Team Based Approaches in Computational Science

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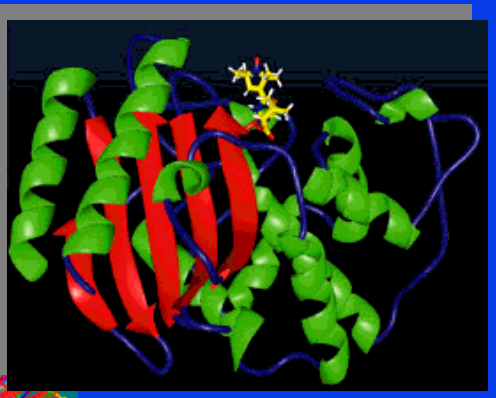
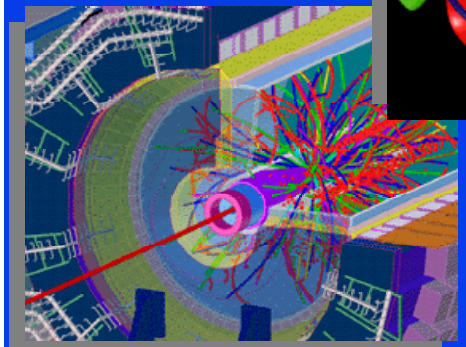
Lawrence Berkeley National Laboratory

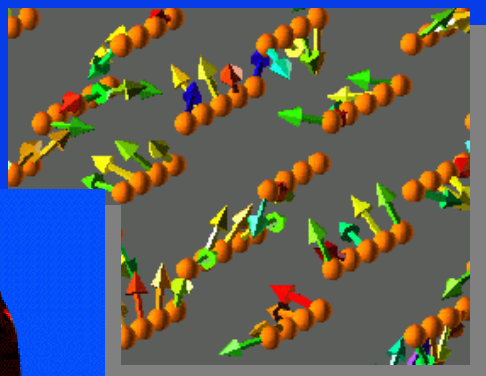
CSUPERB, San Jose, CA, January 16, 2004

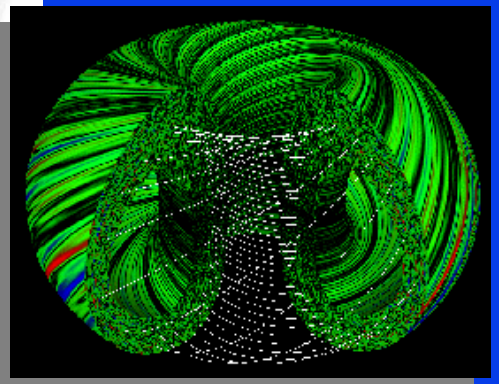
National Energy Research Scientific Computing Center

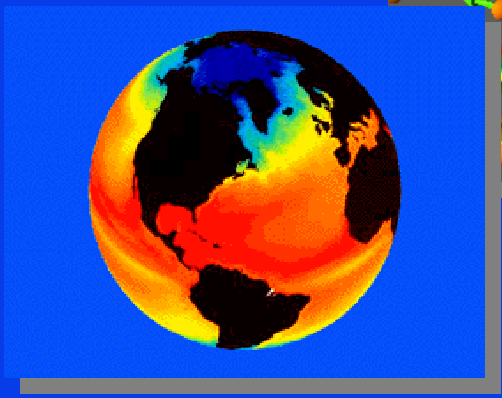




- Serves all disciplines of the DOE Office of Science
- ~2000 Users in ~400 projects
- Focus on large-scale computing







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NERSC Center Overview

BERKELEY LAB

- Funded by DOE, annual budget $28M, about 65 staff
- Supports open, unclassified, basic research
- Located in the hills next to University of California, Berkeley campus
- close collaborations between university and NERSC in computer science and computational science
- close collaboration with about 125 scientists in the Computational Research Division at LBNL

