LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Development of the RIOT Web Service and Information Technologies to Enable Mechanism Reduction for HCCI Simulations

K. Schuchardt, O. Oluwole, W. J. Pitz, L.A. Rahn, W. H. Green, D. Leahy, C. Pancerella, M. Sjöberg, J. Dec

June 15, 2005

Disclaimer

Development of the RIOT Web Service and Information Technologies to Enable Mechanism Reduction for HCCI Simulations

Karen Schuchardt,[1] Oluwayemisi Oluwole,[2] William Pitz, [3] Larry A. Rahn,[4] William H. Green, Jr., [2] David Leahy,[4] Carmen Pancerella,[4] Magnus Sjöberg,[4] John Dec[4]

[1]Pacific Northwest National Laboratory, Richland, WA 99352, [2]Massachusetts Institute of Technology, Cambridge, MA 02139, [3]Lawrence Livermore National Laboratory, Livermore, CA 94551, [4]Sandia National Laboratories, Livermore, CA 94551

E-mail: pitz1@llnl.gov

Abstract. New approaches are being explored to facilitate multidisciplinary collaborative research of Homogenous Charge Compression Ignition (HCCI) combustion processes. In this paper, collaborative sharing of the Range Identification and Optimization Toolkit (RIOT) and related data and models is discussed. RIOT is a developmental approach to reduce the computational of detailed chemical kinetic mechanisms, enabling their use in modeling kinetically controlled combustion applications such as HCCI. These approaches are being developed and piloted as a part of the Collaboratory for Multiscale Chemical Sciences (CMCS) project. The capabilities of the RIOT code are shared through a portlet in the CMCS portal that allows easy specification and processing of RIOT inputs, remote execution of RIOT, tracking of data pedigree, and translation of RIOT outputs to a table view and to a commonly-used mechanism format.

1. Introduction

The urgent need for high-efficiency, low-emission energy utilization technologies for transportation, power generation, and manufacturing processes presents difficult challenges to the combustion research community. The needed predictive understanding requires systematic knowledge across the full range of physical scales involved in combustion processes – from the properties and interactions of individual molecules to the dynamics and products of turbulent multi-phase reacting flows. Innovative experimental techniques and computational approaches are revolutionizing the rate at which chemical science research can produce the new information necessary to advance our combustion knowledge. But the increased volume and complexity of this information often makes it even more difficult to derive the systems-level knowledge we need. Combustion researchers have responded by forming interdisciplinary communities intent on sharing information and coordinating research priorities. Such efforts face many barriers, however, including lack of data accessibility and interoperability, missing metadata and pedigree information, efficient approaches for sharing data and analysis tools, and the challenges of working together across geography, disciplines, and a very diverse spectrum of applications and funding.

This challenge is especially difficult for those developing, sharing and/or using detailed chemical models of combustion to treat the oxidation of practical fuels. This is a very complex problem, and the development of new chemistry models requires a series of steps that involve acquiring and keeping track of a large amount of data and its pedigree. Also, this data is developed using a diverse range of codes and experiments spanning *ab initio* chemistry codes, laboratory kinetics and flame experiments, all the way to reacting flow simulations on massively parallel computers. Each of these processes typically requires different data formats, and often the data and/or analysis codes are only accessible by personally contacting the creator. Chemical models are usually shared in a legacy file format, such as Chemkin [1], often without needed metadata and pedigree information. Detailed reaction

mechanisms [2] are usually too large for efficient operation of chemical reacting flow solvers so there is also much work aimed at reducing number of species and reactions in a fashion consistent with the accuracy needs of the simulation. In the best of cases, this results in a proliferation of diverse models that are difficult to find or trace to their origins.

The Collaboratory for Multi-scale Chemical Science (CMCS) is using advanced collaboration and metadata-based data management concepts and technologies to develop an open source multi-scale informatics toolkit serving as the basis for a CMCS web portal. The portal enables cross-scale data discovery, viewing, comparison, transformation and exchange while facilitating community formation, communication, and data development. The portal also includes tools for browsing cross-scale data dependencies and mechanisms to integrate custom and community resources into active research projects. Of particular interest here, is that the CMCS team is developing new approaches that facilitate collaborative sharing of chemical model data and analysis codes. In this paper, we will briefly describe the relevant CMCS infrastructure and tools in the context of an ongoing collaboration motivated by the desire to understand and control Homogenous Charge Compression Ignition (HCCI) in internal combustion engines. We focus here on the Range Identification and Optimization Tool (RIOT). RIOT is a software tool designed to reduce the number of reactions in a reaction mechanism to just those needed to maintain a specified chemical accuracy in the predictions of the resulting reduced mechanism [3,4]. The approach for the ultimate use of such reduced models in HCCI research will also be briefly described.

