ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ

ΔΙΑΤΜΗΜΑΤΙΚΟ ΠΡΟΓΡΑΜΜΑ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ

"Υπολογιστική Μηχανική"

ΣΕΜΙΝΑΡΙΟ

Dimension Reduction Methods for Nonlinear Multiscale Problems

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Abstract: Detailed modeling of complex physical and biological processes often leads to large systems of nonlinear Ordinary Differential Equations (ODEs) whose dynamics is spread over a broad range of timescales. Multiscale reduction methods exploit such timescale disparities by obtaining simplified descriptions of the system under investigation, which capture the eventual dynamics. In this manner, numerical stiffness may be removed and simulation times radically decreased, paving the way to the efficient simulation of many complex systems. In this talk, I will review some of the better-known nonlinear reduction methods. I will start from the classic Quasi-Steady State Assumption (QSSA), end with my own work on the Zero-derivative Principle (ZDP) and span nearly a century of work in at least four different disciplines. The first challenge facing the applied mathematician is to develop a common analytical framework for these methods. The second challenge is to quantify their approximation properties when applied to realistic problems. The talk will conclude with the insight gleaned from particular application to biochemical pathways. Such an application on a moderately large phosphorylation model will be employed to introduce the need for critical use of QSSA for large biochemical networks. I will finish with the presentation of certain guidelines for the selection of QSSA variables for such networks where insight is de facto limited.

> **Πέμπτη, 18/10/2012, ώρα 1:00 μμ** Αίθουσα "Κουμούτσου" Σχολής Χημικών Μηχανικών