Forward Looking Panel Discussion

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Background

- Development of a **cyber-infrastructure** (Information Technologies for computation, storage, communication, and data processing services) driven by:

  ➢ Fast development of computer and network technologies

  ➢ Dissemination of these technologies on a global scale
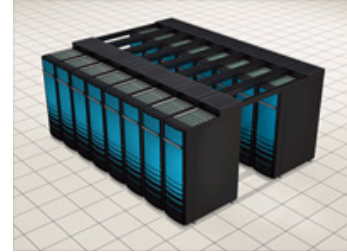
  ➢ Rapid decrease in cost (< $1/MFlops)

Moore's law
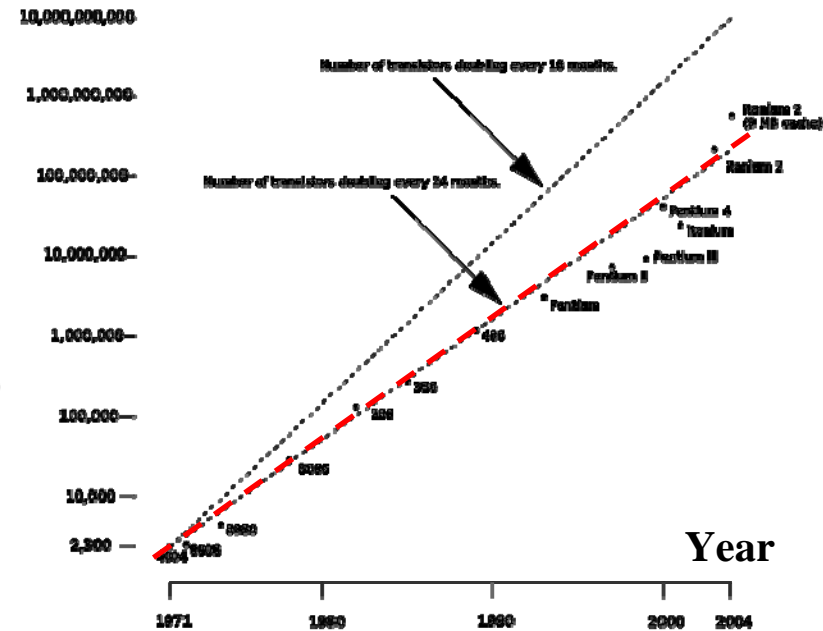
Background

- Current status of cyber-infrastructure technologies:

  - ➤ High-performance computing (HPC) facilities (Government Research Laboratories, Universities)

    - Massively **parallel computing** systems (super-computers) with computational rates between 1 Tera- (10^{12}) and 1 Peta- (10^{15}) Flops

    - Storage capacity up to 1 Peta-bytes

    - Network bandwidth up to 1 Tera-bits per second

  - ➤ Small-to-mid-scale computing facilities (large, medium, small Businesses)

    - Medium-scale parallel computing systems (clusters)

  - ➤ **Grid** infrastructure (coupling of distributed and heterogeneous computational resources and data stores via high-speed networks)

    - Application to: real-time simulations of complex systems, and coupling of sensor technologies with HPC resources

Background

- Changes brought by the cyber-infrastructure:

  ➢ Development of **computational research** as a new scientific approach (DNS, fine-grained LES, MD, KMC, *etc*)

  ➢ Development of computational research as a new engineering approach (ANSYS-CFX, FLUENT, STAR-CD, *etc*)

  ➢ Development of open-source data and software **digital libraries** (CHEMKIN, GRI-Mech, TNF Workshop, Cantera, PRIME, *etc*)

  ➢ Development of distance collaborations and the formation of new **cyber-based communities** (community-wide projects/vision)
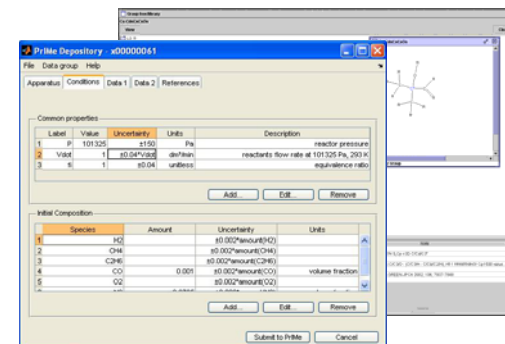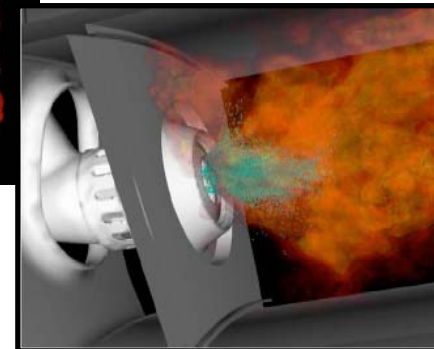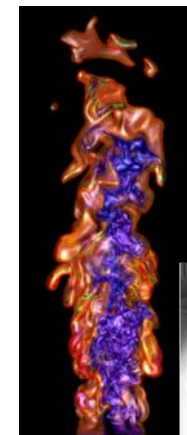
Challenges

