Accelerating Innovation in DOE through R&D Integration: The Role of Advanced Computing

Portfolio Working Group Review of R&D Integration Opportunities

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Background

- **Integrated planning, investment and assessment of R&D programs across the science and technology programs at DOE has several strategic purposes**
  - **Reduce risk**
  - **Accelerate achievement**
  - **Help enable the U.S. to capitalize on investments in R&D**
  - **Create domestic economic advantage**
- **Bridging the "valley of death" between basic science and technology development**

Background

- **Over the last year and a half, the three DOE Under Secretaries formed a Science & Technology Council (S&T Council) and initiated a process to identify high impact R&D areas ripe for integrated investment.**
- **Subsequent discussions between programs have identified a number of R&D areas which may benefit from better integration across DOE.**
- **The S&T Council highlighted six areas of opportunity for R&D integration in order to accelerate the pace of S&T development in support of DOE mission goals.**

R&D Integration Areas Reviewed by PWG

- **The PWG reviewed the opportunities and resources across DOE relevant to these areas.**
  - **Advanced Mathematics for Optimization of Complex Systems, Control Theory, & Risk Assessment**
  - **Electrical Energy Storage**
  - **Carbon Dioxide Capture and Storage**
  - **Characterization of Radioactive Waste**
  - **Predicting High Level Waste System Performance over Extreme Time Horizons**
  - **High Energy Density Laboratory Plasmas**

PWG Review

The PWG focused on the FY09-13 DOE budget:

- **Examples of integration activities within targeted budget**
- **Examples of potential integration activities which could benefit from additional funding through coordinated investments**
- **Ways to improve integration planning for the FY10-14 budget cycle**

PWG Review: Integration Opportunities

- **The PWG provided an overview of R&D efforts across the Department in each area enabling integrated decision making at the corporate level.**
- **In all the areas reviewed, opportunities for coordinated investment have been identified through recent joint technical workshops and reports.**
- **Discussions between programs have occurred in each of these areas, but to varying degrees.**
- **The production and strategic management of a joint roadmap for basic and applied R&D in each of these areas would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**

PWG Recommendations: Improving the planning/budget cycle

1. **S&T Council should establish structures to promote integrated planning such as joint roadmaps and coordinating councils**
2. **S&T Council should develop an independent review of FY10 integration efforts that is distanced from any single program office**
3. **Prioritization/identification of the DOE R&D integration activities that will be analyzed during the FY10 budget cycle should be completed by the S&T Council in September 2007**
4. **R&D integration planning for the FY10-14 budget should begin in September 2007**
5. **Budget guidance issued by Deputy Secretary and CFO should include a stronger focus on integration activities**

The Role of Advanced Computing in R&D Integration across DOE

- **Computation has emerged as one of the central mechanisms to promote improved R&D integration**
- **How can SC and ASCR better work with the applied programs at DOE to help transfer its expertise and know-how regarding computational tools, algorithms and methods across the "valley of death" between basic science and applied science and technology?**

The Role of Advanced Computing in R&D Integration across DOE

- **In program reviews and lab visits over the last year, Under Secretary Orbach often found that a primary impediment to substantial progress in various DOE applied programs arose from obsolete computational methods / resources:**
  - **Not utilizing first principles models**
  - **Not utilizing state of the art computational facilities**
  - **Not utilizing modern algorithms**
  - **Not maintaining resources (technical staff and funding) to implement methods**
- **Best Practices (so far) for R&D Integration:**
  - **Substantive SC/Applied Program discussions**
  - **Technical Workshops**
  - **R&D Roadmap**
  - **Active Coordinating Committee (e.g., EMaCC)**
  - **Coordinated budgeting**

The Role of Advanced Computing in R&D Integration across DOE

- **Important first step – recent ASCR workshops have highlighted some of these opportunities:**
  - **Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems, August 15-17, 2006**
  - **Mathematical Research Challenges in Optimization of Complex Systems Workshop, December 7-8, 2006**
  - **Computational Subsurface Sciences Workshop, January 9-12, 2007**
- **They helped to shape opportunities relevant to:**
  - **Characterization of Radioactive Waste**
  - **Advanced Mathematics for Optimization of Complex Systems, Control Theory, & Risk Assessment**
  - **Carbon Dioxide Capture and Storage *and* Predicting High Level Waste System Performance over Extreme Time Horizons**

