Overview of CLEERS (Diesel Cross-Cut Lean Exhaust Emissions Reduction Simulation) Program

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D.O.E. Crosscut Workshop on Lean Emissions Reduction Simulation
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GOAL

Simulate emission control systems under realistic conditions to optimize the engine/aftertreatment integration

- Issues
  - -Accessible, reliable component submodels
  - •Integration of submodels
  - •Realistic engine out data for Federal Test Proceedure (FTP) driving cycles

Advantages of System Modeling

- Reduced cost and time for system optimization
- Identification of bottlenecks and opportunites
- Improved/tailored component design
  - engines
  - catalysts
  - sensors
  - control strategies
- Vehicle test planning

Outline

- The organization
- The “issue”
  - Integration between aftertreatment and engine
- Approach-Provide a common ground for industry and “the outside world” to develop the tools for aftertreatment simulation
  - Develop a center for computational comparision
    - Provide a baseline modeling environmemt
    - Develop a “library” of engine out measurements for the testing of simulation components
    - Gather a library of simulation and experimental results to serve as technical benchmarks for evaluating new component submodels
  - Technical exchange
    - Web based information
    - Technical meetings to get the “right” people in the same room
    - Web based information exchange on collaborative programs
- What we expect from this meeting
- Wrap-up

Sponsorship

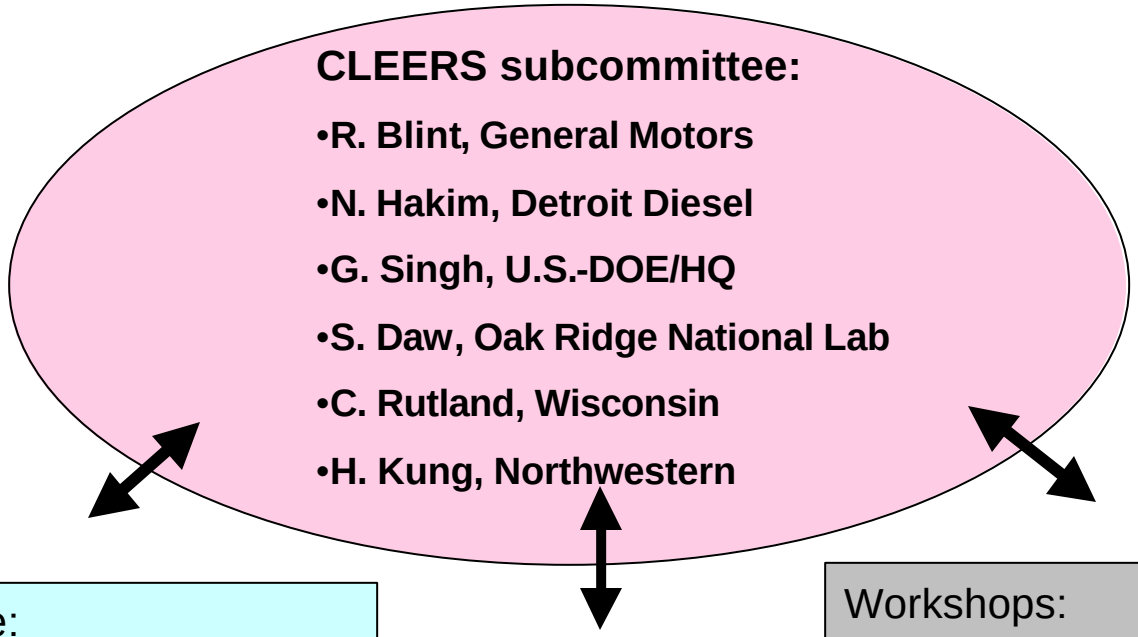
Diesel Cross Cut Team

(organized by the DOE)

Members

- DaimlerChrylser
- Ford
- GM
- Caterpillar
- Cummins
- DDC
- DOE (OHVT)

CLEERS is coordinated by a subcommittee appointed by the Diesel Cross-Cut Team



Website:

- General information about emissions control simulation
- Technical information and benchmark data base
- Data and model exchange forum

