Leadership Computing Facility (LCF) Roadmap

Presented by

Buddy Bland

Leadership Computing Facility Project Director
National Center for Computational Sciences

SC07

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Outline

- Systems
- Facilities upgrade
- Systems infrastructure
  - Overview
  - Networking
  - Storage
- Software and science

Systems
CCS firsts (1991–2008)

1991
KSR1-64
CCS formed

1992
Paragon XP/S 35 installed

1993
PVM used to create first international grid
HPSS development begins

1994
PVM wins R&D 100

1995
Install Paragon XP/S 150-MP
Worlds fastest computer connected by fastest network–OC-12–to Sandia

First T170 climate run

1996
ORNL-SNL create first high-performance computational grid

1997
R&D 100 Award for successful development and deployment of HPSS

Long-standing climate simulation milestone first met on CCS Compaq

1998
Developed first application to sustain 1TF wins Gordon Bell prize

1999
NetSolve wins R&D 100
ATLAS wins R&D 100

2000
First OSC teraflop peak system

2001

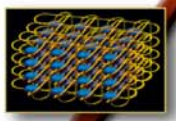
First IBM Power4
SciDAC leadership
Human Genome Project
Jack Dongarra elected to National Academy of Engineering

2002
Partnership with Cray on X1 begins

Neutron Sciences Teragrid Award

2003
GSN testing
Record TCP/IP speed
OC192 to Atlanta

IBM Blue Gene CRADA to develop super scalar algorithms begins



2004

Leadership Computing Facility awarded to ORNL
World's largest Cray X1
ORNL provides bulk of runs of IPCC 4th assessment
OSCAR becomes world's most popular cluster management system

Robert Harrison wins Sidney Fernbach Award
World-class DOE facility

2005

EVEREST facility opens
Cray X1 upgraded to X1E
Cray XT3 installed
Largest fusion simulation using AORSA
UltraScienceNet operational
Production use of LCF

Deploy unified Lustre file system for CCS systems

l·u·s·t·r·e

XT3 upgraded to 100 TF
Breakthrough science from LCF applications

2006

2007
250 Tflop XT3 System

2008
1 Petaflop System

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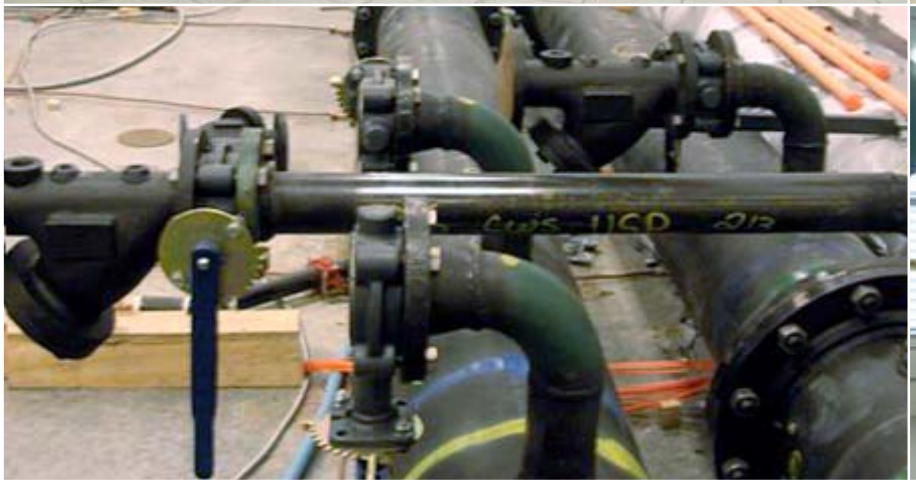
Facilities upgrade

Preparing computer center for petascale computing

Clear 7,000 ft² for the computer

Add 10 MW of power



Install taps for liquid cooling

Upgrade chilled water plant

Systems infrastructure: Overview
Current and projected

Networking	FY 2007	FY 2008	FY 2009
External B/W (GB/s)	3	4	5
LAN B/W (GB/s)	60	140	240