The Role of Advanced Computing in R&D Integration across DOE

- **Under Secretary Orbach expects that through integrated planning and budgeting following current best practices, the opportunities identified can lead to additional, integrated programmatic initiatives in coordination with applied programs in the future**
- **However, having a transformational impact on the strategic goals of the applied programs requires integration that goes beyond this programmatic coordination.**

The Role of Advanced Computing in R&D Integration across DOE

- **What is the appropriate role of ASCR and its facilities in knowledge transfer to DOE programs outside of SC?**
- **How can we help improve the state of computation in the rest of the department without compromising core research?**
- **How do we explain any such role to decision makers in OMB and Congress without complaints of mission creep?**
- **How do we realize the *ASCR 10-year Vision* for exascale computation in support of the energy, environmental, and security missions of DOE?**

Backup Slides

Portfolio Reviews: 2005-2007

- **Laboratory Working Group (Senior Managers of DOE national labs)**
  - **Created by the Undersecretary for Energy in 2005 to examine applied technology portfolio**
- **Integration Working Group (Federal Managers)**
  - **Created by Undersecretary for Energy in 2005 to model the benefits of the applied technology portfolio**
- **Portfolio Working Group (PWG)**
  - **Created by Undersecretary for Science in 2006 in response to the Program Reviews mandated by Energy Policy Act 2005**
- **A-Teams (CFO, HR, OECM, and PI)**
  - **Created annually to review program office budget proposals during DOE's Corporate Program Review. Designed to bring a diversity of opinions and analytical perspectives to support decisions made by senior leadership**

Disclaimers

- **Funding by multiple programs in a given integration area does not necessarily imply planned joint solicitations.**
- **Common funding also does not necessarily imply that prior discussions or coordination beyond technical workshops has occurred.**
- **The six areas reviewed do not all currently have effective coordination efforts, nor do they represent an exhaustive list of coordination efforts underway in the Department.**

Advanced Mathematics for Optimization of Complex Systems, Control Theory, & Risk Assessment

Advanced math for understanding, controlling, and optimizing complex systems such as the electric grid, novel combustion systems and industrial processes, and advanced nuclear reactors.

Relevant workshops & reports

- ***Breaking the Biological Barriers to Cellulosic Ethanol: A Joint Research Agenda*** (December, 2005 - BER, BES, EE)
- ***Workshop on Simulation and Modeling for Advanced Energy Systems*** (August, 2006 - NE, ASCR)
- ***Report on the Mathematical Research Challenges in Optimization of Complex Systems*** (December 2006 Workshop - ASCR, NE, OE, FE, EM)
- **6 other workshops and reports**

At Target

- Basic mathematical and computational research (SC/ASCR)
- Models for materials relevant to biofuels, hydrogen fuel cells, vehicle electrical energy storage (EERE)
- Grid control and optimization (OE)
- Uncertainty analysis for advanced nuclear fuel cycles (NE)

Additional Opportunities

- Models for materials relevant to hydrogen production, advanced vehicles (EERE)
- Increase the pace of development of nuclear fuel cycle simulation codes (NE)

Advanced Mathematics for Optimization of Complex Systems, Control Theory, & Risk Assessment

Conclusions

- **Opportunities for coordinated investment have been identified in this area through recent joint technical workshops and reports.**
- **The production and strategic management of a joint roadmap for basic and applied R&D in this area would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**
- **R&D coordination discussions between SC/ASCR and several applied programs have been initiated.**
- **Additional funding to NE and EE could significantly enhance their ability to conduct basic science handoffs.**

Electrical Energy Storage

Electrical energy storage is critical at the largest scales for the electric grid, at a mid-scale for novel hybrid and plug-in electric vehicles, as well at a small-scale for electronics and sensors.