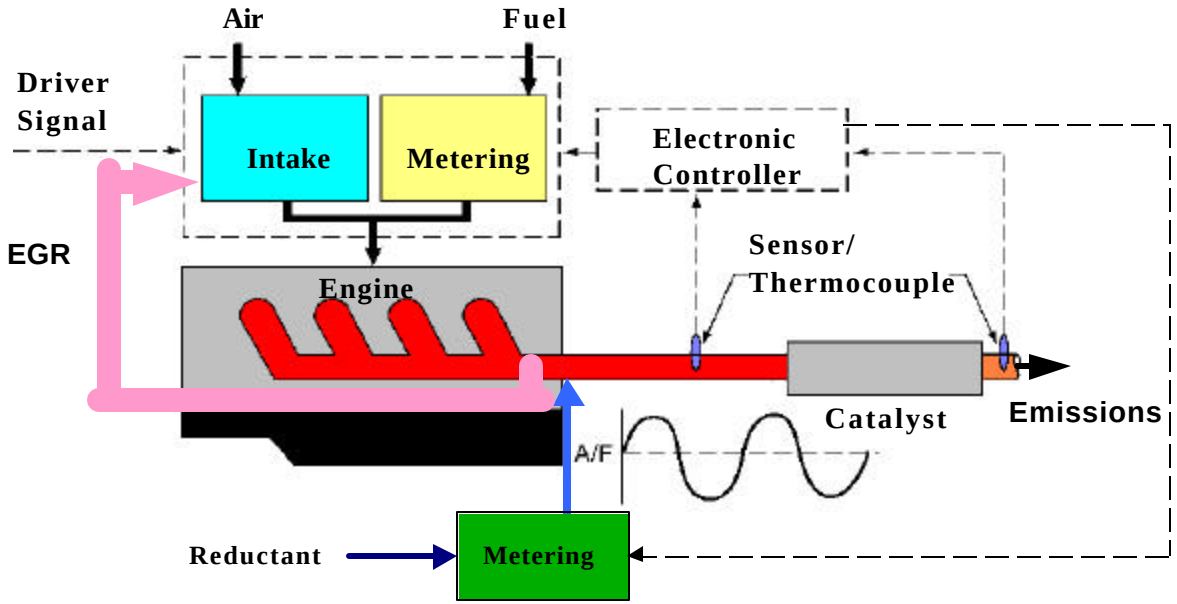
Simulation Testbed

Workshops:

- Focused 2-day meetings on emissions control topics
- Invited and contributed technical presentations on specific topics
- Overview presentations and panel discussions

Closed Loop Operation

Time scale: 1s to minutes



- Engine Control Unit (ECU) controls engine
- ECU responds to aftertreatment requirements
- Aftertreatment “determines” engine response