Archival storage	FY 2007	FY 2008	FY 2009
Capacity (PB)	4	10	18
Bandwidth (GB/s)	4	10	19

Central storage	FY 2007	FY 2008	FY 2009
Capacity (PB)	0.22	1.0	10.0
Bandwidth (GB/s)	10	60	240

Systems infrastructure: Network

- Shifting to a hybrid InfiniBand/Ethernet network.
- InfiniBand-based network helps meet the bandwidth and scaling needs for the center.
- Wide-area network will scale to meet user demand using currently deployed routers and switches.

2007
100 TF
60 GB/s LAN
3 GB/s WAN

2008
1000 TF
240 GB/s LAN
5 GB/s WAN

2009
1000 TF
240 GB/s LAN
5 GB/s WAN

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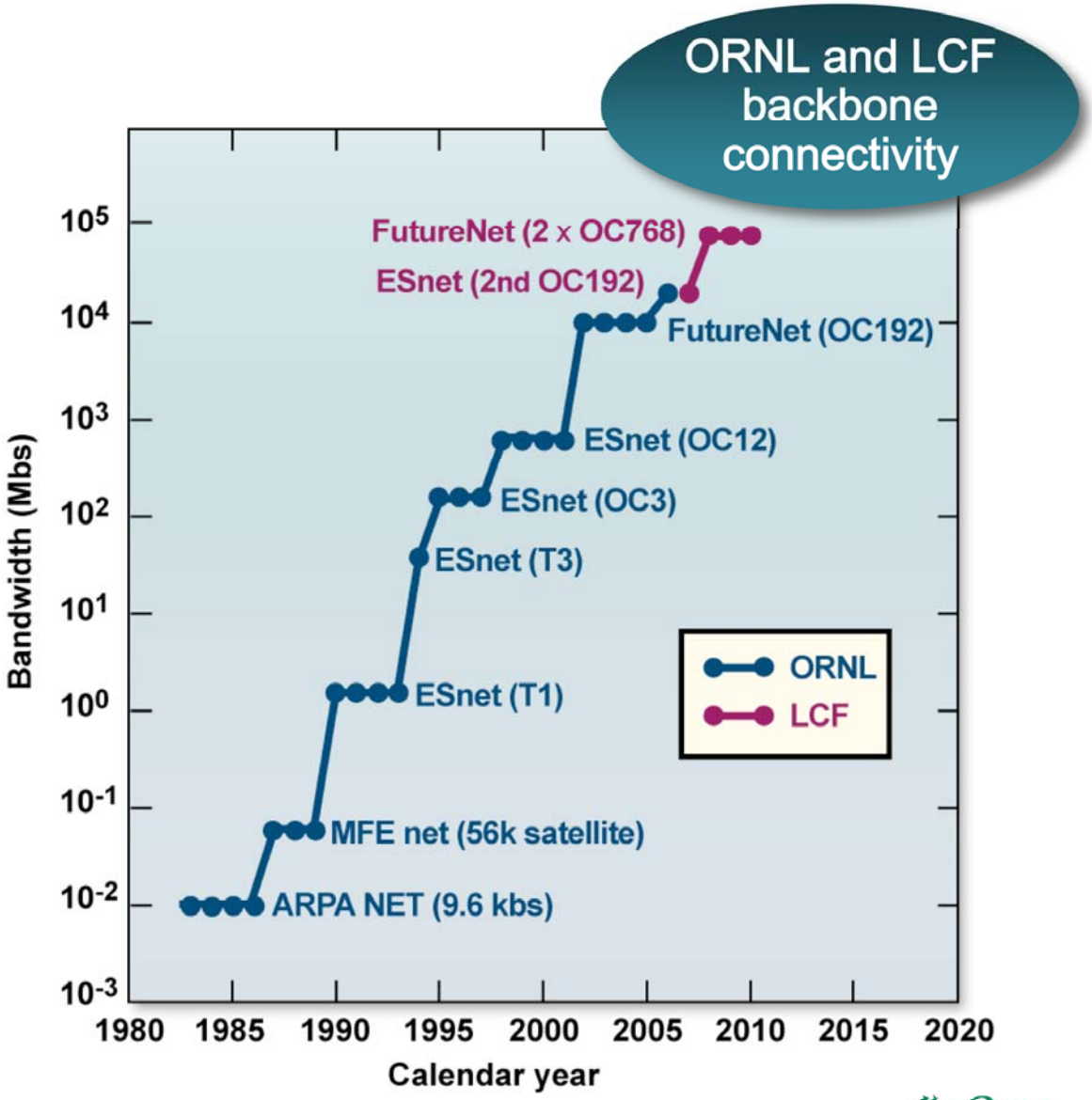
Systems infrastructure: Network (continued)

