

Introduction to NETL Computational & Basic Sciences

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Morgantown, WV

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Focus Area Leader

National Energy Technology Laboratory
Morgantown, WV



National Energy Technology Laboratory

Morgantown, WV



Pittsburgh, PA



Tulsa, OK



- One of DOE's 17 national labs
- Sites in West Virginia, Pennsylvania, Oklahoma, and Alaska
- Implements DOE's R&D programs in coal, oil, and natural gas
- 1,100 Federal and contractor employees
- \$750 million per year budget



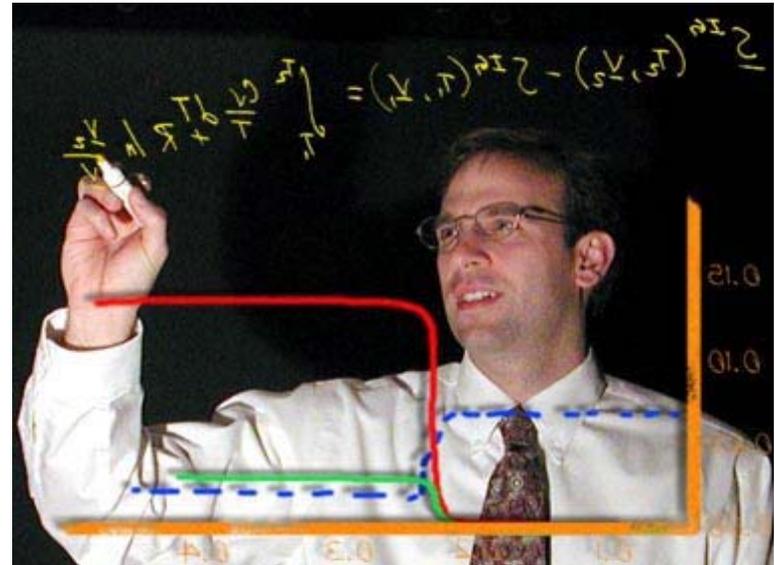
NETL Mission

Implement a science and technology development program to resolve the environmental, supply, and reliability constraints of producing and using fossil resources



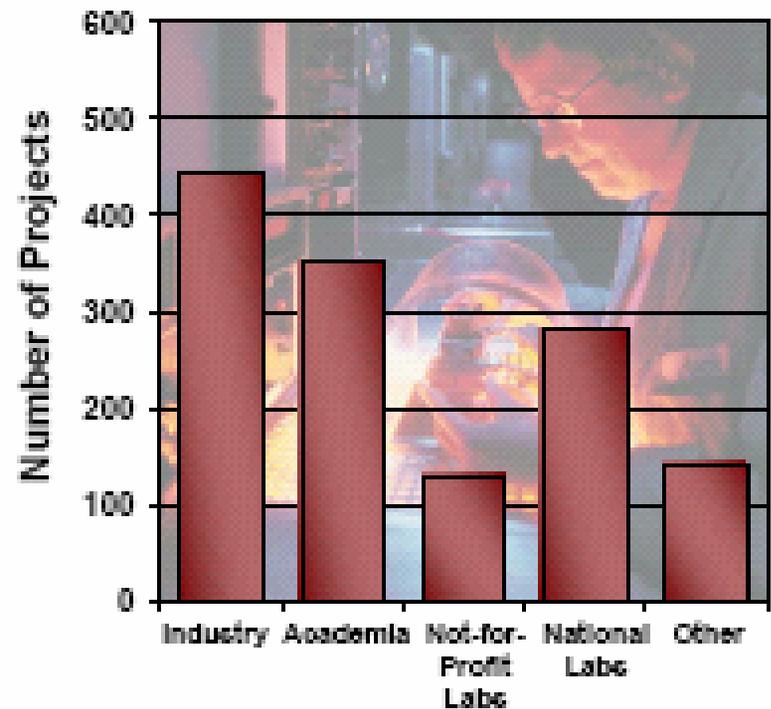
What We Do

- Shape, fund, and manage extramural RD&D
- Conduct onsite research
- Support energy policy development



Shape, Fund, and Manage Extramural RD&D

- 1,400 research activities in 47 states and more than 40 foreign countries
- Total award value of \$8 billion
- Private sector cost-sharing of over \$4 billion
 - Leverages DOE funding
 - Ensures relevance
 - Accomplishes mission through commercialization
- Nearly 60 active memoranda of understanding with industry, universities, and other national laboratories



