Workshop Goals & Process

Large Scale Computing and Storage Requirements for Fusion Energy Sciences

Joint FES / ASCR / NERSC Workshop

August 3-4, 2010
Logistics: Schedule

• Agenda on workshop web page

• Mid-morning / afternoon break, lunch

• Self-organization for dinner

• 9 “science areas,” one workshop
  – Science-focused but cross-science discussion
  – Explore areas of common need (within FES)

• Breakout sessions Weds AM
Why is NERSC Collecting Computational Requirements?

• Help ASCR and NERSC make informed decisions for technology and services.

• Input is used to guide procurements, staffing, and to improve the effectiveness of NERSC services.
  – Includes hardware, software, support, data, storage, analysis, work flow
  – Time frame: 2014

• Result: NERSC can better provide what you need for your work.
Logistics: Case Studies

• One co-lead (for each science area)
  – help roll up discussions into major case studies

• Case Studies:
  – Narrative describing science & NERSC reqmts
  – Audience is NERSC, DOE program managers
  – Initial set suggested by John Mandrekas
    • Minimum set to capture FES mission and unique NERSC requirements
  – Encourage participation by all; roundtable
Logistics: Worksheets

• Web Worksheets: “Reference Material”
  – Based on NERSC info
  – Summary of projects as we know them
  – Good point of departure
  • A framework for discussion
  • But not necessarily the entire story
Logistics: Final Report Content

• Format similar to ESnet
  – But NERSC requirement space much broader than Esnet
  – See “Reference Material” on web site
  – Contents
    • Executive summary,
    • ~2-page case study reports,
    • NERSC synthesis of all results
Logistics: Final Report Schedule

• Case studies due to NERSC ........ Aug 27
• NERSC draft report ..................... Oct 1
• Participants review period ............. Oct 22
• NERSC Near final ........................ Nov 5
• BES AD approval ........................
• NERSC Revisions .......................
• Final Report posted on Workshop Webpage
Examples of Information Sought

• Type of simulation, #, reason for #, algorithms, solver
• Parallelism: method, weak or strong scaling, implementation, concurrency, limits
• Key physical parameters and their limits:
  – spatial resolution, # of atoms/energy levels, integration range, …
• Representative code
• Key science result metrics and goals
Examples of Information Sought

• Typical science process (workflow)
• Data: amount stored / transferred for input, results, and fault mitigation
• Special needs for data intensive projects
  – Grids, gateways, workflows, provenance,`
• Special query regarding multicore/manycore

• How all of this is
  – Driven by the science
  – Likely to change and why
Final Thoughts

• Requirements characterization process is not complicated.

• Mutually beneficial.

Length, Spatial extent, #Atoms, Weak scaling

Time scale Optimizations, Strong scaling

Convergence, systematic errors due to cutoffs, etc.

Initial Conditions, e.g. molecule, boundaries, Ensembles

Simulation method, e.g. DFT, QMC or HF/SCF; LES or DNS