- Consistent planned growth in ORNL external network bandwidth



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Systems infrastructure: Storage
Archival storage

- HPSS software has already demonstrated ability to scale to many PB.
- Add two silos/year.
- Tape capacity and bandwidth, disk capacity and bandwidth are all scaled to maintain a balanced system.
- Use new methods to improve data transfer speeds between parallel file systems and archival system.

2007: 100 TF, 4 PB, 4 GB/s

2008: 1000 TF, 10 PB, 10 GB/s

2009: 1000 TF, 18 PB, 19 GB/s

Systems infrastructure: Storage
Central storage

- Increase scientific productivity by providing single repository for simulation data
- Connect to all major LCF resources
- Connect to both InfiniBand and Ethernet networks
- Potentially becomes the primary file system for the 1000 TF system

2007
100 TF
250 TB
10 GB/s

2008

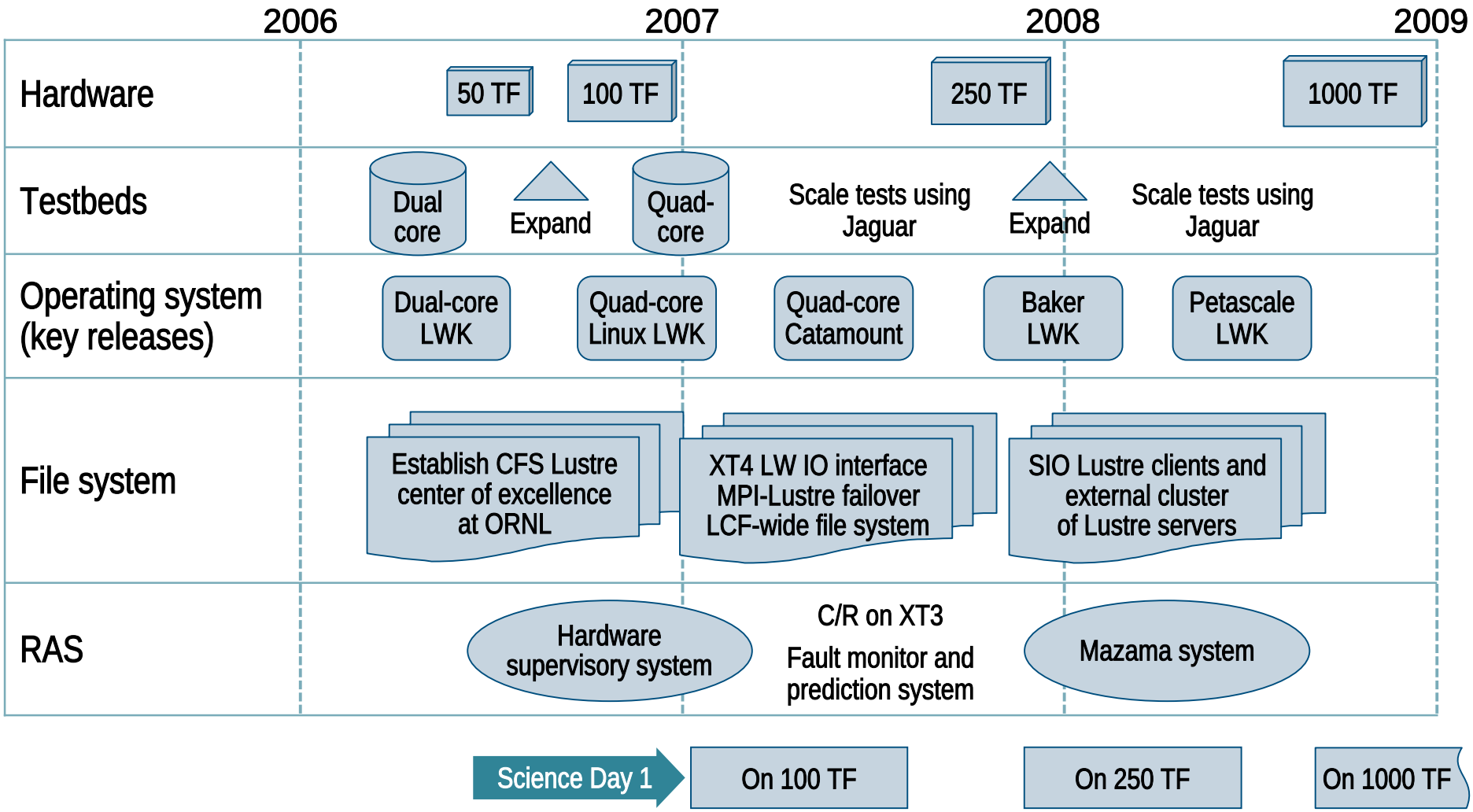
2009
1000 TF
10 PB
240 GB/s

1000 TF
1 PB
60 GB/s

Software and science: Overview

- Cutting-edge hardware lays the foundation for science at the petascale—scientists using a production petascale system with petascale application development software.
  - Establishing fully integrated computing environment.
  - Developing software infrastructure to enable productive utilization and system management.
  - Empowering scientific and engineering progress and allied educational activities using petascale system.
  - Developing and educating the next generation of computational scientists to use petascale system.
- NCCS Management Plan coordinates the transition to petascale production.