Conduct Onsite Research

NETL Focus Areas



- **Energy System Dynamics**

- Fuel Cells / Hybrids
- Gas Combustion
- FutureGen



- **Geological and Environmental Science**

- Carbon Sequestration
- Clean Air Technology
- Water & Coal Utilization Byproducts



- **Computational and Basic Sciences**

- Computational Chemistry
- Device/Systems Modeling
- Multiphase Flow
- Energy Infrastructure



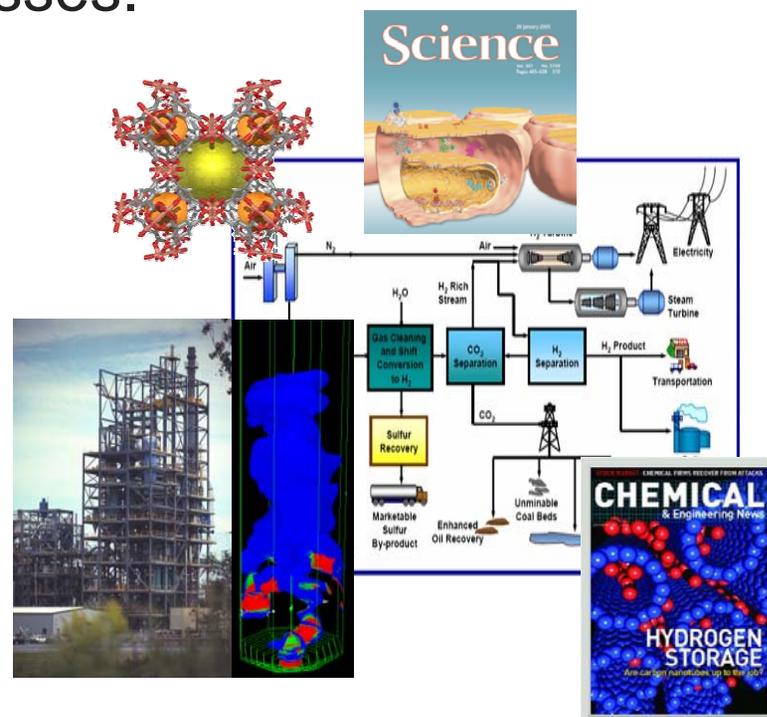
Computational and Basic Sciences Focus Area

- **Mission**

Overcome the technical barriers associated with the development of the next generation of highly efficient, environmentally acceptable Fossil Energy (FE) technologies and processes.

- **Strategy**

- Conduct computational engineering and science research
- Validate models with experimental research
- Apply to FE systems

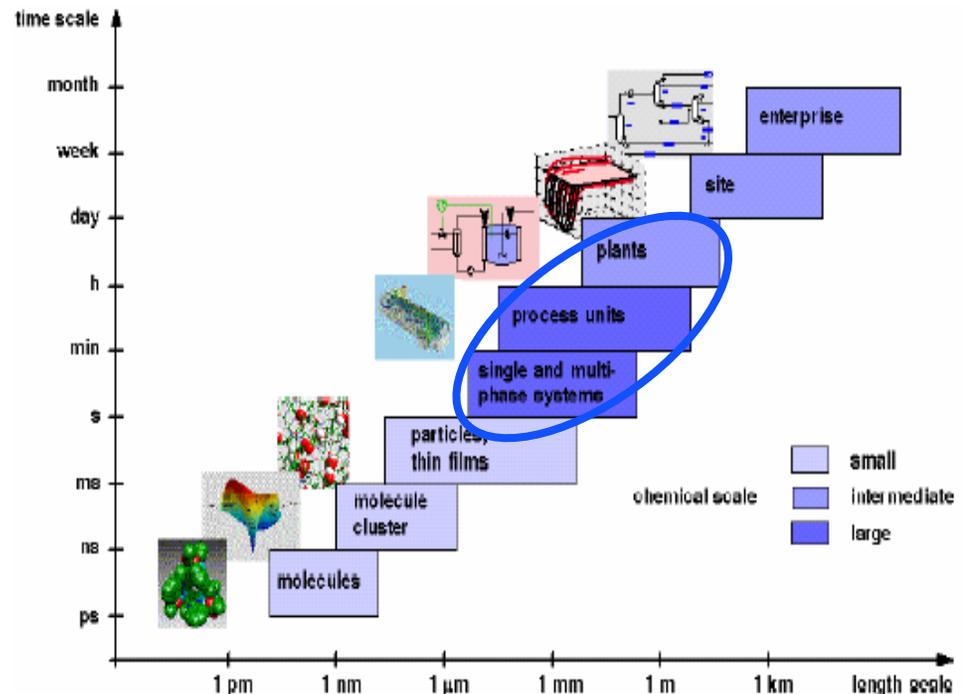


Computational & Basic Sciences Focus Area

Multiscale and Multiphysics Modeling

- **Scope**

- Quantum Mechanical Simulations
- Atomistic/Molecular Dynamics
- Advanced Materials
- Device-Scale Simulations
- Multiphase Flow
- Hydrogen Technology
- Integrated Virtual Plant Co-Simulations
- Energy Infrastructure Analysis



