ASCR Applied Mathematical Sciences Program: *Planning for the Future*

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Presentation to ASCR Advisory Committee

Washington D.C.

February 27, 2007

Revitalizing the AMS Program

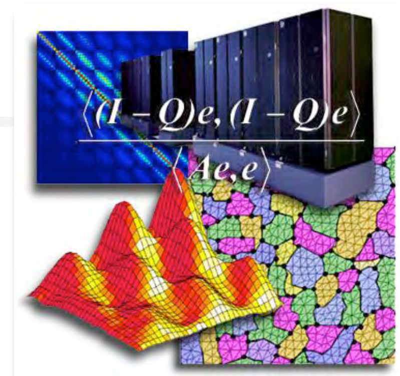
- What do we need to do to ensure that the AMS program is as successful for the next 50 years as it has been for the last 50?
- Determining strategic directions is important, but success will also depend on how the program is structured and managed.
- Working with ASCR program management and the DOE applied math community

We must build on a 50 year history of unprecedented advances in math models, math understanding and algorithmic performance

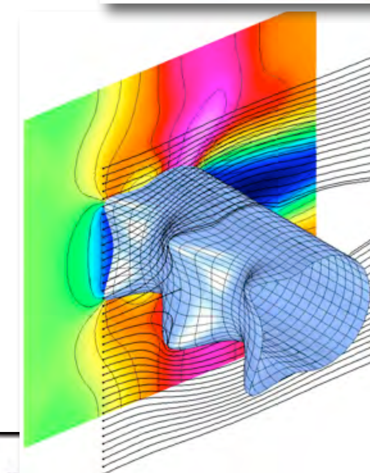
John von Neumann suggested the creation of the AEC *applied math research* program in the early 1950's

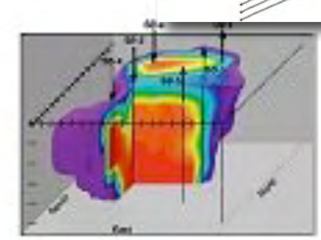
- Sustained support of world-class math PI's has resulted in models, analysis and algorithms for PDE-based science
  - Theory and numerical simulation of partial differential equations
    - fluid, solid mechanics, electromagnetism, radiation transport, atomic and molecular systems
  - Fundamental stability and accuracy of difference methods for PDEs
  - Numerical methods for shock physics
  - Scalable methods for solving large systems of linear and nonlinear equations
  - Methods for handling complex geometries, problems with sharp fronts, complex chemistry
- Other areas as well: optimization, discrete math, …

AMS deploys these advances to users through robust math software libraries



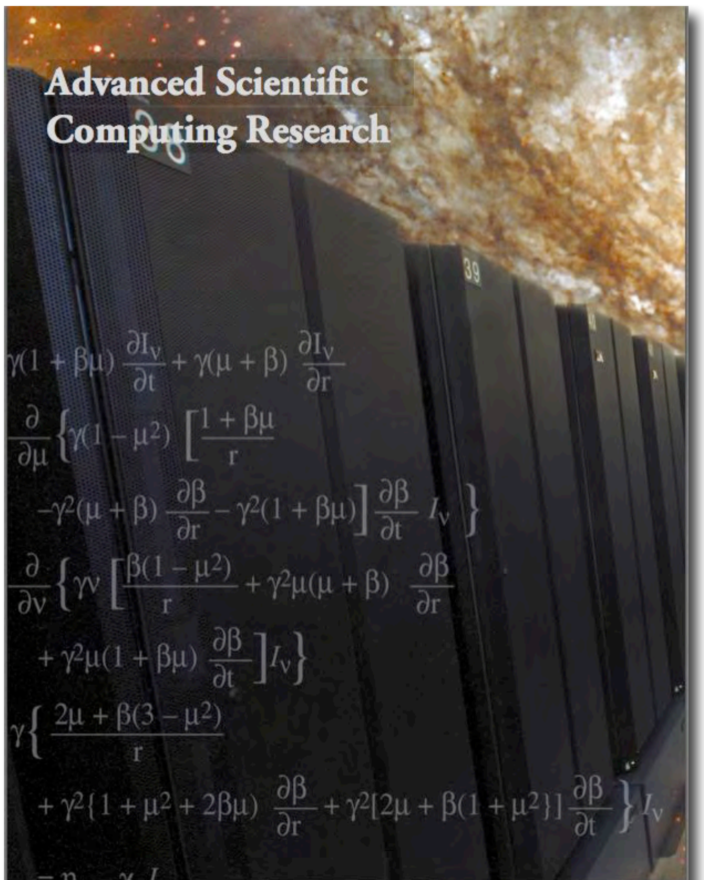
- Software libraries have crosscutting impact on multiple science and engineering applications
- Development of libraries with complex functionality enable insertion of advanced algorithms into science codes
  - Linear solvers: PetSC, hypre, Trilinos
  - AMR/PDE frameworks: Chombo, Overture
  - ITAPS suite of meshing tools, e.g. Mesquite
  - TAO: Toolkit for Advanced Optimization
- Modern software engineering approaches have become essential





