STATUS AND NEEDS FOR DOE COMPUTING:
A MISSION DRIVEN PERSPECTIVE

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OUTLINE

• Mission needs for DOE computing facilities
  • Example: Fusion Energy Sciences

• Background: The development of DOE computing within the fusion program (OFES)

• How computing relates to the present OFES mission

• Computational Projects within OFES
  • Example: The NIMROD Project

• Are present DOE facilities meeting our mission needs?

• A vision for the direction of computing to support DOE missions
PERSONAL EXPERIENCE WITH DOE COMPUTING

- Continuous user of DOE computing facilities since 1973
  - pre-history => CTRCC => MFECC => NERSC => ???
- Staff member of CTRCC and MFECC at LLNL
- Personally developed many large scale computational models that used these facilities
- Project leader for the NIMROD Project
  - Large scale, multi-disciplinary, multi-institutional computational project within OFES
- I am not a computer scientist, but I must solve real programmatic problems that require advanced computing resources
The mission of the U.S. Fusion Energy Sciences Program is to advance plasma science, fusion science, and fusion technology -- the knowledge base needed for an economically and environmentally attractive fusion energy source.

Fusion plasmas present an extreme scientific challenge

- The fundamental laws of physics are known, but the collective nonlinear dynamical behavior is very complicated
- Dynamics characterized by extreme separation of space and time scales, and extreme anisotropy
- Science problems are as challenging as fluid turbulence
- Scientific uncertainties can have large impact on program costs
- Relevant experiments are very expensive
- Realistic simulation using large scale computing is cost effective
• Advanced fusion experiment will cost ~ $2-10 B
• Cost proportional to volume: $ \sim V$
• Power density proportional to square of max. pressure: $P/V \sim p_{\text{max}}^2$
  $\Rightarrow$ $\sim 1/p_{\text{max}}^2$ for fixed $P$ and $B$ (engineering constraints)
• Physics uncertainties (e.g., neo-classical tearing modes) limit max. pressure to $\sim 2/3 p_{\text{max-theoretical}}$

Uncertainties in nonlinear physics account for $\sim 1/2$ the cost of advanced fusion experiment!

Predictive fluid simulation with realistic parameters has high leverage to remove this uncertainty
• Fusion is a decentralized program

• In the 1970s it was recognized that the required simulation capability could only be obtained with a centralized computer center and high speed long distance networking

• Reduced duplication of effort, eliminated institutional monopolies, facilitated collaborations

  *It was revolutionary!*

• This model has been subsequently adopted by other programs and other agencies

• Evolved into the present DOE computing environment
IMPORTANT FUSION PROBLEMS NOT REQUIRING SUPERCOMPUTING

- Programmatically important, but not requiring the most advanced computing facilities
  - *Equilibrium*: static balance between magnetic and pressure forces in experimental geometry (solving a complicated PDE)
  - *Stability*: Is the equilibrium stable to small displacements? (solving a complicated eigenvalue problem)
  - *Transport*: diffusion of mass and energy in response to microscopic processes (solving a time dependent PDE)

*The majority of fusion computing problems do not require the most advanced supercomputers*

ESSENTIAL PROBLEMS REQUIRE SUPERCOMPUTING
• Problems whose solution is essential to the OFES mission:

  • *Turbulent transport*:
    • Computing diffusion coefficients from first principles => a fundamental understanding of the basic confinement properties of fusion plasmas

  • *Long time scale fluid dynamics* (extended MHD):
    • Nonlinear evolution of slowly evolving plasma instabilities => a fundamental understanding of consequences of operating near stability boundaries

*These problems require the largest, fastest supercomputers imaginable!*
The important fusion problems are time dependent, and therefore 4-dimensional.

- They require many thousands of time steps.
- Often a large, ill-conditioned linear algebra problem must be solved at each time step.
- Parallelization can be applied to the 3 spatial dimensions.
- Parallelization cannot be applied to time.
  - Prohibited by causality.

