Computer Science and Mathematics Division Offsite

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Division Director

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Agenda: Background

9:00  The Division
      Overview of the division  Maccabe

9:30  Key Activities
      IAA, XLab & Math/CS Institute  Geist
      Exascale (OLCF-3, ASCR, DARPA UHPC, etc)  Geist
      ESSC  Poole
      Climate Modeling  Drake
      Keeneland  Vetter

10:45  BREAK

11:15  Key Activities
      Hybrid Multicore Consortium  Maccabe
      CAAR  Turner
      Hubs (NE Modeling and Simulation)  Turner
Agenda: Planning

12:00   SWOT
  Think about these throughout the morning
  *Document*: lists of strengths, weaknesses, threats and opportunities

1:00    BREAK

1:30    Relationships outside of the division
  Other directorates, other labs, universities, sponsors
  *Document*: list of key relationships to be managed

2:15    Vision and Mission
  Vision: what are we trying to accomplish as an organization
  Mission: critical things to work on and not to work on
  *Document*: updated vision and mission statements

3:00    BREAK
Agenda: Conclusions

3:30 Administrative Support
   Needs and expectations
   Hiring – how are we doing?
   Communication tools and mechanisms
   Calendar/schedule for significant activities

4:30 Path Forward
   Document: tangible steps with measurable outcomes

What are the three most important things for us to do as a division?
Goals for today

• Why does CSMD exist?
  – What are we trying to accomplish?
  – How do we relate to other groups in CCSD?
  – How do we relate to other groups at ORNL?
  – How do we relate to the broader community

• Planning
  – alignment of strategy, tactics, and funding
    • decide what you want to do
    • decide what you can get funded
  – communication tool

• Broad context
  – Exascale computing
  – Climate change research
  – Nuclear energy
• This is a complex organization
  – there are no simple relationships
  – you have to know everything to know anything

• This is good
  – discourage stove pipes
  – encourage inter- (cross-, multi-) disciplinary research

• Lots of challenges in supporting all of the activities
  – my day job is facilitation
Conceptual Organization of CSMD

Scale (Massive Parallelism)

- Computational Astrophysics
- Computational Earth Sciences
- Comp Materials Sciences
- Molecular Biophysics

Systems

- Computational Engineering and Energy Sciences
- Complex Systems

Apply

- Computational Chemistry
- Computer Science Research
- Future Technologies

Build

- Performance Tools
- Applied Mathematics
- Statistics and Data Science

Think
Supporting Computational Science

• Computational science belongs in CSMD
  – provide a common context for supporting the needs of scientific research based on computation
    • this is easily lost without a centralized focus on computation
  – maintain focus on computation at scale
    • lots more computation can (and should) be done in the (non-computation) science divisions
  – provides the essential context for computer science and mathematics research

• Funding and other forms of support is challenging
  – OASCR doesn’t fund science
  – Other parts of SC don’t fund computing
  – Really need support across multiple organizations
## CSMD and CSED
the two CCSD Research Divisions

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<thead>
<tr>
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<th>CSMD</th>
<th>CSED</th>
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</thead>
<tbody>
<tr>
<td><strong>Primary Funding</strong></td>
<td>DoE then DoD</td>
<td>DHS, DoD, IC, and then DoE</td>
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<tr>
<td><strong>Conceptual Focus</strong></td>
<td>Computation at Scale</td>
<td>Broad applications of computation</td>
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<td><strong>Primary Activity</strong></td>
<td>Development and application of methods and tools Utility-driven</td>
<td>Application and development of methods and tools Applied</td>
</tr>
<tr>
<td><strong>Relation to Universities</strong></td>
<td>Partners in changing the world</td>
<td>Providers of unique talents and skills</td>
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Complex Systems group is a critical bridge between these divisions
CSMD and NCCS
Both focus on DoE Computation at Scale

• NCCS: operation of a computing facility
• CSMD: research in fundamental methods and tools used in computation

• Guiding principles
  – research activity is managed in CSMD
  – operation activity is managed in NCCS

• General observations
  – much of the work in CCSD is advanced development which falls in the “excluded middle”
  – contracting between divisions can support projects that have aspects of research and operations (need to be careful about asymmetry)
  – matrixed reporting allows individuals to move between roles easily
Is ORNL Facilities for Science?

• OMB: SC Labs provide facilities for the national and international research community
• Facilities are certainly a big part of the ORNL mission: we do computing and neutrons
• Traditional facilities model:
  – research community decides what they need,
  – someone wins a proposal to site the facility,
  – the community spends 5 years designing the facility,
  – the facility is built to the specifications,
  – the facility operates for 20+ years
• Computing facilities defy this model
  – rate of change in computing capabilities
  – commodity shifts, but drives our designs
  – research community must be part of the team
CSMD and Academics

• Relations with universities are critical to CSMD
• Academics are partners
  – shared goal of advancing disciplines
  – we need to have impact on curriculum
  – source of the next generation of scientists
• Contrasts: Academics have:
  – state funding for base pay and offices
  – more autonomy in pursuit, less autonomy in activity
  – divided responsibilities
• The NSF problem: NSF doesn’t fund 12 months
• Joint appointments are important continuing these relationships
Key challenges

• Computational Sciences
  – maintaining visibility and contributions to science
  – true multidisciplinary funding

• Computer Sciences
  – relationship to operations (NCCS)
  – lack of consistent program support in Washington (appears to be getting worse)

• Mathematics
  – visibility – embedded not entrenched
  – lack of consistent program support in Washington (but improving)
CCSD Level 1 Plan

• Cynical Perspective
  – 38 pages that no one reads
  – 15 objectives on 5 pages
  – 12+ pages on staffing requirements
  – very easy to miss the forest for the trees

• Why this matters
  – laboratory process for managing resources and risks
  – tool for communicating activities and needs
  – provides documentation to support decisions

• Part of understanding where CSMD fits
ORNL Scientific Core Capabilities

1. Condensed Matter Physics and Materials Science
2. Accelerator Science and Technology
3. Computational Science
4. Climate Change Science
5. Chemical and Molecular Science
6. Biological Systems Science
7. Environmental Subsurface Science
8. Plasma and Fusion Energy Sciences
9. Nuclear Physics
10. Applied Materials Science and Engineering
11. Advanced Computer Science, Visualization, and Data
12. Applied Nuclear Science and Technology
13. Chemical Engineering
14. Systems Engineering and Integration
15. Large-Scale User Facilities/Advanced Instrumentation

Modeling and simulation is relevant to virtually every capability
Managing Management Activities

• Managing
  – Time sheets (cost accounting)
  – Performance evaluation
  – Business plans
  – Finding funding: the almighty dollar

• Mentoring
  – Participation in broad research community
  – Developing and following your scientific intuition
    • encouraging “play time”
  – Defining the discipline
Key points

- Computational Science provides the essential foundation for this division
- Utility-based (mission focused) research, emphasis on “products”
- Computation at scale
- Development of fundamental methods and tools
- Inter-disciplinary: contribute to both disciplines
- Balance between academic and industrial styles
- Matrixing is everywhere
  - Line management: similar roles (research or operations)
  - Project management: distinct roles (operations and research)