מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Faculty of Mathematics and Computer Science
The Weizmann Institute of Science

Distinguished Lecturer Series

Sponsored by the Arthur and Rochelle Belfer
Institute of Mathematics and Computer Science

Professor Yannis G. Kevrekidis

Department of Chemical Engineering
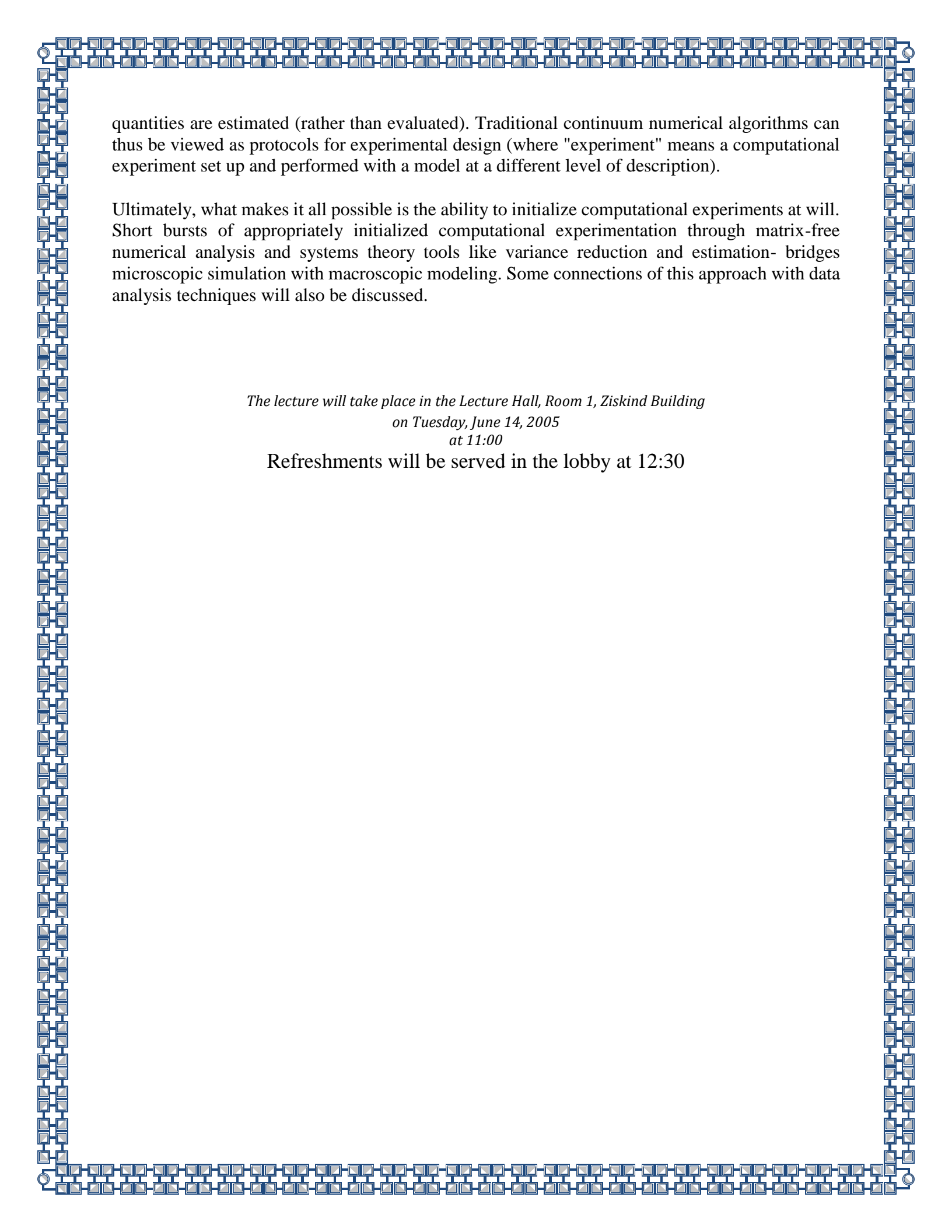*Princeton University*

will speak on

Equation-free Modeling for Complex/Multiscale Systems

Abstract

In current modeling, the best available descriptions of a system often come at a fine level (atomistic, stochastic, microscopic, individual-based) while the questions asked and the tasks required by the modeler (prediction, parametric analysis, optimization and control) are at a much coarser, averaged, macroscopic level. Traditional modeling approaches start by first deriving macroscopic evolution equations from the microscopic models, and then bringing our arsenal of mathematical and algorithmic tools to bear on these macroscopic descriptions.

Over the last few years, and with several collaborators, we have developed and validated a mathematically inspired, computational enabling technology that allows the modeler to perform macroscopic tasks acting on the microscopic models directly. We call this the "equation-free" approach, since it circumvents the step of obtaining accurate macroscopic descriptions.

We will argue that the backbone of this approach is the design of (computational) experiments. In traditional numerical analysis, the main code "pings" a sub routine containing the model, and uses the returned information (time derivatives, function evaluations, functional derivatives) to perform computer-assisted analysis. In our approach the same main code "pings" a subroutine that sets up a short ensemble of appropriately initialized computational experiments from which the same

quantities are estimated (rather than evaluated). Traditional continuum numerical algorithms can thus be viewed as protocols for experimental design (where "experiment" means a computational experiment set up and performed with a model at a different level of description).

Ultimately, what makes it all possible is the ability to initialize computational experiments at will. Short bursts of appropriately initialized computational experimentation through matrix-free numerical analysis and systems theory tools like variance reduction and estimation- bridges microscopic simulation with macroscopic modeling. Some connections of this approach with data analysis techniques will also be discussed.

The lecture will take place in the Lecture Hall, Room 1, Ziskind Building
on Tuesday, June 14, 2005
at 11:00
Refreshments will be served in the lobby at 12:30