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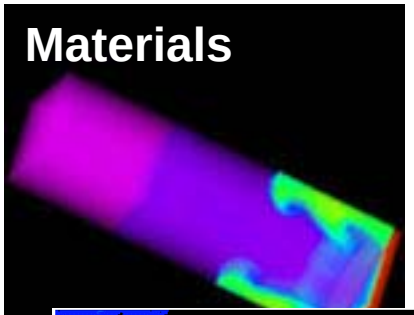
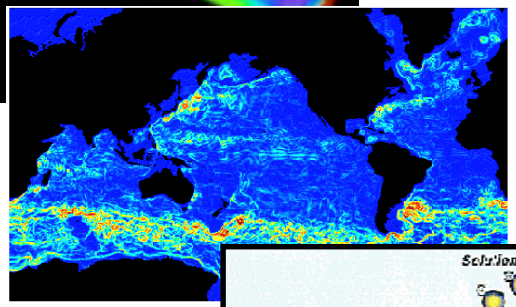
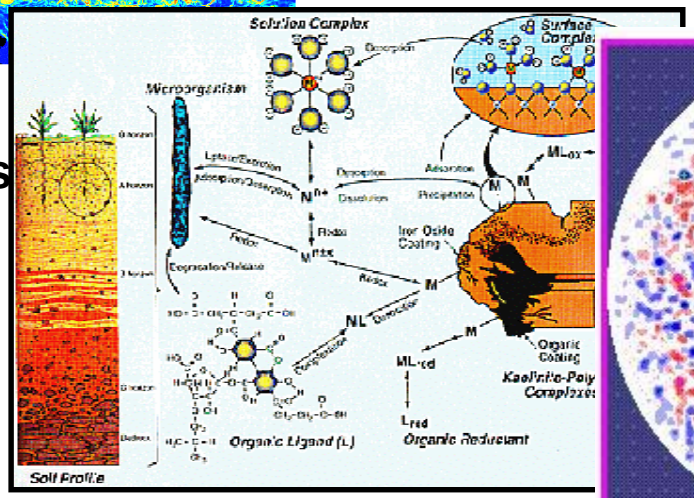
Scientific Discovery Through Advanced Computing

DOE Science Programs Need Dramatic Advances in Simulation Capabilities To Meet Their Mission Goals