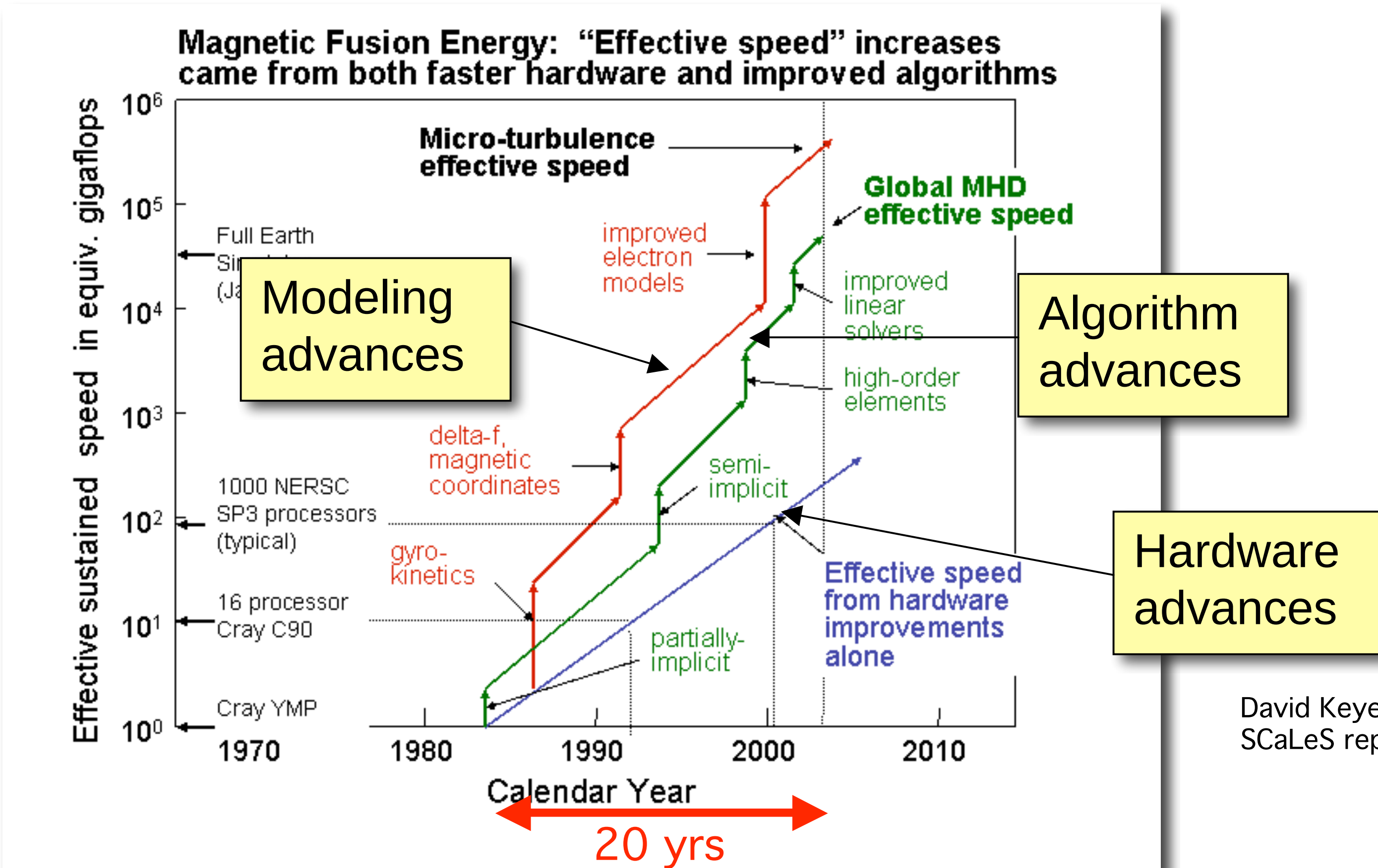
Multiphase flow, 4 million cell blocks, 32 million DOF, over 10.6 Gflops on an IBM SP (128 nodes), entire simulation runs in less than 30 minutes (Pope, Gropp, Morgan, Sepehrnoori, Smith and Wheeler).

