## 数学与系统科学研究院 计算数学所学术报告

报告人: Prof. Jinyun Yuan

( 巴西巴拉那联邦大学 )

报告题目:

Modeling and Optimization of an Ammonia Reactor using a Penalty-like Method

邀请人: 袁亚湘 院士

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计算数学所报告厅

## **Abstract**:

Ammonia is one of the most important chemicals produced in the world. Due to its broad applicability, modeling and simulation of process of Ammonia has received considerable attention among the industrial processes. Ammonia is produced from the reaction of hydrogen and nitrogen at high temperature and high pressure along with a catalyst. Its production depends on temperature of feed gas at the top of the reactor, the partial pressures of the reactants and the reactor length. The optimal design problem requires obtaining the optimal reactor length with maximum economic return subject to a number of equality constraints involving solution of coupled nonlinear differential equations. A more efficient algorithm for the solution of optimization-constrained differential equations is proposed by coupling numerical techniques (barrier function with a direct search method) with Runge-Kutta method. The global convergence of the proposed algorithm is established under some usual conditions. Numerical results showed that the resulting algorithm, based only on function values, is highly competitive with other global optimization methods.

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