2. HCCI Combustion Challenge

Homogeneous charge, compression ignition is a piston-engine combustion process that has emerged as a high-efficiency alternative to traditional spark-ignition (SI) combustion and a low-emissions alternative to traditional diesel combustion. It offers good fuel economy, similar to a diesel engine, while producing very low emissions of NO_X and soot particulate matter (PM). However, before HCCI can be implemented in production engines, several technical barriers must be overcome. Research and development are being pursued in a number of areas, including: control of ignition timing over the load/speed map, slowing the heat-release rate at higher loads, controlling hydrocarbon (HC) and carbon monoxide (CO) emissions, maintaining combustion stability, cold starting, and response to load and speed transients.

Computer modeling of the in-cylinder processes in an HCCI engine is a key element in this research and development effort. Modeling methodologies for HCCI range from adiabatic single-zone models [5] to integrated multi-dimensional CFD/kinetics engine models [6]. Due to the nature of HCCI, the ignition, combustion heat-release, and pollutant formation processes are much more highly coupled to the chemical-kinetics of the charge mixture than they are for traditional SI or diesel combustion. Therefore, the usefulness of HCCI modeling results relies heavily on the accuracy of the chemical-kinetics mechanism employed and its ability to match the behavior of the specific fuel in use. For a limited number of reference fuels, detailed chemical mechanisms have been developed [3,7]. These mechanisms often contain many hundreds of species and thousands of reactions, and have provided useful understanding of the in-cylinder processes [6]. Yet, even these detailed mechanisms sometimes fail to describe important changes to the autoignition with changes in engine operation conditions [5]. Thus, there is a strong need for improvement and further development of these detailed chemical kinetics mechanisms.

Such detailed chemical kinetics models are complex however, and their direct implementation in CFD codes can result in computational times that are impractical. Not only are improved kinetic mechanisms needed, but also new approaches to their implementation in CFD that maintain accuracy while increasing computational efficiency. Such an approach would substantially improve our ability to simulate HCCI combustion, and therefore, provide a valuable component in overcoming the technical barriers to HCCI.

3. Enabling HCCI Science With New Tools and Approaches

A more efficient combination of multi-dimensional CFD and chemical-kinetics modeling is required to facilitate research, for example, on the effects of non-uniformities in the charge mixture and temperature in HCCI. We are exploring, therefore, the adaptation of detailed mechanisms to specific conditions or sub-problems to enable their reduction to a more tractable size without sacrificing the ability to capture the important chemistry of the conditions studied. Individual zones in a combustion chamber experience a smaller range of conditions than the entire combustion chamber as illustrated in Fig. 1 depicting the computational domain for an HCCI simulation. The idea is to then reduce the model to a much less complex, but different, version that is still accurate over each zone to which it is applied.

However, kinetic model reduction is normally a complex and slow process, resulting in models that may not be applicable across the full range of conditions in the process being studied. This approach embarks on a new paradigm in which many specified model reductions are rapidly computed, with specified accuracy, for sub-problems that encompass a smaller range of conditions. The approach requires access to new, developmental, tools and ways for researchers to manage and efficiently use the resulting proliferation of model data and metadata. These researchers are collaborating from multiple disciplines and locations, and must be able to work together efficiently with developmental tools and evolving data.
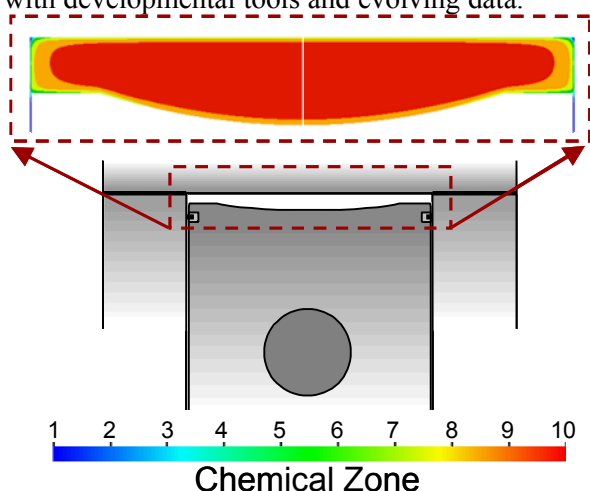

Figure 1: An expanded view of a model HCCI engine combustion chamber divided up into zones (indicated by color) so that each can be assigned a different chemical model by the Range Identification and Optimization Toolkit. (Figure courtesy D. L. Flowers, LLNL)