Software and science Roadmap to deliver Science Day 1



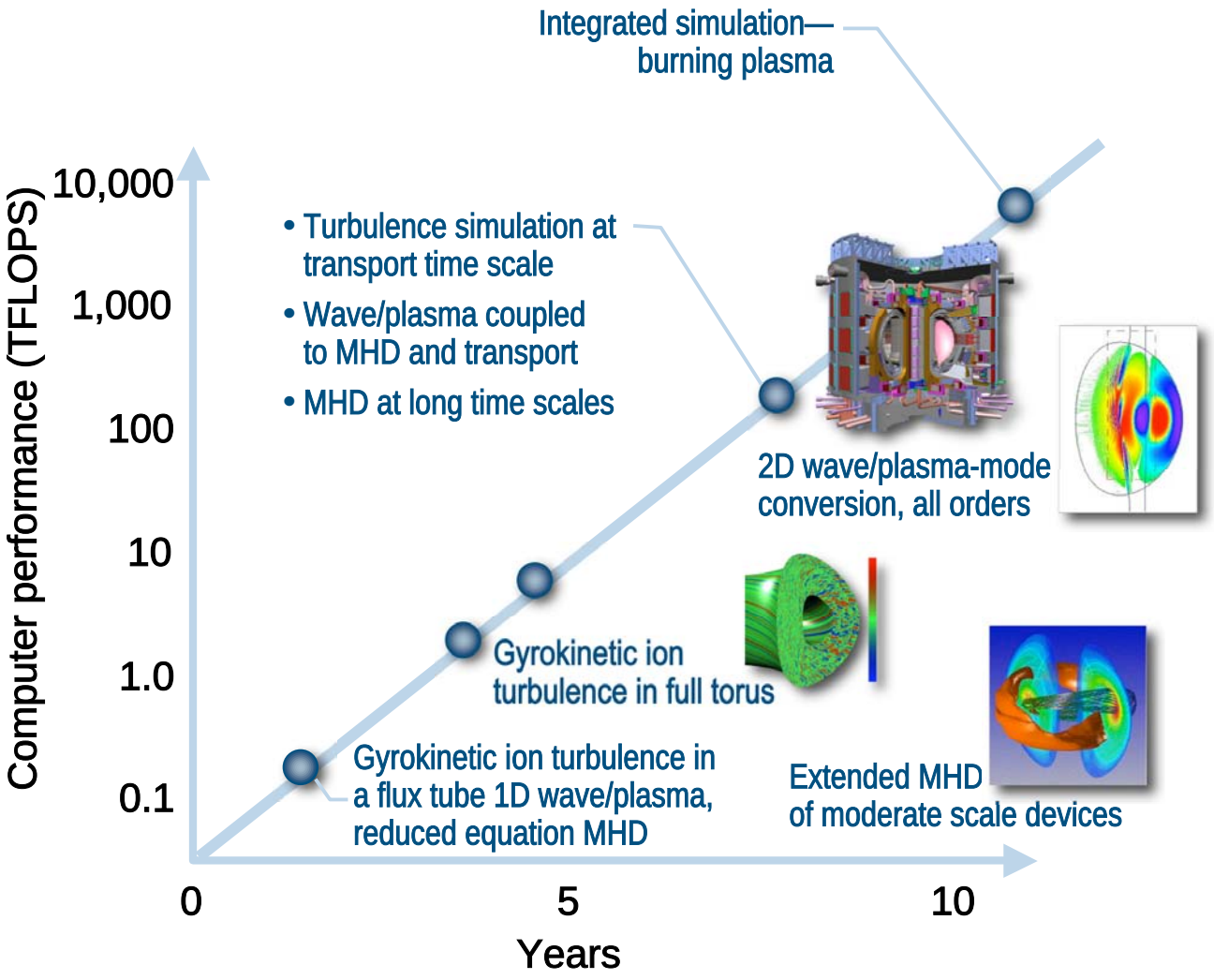
Science drivers

- Advanced energy systems
  - Fuel cells
  - Fusion and fission energy
- Bioenergy
  - Ethanol production
- Environmental modeling
  - Climate prediction
  - Pollution remediation
- Nanotechnology
  - Sensors
  - Storage devices

"University, laboratory, and industrial researchers using a broad array of disciplinary perspectives are making use of the leadership computing resources to generate remarkable consequences for American competitiveness."