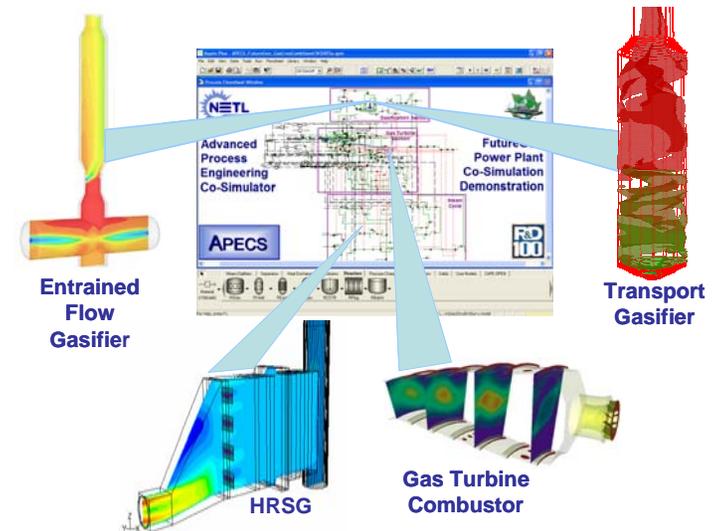
Multiscale Modeling and Simulation

Computational & Basic Sciences Focus Area

Device-Scale & Systems Modeling Research Group

• Objectives

- Apply wide range of modeling and simulation technology
 - CFD, PDE multiphysics modeling, process simulation
- Develop integrated, multiscale simulation capabilities
 - Use co-simulation frameworks
 - Exploit open standards
 - e.g., CAPE-OPEN
- Couple with advanced visualization and high-performance computing
- Demonstrate virtual power plant simulations



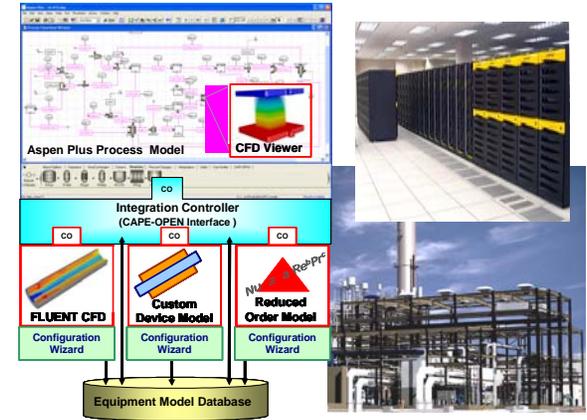
Advanced Process Engineering Co-Simulator (APECS)





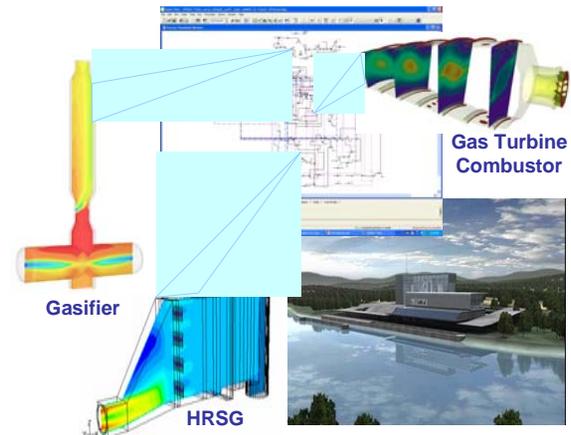
Advanced Process Engineering Co-Simulator (APECS)

- **APECS combines process simulation with detailed equipment models, advanced visualization, and high-performance computing**
 - First of a kind development by NETL and its R&D technology partners
 - Relies heavily on **CAPE-OPEN** standard
 - Recognized with **2004 R&D 100 Award**



APECS Integration Framework

- **APECS enables high-fidelity power plant design, analysis, and optimization**
 - Provides the necessary level of detail and accuracy essential for advanced power plant simulation
 - Applies to high-efficiency, zero-emission systems, including the **FutureGen** plant



APECS FutureGen Plant Simulation



Contact Information

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