



## **CYCLE DE CONFÉRENCES DE CHIMIE**

*Avec le concours de : Manufacture Française des Pneumatiques MICHELIN  
Ecole Nationale Supérieure de Chimie de Clermont-Ferrand  
Institut de Chimie de Clermont-Ferrand (ICCF UMR 6296)  
U.F.R.S.T. / Master de Chimie / Département de Chimie*

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**Jeudi 22 Mars 2012 à 16 h**

**Amphi de Chimie Paul REMI - (Site des Cézeaux)**

**MICHAEL FRENKEL**

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### **GLOBAL INFORMATION SYSTEMS IN SCIENCE: APPLICATION TO THE FIELD OF THERMODYNAMICS**

Global Information Systems can be defined as information systems designed to collect, process, integrate, evaluate, and communicate the entire “body of knowledge” pertaining to a field and to support any application requiring this knowledge in an “on-demand” mode with definitive information quality assessments. Recent advances in computer hardware technology, development of relational data management systems capable of reliably supporting storage of enormous amounts of information pertaining to specific areas of science, new interoperable means of standardizing data communications based on the Extensible Markup Language (XML) ontologies, new generation software expert systems, and secure on-line networks have created unprecedented opportunities for defining and implementing a new paradigm of Global Information Systems in Science. Global Information Systems have a profound impact on the scientific discovery process, industrial development, and knowledge communication.

Within the last 10 years, one of the first Global Information Systems in Science has been developed for the field of Thermodynamics (ThermoGlobe) at the Thermodynamics Research Center (TRC) of the U. S. National Institute of Standards and Technology (NIST). The components of this system include software tools for mass-scale data capture (Guided Data Capture Software), a comprehensive data storage facility (SOURCE Data Archival System), the NIST/TRC Data Entry Facility, a data communication standard (ThermoML – IUPAC standard for thermodynamic data communications), data “reader” software (ThermoML opener into Microsoft Excel), expert system software (NIST ThermoData Engine), and a Web communication portal (NIST Web-Oracle data dissemination channel). The role and principle structure of all the components will be discussed with the emphasis on the profound impact of the ThermoGlobe implementation on various areas of research and engineering including, but not limited to, efficiency of information delivery, journal publication quality, and chemical process design.

Technology of the TDE (NIST ThermoData Engine), one of the critical elements of the ThermoGlobe system, is incorporated into online software to aid the process of experimental planning for property measurements (ThermoPlan). This software is to be used by experimentalists through open domain free Web access worldwide. The capabilities of the ThermoPlan will be demonstrated.

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