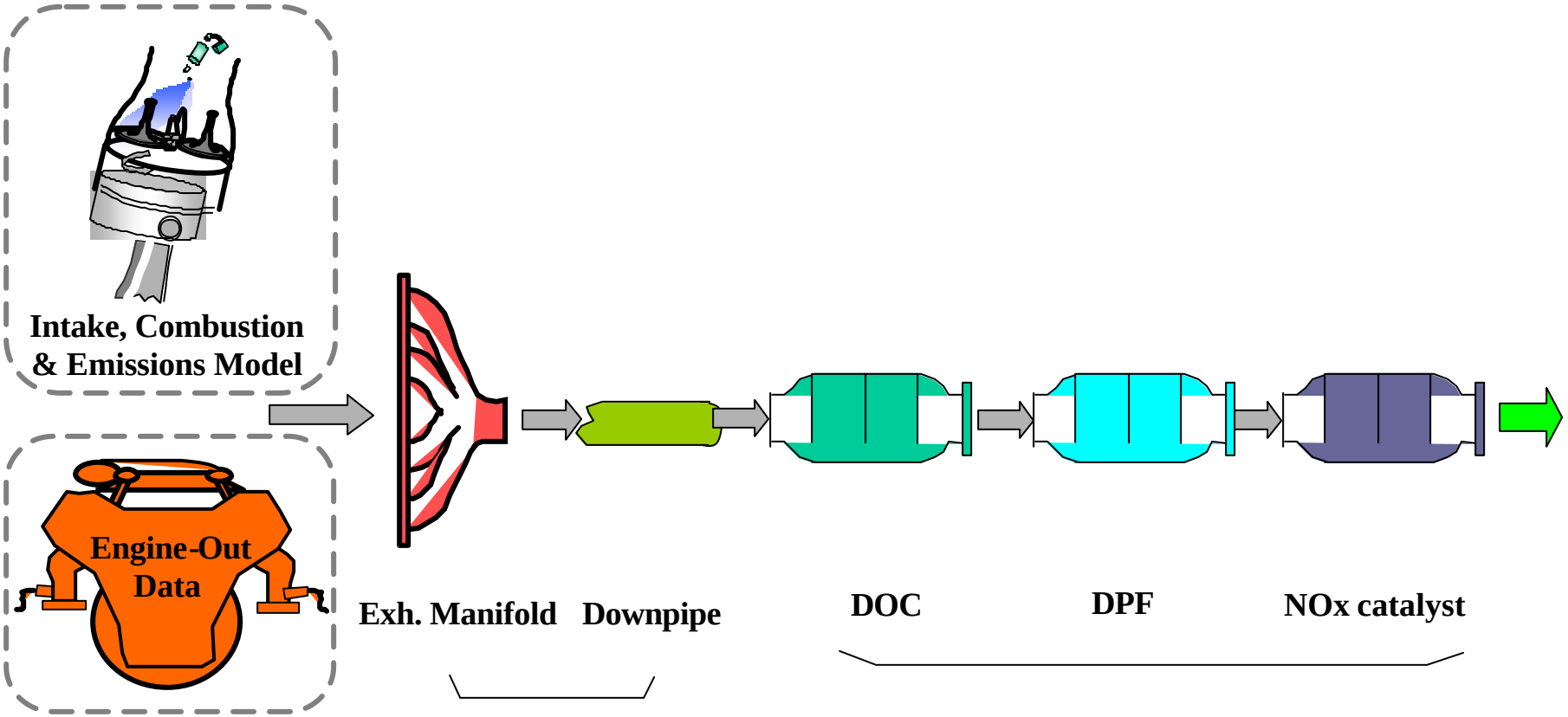
System Modeling Requirements

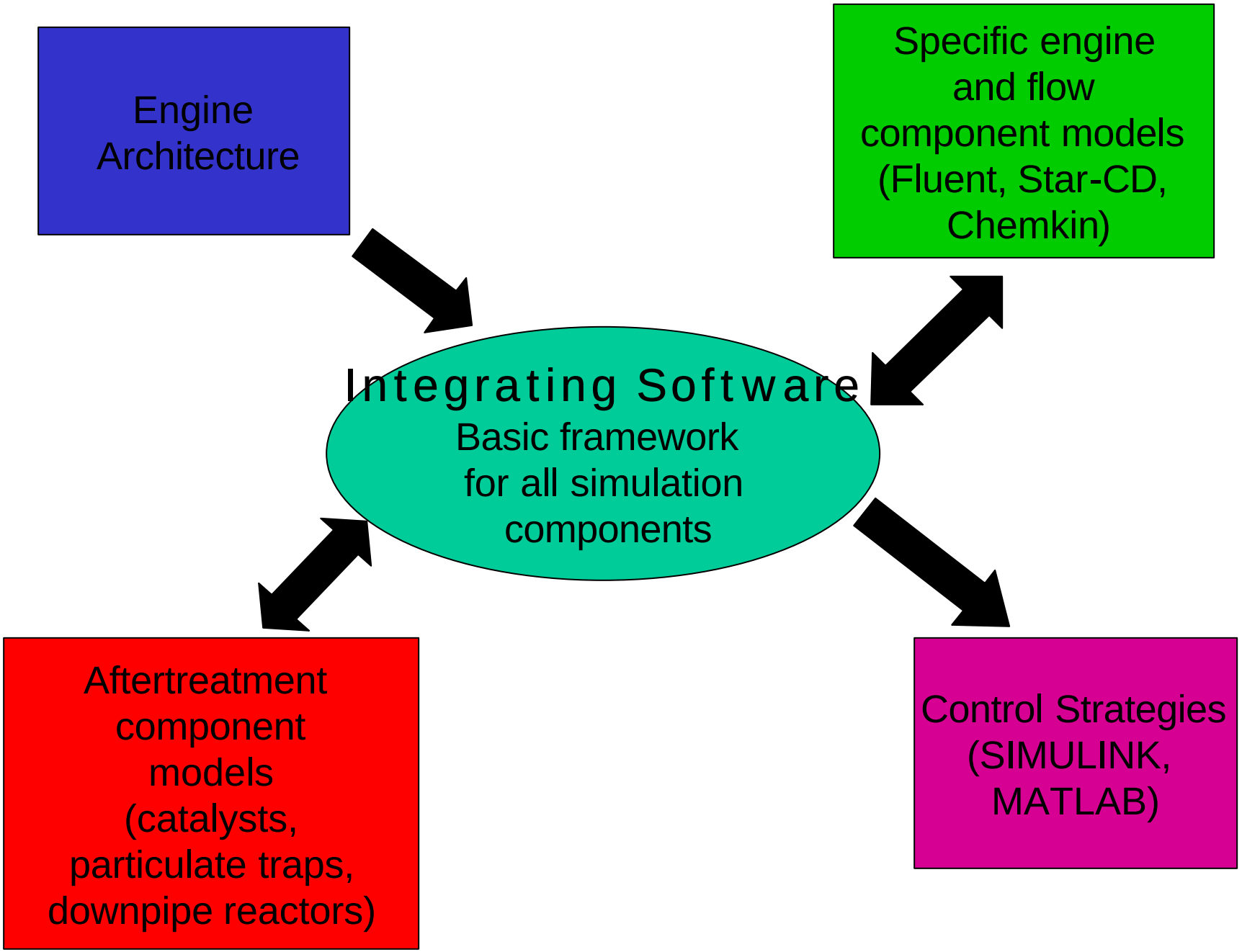
- Must be compatible with industry engine modeling systems to enable testing on relevant engine systems
- Allow interchangeable submodels for research and development purposes
- Should be supported and generally available (most likely proprietary)