- **Goal:** achieve quantitative (predictive) capabilities for engineering-level simulations of combustion systems

- **Needs:** HPC, theory/modeling, self-organization

  - ➢ Establish DNS as the computational companion of detailed experimental studies of laboratory-scale flames – requires adapting high-end numerical combustion solvers to **Peta-scale computing**
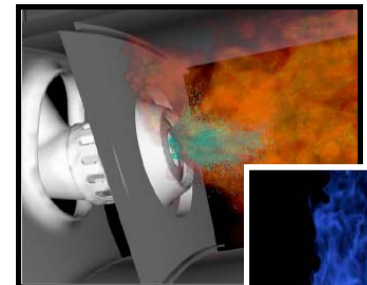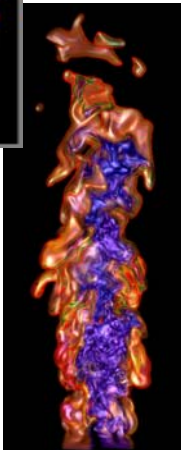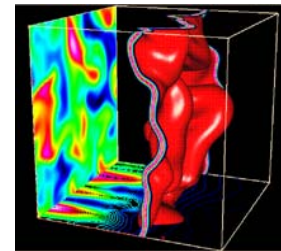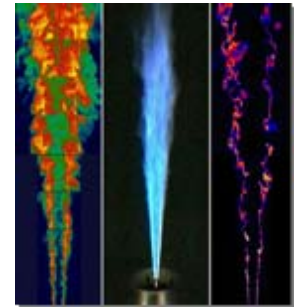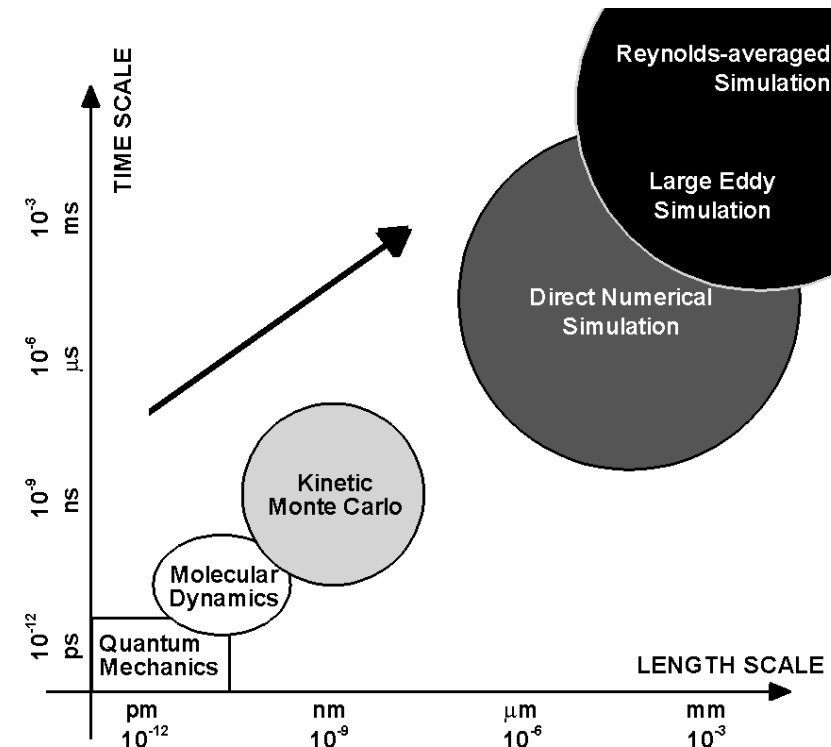
Challenges

- **Goal:** achieve quantitative (predictive) capabilities for engineering-level simulations of combustion systems

- **Needs:** HPC, theory/modeling, self-organization

  ➢ Extend knowledge base of soot physical/chemical processes – requires nano- and continuum-scale tools and a **multi-scale modeling** approach

Challenges

- **Goal:** achieve quantitative (predictive) capabilities for engineering-level simulations of combustion systems

- **Needs:** HPC, theory/modeling, self-organization

  - ➢ Integrate into a common framework different areas of combustion expertise (from nano-scales to engineering device scales), skill sets (theoretical, experimental or computational), and research interests (from fundamental sciences to practical applications) – requires further development of **collaborative science** infrastructure