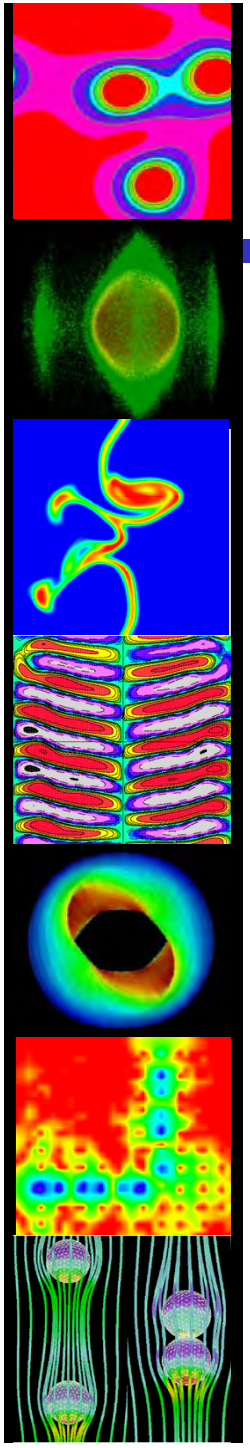


SciDAC
Scientific Discovery through Advanced Computing

DOE Office of Science

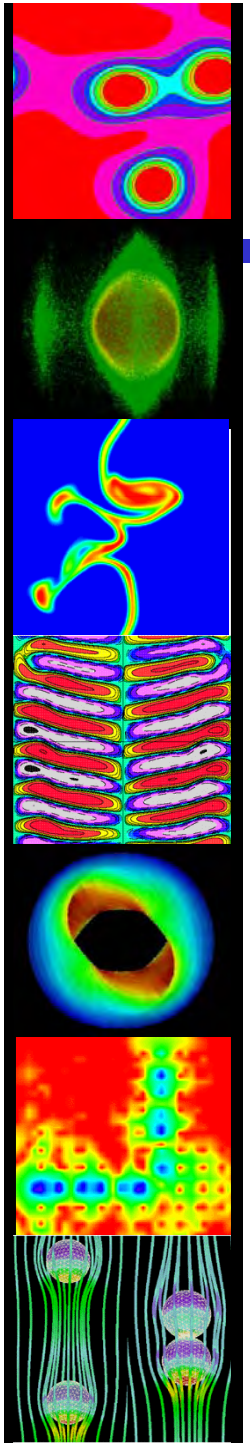
SciDAC Update

Scientific Discovery through Advanced Computing

Alan J. Laub, Director

March 14, 2003

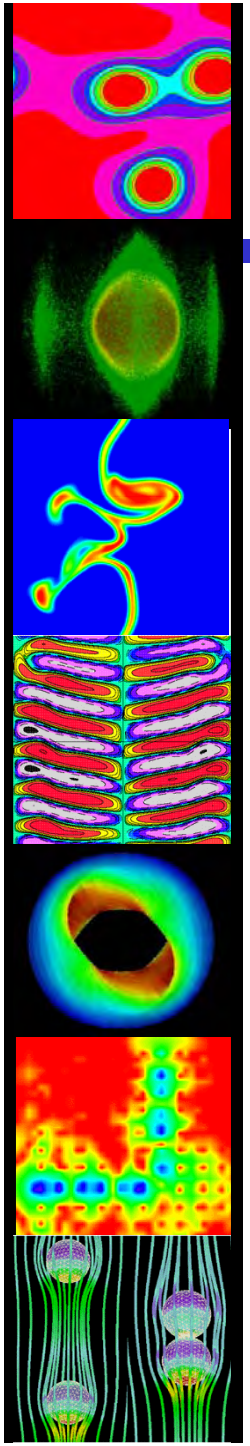
www.science.doe.gov/scidac



SciDAC Goals

- an INTEGRATED program to:
  - (1) create a new generation of scientific simulation codes that take full advantage of the extraordinary capabilities of terascale computers
  - (2) create the mathematical and computing systems software to enable scientific simulation codes to effectively and efficiently use terascale computers
  - (3) create a collaboratory software environment to enable geographically distributed scientists to work effectively together as a TEAM and to facilitate remote access, through appropriate hardware and middleware infrastructure, to both facilities and data

