Process Informatics Model (PrIMe)

Applications to Combustion Chemistry

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GCEP

Meeting the Challenge of Reducing Global GHG Emissions Through Energy Research

- **Policymaker to PrIMe:** *How much longer will there be an Antarctic ozone hole?*
- **PrIMe to Policymaker:** *50 to 150 years.*
- **Policymaker to PrIMe:** *Can I get the answer more accurately, within at worst a 5 year interval, and what would it take?*
- **PrIMe to Policymaker:** *The result is the best current estimate based on all available data and scientific community consensus. To get to the requested level of certainty the heat of formation of Cl_2O_2 has to be known to within 1 kJ/mol and the rate coefficient for the reaction between two ClO radicals to within 10%.*
- **Policymaker to Chemists (via funding agency):** *Please (re)measure/(re)calculate the heat of formation of Cl_2O_2 and the rate coefficient for the reaction between two ClO radicals to the above accuracy.*

- **Engineer to PrIMe:** *What fueling rate produces peak output power while holding NOx yields within the EPA prescribed limits in a HCCI engine running GTL prescribed fuel #22 with the following design and operating parameters: xx,yy, …*

- **PrIMe to Engineer:** *How well do you want to know this?*

- **Engineer to PrIMe:** *I need 5% accuracy!*

- **PrIMe to Engineer:** *This accuracy is not achievable. The uncertainty range on the fueling rate runs from 1.22 to 1.35 g/s.*

- **Engineer to PrIMe:** *What is the dominant source of this uncertainty?*

- **PrIMe to Engineer:** *80% of the uncertainty is caused by the uncertainty in the estimated rate constant for the reaction $(CH_3)_2CCHCH_2+O_2 \rightarrow (CH_3)_2CCCH_2 + HO_2$. There are no literature data on this reaction, only indirect estimates. The needed data can be obtained via quantum chemistry calculations (time 2 days, cost $$) or by experiments (time 2 years, cost $$$$); what is your choice?*

- **Engineer to PrIMe:** *The quantum chemistry calculations right away and start experiments as well.*

- **PrIMe to Engineer (2 days later):** *Optimal fueling rate needed is 1.31 g/s, based on computed rate constant of 5E9 cc/mol s. Uncertainty range is 1.29 – 1.33 g/s.*

- **PrIMe to Chemists:** *Perform measurements to determine the rate constant for the reaction $(CH_3)_2CCHCH_2+O_2 \rightarrow (CH_3)_2CCCH_2 + HO_2$.*

PrIMe Goal

- Create *infrastructure and tools* for the development of predictive reaction models of *combustion*
  - by extracting *all possible information* from all available data, and converting this knowledge into predictive models
  - by establishing and demonstrating a *community approach* to kinetic-model development and most importantly, establishing a means for reaching community consensus on the models and data

Motivation for PrIMe

- Chemical models can be a vital ingredient in optimizing industrial processes
- Reduction in the elapsed time to obtain solutions to science/engineering problems
- Converting model building into science rather than “art”
- A formal framework for making resource allocation decisions

History

- PrIMe: Collaborative effort; Stanford; UC Berkeley; MIT; NIST; Sandia; and Leeds University, UK.
- Informal meeting in Sapporo 2002
- Presentation to DOE contractor's meeting 2003
  - Sandia CMCS (Colaboratory for Multiscale Chemical Science) project adopts PrIMe as a main task
- Presentations at "Real Fuels" Workshop at NIST
  - NIST becomes "home" for PrIMe
- Presentation at ACS Meeting 2004
- Large scale Multi-Institution support (Stanford; UC Berkeley; MIT) being sought from NSF 2005
- Discussions at DOE contractor's meeting 2005