– Dr. Raymond L. Orbach, Undersecretary for Science, U.S. Department of Energy

Software and science: Fusion



Expected outcomes

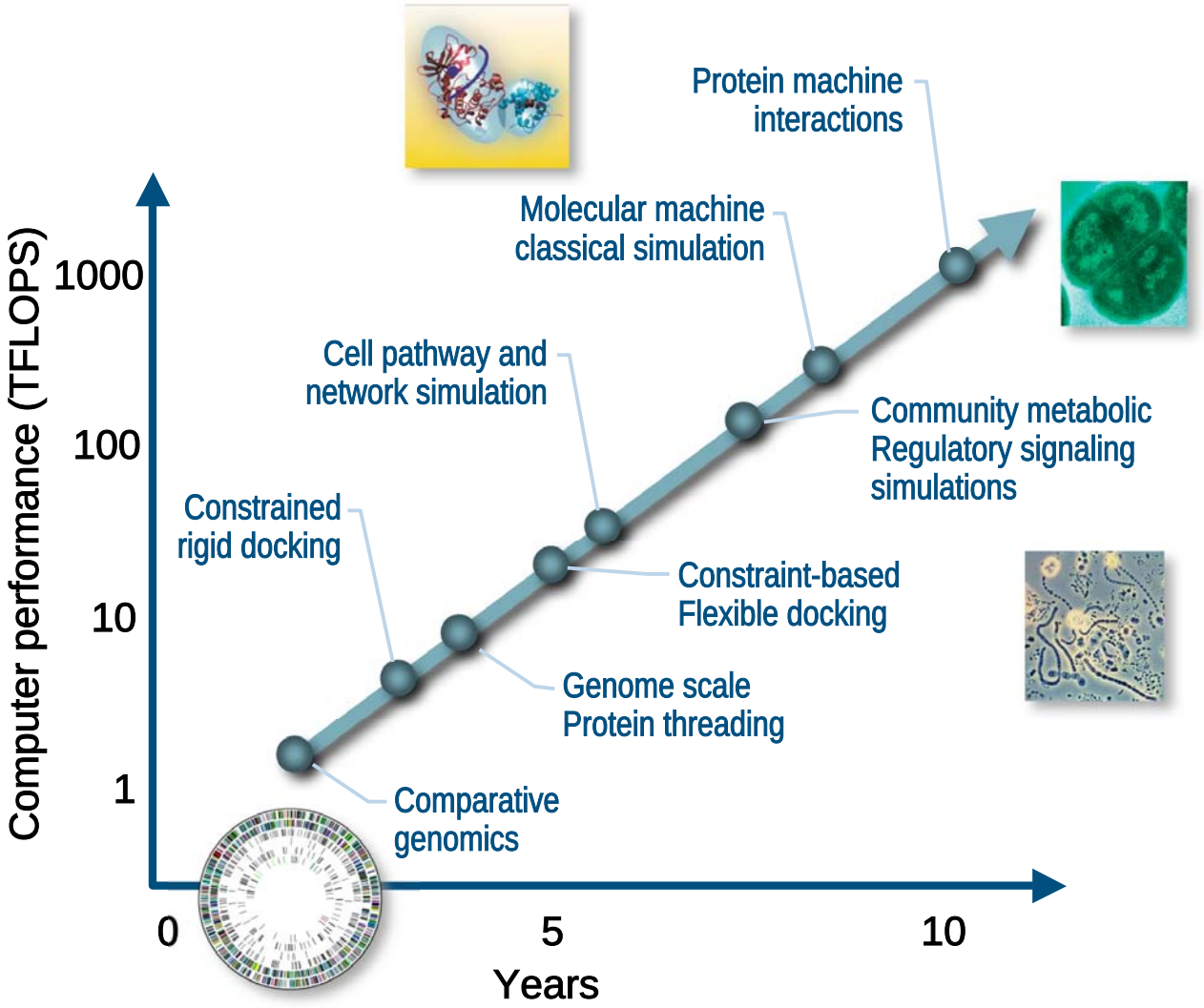
5 Years

- Full-torus, electromagnetic simulation of turbulent transport with kinetic electrons for simulation times approaching transport time-scale
- Develop understanding of internal reconnection events in extended MHD, with assessment of RF heating and current drive techniques for mitigation

10 years

- Develop quantitative, predictive understanding of disruption events in large tokamaks
- Begin integrated simulation of burning plasma devices – multi-physics predictions for ITER

