



27TH ANNUAL JAMES F. BELL MEMORIAL LECTURE IN CONTINUUM MECHANICS

Thursday, October 28, 2021 | 3:00 pm on Zoom

In-person viewing held in Malone G33/35 (open to first 50 people)

[REGISTRATION LINK](#)

“NUMERICAL SIMULATIONS OF ENTANGLED POLYMER MELTS: FROM SEGMENTAL DYNAMICS TO VISCOELASTIC RESPONSE”

PRESENTED BY GARY S. GREST | SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, NM

From the first numerical simulations of single polymer chains in dilute solution to current exascale simulations of highly entangled polymer melts, computer simulations have played a critical role in polymer physics. Numerical simulations have provided microscopic insight into macroscopic behavior. Here the potential of computations to polymer physics in the realm of new computer architectures will be introduced in view of the fundamental insight connecting theory and experiments attained thus far. Capturing the wide range of coupled length and time scales that govern the unique macroscopic, viscoelastic behavior of polymers has been one of the major challenges to surmount. Starting with the simple bead-spring models, through atomistically inspired coarse-grained approaches, it is now possible to capture not only chain mobility but also the mechanic response of entangled polymers melts and suspensions. With current and future computational resources, numerical simulations provide a unique understanding of viscoelastic response and shear and extensional flow of entangled melts for complex architectures bridging the dynamics on the atomic length scale with the macroscopic response.



GARY GREST is a computational physicist at Sandia National Laboratories. He was awarded a B.Sc in physics (1971), an M.S in physics (1973) and a Ph.D in physics (1974) by the Louisiana State University. His interest is the theory and simulation of nanoscale phenomena. Since 1998 he has been a member of the technical staff of Sandia Laboratories, since 2009 an Adjunct Professor in Department of Chemistry, Clemson University and since 2013 a Distinguished Sandia National Laboratories Professor in the Department of Chemical and Biological Engineering, University of New Mexico. He was elected a Fellow of the American Physical Society in 1989 "for contributions to the understanding of the kinetics of domain growth, amorphous glasses, disordered magnets, and polymer dynamics". He was elected to the National Academy of Engineering in 2008. He received the Aneesur Rahman Prize for Computational Physics from the American Physical Society in 2008 for his work in computational physics and the American Physical Society Polymer Physics Prize in 2011.