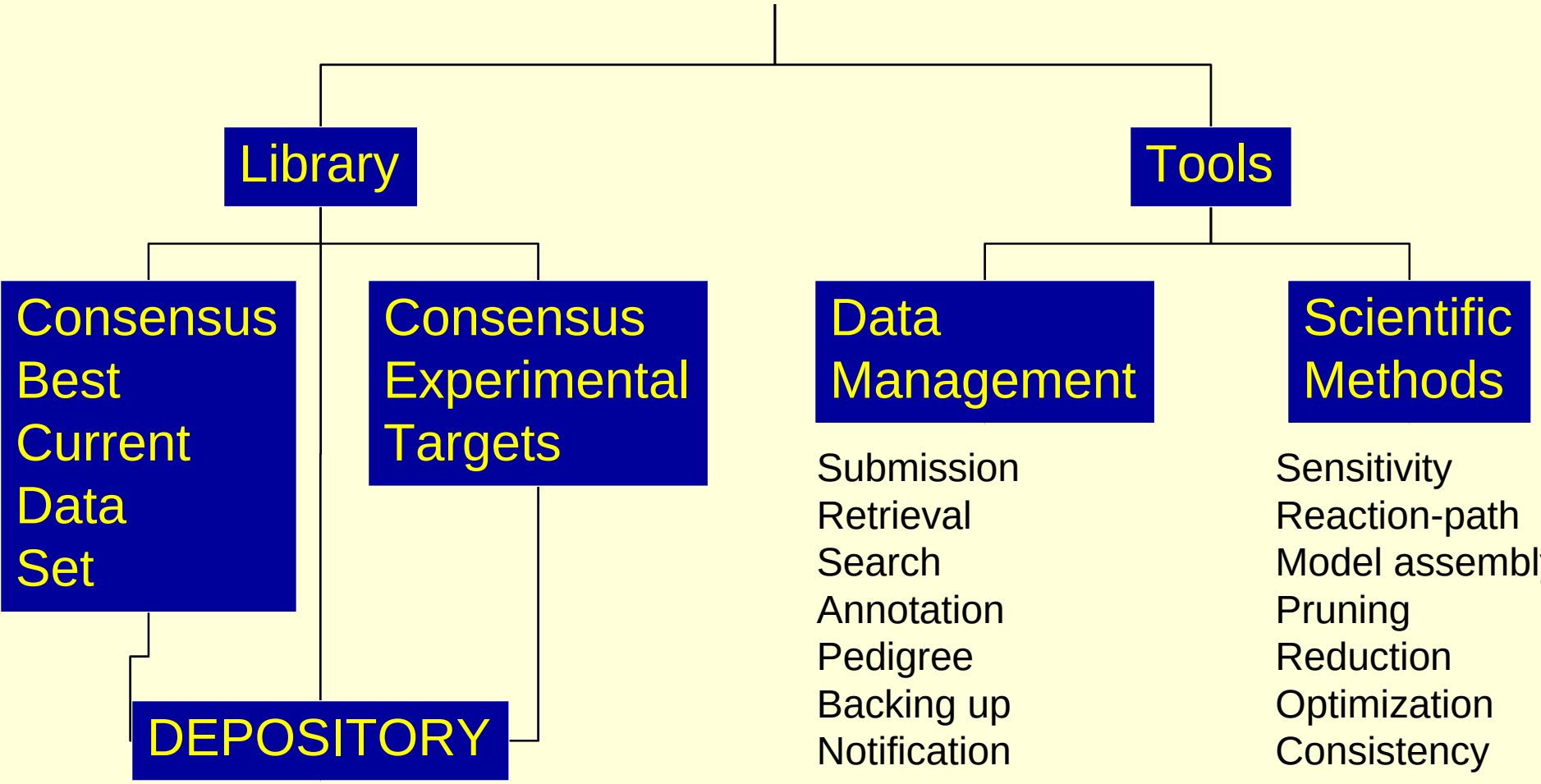
Precursors to PrIMe

- Data gathering-NIST Database
- Evaluated data gathering-NASA Panel
- Evaluated data gathering and optimization to produce “best current set”-GRI-Mech
- *All would be simpler and more reliable if tools were to be developed to aid in acquiring and processing data and assuring the data completeness and mutual consistency*