Key requirements for realistic simulations

- Accurate prediction of engine-out conditions
  - Variable flow, composition, temperature
  - Normal operation (cold start, acceleration, load change)
  - Anomalous operation (misfire, cylinder cut-out)
- Predict component response under engine conditions
  - Translate reactor measurements to simulation parameters
  - Correlate/refine reactor response to component engine response over the range of conditions
- Federal Test Procedure (FTP) prediction
  - Ultimate standard for the simulation
  - Evaluate engine control algorithm for effect on catalyst efficiency

Elements of the System




Engine Architecture
Specific engine and flow component models (Fluent, Star-CD, Chemkin)
Integrating Software
Basic framework for all simulation components
Aftertreatment component models (catalysts, particulate traps, downpipe reactors)
Control Strategies (SIMULINK, MATLAB)

Simulation Framework

- Integrating Software
  - –MATLAB/SIMULINK
  - –GT-POWER
  - –WAVE
  - –? KIVA, CHAD

Simulation Center (Goals)

- ORNL Home (Stuart Daw, Coordinator)
- Central system for evaluating aftertreatment models with a complete set of aftertreatment model
- Suite of baseline models for comparison Library of benchmark case inputs (e.g., OEM engine out data and catalyst out if possible)
- Library of benchmark case results for public, private models
- Web-based simulation access

Crosscut Aftertreatment Simulation Website

- Downloadable case results, public/private models
- Remote job submission to access engine data or simulation code
- Tutorial and education pages
- Security controls to limit access according to the users (e.g., public, crosscut member, proprietary)
- Workshop announcements and downloadable presentations/proceedings
- Public forum, bulletin board

Framework Codes

- GT-Power
  - Full engine simulation suite
  - Point and click construction of full powertrain including aftertreatment
  - Proprietary simulation environment, but accepts submodels in fortran or C.
  - Aftertreatment models can interact with engine simulation
- MATLAB
  - Industry standard simulation environment
  - Engine simulation codes can be brought in as separate entities
  - No feedback from aftertreatment to engine simulation

License Plan

- Tentative ORNL License Plan
  - GT-Power on UNIX machine with Flexlm license
  - GT-Power copy on Windows PC with node-locked license
  - MATLAB generally available
  - Component models available with individual restrictions
  - Direct access by crosscut members holding GT Power and/or MATLAB licenses
  - Non crosscut members are enabled based on project
    - Non-crosscut exploratory
    - Non-crosscut development
    - Non-crosscut industrial collaboration

Industrial Strengths for the program

- Product relevant systems modeling
- Exhaust measurements from production engines
- Emission engineers
- Catalyst suppliers
- Customer driven focus

