DR. JUAN MEZA

DIRECTOR, NSF DIVISION OF MATHEMATICAL SCIENCES
PROFESSOR, DEPT OF APPLIED MATHEMATICS,
UNIVERSITY OF CALIFORNIA-MERCED

DISTINGUISHED COLLOQUIA TALK

A TRUST-REGION DIRECT CONSTRAINED OPTIMIZATION METHOD FOR SOLVING THE KOHN-SHAM EQUATIONS

With the advance of new mathematical algorithms and supercomputers, we can now study many thousand-atom systems, with applications including the study of solar cells for renewable energy, biomedical imaging, and the design of novel materials. One of the most widely used techniques in computational chemistry and material simulations is based on Density functional theory (DFT). Using DFT codes, one can calculate many properties including the electronic structure, the charge density, and the total energy of an electronic system. At the heart of many of these codes, one typically finds a Self Consistent Field (SCF) iteration for solving the resulting Kohn-Sham DFT equations. In this talk, I will discuss an alternative approach based on an optimization method that minimizes the Kohn-Sham total energy directly. I will also discuss several acceleration and globalization techniques to improve convergence of the overall method. Numerical experiments demonstrate that the combination of these approaches is more efficient and robust than SCF alone, which can be shown to fail in certain cases.

FRIDAY, MARCH 29

1:00 pm - 2:00 pm

Room: EMAGC 1.302 / BLHSB 1.312

ZOOM: HTTPS://UTRGV.ZOOM.US/J/521329985

NSF

UTRGV
SCHOOL OF
MATHEMATICAL
& STATISTICAL
SCIENCES

STEM