More Chemistry, Faster Computation in Models of Internal Combustion Engines

Scientists researching Homogeneous Charge Compression Ignition (HCCI) engines are turning to a new Range Identification and Optimization Tool (RIOT) to tackle this complex problem. RIOT is being developed at MIT as a part of the Collaboratory for Multi-scale Chemical Science (CMCS). HCCI offers the potential for high-efficiency low-emission power sources for transportation, but developing a detailed enough understanding of the ignition process to allow control of HCCI combustion has so far eluded the research community. The HCCI researchers, part of a university consortium sponsored by DOE Office of Transportation Technology, typically must compromise the complexity of the chemical models and divide the combustion chamber into only a few zones so that computational costs are not prohibitive.

The availability of RIOT through the CMCS web-portal attracted the HCCI scientists and engineers to this new way to compute such chemically complex problems. RIOT converts a highly detailed chemical model to many smaller ones, each reduced to just the size that needed by conditions in a particular spatial/temporal zone by eliminating reactions that are not needed for the desired accuracy. The smaller models can then be automatically translated to the required format using other CMCS portal features resulting in a simulation having more simulation zones, each with a controlled chemical accuracy, and higher computational efficiency,

The result is a current project with an HCCI scientist who is using Lawrence Livermore National Laboratory's reaction mechanism for iso-octane containing 857 species and 3606 reactions. It takes one week to run a five-zone simulation of an HCCI engine with this model. The results of the first RIOT application are now being validated, with the expectation that the computational efficiency will be improved by nearly a factor 10, while at the same time using a state-of-the-art model approximated with a known and controllable accuracy.