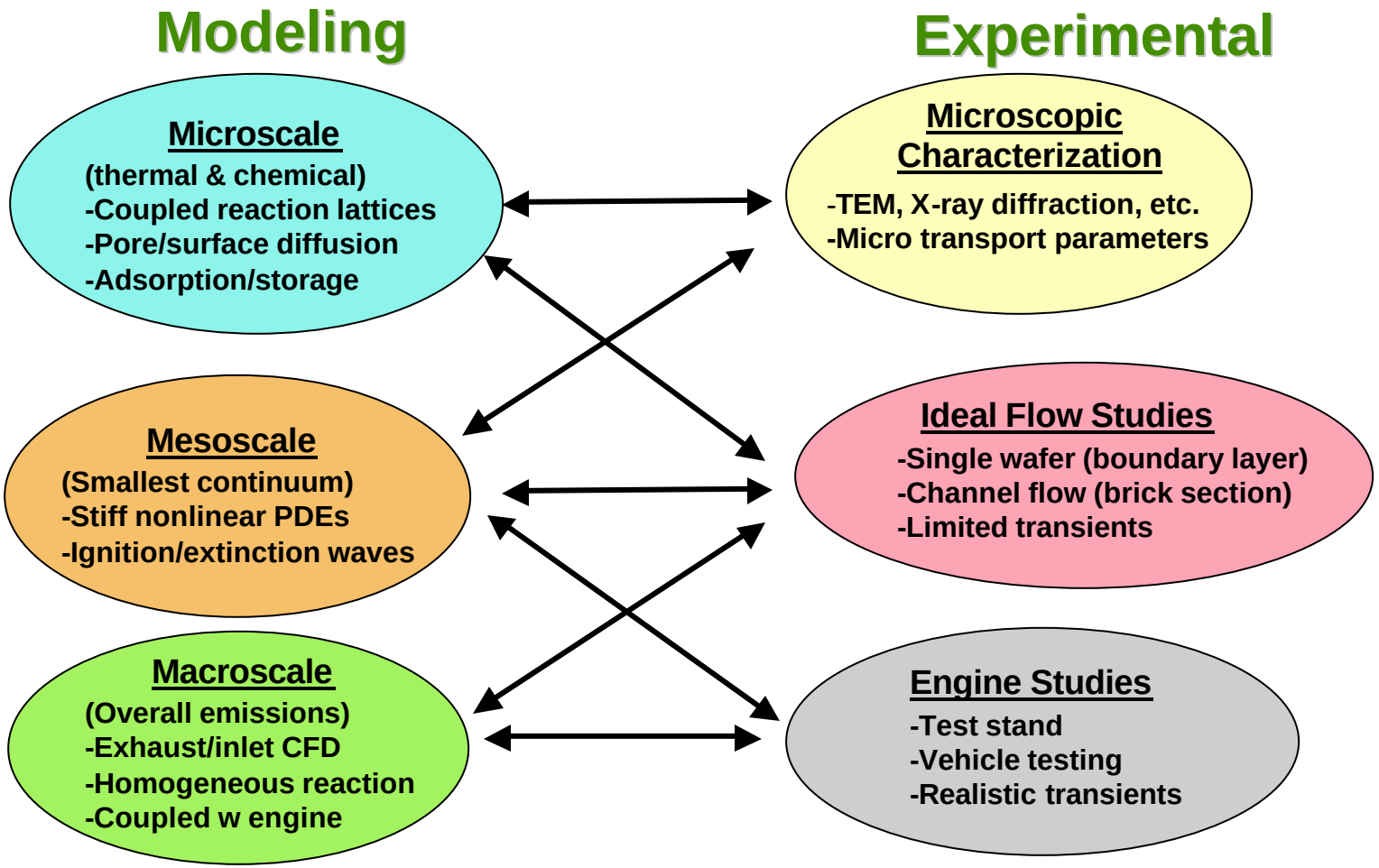
Non Proprietary Needs I.

- First principles modeling
  - detailed flow field
  - catalyst surface morphology
  - gas-surface reactions (morphology dependence)
  - unsteady dynamics both flow and reactive
  - mathematics for sensitivity analysis

Non Proprietary Needs II.

- Measurement verification of simulations
  - detailed flow field
  - catalyst surface morphology
  - gas-surface reactions (morphology dependence)
  - unsteady dynamics both flow and reactive
  - to be determined needs

Multidisciplinary Projects Can Provide Faster Track to Improved Catalysts



Technical Workshops

- Overall Concept
  - Promote research collaborations in emission controls simulation
  - Identify state-of-the-art for various technologies and models
  - Identify key unresolved issues, technical paths to solutions
- Approach
  - Sponsor workshops focused on specific simulation topics
  - Workshop parameters
    - 2 days each, 3/yr at accessible locations (e.g., Detroit, Chicago)
    - Participation by industry, academia, national labs
    - Specific topic, 3-4 invited talks, 8-10 contributed talks
    - Published proceedings (Website)

What do we want from this workshop?

