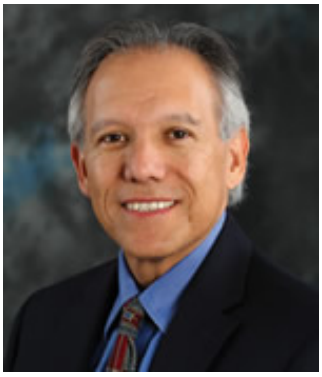
School of Natural Sciences Applied Math Seminar Series

UCMERCED

Derivative-free Optimization Methods for a Surface Structure Determination Problem



By Juan Meza
Dean of the School of Natural Sciences
University of California, Merced

Date:

Friday,

10/07/16

Time:

3:00 pm

Location:

SSB 120

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Abstract:

Many material and electronic properties of systems depend on the atomic configuration at the surface. This problem can be viewed as a mixed variable optimization problem for the chemical identity of the atoms as well as their spatial coordinates. One common technique used for determining surface structures is based on solving an inverse problem to match some known data. An example arises in the determination of nanostructures where a technique known as low energy electron diffraction (LEED) method is used. We will describe the use of pattern search methods and simplified physics surrogates for determining the surface structure of nanosystems. The pattern search methods have the property of being able to handle both continuous and categorical variables, which allows the simultaneous optimization of the atomic coordinates as well as the chemical identity.

Bio:

Juan Meza is the current Dean of the School of Natural Sciences and studied at Rice University — earning bachelor's and master's degrees in electrical engineering and a Ph.D. in computational and applied mathematics — and formerly worked at Lawrence Berkeley National Laboratory (LBNL) as head of the High Performance Computing Research Department and acting director of the Computational Research Division.

At LBNL, Meza helped grow research funding levels and established collaborations with the lab's earth sciences, environmental energy technologies, physics and genomics divisions.

Meza's own research interests include applied mathematics and computer science with an eye toward computational research, including nonlinear optimization and parallel computing methods. He has also done work on a variety of other scientific applications, such as scalable methods for nanoscience, power grid reliability, molecular conformation problems, optimal design of chemical vapor deposition furnaces, and semiconductor device modeling.

He was drawn to UC Merced by the interdisciplinary spirit of its research — something that has been a hallmark of his own research career — and its inherent diversity.

Education:

1986 Ph.D., M.S., Rice University, Computational and Applied Mathematics 1979 M.S., Rice University, Electrical Engineering/Computer Science 1978 B.S., Rice University, Electrical Engineering/Computer Science