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SciDAC-e: Updates, Highlights, and Lessons Learned

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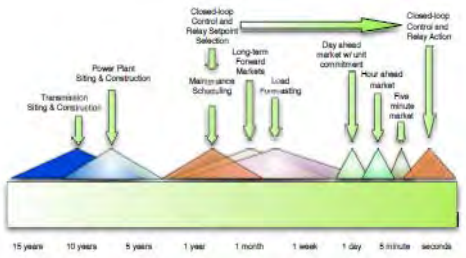
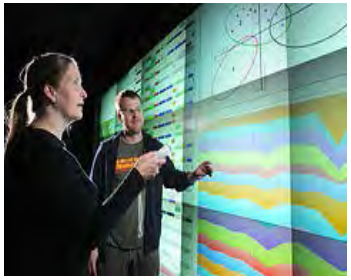
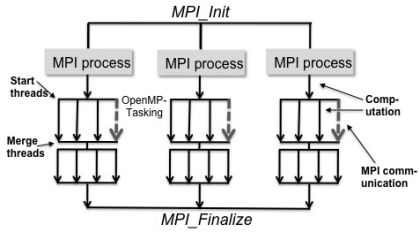
SciDAC-e is in Three Parts

- What it is:
  - One-time stimulus of applied mathematics & computer science research efforts to establish computational foundation to advance the DOE mission across a wide range, including developing renewable energy sources and developing smart grids.

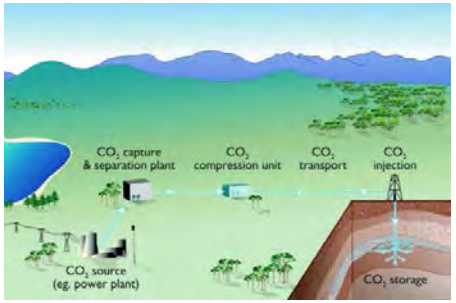


- Components of SciDAC-e
  - Research grants and national lab projects to develop mathematical techniques and algorithms to enable a bigger, better, and a smarter electric grid ($8.3M)
  - Approximately new 30 postdoctoral at ASCR facilities to offer assistance to SciDAC-e projects and other energy users awarded ASCR Leadership Computing Challenge (ALCC) allocation process ($10M)
  - Supplemental awards to ASCR SciDAC Centers and Institutes to support BES EFRCs to develop a high-performance computing capability relevant to the goals of the EFRC ($10.86M)





- Expected Impact:
  - Algorithms to simulate performance of electrical grids over a full range of operating conditions
  - Provide software environment and intellectual resources to EFRCs to meet computational goals



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SciDAC-e: applied math in support of DOE smart grid efforts

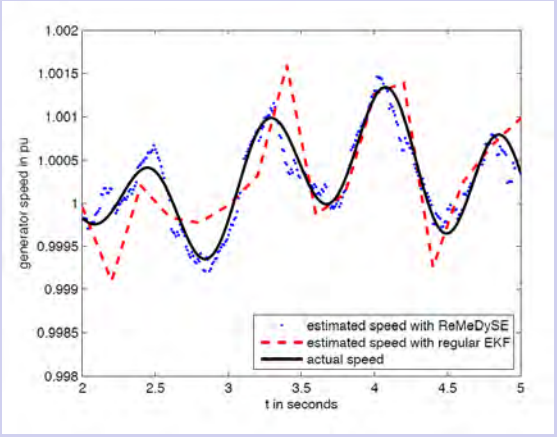
- Seven applied mathematics research projects funded since 2009
  - *Robust Optimization for Connectivity and Flows in Dynamic Complex Networks, Lead PI: Balasundaram (Oklahoma State)*
  - *Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms, Co-PIs: Bienstock (Columbia), Wright (UW-Madison)*
  - *Approaches for Rare-event Simulation and Decision Making, Lead PI: Shortle (GMU)*
  - *Analysis and Reduction of Complex Networks under Uncertainty, Marzouk (MIT), Knio (JHU), Ghanem (USC), Najm (SNL)*
  - *Optimization and Control of the Electric Power Systems, Co-PIs: Meza (LBNL), Thomas (Cornell), Lesieutre (UW-Madison)*
  - *Advanced Kalman Filter for Real-Time Responsiveness in Complex Systems, Co-PIs: Huang (PNNL), Welch (UNC-Chapel Hill)*
  - *Extending the Realm of Optimization for Complex Systems: Uncertainty, Competition and Dynamics, Lead PI: Shanbhag (UIUC)*