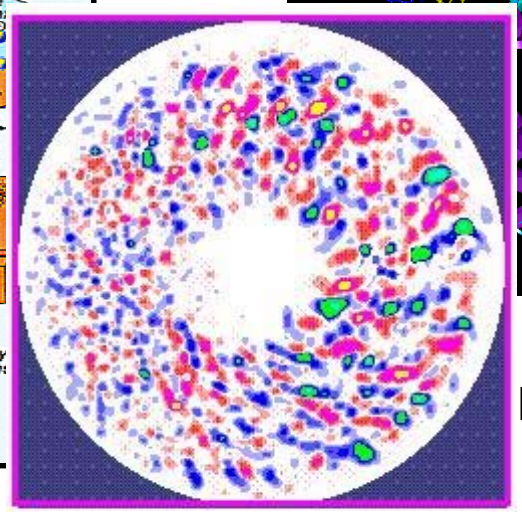




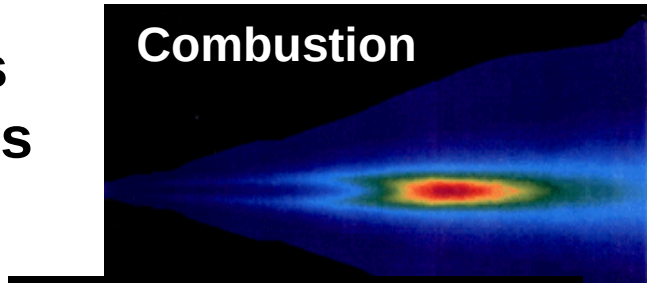
Global Systems

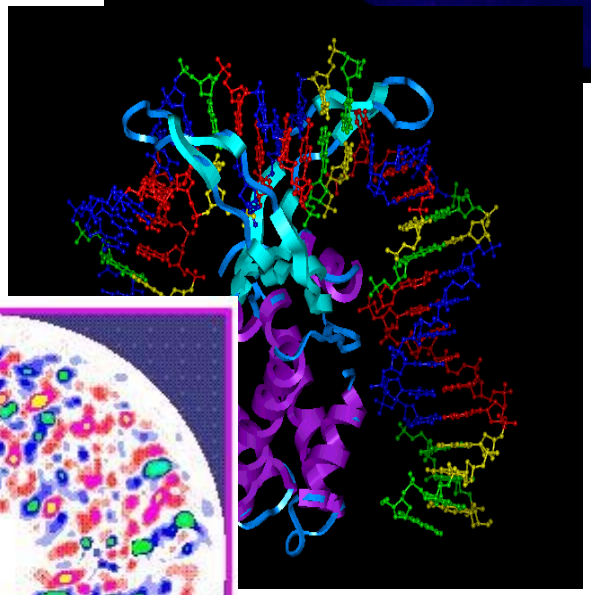


Subsurface Transport



Fusion Energy





Health Effects, Bioremediation

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Introduction – What is SciDAC?

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- SciDAC is a pilot program for a “new way of doing science”
- first Federal program to support and enable “CSE” and (terascale) computational modeling and simulation as the third pillar of science (relevant to the DOE mission)
- involves all DOE labs and many universities

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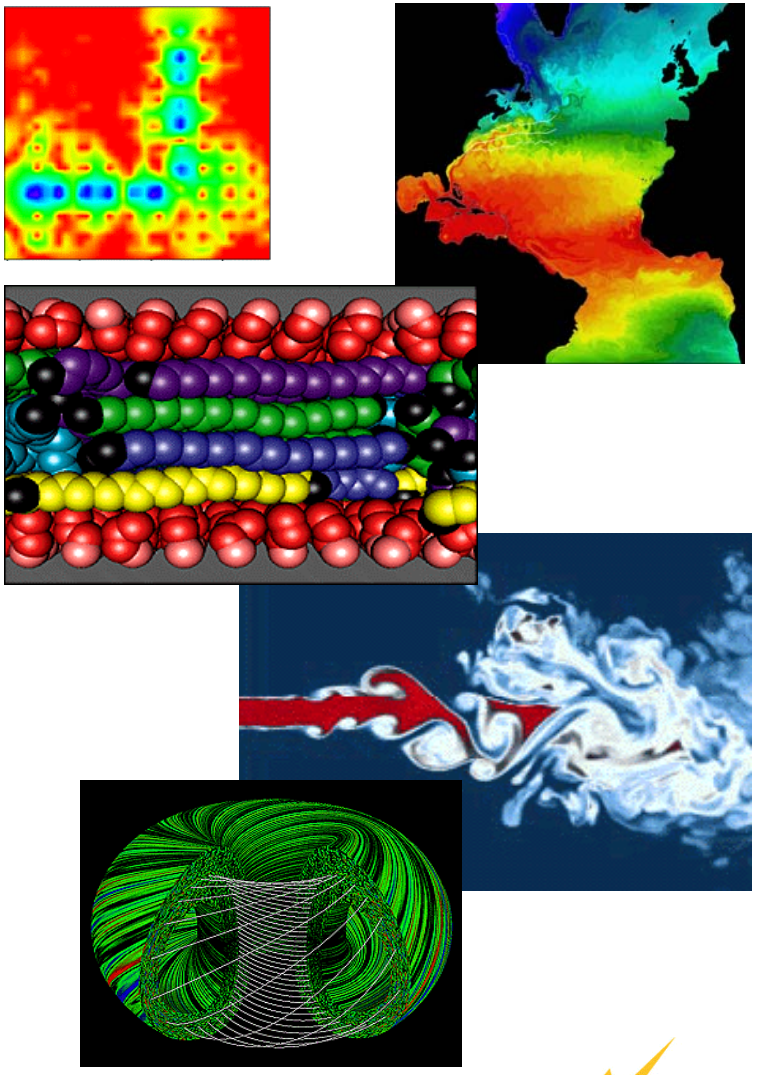
SciDAC

Berkeley Lab

- **Harness the power of terascale super-computers for scientific discovery:**
  - Form multidisciplinary teams of computer scientists, mathematicians, and researchers from other disciplines to develop a new generation of scientific simulation codes.
  - Create new software tools and mathematical modeling techniques to support these teams.
  - Provide computing & networking resources.