Software and science: Biology



Expected outcomes

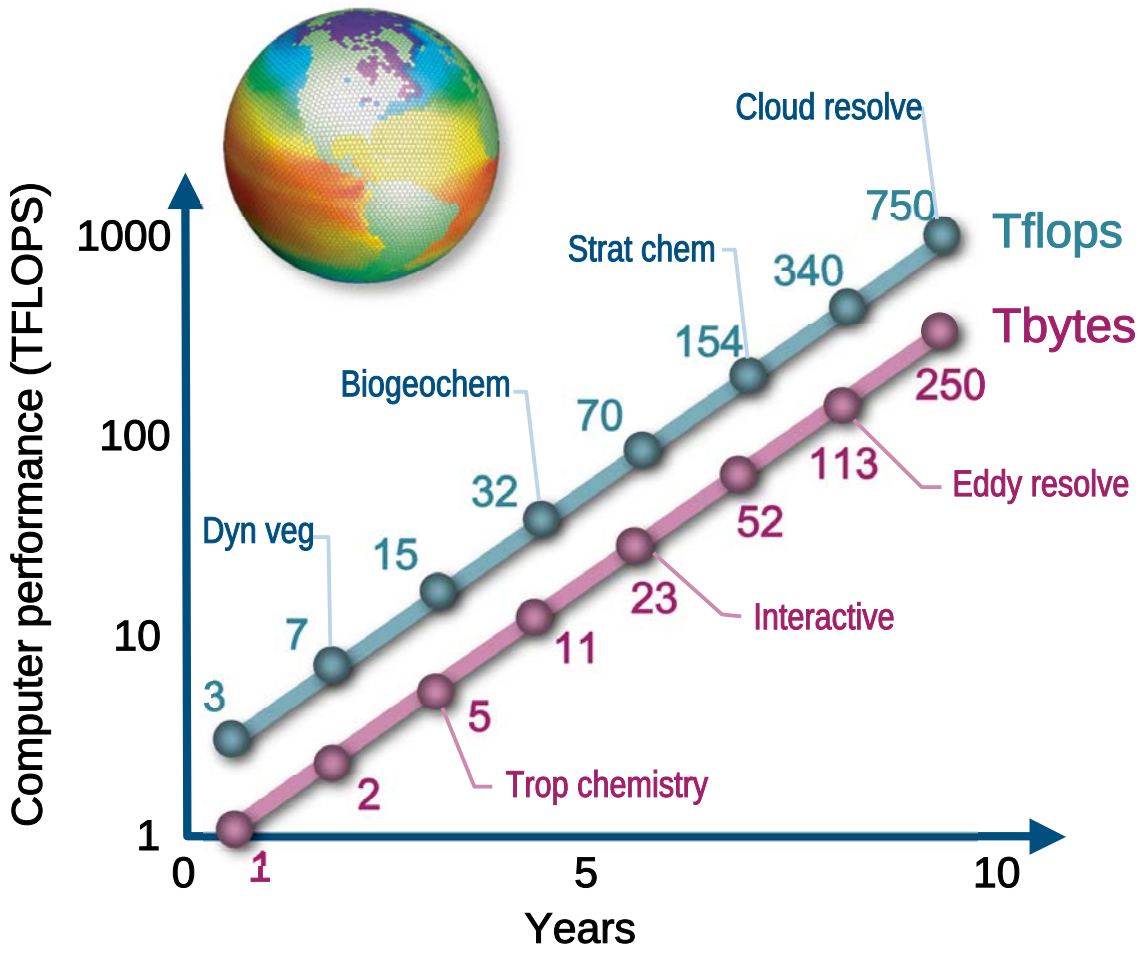
5 years

- Metabolic flux modeling for hydrogen and carbon fixation pathways
- Constrained flexible docking simulations of interacting proteins

10 years

- Multiscale stochastic simulations of microbial metabolic, regulatory, and protein interaction networks
- Dynamic simulations of complex molecular machines