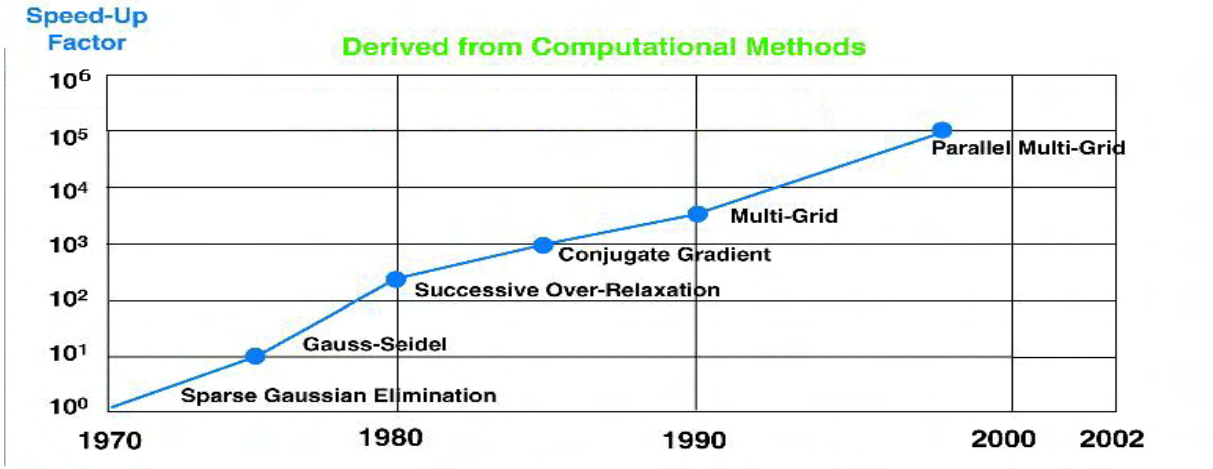
with the ultimate goal of advancing fundamental research in science central to the DOE mission

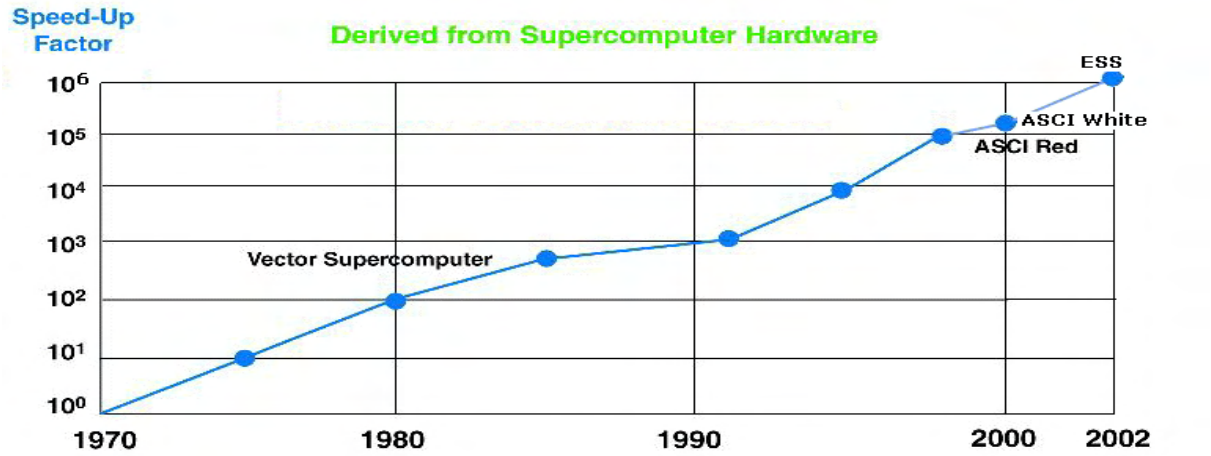


SciDAC
Scientific Discovery through Advanced Computing

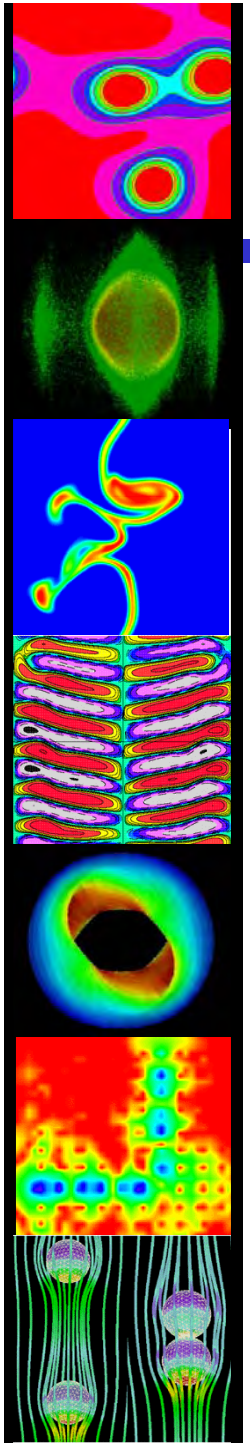
OFFICE OF SCIENCE
U.S. DEPARTMENT of ENERGY

It's Not Only Hardware!