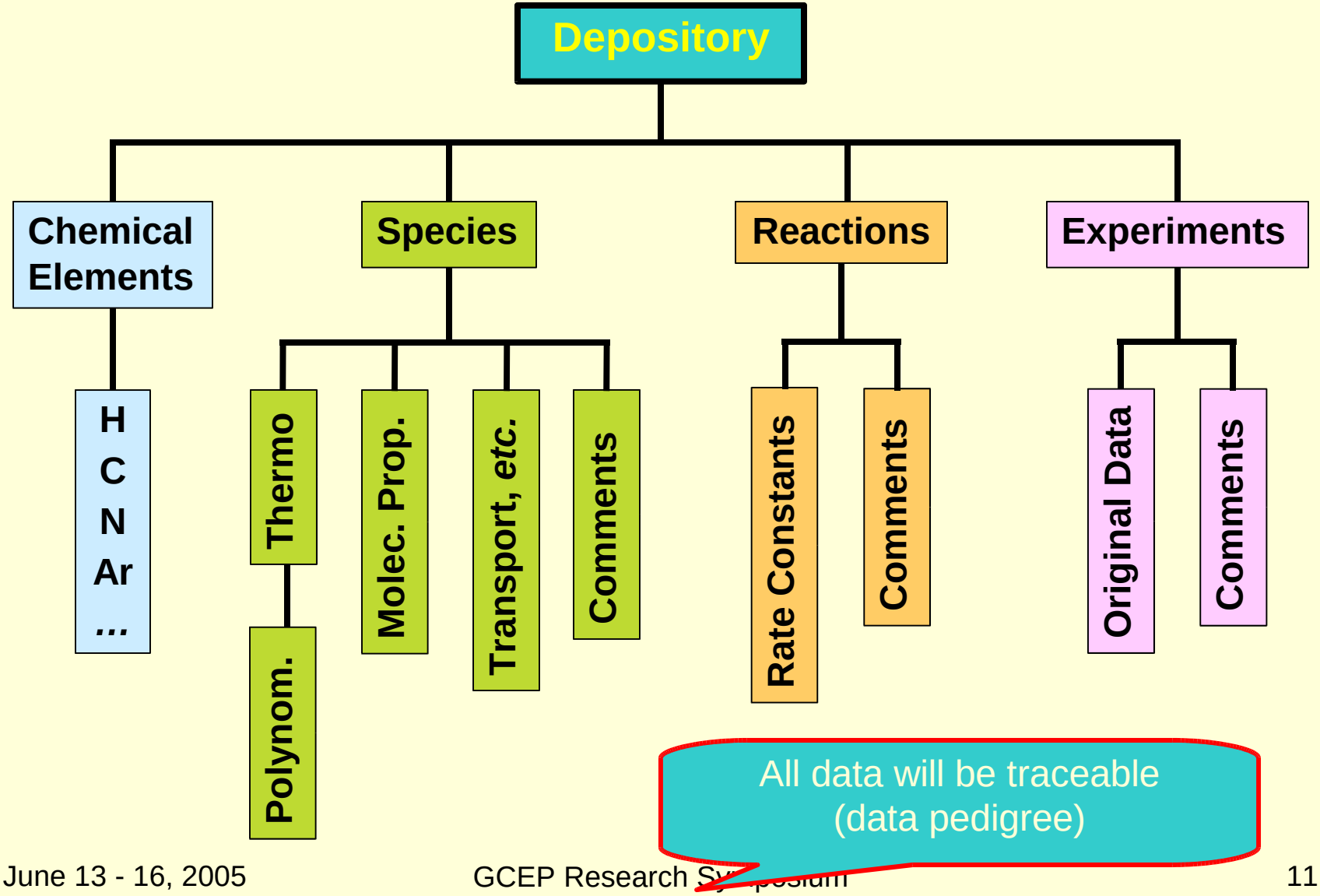
PrIMe Structure

- Warehouse
  - --*Data Depository*-All Traceable Data (Good & Bad)
  - --*Library*-“Best Current Set” of values with uncertainties
- Tools