SciDAC-e Applied Math Highlights

Outage lines after a simulated failure of the US Eastern Interconnect grid

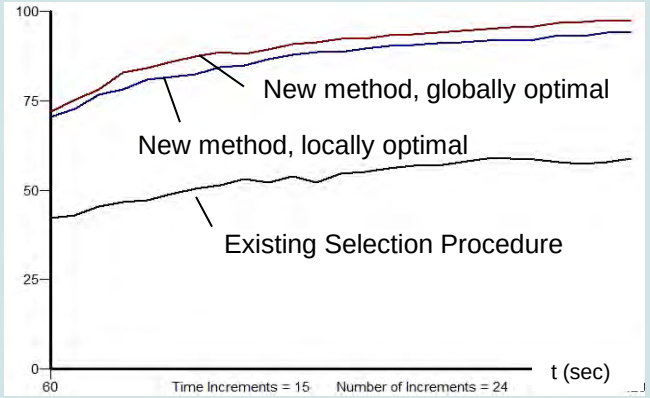
"Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms" (Bienstock et al) developed tools for simulating effect of grid design on cascade size and efficient methods for identifying weaknesses of a grid; software suite for simulating cascades and computing optimal controls on a parallel platform will be released soon.

"Power Grid Dynamic State Estimation Using Kalman Filter" (Huang, Welch, et al) developed a lightweight yet efficient reduced measurement-space dynamic state estimation method to capture the dynamic states in power systems, with a parallelized dynamic measurement selection procedure which incorporates only the most critical measurements into computation for higher reporting rates and accuracy.



Estimated generator rotor speed using ReMeDySE and regular Extended Kalman Filter

"New Approaches for Rare-Event Simulation and Decision Making" (Shortle et al) developed method for optimally allocating simulation budget (a) among alternate designs and (b) within splitting levels of each design



Probability of Selecting Design with Lowest Rare-Event Probability among 3 Designs

Petascale Initiative: ALCC Postdocs

As of 9/15/2011:

- ALCF: 11 postdocs total; one left after one year
- OLCF: 10 postdocs total; one resigned after 4 months
- NERSC: 9 postdocs total; one completed the two-year term and has started a new job

Some of the postdocs at NERSC and their coordinator, Alice Koniges.
http://www.nersc.gov/research-and-development/petascale-initiative/

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Petascale Initiative – ALCC Postdocs Review

- Project reports due 9/15/2011 were reviewed by ASCR, FES, and BES PMs in October
- Program leads at NERSC, ALCF, and OLCF have been apprised of our assessments, both kudos and requests for further information

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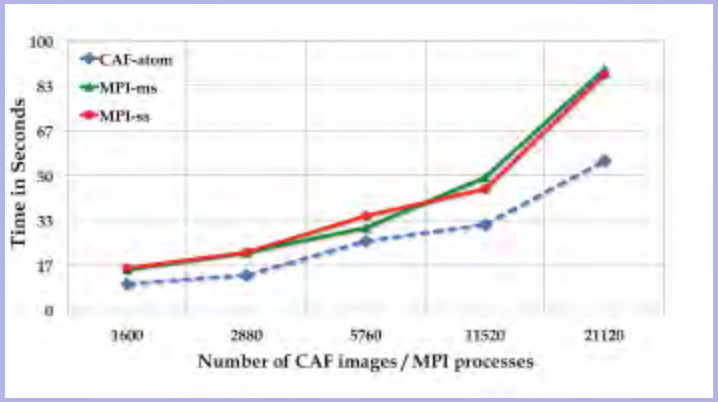
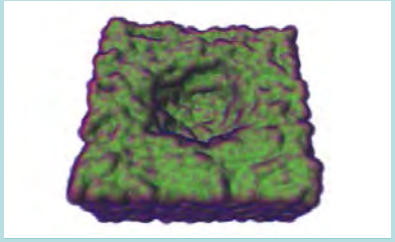
Petascale Initiative Highlights