- Introduce the program
  - What, where, when and how
- Bring the players together
- Get feedback on the direction of the program
  - Especially the common computing environment
- Get feedback on technical priorities
  - Tuesday afternoon prioritization will direct future technical meetings and help define the structure of the center

Wrap-Up

- This program:
  - could be the common ground for math based emission system development (code formats, types of applications….)
  - provides an environment for future R & D on emissions simulation (technical meetings and collaborations)
  - could define industry wide standards for interchangeable simulations modules (participation by the catalyst manufacturers may standardize “new catalyst” simulation modules)

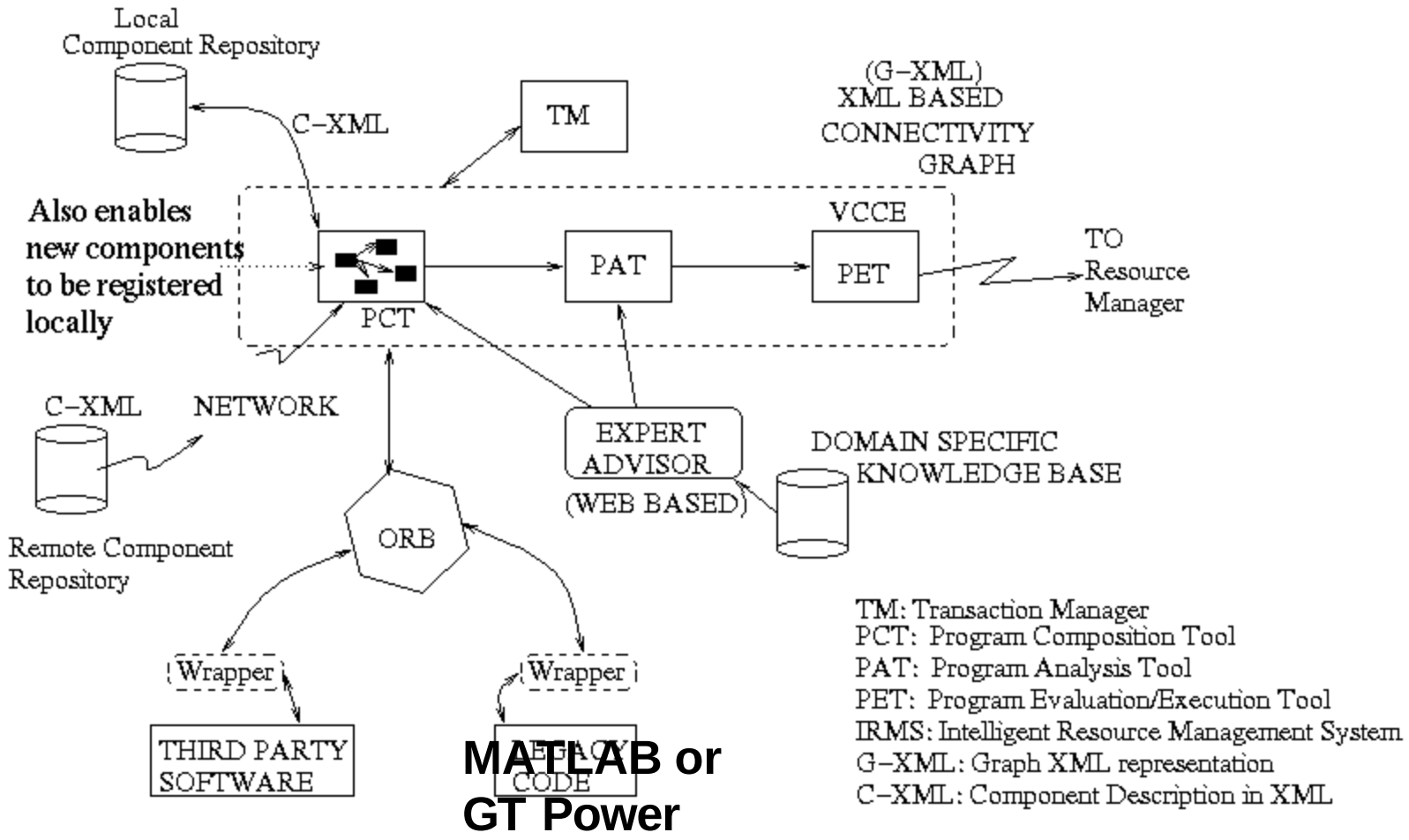
Website

- General Approach
  - Construct and maintain a website at ORNL through which external users can meet previous objectives
  - Provide tutorial and education
  - Institute security controls to limit access according to the users (e.g., public, crosscut member, proprietary)

Website

- Objectives
  - Encourage information transfer, collaboration
  - Interface for crosscut members to access simulation framework, benchmark case parameters, benchmark results
  - Access to publicly shared component codes
  - Workshop announcements, distribution of proceedings
  - On-line discussions
  - Posting of important research results
  - Possible access to advanced DOE computing resources for industry, universities