PrIMe


Library
Tools
Consensus Best Current Data Set
Consensus Experimental Targets
Data Management
Scientific Methods
DEPOSITORY
a *liquid* database
Submission
Retrieval
Search
Annotation
Pedigree
Backing up
Notification
Team management
…
Sensitivity
Reaction-path
Model assembly
Pruning
Reduction
Optimization
Consistency
…

Organization of Data Depository



Guiding Principles

- Open membership to all qualified people
- “Open-source” data sharing
- Distributed management and shared scientific leadership
- Data integration
- Single copy of each data entry in the *Data Depository*
- Periodic updates of “best current set” in the *Library*
- On-the-fly model building

PrIMe Organization

- PriMe team organized into work groups
- Each group has responsibility for “monitoring” specific parts of *Data Depository*
- Group activities include reviewing comments, recommendations, opinions, and new data, as submitted by the community at large
- Assessing their merits and completeness, and making a recommendation to PrIMe team
- Membership in PrIMe work groups is open to all qualified individuals

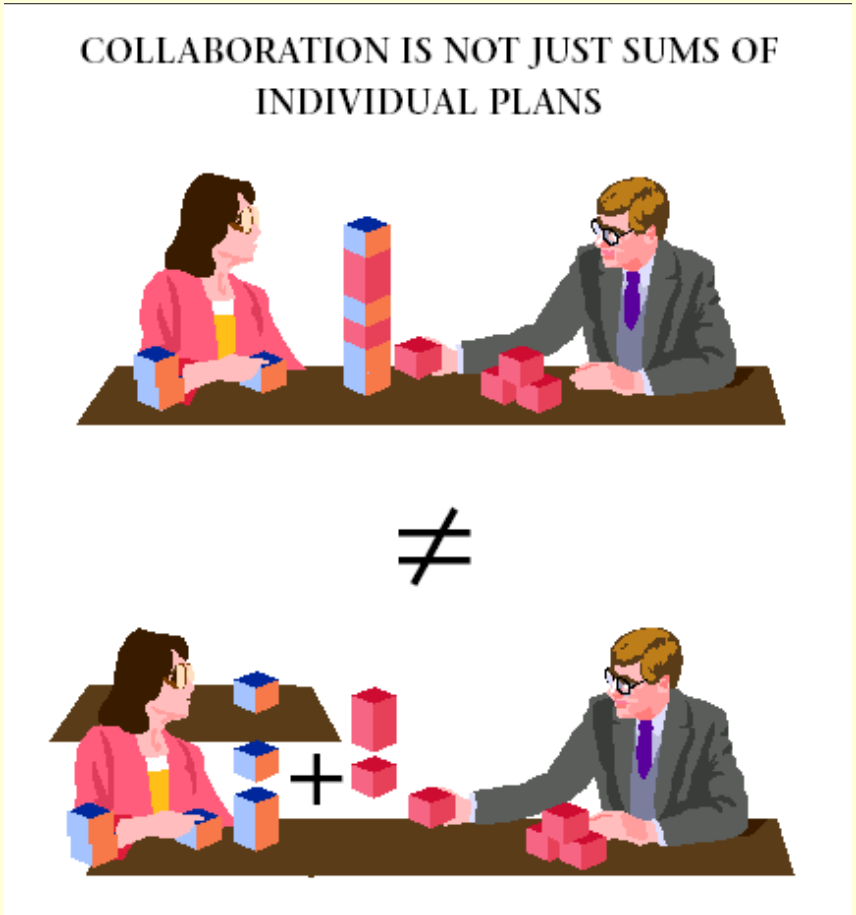
PrIMe Customers: *Data Provider*

- Experimenter (theorist) submits new measurement (calculations) to the *Depository*
- Protocol assures completeness of data
- Submitted data analyzed for consistency with *Library* and the results are reported both to the *Data Provider* and PrIMe team
- Upon consensus of PrIMe team data “deposited” and *Library* modified and/or feedback given to *Data Provider* on what may need to be checked (The possibility that new data at odds with the *Library* may be better than the extant values, will not be ignored!)