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Science in the 21st Century is Distributed!

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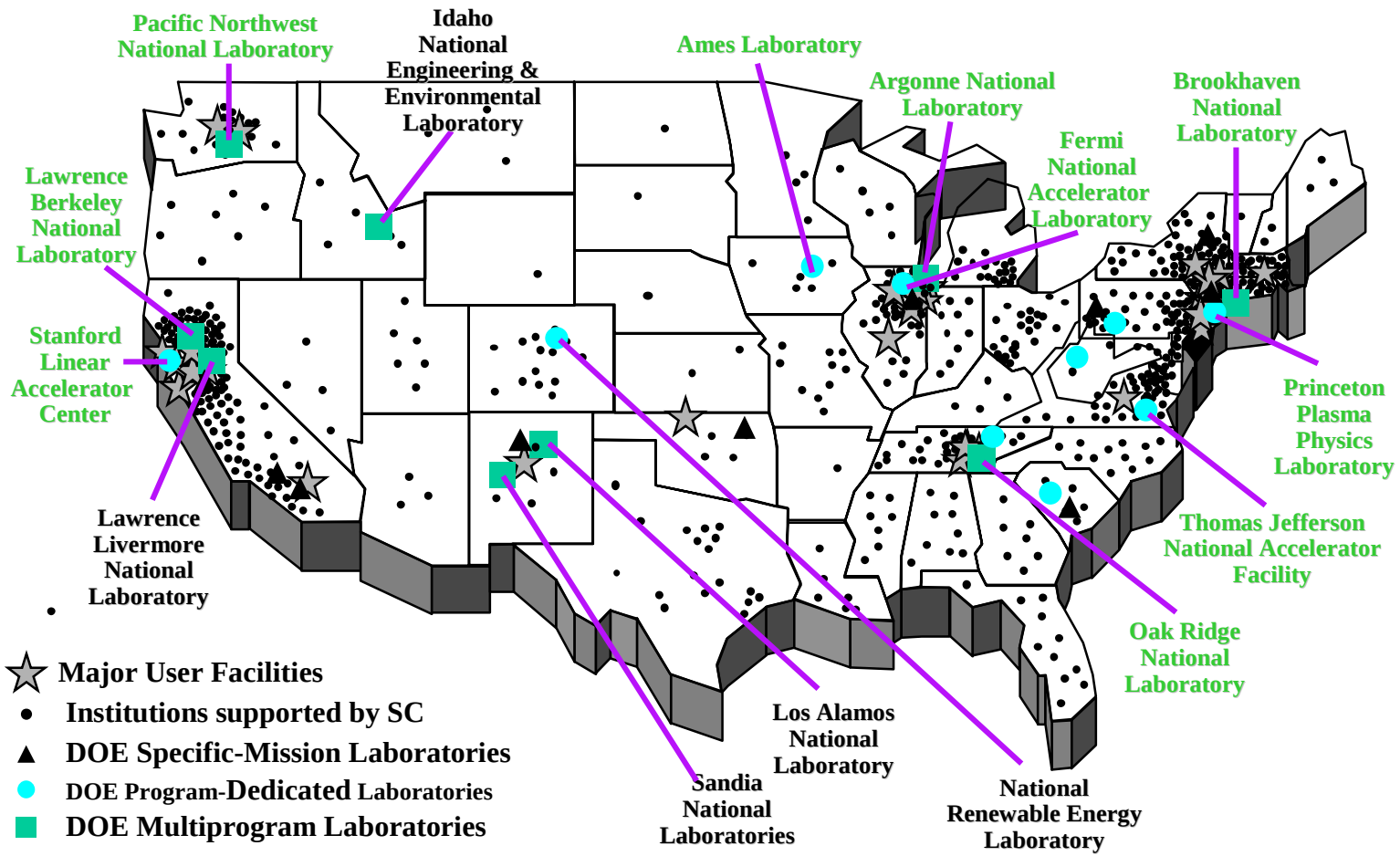
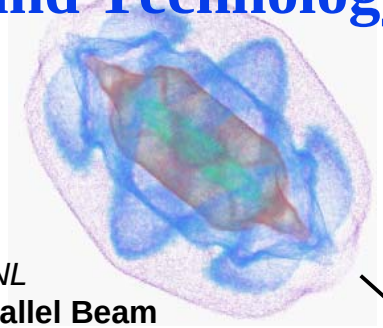
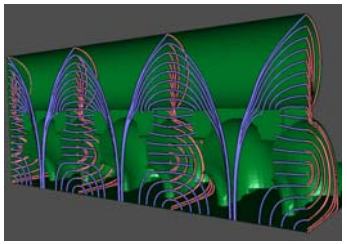


