

Lecture from SKIPER College

Speaker: Prof. Christodoulos A. Floudas

NAE member,

Stephen C. Macaleer '63 Professor

in Engineering and Applied Science,

Professor of Chemical and

Biological Engineering



Presided by Prof. Xiao Xin

Place: Meeting Room 312, IPE mansion

Language: English

Brief Introduction:

Prof. Christodoulos A. Floudas' research interests are in the area of Chemical Process Systems Engineering and lie at the interface of chemical engineering, applied mathematics, and operations research, with principal areas of focus including chemical process synthesis and design, process control and operations, discrete-continuous nonlinear optimization, local and global optimization, bioinformatics, computational genomics, computational chemistry and molecular biology. He was selected to the National Academy of Engineering (NAE) on Feb 8, 2011

For more information see <http://titan.princeton.edu>

Report 1

Time: 10:20 – 11:40(am), Apr 12, 2011(Tuesday)

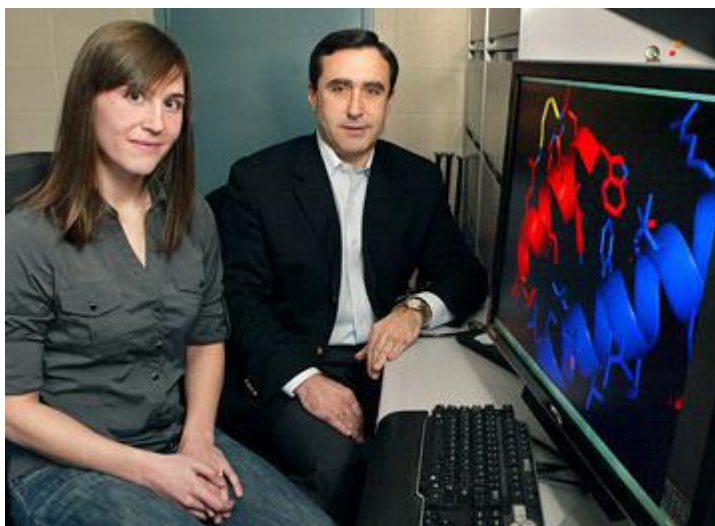
Title: Towards Large Scale Deterministic Global Optimization

Abstract

In this presentation, we will provide an overview of the research progress in global optimization. The focus will be on important contributions during the last five years, and will provide a perspective for future research opportunities. The overview will cover the areas of (a) twice continuously differentiable constrained nonlinear optimization, and (b) mixed-integer nonlinear optimization models. Subsequently, we will present our recent fundamental advances in (i) convex envelope results for multi-linear functions, (ii) a piecewise quadratic convex underestimator for twice continuously differentiable functions, (iii) piecewise linear relaxations of bilinear functions, (iv) large scale extended pooling problems, and (v) large scale generalized pooling problems. Computational studies on medium and large scale global optimization applications will illustrate the potential of these advances.

Application Example

Global Optimization has wide applications from molecule to system, from material to policy and from static to dynamic almost in all aspects of science and engineering. Prof. Floudas (right) and his Ph.D student Meghan Bellows-Peterson have innovated a new way based on global optimization to take some of the guesswork out of discovering new drugs. Using the technique, they have identified several potential drugs for fighting HIV. The image



reported as headline news on Princeton University home page shows a graphic of their drug candidate (red) attached to HIV (blue). (Photo by Frank Wojciechowski)

For detail:

<http://www.princeton.edu/main/news/archive/S29/66/70K88/index.xml?section-topstories>

Report 2

Time: 10:30 – 11:40(am), Apr 13, 2011(Wednesday)

**Title: Hybrid Biomass, Coal, and Natural Gas to Liquids
(CBGTL) Systems: Design, Simulation, and Supply
Chain Optimization**

Abstract

Heavy dependence on petroleum and high greenhouse gas (GHG) emissions from the production, distribution, and consumption of hydrocarbon fuels pose serious challenges for the United States (US) transportation sector. Depletion of domestic petroleum sources combined with a volatile global oil market prompt the need to discover alternative fuel-producing technologies that utilize domestically abundant sources. The primary aim in the discovery of hybrid energy processes is to combine coal, biomass, and natural gas to meet the United States transportation fuel demand.

The first part of this presentation will outline the needs and introduce novel coal, biomass, and natural gas to liquids (CBGTL) hybrid energy process alternatives which employ the reverse water-gas-shift reaction along with a non-carbon based source of hydrogen, and attain a near 100% conversion. Mathematical models for biomass and coal gasification are developed to model the nonequilibrium effluent conditions using a stoichiometry-based method. Steady-state process simulation results coupled with heat and power integration, and economic analysis determine the break-even price of crude oil (BEOP) and suggest that the CBGTL process is competitive with petroleum-based processes.

The second part will present a novel framework for the optimal energy supply chain of CBGTL processes. A mathematical model will be introduced that minimizes the total network cost while simultaneously evaluates the environmental performance through a life cycle analysis of each individual plant. The optimal network topology provides information on (i) the optimal plant locations throughout the country, (ii) the locations of feedstock sources, (iii) the interconnectivity between the feedstock source locations, CBGTL plants locations, and the demand locations, (iv) the modes of transportation used in each connection, and (v) the flow rate amounts of each feedstock and product type.