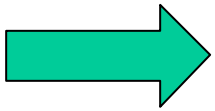
Website Implementation of Shared Simulation Environment



Aftertreatment System Modeling

Support prediction, analysis, and collaboration in an integrated web-accessible environment that:

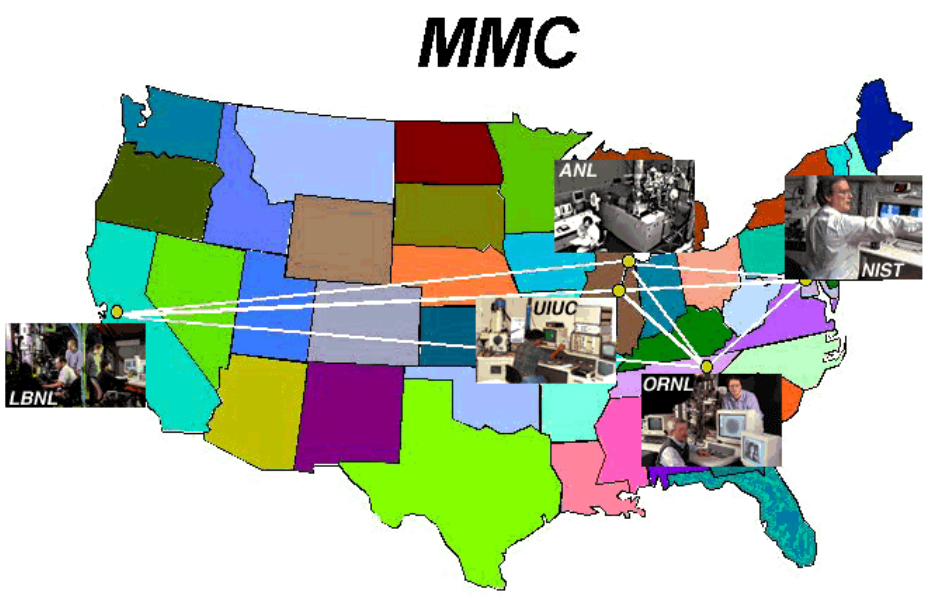
- Gives transparent access to heterogeneous distributed resources
- Supports new component creation and use
- Seamlessly incorporates new hardware and software

