A Newton-Krylov based Computational Fluid Dynamic (CFD) modeling tool is being developed for performing engineering calculations of turbulent reacting flows in which finite rate chemistry effects are important. The near term target applications are simulations of NOx emissions from industrial combustion systems.

The finite rate chemistry effects are modeled using reduced chemical kinetic mechanisms. Reduced mechanisms are noted for being able to faithfully reproduce the reactions of a detailed kinetic mechanism while tracking only a relatively small number of species. However, the disadvantage to using reduced mechanisms is the (sometimes) severe non-linearity and corresponding \textit{numerical stiffness} they induce in the governing equations.

The new tool employs a matrix free Newton-Krylov iteration scheme which is suitable for solving large scale systems containing severe non-linearity. A GMRES method is used to solve for the inexact Newton step. Experience has taught us that a pre-conditioner must be used in the linear solves within the GMRES method due to the stiffness problem. In our current research, an Algebraic Multi-Grid (AMG) solver has been integrated into the pre-conditioning calls of the Newton-Krylov solver. The AMG preconditioner uses a generalized method for agglomerating fine grid cells to create the coarse grid problem. Preliminary results have shown the improvement in the overall efficiency and robustness of the new solver.

In this presentation, we will describe the formulation for our Newton-Krylov solver with the AMG pre-conditioner. Performance of the new solver will be highlighted through NOx simulations for a simple, \textit{hotbox} furnace and a full scale coal fired electric utility boiler.
Acknowledgements: This work was performed under support from the National Science Foundation under SBIR Phase II grant no. DMI-0216590 (NSF Program Manager Dr. Errol Arkilic). The authors would like to thank Dr. Michael Pernice (Los Alamos National Laboratory) and Prof. J.-Y. Chen (U. of California-Berkeley) for their input and guidance in this work.