PrIMe Customers: *User*

- *User* needs chemical model as CFD input
- *User* specifies model requirements: type, size, accuracy, ranges of conditions, etc
- PrIMe Tools generate such a model, if possible, built on the fly
- If not enough data are available, PrIMe provides choices to generate required data

Bringing-in the Community



- *Pulling* rather than *pushing*
- Moving via “lowest levels of mutual agreement”
- Currently this means creating the *Warehouse*, in particular, the *Depository*

Examples of Tools for PrIMe

- Reaction mechanism generation/reduction
- Estimation of thermochemistry data
- Dataset consistency
- Parameter/state estimation
- Uncertainty propagation
- Advanced numerics for stiff systems
- Design optimization/parametric analysis

Major Benefits

- Development of reaction models in a systematic, scientifically rigorous way
- Better utilization of resources
- Availability of best possible working model at any given time
- Clear identification of future programmatic needs
- Establishing of a new paradigm in the field of complex model development

Current Status of PrIMe

- *Building and launching of PrIMe (CMCS + NIST)*
  - XML data formats have been developed (nearly completed)
  - Data are being prepared in those formats (nearly completed)
- *Data Depository* is being populated with data (beginning)
  - Submission forms are being developed (almost complete)
- Working group collaborative environment (~90% complete)
- *Tool development – through individual efforts*
- *Community support*
  - US “major players”, Utah–Sandia, Albuquerque,…
  - Companies: Caterpillar, (GCEP, …)
  - International: UK (Leeds), Germany, Sweden, …
- *Other fields*
  - Atmospheric chemistry, astrophysics/astrochemistry,…

Tentative Timeline: PHASE I

- Building for initial launch of PrIMe
  - *Depository* populated with initial set of data based on the NIST library and GRI-Mech release 3.0
  - Data submission forms developed and integrated through CMCS infrastructure
  - Operation of PrIMe working groups is enabled through CMCS
- Activation of PrIMe group leaders and the “formulation” of PrIMe groups
- Official launch of PrIMe: announcement to entire community and inviting submission of “individual” data
- Organizational meeting of PrIMe team, and setting objectives for next year (i.e., what PrIMe 1.0 release should include; perhaps starting with natural gas system as an update and revision of GRI-Mech)

Tentative Timeline: PHASE II

- Addition of data to *Depository* (Leeds, …)
- Incorporation of simulation and analysis (sensitivity, optimization, …) tools into PrIMe infrastructure, through CMCS tools (ActiveTables, ReactionLab, RIOT, …)
- Release of the first “best current data set” (i.e., the *PrIMe Library* 1.0)
- Annual PrIMe team meeting, and so on.

FAQ

- To what detail will experiments have to be entered?
  - *Eventually it would be good to have all details. We will begin with some relatively obvious "standards" that we have developed over the past few years.*
- How do you support what is essentially an infrastructure with research funds?
  - *This will require explaining how PrIMe will enhance research.*
- Is there an analogy with projects like the Advanced Light Source (ALS)?
  - *This is an example of funds spent on infrastructure to enhance research.*

FAQ

- How long before anything emerges?
  - *We are working hard to launch the Depository, and expect it to happen within the current year*
- How do we get and demonstrate community support?
  - *All aspects are open to the entire community. Nobody will be left out. The advantages of a single location for all data will be clear.*
- How do we interact with users?
  - *Mainly through the internet --- using the CMCS Portal. Meetings will also be required from time to time, and we hope that they will occur under the umbrella of the Combustion Institute*