Final Technical Report
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Collaboratory for Multiscale Chemical Science (CMCS)
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The involvement of NIST in the CMCS project centered around its leadership in chemical data. In particular, the contents of the NIST Chemical Kinetics Database were of particular interest due to its relevance in the CMCS pilot project that was focused on combustion problems. Contributions from NIST included

- developed a database of chemical identifiers for compounds of interest in the CMCS pilot project on combustion (PrIMe)
- developed a SOAP-based system for looking up chemical names, chemical formulas, and CAS registry numbers and returning these to the CMCS software
- developed XML Schema in support of the PrIMe pilot project
- created XML data files to support the PrIMe pilot project from the NIST Chemical Kinetics Database
- created data entry software in support of the PrIMe pilot project
- made other contributions to the CMCS software infrastructure

A peer-reviewed publication was produced as part of the funded work:

“A Collaborative Informatics Infrastructure for Multi-Scale Science,” J. D. Myers, T. C. Allison, S. Bittner, B. Didier, M. Frenklach, W. H. Green Jr., Y.-L. Ho, J. Hewson, W. Koegler, C. Lansing, D. Leahy, M. Lee, R. McCoy, M. Minkoff, S. Nijsure, G. von Laszewski, D. Montoya, L. Oluwole, C. Pancerella, R. Pinzon, W. Pitz, L. A. Rahn, B. Ruscic, K. Schuchardt, E. Stephan, A. Wagner, T. Windus, and C. Yang, *Cluster Computing*, 2005, 8, 243–253.