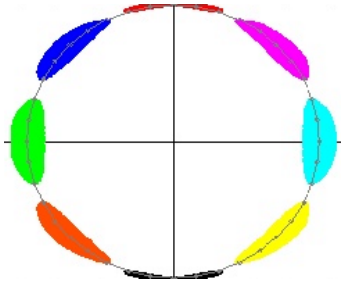
Typical SciDAC Application Project: Advanced Computing for Twenty-First Century Accelerator Science and Technology



LBNL
Parallel Beam Dynamics Simulation



UC Davis
Particle & Mesh Visualization

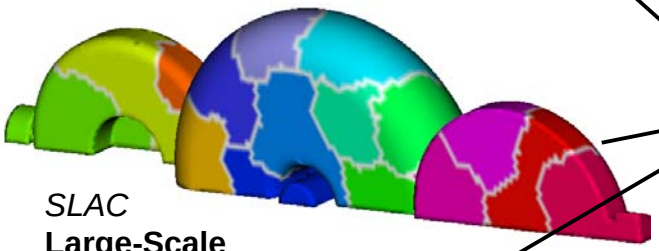


FNAL, BNL
High Intensity Beams in Circular Machines

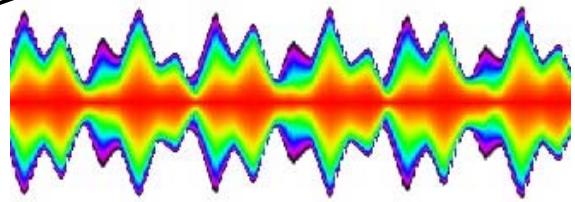
$$M = e^{:f_2:}\ e^{:f_3:}\ e^{:f_4:} \ldots$$
$$N = A^{-1}\, M\, A$$

U. Maryland
Lie Methods in Accelerator Physics

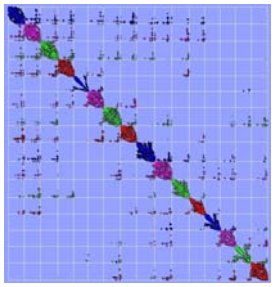
Jefferson Lab.
Coherent Synchrotron Radiation Modeling

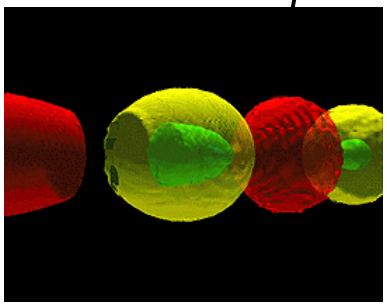


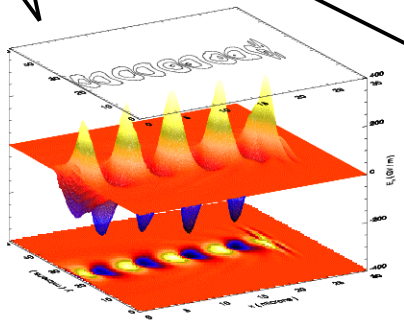
SLAC
Large-Scale Electromagnetic Modeling

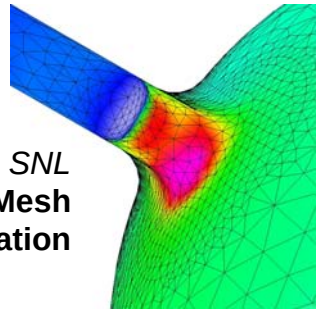


LANL
High Intensity Linacs, Computer Model Evaluation









Stanford, NERSC
Parallel Linear Solvers & Eigensolvers

UCLA, USC, UCB, Tech-X, U. Colorado
Plasma-Based Accelerator Modeling

SNL
Mesh Generation

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Success Story: SCIDAC Collaboration Speeds Up Fusion Code By Factor of 10