Relevant workshops & reports

- ***Basic Research Needs Workshop for Electrical Energy Storage*** (April, 2007 - BES, OE, EE)

At Target

- Basic research in some areas of chemical and capacitive storage sciences (SC/BES)
- Limited application of basic research to novel, high energy density storage technologies, and incorporating them into devices and systems (OE - grid, EERE – vehicles)

Additional Opportunities

- Can address all relevant areas of chemical and capacitive storage sciences discussed in recent energy storage workshop (SC/BES)
- Can address all research areas identified for utility scale energy storage (OE) and hybrid electric vehicle energy storage (EERE) in recent energy storage workshop

Electrical Energy Storage

Conclusions

- **Opportunities for coordinated investment have been identified in this area through a recent joint technical workshop and report.**
- **The production and strategic management of a joint roadmap for basic and applied R&D in this area would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**
- **R&D integration between SC/BES, OE and EE has been initiated through discussions at the program level and should be sustained.**
- **The basic (SC/BES) and applied (OE and EE) programs have agreed that integration efforts which are now underway could be greatly enhanced through coordinated additional funding in this area.**

Carbon Dioxide Capture and Storage

Achieving the goal of zero carbon emissions from fossil fuel usage requires efficient and cost-effective capture of CO_2 as well as safe and reliable storage, posing substantial science and technology challenges.

Relevant workshops & reports

- ***Carbon Sequestration Research and Development*** (December, 1999 – FE, SC)
- ***Computational Subsurface Sciences Workshop Report*** (January, 2007)
- ***Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems*** (February, 2007)
- ***Carbon Sequestration Technology Roadmap and Program Plan 2007*** (May 2007, FE)
- ***One other report/workshop***

At Target

- Subsurface carbon storage, role of microbes and biomass in carbon cycling, GTL Research Center for Carbon Cycling (SC/BER)
- Basic geosciences relevant to geological storage of carbon, novel materials for combustion (SC/BES)
- Development of technologies for direct capture and geologic storage. (FE)

Additional Opportunities

- Pilot scale testing of new capture technologies, simulation of full scale plant with capture (FE)
- Accelerate large scale field tests of geological storage, use field tests to verify risk assessment methodologies, predictive models and monitoring approaches (FE)

Carbon Dioxide Capture and Storage

Conclusions

- **Opportunities for coordinated investment have been identified in this area through recent joint technical workshops and reports.**
- **An update of a joint SC-FE roadmap for R&D in this area produced in 1999 would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**
- **R&D cooperation activities in the area of S&T Needs for Risk Assessment for Geological Carbon Storage have been initiated.**
- **Several R&D integration areas identified by workshops and reports are supported at the Target level in the outyears in SC/BES and SC/BER.**
- **Additional funding to FE can greatly accelerate innovation in this area, particularly if further leveraged by coordinating investments in the relevant basic sciences.**

Characterization of Radioactive Waste

Address critical unanswered scientific questions to facilitate the stabilization, long-term storage, treatment, and ultimate disposal of radioactive waste.

Relevant workshops & reports

- ***The Path to Sustainable Nuclear Energy***
  Basic and Applied Research Opportunities for Advanced Fuel Cycles (September, 2005)
- ***Basic Research Needs for Advanced Nuclear Energy Systems*** (July, 2006 - NE, BES)
- ***Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop*** (August, 2006 - NE, NP, ASCR)
- ***National Academy of Sciences: Science and Technology Needs for DOE Site Cleanup, EM Roadmap*** (March, 2007- EM)
- ***2 other workshops or reports***

At Target

- Understand basic science relevant to transport and fate of contaminants at Savannah River Site (SC/BER)
- Physics and chemistry of the heavy elements for nuclear energy (SC/BES)
- Nuclear physics and data to support advanced nuclear fuel cycles (SC/NP)
- Enhance understanding of subsurface fate and transport and tank waste chemistry. (EM)
- Characterize fuel cycle waste streams (NE)