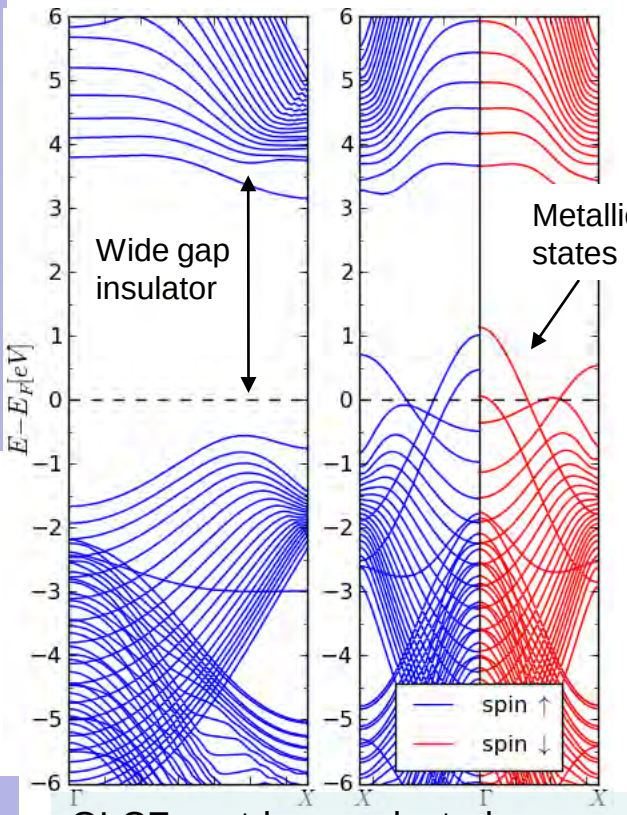
NERSC postdoc Robert Preissl optimized the performance of GTS, a fusion code, by improved concurrency using hybrid programming models and demonstrated weak scaling. Robert's paper is a finalist for SC11 best paper.



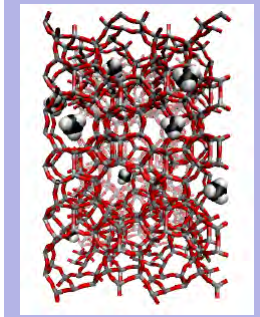
ALCF postdoc Aaron Knoll developed volume rendering techniques for EFRCs IACT and CEES to visualize material interfaces according to physical quantities (measured atomic radii)



Hydrogen vs Oxygen



OLCF postdoc Josh Hursey proposed Run-Through Stabilization (RTS) that enables an MPI application to continue execution even if one or more MPI processes fail. The RTS proposal is a candidate for inclusion in the next MPI standard.



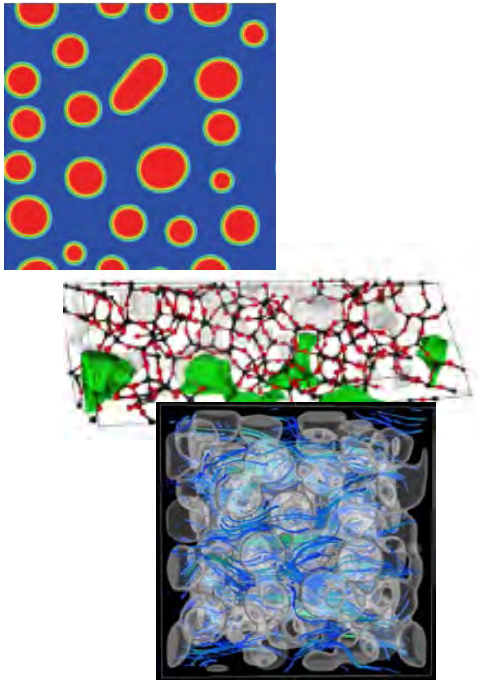
(former) NERSC postdoc Jihan Kim improved the CPU time an EFRC took to screen a dataset of 5 million materials from several years to a few weeks.

OLCF postdoc conducted theoretical study to discover that boron nitride nanoribbon, an insulator, may become metallic depending on how the ribbon terminates. This may have implications on engineering graphene nanoelectronics.

SciDAC-e Collaborations with Energy Frontier Research Centers (EFRCs)

Supplemental awards to SciDAC-2 Centers and Institutes to support BES EFRCs to develop a high-performance computing capability relevant to the goals of the EFRC

- 14 projects awarded in 2010 to APDEC, VACET, IUSV, TOPS, ITAPS, PERI, SDM
- Requests for no-funds extensions (NFEs) from University SciDAC-2 PIs with SciDAC-e projects have been approved; Laboratory SciDAC-e authorizations have been extended to August 2014
- Interim progress reports received & reviewed internally



EFRC Category	# Unique EFRCs	# EFRC Collaborations	Awards ($K)
Materials Under Extreme Conditions	2	3	1,095
Geological Flows & Carbon Storage	3	6	3,931
Solar & Photovoltaics	5	5	3,379
Material Design	1	2	951
Others	4	4	1,540
TOTAL	15	20	10,895

SciDAC-e EFRC Project Review

- Interim reports due 8/15/2011 were reviewed by ASCR & BES PMs in early September
- Project PIs have been informed of our assessment
- Of the 14 projects,
  - 9 projects considered making good progress
  - Clarifications and further information were requested from 4 projects (3 of the 4 have responded)
  - One project did not report substantial results; PI has been encouraged to take on bigger challenges
  - In addition, two projects have been requested to submit new letters of commitment from new EFRC Center Director (one has complied)