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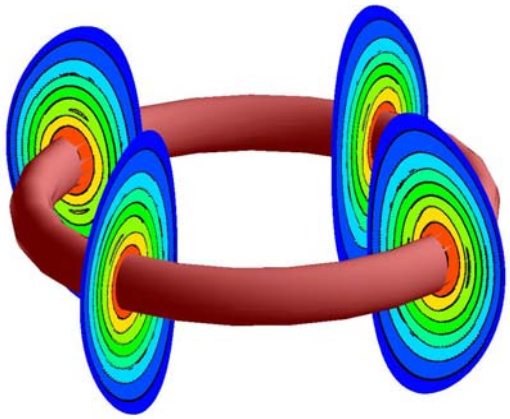
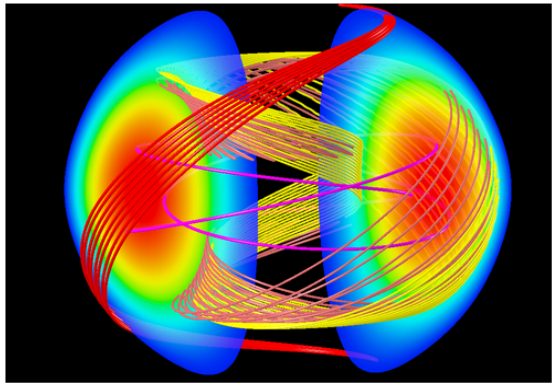


- NIMROD is a parallel fusion plasma modeling code using fluid-based nonlinear macroscopic electromagnetic dynamics.
- Joint work between CEMM and TOPS led to an improvement in NIMROD execution time by a factor of 5-10 on the NERSC IBM SP.
- This would be the equivalent of 3-5 years progress in computing hardware.

- Parallel SuperLU, developed at LBNL, has been incorporated into NIMROD as an alternative linear solver.
  - Physical fields are updated separately in all but the last time advances, allowing the use of direct solvers. SuperLU is >100x and 64x faster on 1 and 9 processors, respectively.
  - A much larger linear system must be solved using the conjugate gradient method in the last time-advance. SuperLU is used to factor a preconditioning matrix resulting in a 10-fold improvement in speed.



http://w3.pppl.gov/CEMM

http://www.tops-scidac.org

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Team Science Education

- SciDAC is first Full Implementation of Computational Science and Engineering (CSE)
- CSE is a widely accepted label for an evolving field concerned with the science of and the engineering of systems and methodologies to solve computational problems arising throughout science and engineering
- CSE is characterized by
  - Multi - disciplinary
  - Multi - institutional
  - Requiring high end resources
  - Large teams
  - Focus on community software
- CSE is not “just programming” (and not CS)
- References:
  - Petzold, L., *et al*., Graduate Education in CSE, *SIAM Rev*., 43(2001), 163-177
  - Osman, Y. et al., SIAM Rev., 45 (2003)
- CSE is an emerging department/program at universities

How do we manage team science?

Lessons learned:

- technology transfer
  - Build it into the project from the beginning
  - Provide explicit funding for tech transfer activities
  - Provide recognition
- consortium with other institutions
  - Clearly define roles and responsibilities up front (management plan)
  - Define lead institution, and provide resources for the lead institution to carry out responsibilities (e.g. administrative help for developing progress reports, funding for mandated progress reviews, advisory groups)
  - Define mechanism for re-allocation of resources and funding as the project progresses

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Career Issues

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- Recognition and Promotion
  - Recognize direct contribution to project in annual performance appraisals
  - Lab culture recognizes and rewards good team work
  - Publications are a positive indicator, but not the exclusive or most important measure of success
- Issue: overall success (or failure) of a team project biases the evaluation of the individual team member

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Publications

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Current practice in computational science is in flux:

- all contributors listed in alphabetical order
- key contributor(s) listed first, all others in alphabetical order
- publish different aspects of the project with different lead authors in different discipline journals