*Programmatically important fusion problems are not optimally suited to massive parallelization!*
FACTORS AFFECTING FUSION COMPUTING

• Ascendancy of massively parallel computer architecture over serial vector machines, and associated conversion costs

• Uncertainty in configuration of future computer architecture, and anticipated costs of additional future code conversions

• High cost and long time line of individual (superhero) code development, and general inaccessibility of resulting codes by the fusion community

• Increasing programmatic importance of physics problems that require extensions of the capability of existing computational tools
NEEDS OF FUSION COMPUTING

• The need to lower the future cost of application development, maintenance, and use

• The need to implement computational and programming methods that isolate architecture dependencies so that future codes will be more efficiently adapted to evolving new architectures

• The need to make applications codes more readily available to, and usable by, the overall fusion science community

• The need for advanced simulation codes to address physics problems of immediate programmatic interest

   OFES responded with Project-based Computing
PROJECT-BASED COMPUTING

• The *old* way: Code development by individual researcher (the Superhero):
  • Individual or institutional monopolies
  • Non-portable, unreadable, inflexible, non-maintainable code
  • Eventually required expensive rewriting

• The *new* way: Code development by inter-disciplinary, multi-institutional team
  • Publicly available (including source), no monopolies
  • Extensible, modular, portable, maintainable code

*Need for centralized facilities that not only provide high quality CPU cycles, but that also facilitate project function*
The vision of the NIMROD project is to provide the magnetic fusion research community with a useful and widely available computational tool that can be applied to obtain a predictive understanding of the nonlinear dynamics of the most modern and expensive fusion experiments.

- The NIMROD project represents a new paradigm for fusion computing because:
  - It seeks to solve the critical nonlinear physical problems facing the fusion program within a user-friendly, widely available, self-contained structure that allows interaction with commonly available analysis tools and experimental data bases; and,
  - It aims not only to provide this advanced computational capability, but also to change fundamentally the way that capability is developed, deployed, and maintained within the fusion program.
A NIMROD PHYSICS CALCULATION

- Time-dependent, nonlinear evolution of a slowly growing, non-ideal MHD instability at large Reynolds' number \((S \sim 10^6)\)

- Computed on T3E at NERSC:
  - 8 dependent variables on 49,252 vertices
  - 154 PEs
  - 40,870 time steps
  - 64,680 CPU hours => 7.38 CPU years
  - 3.2 months wall clock time

- Increasing number of PEs has little effect because of causality

  This performance is only marginally acceptable
HIGH END NEEDS FOR MISSION PERFORMANCE

• The largest, fastest systems available (can never be too big, or too fast)

• Optimize performance for long runs
  • Specialized systems for time dependent problems?
  • Longer residence time for jobs?
  • Revisit the MP paradigm?

• Maximize memory for large Reynolds' number calculations

• Offload smaller jobs to mid-range systems

• ????
MID-RANGE NEEDS FOR MISSION PERFORMANCE

• Most fusion computing capacity does not require high-end computing

• Lack of generally available mid-range computing systems
  • Beowulf/Linux clusters
  • "Tens of dozens" of processors
  • Much cheaper than supercomputers, but too expensive for small groups/institutions

  Back to pre-CTRCC computing situation

• Needed for debugging, and preparing large problems

• These jobs are clogging the queues on present DOE supercomputers
NETWORKING AND OTHER SUPPORT

- Large data "farms" for archiving data (many Gbytes/run)
- Fast networks for transferring data between central and local facilities
- Software and hardware to enable team interaction
- High end graphics, and the capability to use it remotely (in the real world of firewalls, etc.)
- Debugging and performance analysis tools
- Mathematical software libraries
  - F90. Don't insist on C++
- ???
VISION TO SUPPORT THE FUSION MISSION

• The largest, fastest supercomputer (of course!), but...
  • Configuration optimized for time dependent problems requiring many time steps (inherently sequential)
  • Access limited to only the largest, programmatically important problems

• Centrally available mid-range computing facility
  • Provide needed capacity for majority of fusion applications, and eliminate institutional monopolies
  • Offload jobs from the supercomputer

• Storage, networking, communication, and graphics to facilitate code and data comparisons, and enable remote collaborations
**SUMMARY**

- The fusion mission is not optimally served by the MP computer paradigm
  - Need specialized architectures for time dependent problems
- Present DOE facilities are not configured in a way that well serves the fusion computing mission
- Need for centralized mid-range computing facility
- Remote collaborations are the reality
  - Need networks, hardware, and software that facilitates these efforts