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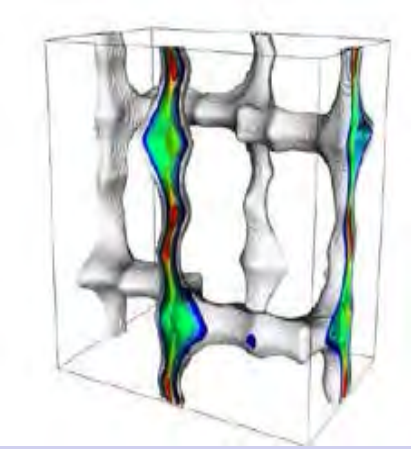
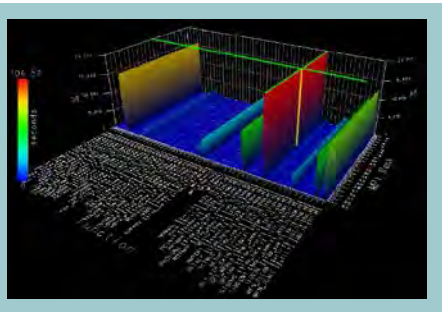
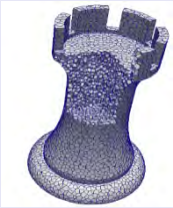
SciDAC-e EFRC Highlights

VACET (PI: Bethel & Haranczyk) visualized material constant (Henry coeff) for EFRC on geologic flows

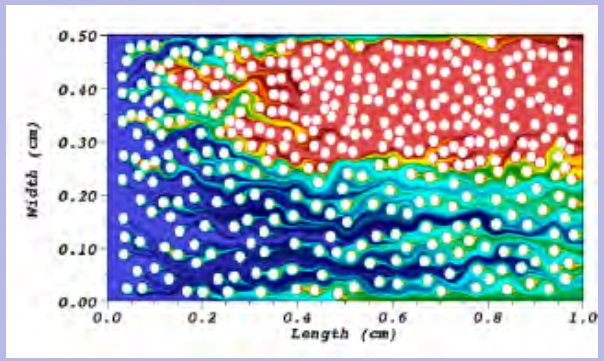


PERI (PI: Lucas) analyzed the performance of the EFRC's quantum MD code to explore tuning and optimizing strategy



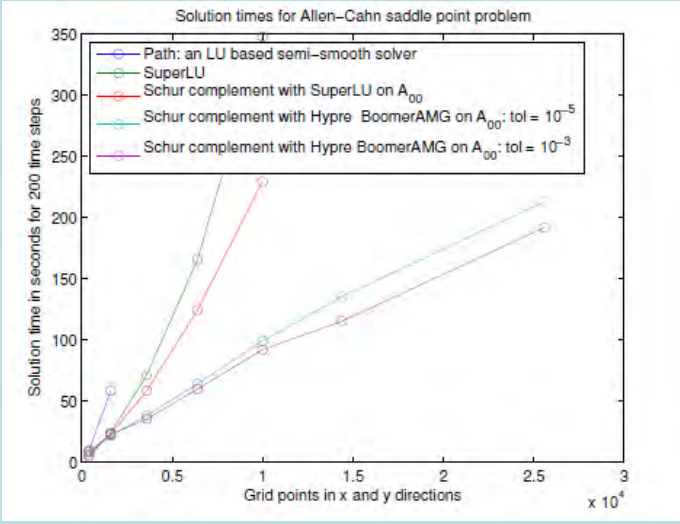


ITAPS (PI: Knupp) provided EFRC the only non-biased, fracture-conforming 3D Voronoi meshes that can be created on nonconvex domains for studies of fractures.



APDEC (PI: Trebotich) developed advanced numerical algorithms at the pore-scale for EFRC to model geologic flows

TOPS (PI: McInnes) demonstrated mesh-independent convergence for preconditioning in solving equations for mesoscale models for nuclear materials EFRC



Lessons Learned

- The SciDAC "infrastructure" (experience, personnel, breadth of technical expertise, organization) allows the rapid transfer of capabilities from ASCR SciDAC Centers and Institutes researchers to collaborating application scientists
  - Corollary: the SciDAC experience has trained ASCR researchers to "speak the language" of application scientists for timely deployment of computational expertise
- It is important to motivate and encourage today's students in computational sciences to acquire a broad set of skills and experiences
  - Corollary: it is also important that aspiring computational scientists be well-mentored and engaged.