinetic and hydrodynamic models, plasmas with complex properties also occur. Dusty plasmas, ultracold plasmas, and dense plasmas differ from common plasmas in that they have liquid-like structure and potentially quantum behavior. Modeling of this class of plasmas requires molecular dynamics techniques, rather than the more common kinetic and hydrodynamic approaches. We are developing new potentials to describe ion-ion interactions in dense plasmas, effective potentials that incorporate quantum aspects of electron dynamics, and modified Coulomb solvers adapted to this class of systems.

2. Multiscale methods. Highly collisional many-body systems are well described at the macroscale by hydrodynamics equations, which are an expansion in small mean-free paths around local equilibrium. Conversely, very weakly collisional systems may have large mean-free paths and deviations from equilibrium that require a kinetic treatment. Between these well defined limits lies the most challenging regime, the "transition regime," where the usual expansions fail. We are developing computational methods that address this need through the use of multiscale methods that combine molecular dynamics at the microscale and kinetic theory at the macroscale.

3. Transport physics. Conservation laws stringently control the dynamics of many-body systems. However, mass, momentum and energy can free flow in time between species and locations, which is the problem of transport physics. We are developing methods to describe such transport for fusion energy problems that employ highly compressed plasmas. We have developed a Vlasov-BGK framework for multispecies, multitemperature plasmas that has computational advantages over other kinetic models. The microphysics enters through an effective scattering approach in which cross sections are computed in effective many-body potentials. Our molecular dynamics tools provide validation not available from incompletely diagnosed experiments.

4. Agent-based modeling. In the same way as our physics modeling approach begins from the "bottom up" by building interparticle interactions at the atomic scale for simulations that reveal the emergent phenomena of dynamics and transport, we apply similar a similar approach to agents. Agents are autonomously defined "particles" that interact with the "many-body" system to generate emergent phenomena at vastly different scales. In analogy with our plasma research, we have developed a multiscale approach for agent based modeling that incorporates a systems dynamics model for each agent, which impacts agent behavior as it interacts with other agents, with community-based set of behaviors among the agents. To date, our work has primarily focussed on influenza pandemics and the optimal use of antiviral drugs.

5. Dynamic density functional theory. Density functional theory (DFT) was developed originally as a question regarding

the minimum information needed to describe the electronic structure of a material. It's main impact, however, is the computational gain it provided in its Kohn-Sham formulation, essentially revolutionizing materials science, chemistry and biology. Less well known is the classical limit of DFT where our group asks: can the Nobel Prize–winning theorems of DFT have a similar impact on classical (or semiclassical) many-body systems? In particular, can time-dependent DFT lead to deeper insights into kinetic processes in liquids and plasmas? Our current approach formulates an exact hydrodynamics in terms of a near equilibrium closure based on the thermodynamic ground state; such approximations are called "dynamic" DFTs because they are DFT based, but with approximate dynamics. For dense systems this approach allows us to incorporate correlations impossible to obtain through moments of kinetic equations. In combination with our efforts on transport physics, we are applying DDFT to the sedimentation problem in late-stage stars, such as white dwarfs and neutron stars.

RESEARCH SUPPORT: Air Force Office of Scientific Research (AFOSR), National Science Foundation (NSF), Department of Energy (DOE)

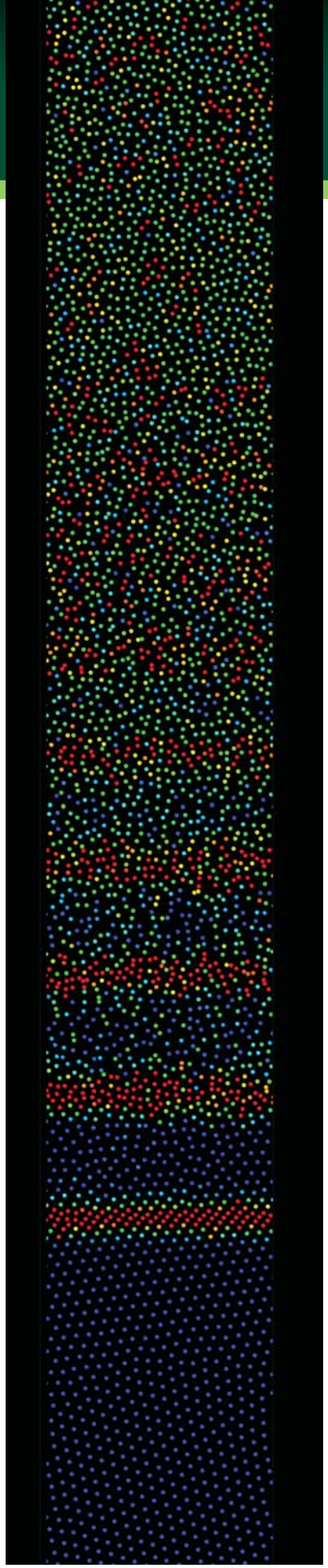

FIGURE 1. Non-equilibrium molecular dynamics reveal the structure of a weak shock at the individual particle level, including dispersive compression waves ahead of the shock.

RECENT PUBLICATIONS

A. Diaw, M.S. Murillo, "Generalized hydrodynamics model for strongly coupled plasmas," *Phys. Rev. E* 93, 069904 (2016).

L.G. Stanton, M.S. Murillo, "Ionic transport in high-energy-density matter," *Phys. Rev. E* 93, 043203 (2016).

M. Lyon, S.D. Bergeson, M.S. Murillo, "Strongly coupled plasmas formed from laser-heated solids," *Scientific Reports* 5, 15693 (2015).

L.G. Stanton, M.S. Murillo, "Unified description of linear screening in dense plasmas," *Phys. Rev. E* 91, 033104 (2015).

M. Lyon, S.D. Bergeson, M.S. Murillo, "Using higher ionization states to increase Coulomb coupling in an ultracold neutral plasma," *Phys. Rev. E* 91, 033101 (2015).

T. Ott, M. Bonitz, L.G. Stanton, M.S. Murillo, "Coupling strength in Coulomb and Yukawa one-component plasmas," *Phys. Plasmas* 22, 19901 (2015).

F.R. Graziani, J.D. Bauer,d M.S. Murillo, "Kinetic theory molecular dynamics and hot dense matter: Theoretical foundations," *Phys. Rev. E* 90, 033104 (2014).

L.N. Murillo, M.S. Murillo, A.S. Perelson, "Towards multiscale modeling of influenza infection," *J. Theor. Biology* 332, 267 (2013).