None of these is satisfactory

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Team Science at Research Labs

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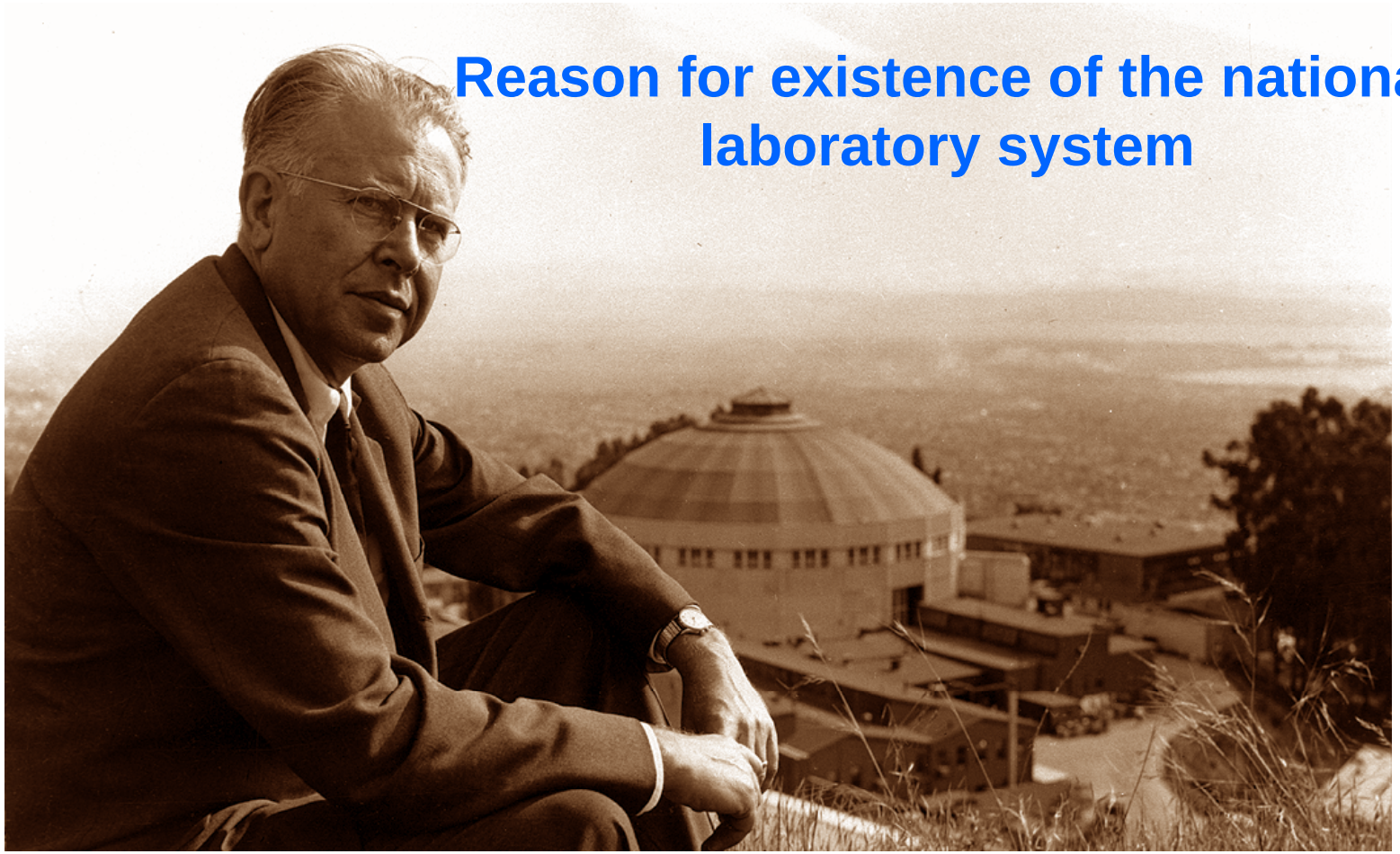

Reason for existence of the national laboratory system

Berkeley Lab Founded in 1931 by E.O. Lawrence on the Berkeley Campus;
Moved to Current Site in 1940