4D02: A DYNAMIC ADAPTIVE CHEMISTRY SCHEME FOR REACTIVE FLOW COMPUTATIONS.

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This paper is one of several at this Symposium and in the recent literature which demonstrate fast methods for reduction from very large chemistry models to skeletal models. These methods have a lot of promise in applications to multidimensional CFD models, and to design applications where zero-d or one-d models must be run repeatedly (e.g. HCCI engine design, or construction of flamelet libraries). We are now at the stage where we need clear benchmark cases and clear error/tolerance measures, so that different methods can be scientifically compared, and the community can learn which reduction technique should be used to meet desired error or model-size constraints. It is hoped that this benchmarking effort will also assist in the development of error control methods and rigorous error bounds which can be incorporated into future uncertainty quantification (UQ) schemes, to put error bars on model predictions.

Reply by Long Liang

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Similar to most of the other methodologies referred to by Professor Green, the DAC scheme controls the error of the reduced mechanisms by limiting the graph search depth using a threshold parameter. In the *n*-heptane HCCI cases shown in the paper, a smaller threshold value generally results in better accuracy but less extent of reduction. However, we do agree that a mathematically or physically more rigorous error control parameter will be highly desirable for easy comparison to the peers. Plus, a better defined error control parameter may allow adaptive adjustment of the threshold value at each reduction condition in the DAC framework, which may further improve the computational efficiency compared to using a fixed threshold value for all reduction conditions. Using the present error control parameter, the DAC scheme can participate in the benchmarking effort via either a comparison of reduced model sizes given an error constraint or a comparison of errors given a reduced model size constraint. But exploring for a better error control parameter will be a key to further improving the DAC method.