What is the vision 50 years hence?



- Computation firmly rooted as the third pillar of scientific discovery, advancing energy, economic and national security of the US
  - Computing will be used to make new discoveries and develop understanding of complex processes
    - Science, Engineering, Social sciences, Economics
- Applied Mathematics a peer to other scientific disciplines

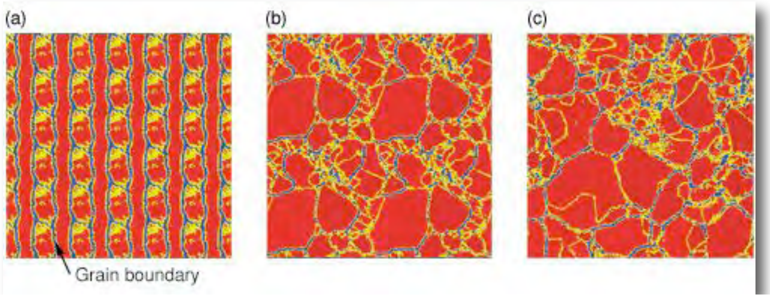
Math advances are essential for the exponential performance increases that will drive scientific discovery through computation



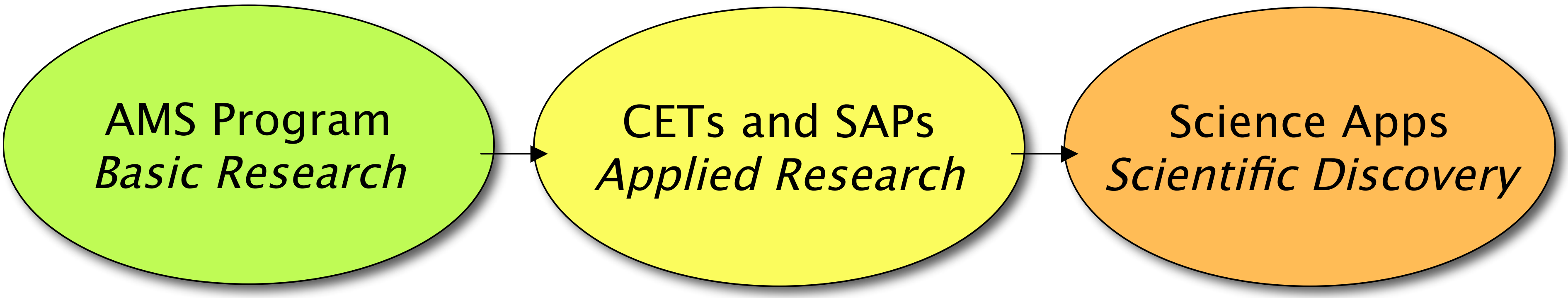
David Keyes
SCaLeS report v. 2

AMS must anticipate changes in future scientific computing habits across the DOE

- Availability of increasingly powerful computers will enable scientific advances and fuel further demand for computing by scientists
- High end simulations and world-class experimental facilities will generate enormous amounts of data that must be analyzed and understood
- As biology becomes a quantitative science, new data analysis challenges must be addressed
- Anticipate emergence of scientific computing needs as sciences become more quantitative