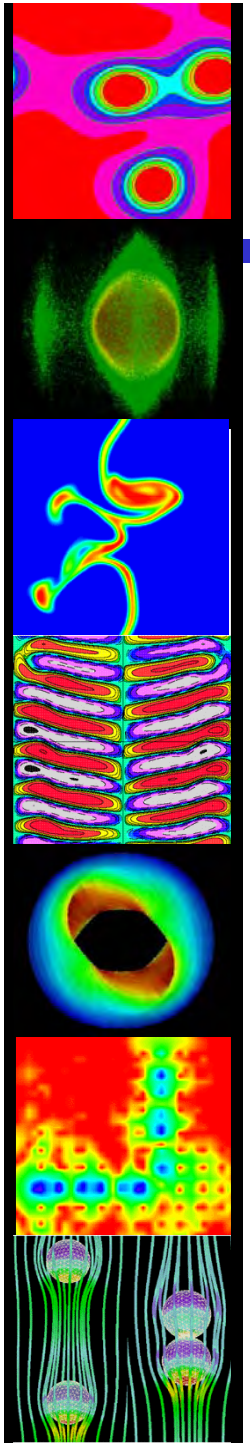


Updated version of chart appearing in "Grand Challenges: High performance computing and communications", OSTP committee on physical, mathematical and Engineering Sciences, 1992.



Successful Launch of Program

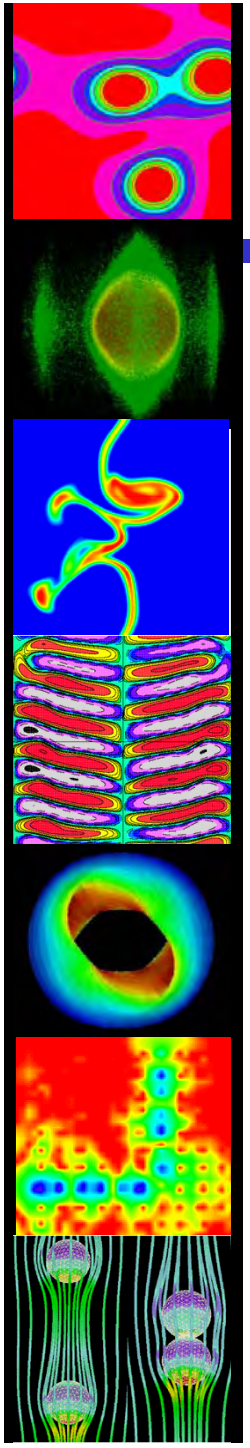
- SciDAC under way for about a year and a half
- first PI meeting January 2002 in Washington DC
- theme: introduction to the integrated SciDAC program; initiation of team building
- second annual PI meeting was held March 10-11, 2003 in Napa, Calif.
- theme: assessing SciDAC progress



Updated Overview of SciDAC

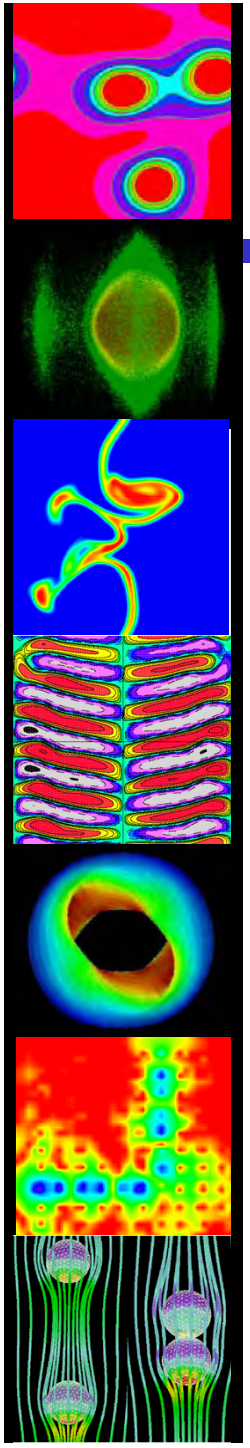
- 76 “two-pagers” now available on SciDAC website: www.science.doe.gov/scidac or at www.osti.gov/scidac

