TITLE: **Mathematically Reduced Chemical Reaction Mechanism Using Neural Networks**

AUTHORS: Nelson K. Butuk and Ken E. Johnson

INSTITUTION: Prairie View A & M University
Department of Mathematics
WR Banks Building Room 328
Prairie View, TX 77446-4189

PHONE NO.: 936-857-4021

FAX NO.: 936-857-2019

E-MAIL: n_Butuk@pvamu.edu

GRANT NO.: DE-FG26-03NT-41913

PERIOD OF PERFORMANCE: October, 2003 – September, 2006

DATE: March 24, 2005

ABSTRACT

Objectives

The aim of the project is to develop an efficient chemistry model for combustion simulations. The reduced chemistry model will be developed mathematically without the need of having extensive knowledge of the chemistry involved. To aid in the development of the model, Neural Networks (NN) will be used via a new network topology know as Non-linear Principal Components Analysis (NPCA).

Many Combustion systems are modeled by very high-dimensional systems of non-linear differential equations. These equations often exhibit solutions which are un-evenly distributed in phase-space, and which may exist as circles, tori or other manifolds. It is desirable to approximate these isolated regions of the phase-space by a mathematical model of lower dimension than the dimension of the original ambient space. NPCA accomplishes this task using NN.

Accomplishments To Date:

In a previous investigation, it was found that the NPCA developed was hard to train as well as slow in converging to the optimal solution. For this reason, the initial objectives of the project, was to develop ways and means of accelerating training and convergence of NPCA. The difficult in training is due to the fact that NN training is an ill-posed non-linear optimization problem and

as such has problems with local minima, slow convergence as well as stability with respect to errors in input data. To address these problems, we have looked that a fast training network architecture known as Generalized Regression Neural Networks (GRNN).

Among the different implementation of Neural Networks (NN), the network structure that posses the fastest training time, is the Generalized Regression Neural Networks (GRNN). Over the past year, we have studied this network with the aim of incorporating its desirable properties into our NPCA-NN data reduction algorithm. Our results so far including current investigations are promising. In the talk, a brief description of GRNN will be given as well as results of the actual implementation on a test problem and highlights of some of its advantages.

Our first step was to implement and thoroughly understand the GRNN. The algorithm to implement GRNN was written and implemented in MATLAB. In order to test the algorithm, we used the following non-linear function.

$$f(x_1, x_2, x_3) = 4x_1^2 + 2x_2^2 + x_3^2 - x_1x_2 + x_2x_3 - 5x_1 - 9x_2 + x_3$$

Promising results were obtained on the test function and work continues to adapt the GRNN to NPCA-NN.

Also accomplished during this period is the development of a simple Euler solver to be used to test the developed NPCA-NN mathematical model.

Future Work

The remaining tasks in this project include**:**

- Continue to develop an efficient training method for NPCA
- Implement Bagging method to generate training data
- Develop the NPCA model on real chemical reaction mechanism data
- Couple NPCA model to a CFD code. Code chosen is the popular KIVA combustion simulation code**.**

2. LIST OF PUBLICATIONS AND STUDENTS SUPPORTED

Publications

- Butuk, N. and Johnson, K., "Investigation of the Use of Kernel Smoothing Techniques in Dimension Reduction of Kinetic Chemical Reaction Mechanism Data," Hawaii International Conference on Statistics, Mathematics and Related Fields, January 9-11, 2005, Honolulu, Hawaii

Students Supported

- Ken Johnson, a graduate student in applied mathematics
- Owen Clark, an undergraduate senior.