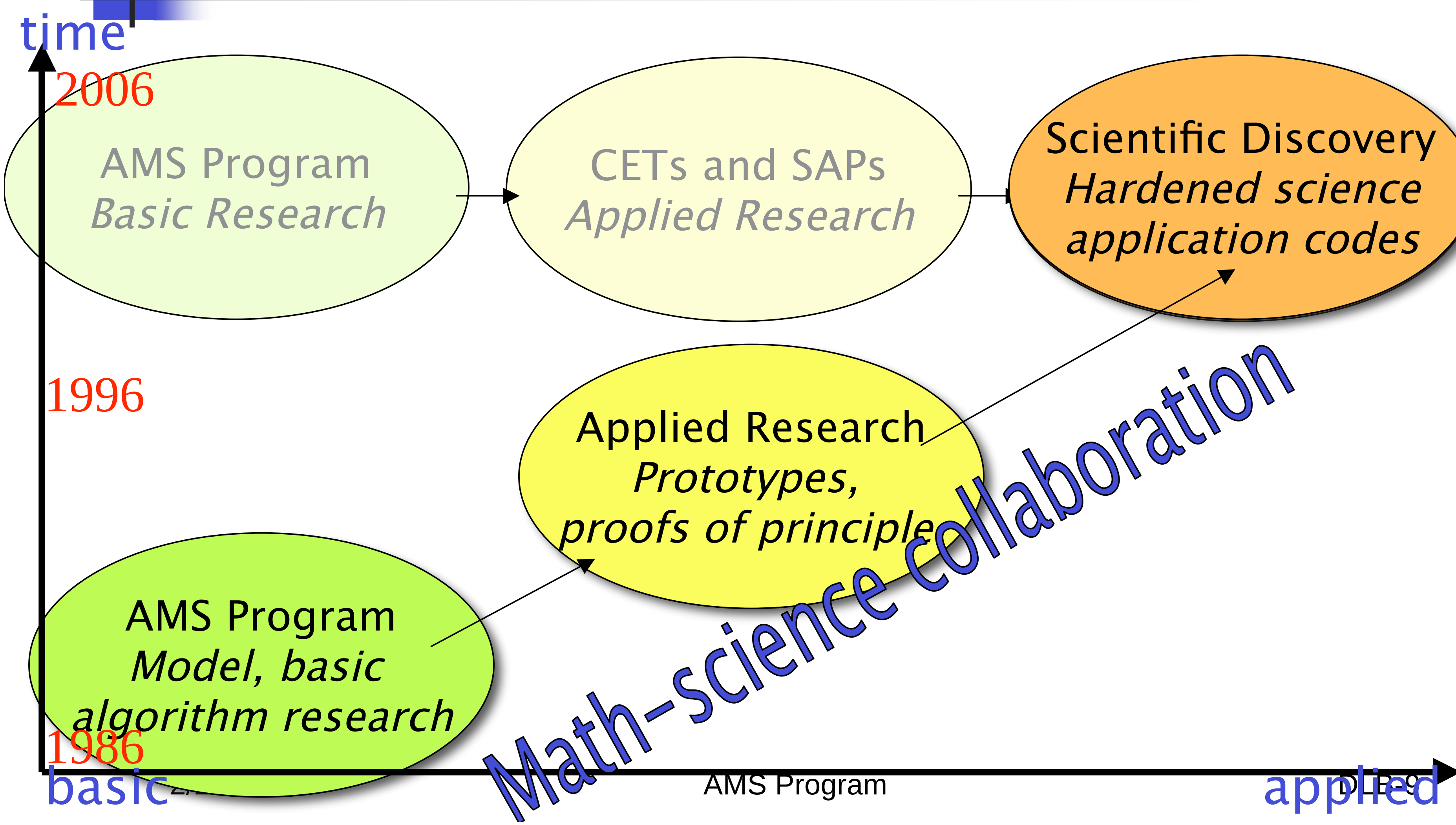


SciDAC science partnerships enable scientific discovery by leveraging math and CS results of last 50 years



- SciDAC model:
  - CETs, SAPs enable scientific discovery by providing technology and assistance to Science Apps
  - CETs, SAPs draw on expertise in AMS program to improve technology near-term
- *Overwhelming success of the SciDAC “brand” threatens to eclipse the base program*

The reality is that today's SciDAC discoveries are enabled by past base program research