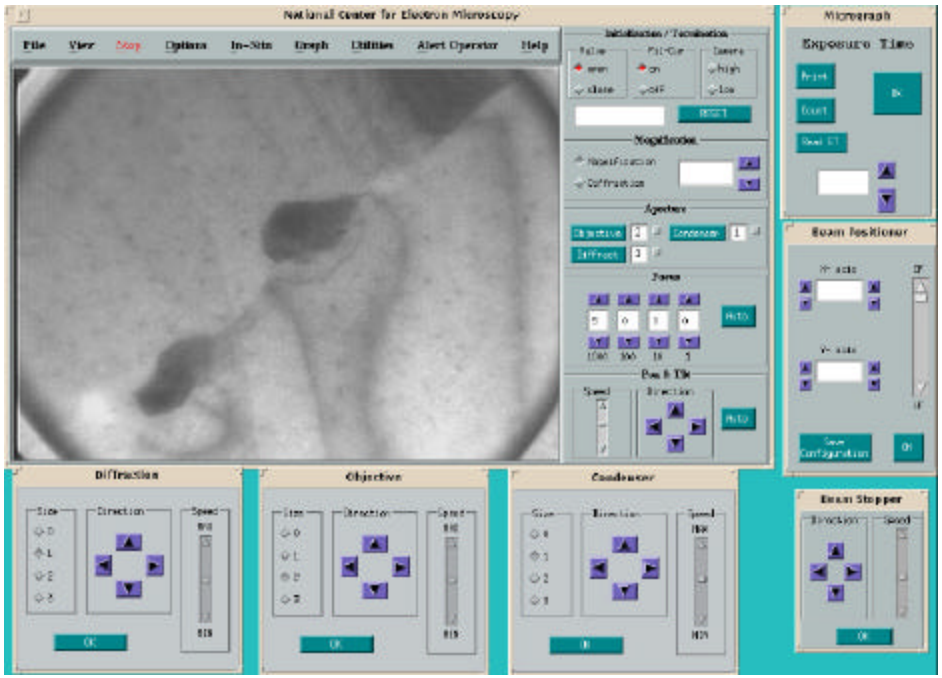


Problem-Solving Environment

Example Website: www.ornl.gov/doe2k/html

DeepView: Remote access to microscope images and controls



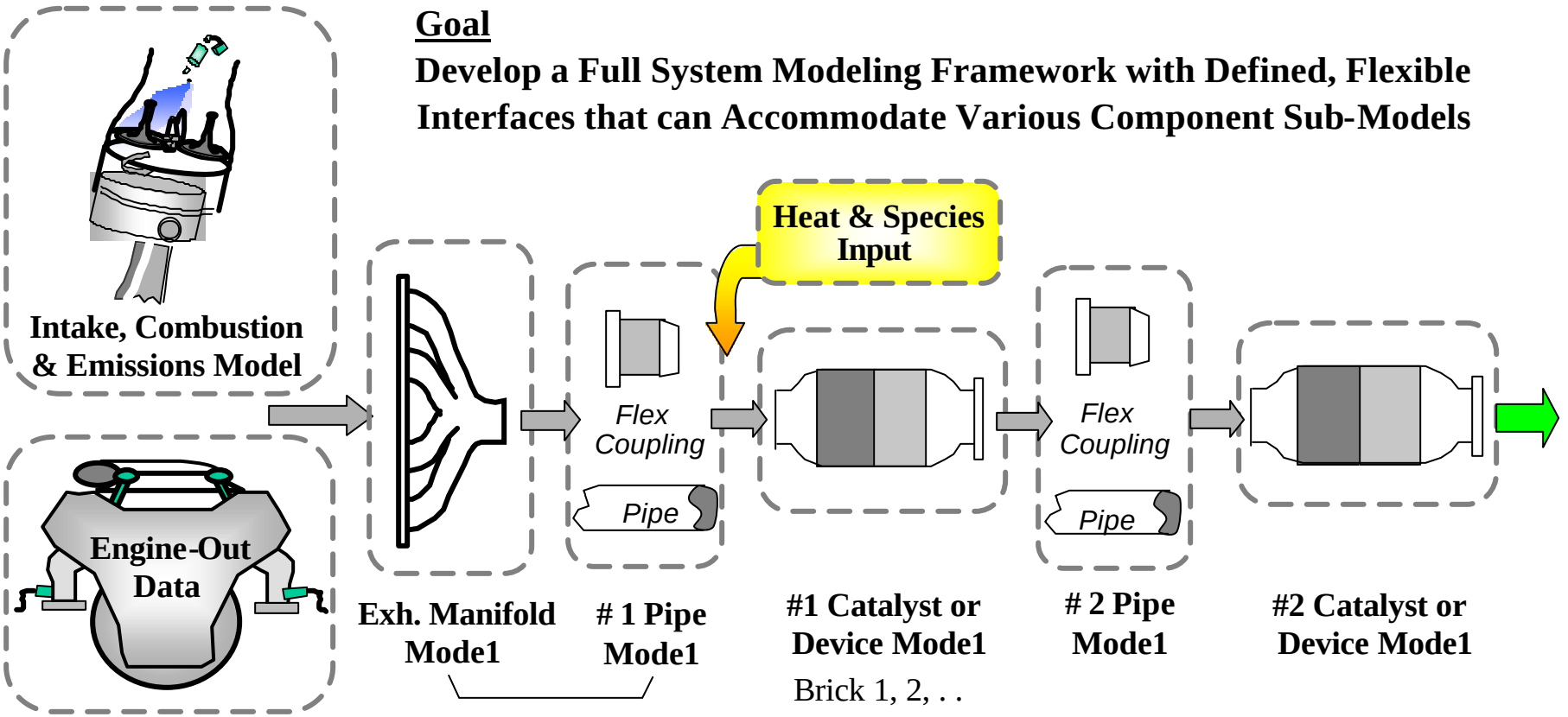


The Full System Modeling Vision

From Air Intake to Tailpipe Exhaust

Goal

Develop a Full System Modeling Framework with Defined, Flexible Interfaces that can Accommodate Various Component Sub-Models



- Exhaust Flow
- Air-Fuel Ratio
- Temperature
- HC & NOx Species
- CO, CO2, etc
- Gas Phase Reactions
- Etc

- Material Properties
- Dimensions
- Flow Distribution -CFD
- Wall Thickness
- Smoothness (Chuff)
- Etc

Brick 1, 2, . .

- Volume, Surface Area
- PGM Loading
- Flow Distribution- CFD
- Substrate Properties
- Chemical Reactions
- Aging, Poisoning
- Etc