Additional Opportunities

- Address many basic research areas in materials, chemistry identified in workshop reports (SC/BES)
- More complete nuclear data and improved integration with energy program (SC/NP)
- New projects for advanced remediation and tank waste cleanup methods (EM)

Characterization of Radioactive Waste

Conclusions

- **Opportunities for coordinated investment have been identified in this area through recent joint technical workshops and reports.**
- **The production and strategic management of a joint roadmap for basic and applied R&D in this area would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**
- **R&D cooperation between SC/BES, SC/BER, SC/NP, EM and NE has progressed and should be sustained and encouraged through funding at the Target level.**
- **Additional funding for SC/NP can enhance coordination with NE.**
- **SC/BES and EM have both indicated that integration efforts which are now underway can be greatly enhanced through coordinated additional funding in this area.**

Predicting High Level Waste System Performance over Extreme Time Horizons

Using science to reduce the uncertainties in the prediction of the performance of engineered and natural containment barriers for high level radioactive waste over extreme time horizons.

Relevant workshops & reports

- ***Basic Research Needs for Advanced Nuclear Energy Systems*** (July, 2006 - NE, BES)
- ***Computational Subsurface Sciences Workshop Report*** (January, 2007)
- ***Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems*** (February, 2007)
- ***National Academy of Sciences: Science and Technology Needs for DOE Site Cleanup, EM Roadmap*** (March, 2007)
- ***2 other reports/workshops***

At Target

- Modeling and simulation of contaminant distribution and flow (SC/ASCR)
- Physics and chemistry of the heavy elements (SC/BES)
- Research to better assess integrated disposal system long-term performance and enhance long-term performance evaluation and monitoring (EM)

Additional Opportunities

- Address many basic research areas in materials, chemistry identified in workshop reports (SC/BES)
- Accelerate development of enhanced long-term performance evaluation and monitoring (EM)

Predicting High Level Waste System Performance over Extreme Time Horizons

Conclusions

- **Opportunities for coordinated investment have been identified in this area through recent joint technical workshops and reports.**
- **The production and strategic management of a joint roadmap for basic and applied R&D in this area would enable productive and timely resource allocation to address significant gaps, overlaps, and emergent opportunities.**
- **R&D cooperation between SC/BES, SC/BER, SC/ASCR, and EM has progressed and should be sustained.**
- **SC/BES and EM have both indicated that integration efforts which are now underway can be greatly enhanced through coordinated additional funding in this area as described in the recent EM technology roadmap.**

High Energy Density Laboratory Plasmas

Laboratory-scale science of matter subjected to extreme conditions of temperature and density, which is expected to enable significant progress in astrophysics, cosmology, nuclear physics, plasma science, inertial fusion energy, and nuclear stockpile stewardship

Relevant workshops & reports

- ***Frontiers for Discovery in High Energy Density Physics*** (July 2004, OSTP)
- ***High-Energy-Density Laboratory Plasma Physics Research Workshop*** (May 2007 – OFES, NNSA/DP)
- ***Interagency Taskforce Report on High Energy Density Physics*** (in press, NRC)
- ***4 other national reports***

At Target

- Inertial fusion fast ignition, high-mach-number plasma jets, dense plasmas in ultrahigh magnetic fields, heavy-ion beam science (SC/FES)
- University grants in HEDLP and support of facility user programs (NNSA/DP)

Additional Opportunities

- Support of focused research on priority scientific activities and expanded user programs, as defined by the workshop process (NNSA/DP)

High Energy Density Laboratory Plasmas

Conclusions

- **Opportunities for coordinated investment have been identified in the science of high-energy-density laboratory plasmas (HEDLP) through recent joint technical workshops and reports.**
- **A joint SC-NNSA program has been established for HEDLP and budget planning to ensure productive and timely resources to address significant gaps, overlaps, and emergent opportunities.**
- **In FY 2008, the joint program will issue a combined solicitation for university activities.**
- **Planning is needed now to capitalize on scientific opportunities enabled by key facilities that that are becoming available in this area, including the National Ignition Facility.**