3.1 Collaborative Research Environment

CMCS is developing open-sourced software called KnECS (Knowledge Environment for Collaborative Science) that offers many features to meet the challenge of tracking large amounts of data and its pedigree while fostering data sharing and development. KnECS is a multi-scale informatics toolkit that addresses issues related to knowledge sharing. The KnECS toolkit has a multi-layer architecture including a web portal interface and underlying services that together provide rich group-level collaboration capabilities, data/metadata organization and management capabilities, data annotation and multiple interfaces for integrating third-party capabilities such as domain specific data viewers and analysis tools, data translators, and experimental or computational data sources. The portal engine is based on CompreHensive collaborativE Framework (CHEF) [8] which uses Apache Jetspeed [9], but has been modified to meet CMCS requirements. Many of the software features are enabled by the KnECS data infrastructure which is provided through integration with the Scientific Annotation Middleware (SAM) software [10]. More about the vision of CMCS and its informatics infrastructure can be found in a recent paper [11] and on the CMCS web site (cmcs.org).

KnECS supports the integration of scientific applications through portlet interfaces that access scientific codes through web services. Examples include Active Thermochemical Tables (ATcT) [12] and RIOT [4] with others planned. CMCS is also developing tools centered around community data sharing and curration processes. Desktop applications can also directly access the KnECS

infrastructure using the Data Service Interface (DSI) library that provides a Java interface to the data middleware. Finally, non-CMCS desktop applications can access data using WebDAV-enabled clients available with or for many operating systems [13].

3.2 RIOT Software

RIOT (Range Identification and Optimization Toolkit) is a software tool that is being developed to allow reduction of the number of species and/or reactions in a reaction mechanism while maintaining user specified tolerances on the accuracy of the reduced mechanism [3,4]. The basic idea is to reduce the model without significantly changing predicted values such as temperature, pressure and species concentrations from the values predicted by using the full model. The computational gain realized by using the reduced model is proportional to the extent of the reduction. Therefore, maximum speedup can be obtained by using optimally-reduced models. CMCS has integrated the RIOT model reduction code into its portal environment by developing a portlet interface that assists the user with specifying inputs to the RIOT code, generates the input file, ships the request to a web service interface to the code, and uploads and presents the results when the reduction completes. We will now describe how this capability can be used through a practical example being worked on by participating CMCS scientists.

3.3 Using the RIOT Portal to Reduce a Mechanism

The RIOT program requires several input files to perform the mechanism reduction. These files include a detailed chemical kinetic mechanism file, a thermodynamics data file and one or more solution files. The first two files are assumed to be in Chemkin format [1]. The solution files contain histories of pressure, temperature, and species concentrations. For HCCI, this would likely be computed histories from a simulation of an HCCI ignition in an engine. In addition to a solution file format specified by RIOT, the portal accepts both Senkin and Aurora [1] solution files from their post processors to provide these histories. The portlet automatically recognizes the file formats (MIME type) if the filenames end with the extension ".senkin-export" or ".aurora-export". This is an example of where we take advantage of the portal capability of recognizing file MIME types and enabling data translations. To support additional file formats, new translators can be written and registered with the CMCS infrastructure. Without changes to the RIOT portlet itself, these new formats will automatically be recognized by the RIOT portlet.

Once the user has assembled the required files, the user uploads them to the portal using the Data Browser portlet. This portlet is the CMCS data and metadata browsing tool providing a full set of basic content management operations including file upload, copy, move, and delete, and the creation of hierarchical directory structures [11]. The portal recognizes the reaction mechanism file and the thermodynamic data file based on their MIME-types (".mech" and ".therm" respectively). Translations to CMCS standard XML-based formats are automatically available to the user enabling further translations through XSLT scripts; one such example is a table view of a mechanism. The user then accesses the RIOT portlet and specifies the set of files to be used for the reduction. One or more solution files can be specified. Multiple solution files may be needed to cover a broad range of conditions (pressure, temperature, fuel composition, equivalence ratio and exhaust gas recirculation) for HCCI.

In the RIOT portlet, the user selects the solution points to be used to reduce the model and specifies the tolerances that affect the accuracy of the model. The user selects the points that have the critical temperatures and pressures where the reduced mechanism should be valid. A "Model Reduction Parameters" button provides access to a portlet page where parameters for which the reduced model should be accurate are specified including tolerance in temperature, species concentrations, and even which reactions should never be removed. The user then presses a "submit" button to reduce the mechanism. The mechanism and all required inputs are sent via an asynchronous web-based service to a server at MIT where the mechanism reduction is performed. When the calculation is finished, an XML-based reduced mechanism file is returned to the CMCS data store where it is available in the

RIOT portlet. When the entire process completes, the user receives an email notification with a link that leads directly to the file in the portal. The XML-formatted results file allows easy XSLT-based automatic conversion to a table view or to a Chemkin formatted file for use with desired reacting flow calculations. As described above for input files, additional translation scripts can be written and registered with CMCS. For example, translation to other reacting-flow code mechanism formats can be added.