SciDAC's turbulent flame success is an example of these principles at work

time

2006

3D Flame simulations matching, predicting, driving expts

1996

Development of AMR software frameworks

SIAM CSE Award 2003
Sidney Fernbach Award 2005

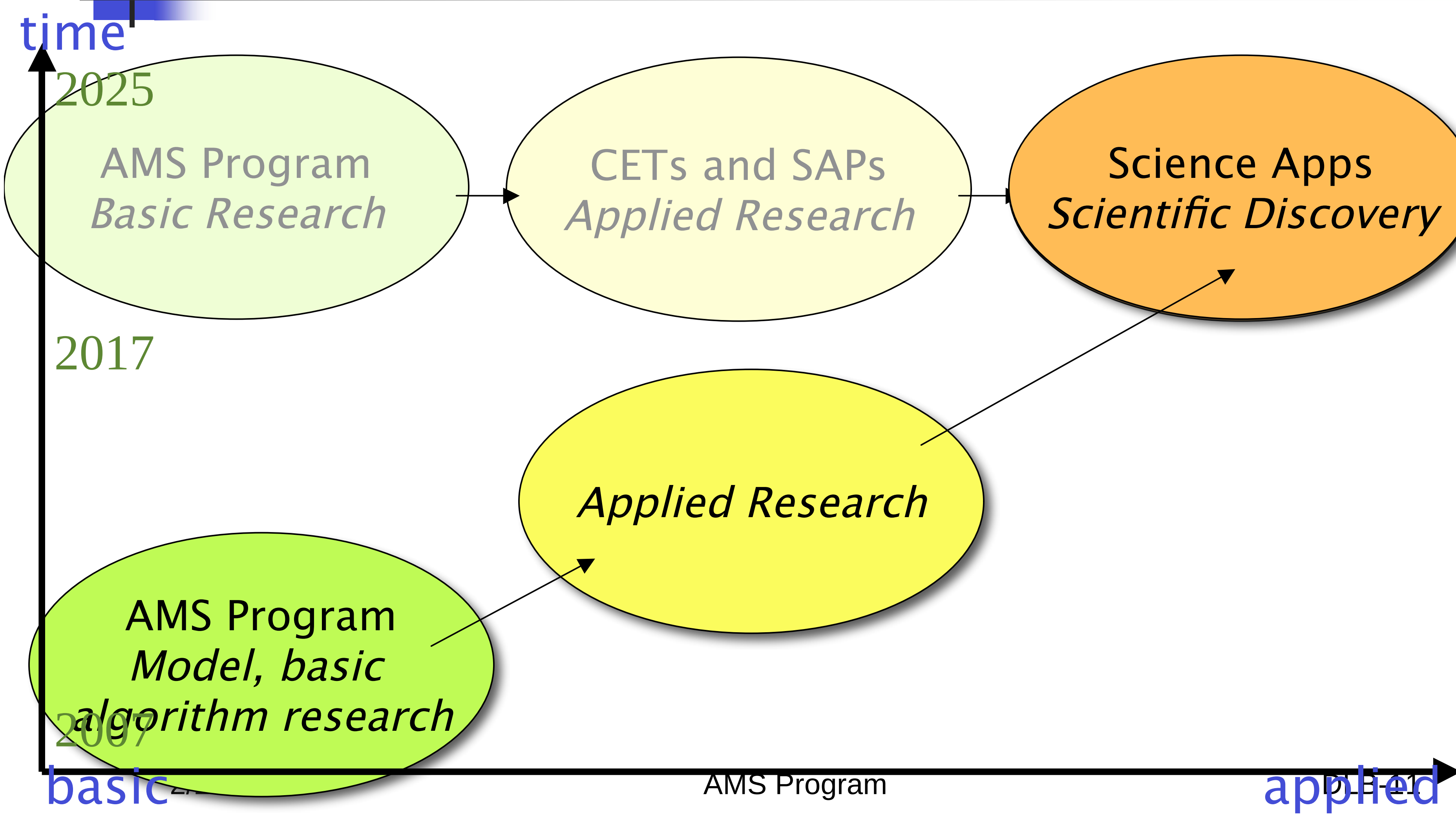
Low-Mach combustion; high-resolution algorithms

1986

basic

applied

Current AMS program developments will impact science in 10 to 20 years



Why is DOE AMS the right place to fund modeling and algorithm development?

