The Role of Simulation in Accelerating Deployment of Clean and Secure Energy Technologies

Philip J. Smith, professor & director
Global Primary Energy Consumption

- Oil: 37%
- Coal: 25%
- Natural Gas: 23%
- Nuclear: 6%
- Biomass: 4%
- Hydro: 3%
- Solar: 2%
- Wind: 1%

Monday, March 21, 2011
Proved Reserves (billion BOE) 2009

- Middle East
- South & Central America
- Africa
- Europe & Eurasia
- North America
- Asia Pacific

- Coal
- NG
- Oil

THE INSTITUTE FOR CLEAN AND SECURE ENERGY

Monday, March 21, 2011
Coal (domestic)

- mines
- reserve
- resource (proven)
- resource (identified)

- 28%
- 64%
- 8%
- 0.3%
Oil Shale (domestic U.S.)
• need new technologies, new solutions - NOW!
  – historically required decades to deploy
  – need environmentally acceptable energy solutions
  – need new fuel sources

• how?
  – high performance computing
  – uncertainty quantification
  – reduce risk
LES

heat flux hazard from liquid fuel fires

resolved turbulence, mixing, and reaction
Strong Scaling for 64 million cells

Figure 17 from previous report

Strong and weak scaling for reacting case for version 5.06.010

number of processors

work (wall clock time)

CCM+ 6.02.007

Monday, March 21, 2011
Reaction & Mixing

\[ E_v(\kappa) \]

\[ \frac{\langle v'v' | \kappa \rangle}{\langle v'^2 \rangle} \]

Nyquist Limit

LES cutoff

DNS

\[ I \]

\[ \kappa(l^{-1}) \]
Reaction & Mixing

\[ E_\Phi(\kappa) \]

\[ \frac{\langle \Phi' \Phi' \mid \kappa \rangle}{\langle \Phi'^2 \rangle} \]

\[ E_v(\kappa) \]

\[ \frac{\langle v'v' \mid \kappa \rangle}{\langle v'^2 \rangle} \]

LES cutoff

\[ Da (t_m/t_r) \]

\[ Sc \]

Nyquist Limit

\[ \kappa (l^{-1}) \]
Reaction & Mixing

- **Reactants** \( \rightarrow \) **Intemediates** \( \rightarrow \) **Products**

\[ E_{\Phi}(\kappa) \]
\[ \frac{\langle \Phi'\Phi' | \kappa \rangle}{\langle \Phi'^2 \rangle} \]
\[ E_{v}(\kappa) \]
\[ \frac{\langle v'v' | \kappa \rangle}{\langle v'^2 \rangle} \]
\[ E_{r}(\kappa) \]
\[ \frac{\langle r_i'r_i' | \kappa \rangle}{\langle r_i'^2 \rangle} \]

**LES cutoff**

**Nyquist Limit**

\[ Da \left( \frac{t_m}{t_r} \right) \]

\[ \kappa(\ell^{-1}) \]
Carbon Capture: Oxy-Coal Combustion with Alstom & Praxair
HPC - LES provides liftoff (ignition/extinction)

- Ignition controlled by:
  - small particles
  - radiation
- High gas radiation absorption from CO₂
- High sensitivity to wall temperature
Coal Gasification

Coal Gasification Validation Collaboratory
U.S.-Canada Bilateral Cooperative Agreement
- expts: Canmet, U of Utah
- sims: Canmet, U of Utah, U.S. DOE-NETL, MIT
HPC - LES provides dynamics (clustering, reaction intermediates)
U.S. oil shale history

High Performance Computer Simulations: to accelerate deployment of new technology

THE INSTITUTE FOR CLEAN AND SECURE ENERGY
use HPC to deploy first commercial U.S. oil shale operation
resolved geometry in rubblized beds, fixed beds, moving beds

- realistic shale structure
  - statistically representative bed
  - 2000+ pieces of shale
convective heat transfer in rubblized beds, fixed beds, moving beds
convective heat transfer in rubblized beds, fixed beds, moving beds
Can we indirectly heat coal in the ground to produce synfuels?
1. “All scientifically relevant data have an uncertainty.”
2. “Data without uncertainty cannot be relevant scientifically”

\[ y_m(x) - y_{\text{exp}} \leq u \]

- Experimental Uncertainty \((y_e \pm u_e)\)
- Verification Error - Numerics \((y_v \pm u_v)\)
- Models / Model Parameters \((x_m \pm u_m)\)
- Scenario Parameters \((x_s \pm u_s)\)
Validation = Uncertainty Quantification = Error Budget

1. “All scientifically relevant data have an uncertainty.”
2. “Data without uncertainty cannot be relevant scientifically”

Manfred Drosg

\[ y_m(x) - y_{\text{exp}} \leq u \]
Validation = Uncertainty Quantification = Error Budget

1. “All scientifically relevant data have an uncertainty.”
2. “Data without uncertainty cannot be relevant scientifically”  

\[ y_m(x) - y_{exp} \leq u \]

\[ C_\mathcal{E} = \max \gamma \text{ subject to constraints:} \]
\[ \beta_i \geq x_i \geq \alpha_i, \text{ for } i = 1, \ldots, n \]
\[ (1 - \gamma)u_e \geq |y_m(x) - y_e| \geq l_e (1 - \gamma), \text{ for each } e \in \mathcal{E} \]
V/UQ: heat flux from large pool fires

Validation

\[ |y_m(x) - y_{\text{exp}}| \leq u \]

Incident Heat Flux (kW/m\(^2\))

Validation

original experimental uncertainty

uncertainty after consistency analysis

Monday, March 21, 2011
Accelerating Deployment of Clean and Secure Energy Technologies

High Performance Computing provides:

- multiscale multiphysics with less modeling approximation
- validation with uncertainty quantification
- risk reduction

Monday, March 21, 2011