- divided into
  - Basic Energy Sciences (BES)
  - Biological and Environmental Research (BER)
  - Fusion Energy Science (FES)
  - High-Energy & Nuclear Physics (HENP)
  - Advanced Scientific Computing Research (ASCR)
    - CS ISICs
    - Math ISICs
    - Collaboratories
    - Networking and Middleware



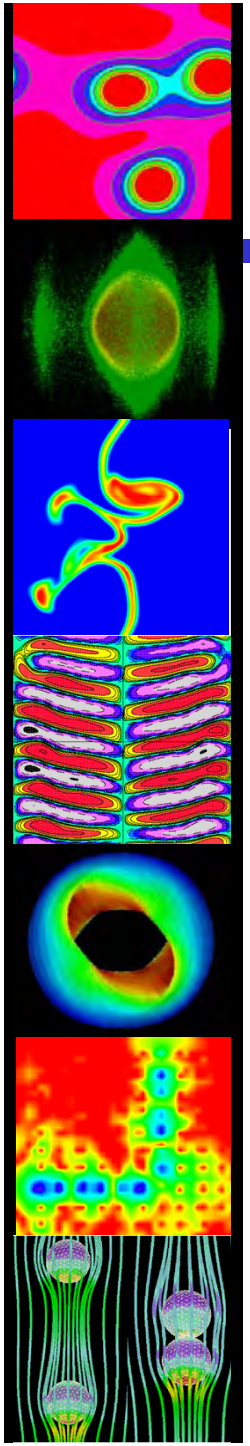
PI Meeting Notes

- keynote addresses by Ray Orbach and Jack Dongarra on first morning
- oral presentations and poster sessions for applications (BES, BER, FES, HENP), CS and math ISICs, and collaboratories/networking/middleware
- spirited final-afternoon discussions at two panels on *Closing the "Performance Gap"* and *Future SC Computing/Infrastructure Needs* (attended by OMB Examiner, Joel Parriott)



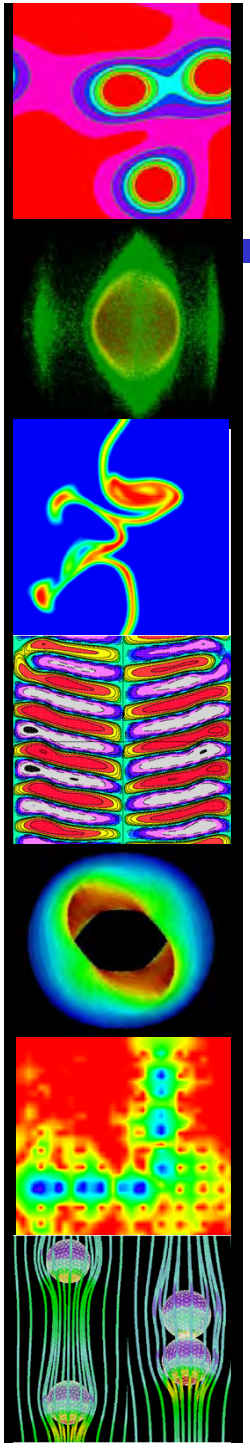
PI Meeting Notes (cont'd.)

- some recurring themes included
  - need for and dealing with architectural diversity
  - need for advances in storage and data handling capability
  - need for advances in interconnect and memory technology



PI Meeting Notes (cont'd.)

- the SciDAC concept is working
  - teams and collaborations are yielding new science (cf. Mezzacappa) that would not otherwise have been obtained (as easily)
  - many discipline scientists are (re)discovering new value in math, CS, and CSE research through application to their problems and codes
- a cultural change is emerging



Future SciDAC Issues

- additional computing and network resources
  - initial SciDAC focus is on software, but new hardware will be needed within the next two years
  - U.S. response to Japanese Earth Simulator?
  - potential synergistic partnerships leveraging off the success of the SciDAC model
  - both capability and capacity computing needs are evolving rapidly
- limited architectural options available in the U.S. today
  - topical computing may be a cost-effective way of providing extra computing resources
  - math and CS research will play a key role
- expansion of SciDAC program
  - many important SC research areas (e.g., materials/nanoscience, functional genomics/proteomics) are not yet included in SciDAC; NSRCs, GTL