Another illustration of the capabilities of CMCS is its ability to follow the pedigree of the data. The portal provides a graph that allows a user to track the pedigree of the reduced model. The user can trace the reduced model back to the detailed model and the specified conditions that were used to create it. It is part of the CMCS vision that users will be able to follow the pedigree of the data without having to contact other scientists who created the data. This feature should help to reduce the time it takes for scientists to understand where data came from and what its limitations are.

4. Conclusion and Acknowledgments

The best reduced model that has been obtained by RIOT for the HCCI problem contains 660 reactions versus 3606 in the full model for the fuel iso-octane. With this reduced model, we have obtained HCCI ignitions that reproduce full model results to within 1.5 crank angle degrees and speed-up the calculations by a factor greater than 6. This accuracy is sufficient for many HCCI engine applications. We plan to continue to test the RIOT reduction software for the HCCI applications.

5. References

[1]   Kee, R. J., Rupley, F.M., Miller, J.A., Coltrin, M.E., Grcar, J.F., Meeks, E., Moffat, H.K., Lutz, A.E., Dixon-Lewis, G., Smooke, M.D., Warnatz, J., Evans, G.H., Larson, R.S., Mitchell, R.E., Petzold, L.R., Reynolds, W.C., Caracotsios, M., Stewart, W.E., Glarborg, P., Wang, C., Adigun, O., Houf, W.G., Chou, C.P., Miller, S.F. Chemkin Collection, 3.7.1, Reaction Design, Inc., San Diego, CA, 2003.

[2]   Pitz, W. J., Westbrook, C. K. and Curran, H. J. LLNL Chemical Kinetic Mechanisms, 2004.

[3]   Bhattacharjee, B., Schwer, D. A., Barton, P. I. and Green, W. H., Combust. Flame 135(3):191-208 (2003).

[4]   Olumwole, O. O., Bhattacharjee, B., Tolsma, J. E., Barton, P. I. and William H. Green, J., "Rigorous Valid Ranges for Optimally-Reduced Kinetic Models", Combust. Flame, submitted, 2005.

[5]   Dec, J. E. and Sjöberg, M., Isolating the Effects of Fuel Chemistry on Combustion Phasing in an HCCI Engine and the Potential of Fuel Stratification for Ignition Control, SAE Paper 2004-01-0557 (2004).

[6]   Aceves, S. M., Flowers, D. L., Espinosa-Loza, F., Martinez-Frias, J., Dec, J. E., Sjöberg, M., R.W. and Hessel, R. P., Spatial Analysis of Emissions Sources for HCCI Combustion at Low Loads Using a Multi-Zone Model, SAE Paper 2004-01-1910, (2004).

[7]   Curran, H. J., Gaffuri, P., Pitz, W. J. and Westbrook, C. K., Combust. Flame 129:253-280 (2002).

[8]   CHEF, Collaborative Portal Framework Website, CHEF Collaborative Portal Framework Website, http://www.chefproject.org/, University of Michigan, University of Michigan,

(2004).

[9]   Jetspeed, an Open Source implementation of an Enterprise Information Portal, using Java and XML, Apache Jakarta Project, http://jakarta.apache.org/jetspeed/site/, (2003).

[10]   Myers, J. D., Chappell, A., M., E., A., G. and Schwidder, J., IEEE Computing in Science and Engineering 5(3):44-50 (2003).

[11]   Myers, J. D., Allison, T. C., Bittner, S., Didier, B., Frenklach, M., William H. Green, J., Ho, Y.-L., Hewson, J., Koegler, W., Lansing, C., Leahy, D., Lee, M., McCoy, R., Minkoff, M., Nijsure, S., Laszewski, G. v., Montoya, D., Pancerella, C., Pinzon, R., Pitz, W., Rahn, L. A., Ruscic, B., Schuchardt, K., Stephan, E., Wagner, A., Windus, T. and Yang, C., "A Collaborative Informatics Infrastructure for Multi-scale Science," Challenges of Large Applications in Distributed Environments (CLADE 04), Honolulu, Hawaii, 2004, p. 24, http://csdl.computer.org/comp/proceedings/clade/2004/2115/00/2115toc.htm.

[12]   Ruscic, B., Pinzon, R. E., Morton, M. L., von Laszevski, G., Bittner, S. J., Nijsure, S. G., Amin, K. A., Minkoff, M. and Wagner, A. F., J. Phys. Chem. A 108(45):9979-9997 (2004).

[13]   WebDrive http://www.webdrive.com/, South River Technologies: 2004.