AMS Program
Model, basic algorithm research

- Cross cutting research: often new math discoveries can be applied broadly to may applications
    - *Adaptive Mesh Refinement broadly applicable to many applications areas; now adaptive model refinement*
- We need models that are computable on high-end platforms
    - *Asymptotically-derived zero-Mach equations allow time-stepping at convective scale instead of acoustic*
- Models for man-made systems will involve new types of math
    - Coupled discrete and continuous models
    - Nonlinear effects

What are the issues for the AMS program going forward?

- Focus of AMS program hasn't changed significantly in 50 years
- AMS program funding stagnant for more than a decade
  - Effective 'buying power' halved since 1990
- Current focus on measuring progress discourages risk taking and innovation
- Applied math is viewed as a "support" discipline for other sciences
- We must anticipate needs 20 years in the future

As new opportunities emerge, AMS program emphasis must adapt

- Predictive multi-physics simulation requires multiscale analysis and algorithms
- Using simulations to inform decision makers requires risk analysis supported by uncertainty quantification
- Increased emphasis on Scientific Data Understanding at the high end for both simulation and experiment
- Statistics has been neglected
- Large scale Optimization becomes possible as computers and algorithms become more powerful
- Discrete math, complex systems will support new areas of energy importance
- Hybrid simulations that combine discrete and continuum models will enable new discovery
- Learning to exploit heterogeneous architectures; hybrid computing models increasingly important in the future

Plan for Action

- Near term: Propose new math initiatives for FY2009 -2010 to infuse increased funding and new ideas into AMS program

- Longer term: Develop AMS Strategic Plan
  - Engage DOE math community
  - Input from scientists knowledgeable about DOE mission and programs
  - Leverage NRC study: Science case for computation
  - DOE Strategic Plan; EPAct report
  - Objective:
    - Articulate 10-20 yr goals for AMS program
    - Map out 5-yr strategies for achieving goals

Future success of math program depends on more than identifying the right topics

- Sustained long-term investments in successful PIs are essential
  - Science-enabling advances don’t happen on a 3 year schedule
  - Expect 10-15 years for impact, but watch for progress
- Need mechanisms that encourage unexpected discovery
- Not every result need have near-term high-end computing impact
- Promote early collaboration with science programs to develop new math models (not just new algorithms)
- Active program management important
  - Create successful research teams, mold programs to ensure DOE impact
- New programs don’t just fund the “best” proposals, they must create a structure than ensures success for DOE
  - Take advantage of unique Lab and university strengths

How math and computation will make inroads into a broader set of DOE programs

- Must engage applied programs to understand their needs
  - “What unsolved problems are most important to you?”
  - *NOT* “How can computing help?”
- Recognize that key math developments for new programs may not have direct high-end computing impact
- Science and engineering practitioners may not immediately recognize the value of HPC
- Not having scientific data now shouldn’t stop development of advanced methods of the future (e.g. biology)
- Engaging new application areas will require AMS to move into new areas of math

How do we train the future workforce?

- Exposure to the national labs essential:
  - We need a “CSGF” for applied math
    - CSGF focuses on HEC impact
  - Apply the CSGF model to ECPI
  - Promote Lab internships for undergrads and grads

AMS Program must recapture the strong sense of community that existed in the ‘80s and ‘90s

- Encourage collaboration, communication
- Develop a community sense of purpose supporting DOE mission
- Annual community meetings
  - Include both lab and university researchers
  - *AMS 2007 PI Meeting: May 22-24, 2007 @ Lawrence Livermore*

AMS must effectively leverage academic expertise

- Recognize that some expertise (e.g. analysis) exists predominantly in the university environment
- Research funded in academia should have a clear insertion path to assure DOE relevance
  - Encourage collaborative work between academia and lab mathematicians and/or scientists
  - Student internships at labs
  - Faculty visits, sabbaticals

It is time to revitalize the ASCR AMS program

- Growth to re-establish a critical mass of AMS research
- Math modeling an essential essential element for future DOE computational science advances
- Effective partnerships between Lab and academic researchers
- Recapture DOE applied math community identity
- Structural changes to promote creativity, innovation, new discoveries
- Identify new directions to prepare for future computational science needs
- Establish applied math as a peer to the other sciences