Software and science: Climate



Expected outcomes

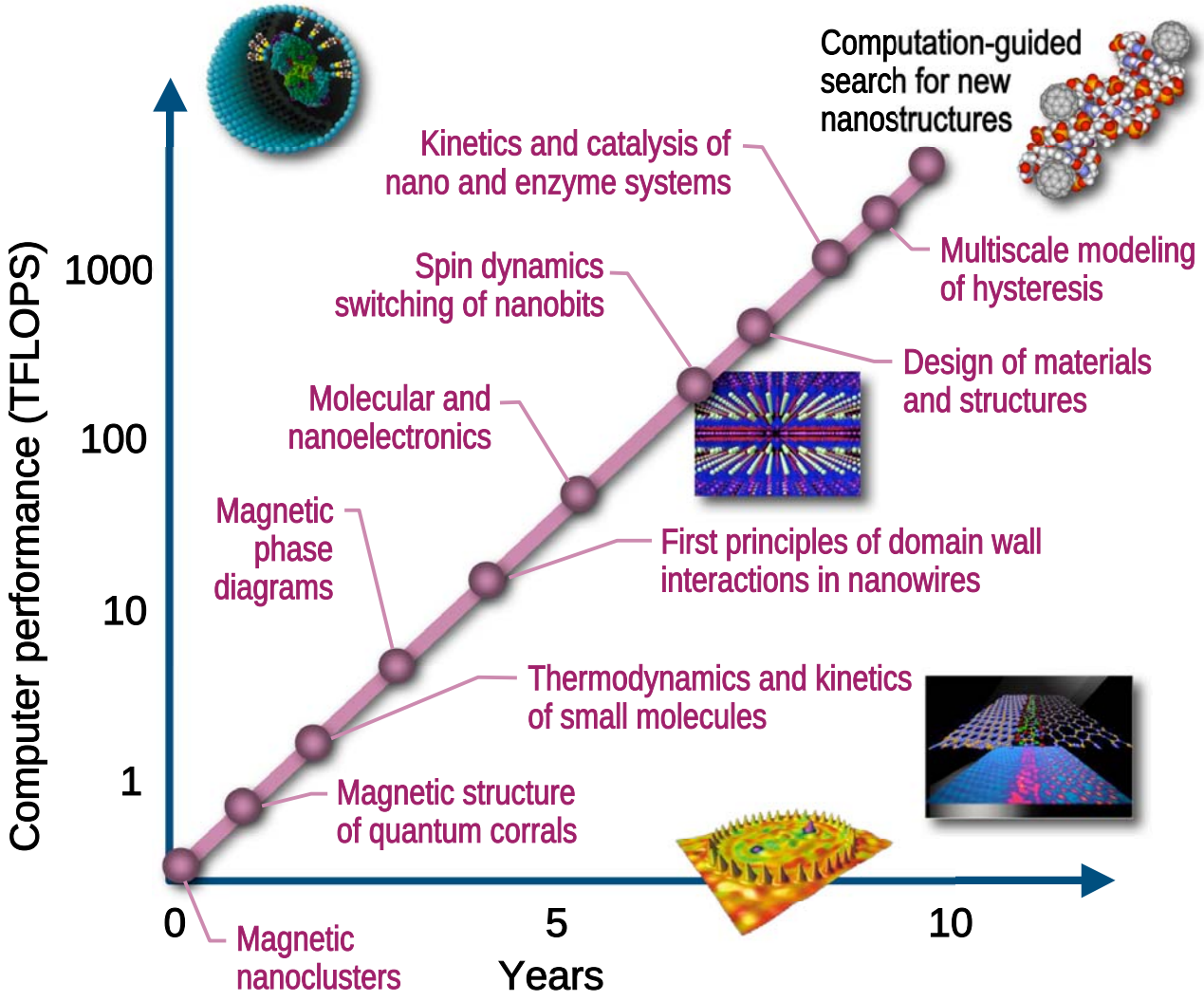
5 years

- Fully coupled carbon-climate simulation
- Fully coupled sulfur-atmospheric chemistry simulation

10 years

- Cloud-resolving 30-km spatial resolution atmosphere climate simulation
- Fully coupled, physics, chemistry, biology earth system model

Software and science: Nanoscience



Expected outcomes

5 years

- Realistic simulation of self-assembly and single-molecule electron transport
- Finite-temperature properties of nanoparticles/quantum corrals

10 years

- Multiscale modeling of molecular electronic devices
- Computation-guided search for new materials/nanostructures

Contact

Arthur S. (Buddy) Bland

Leadership Computing Facility Project Director
National Center for Computational Sciences
(865) 576-6727
blandas@ornl.gov

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