Cyberinfrastructure: Enabling New Research Frontiers

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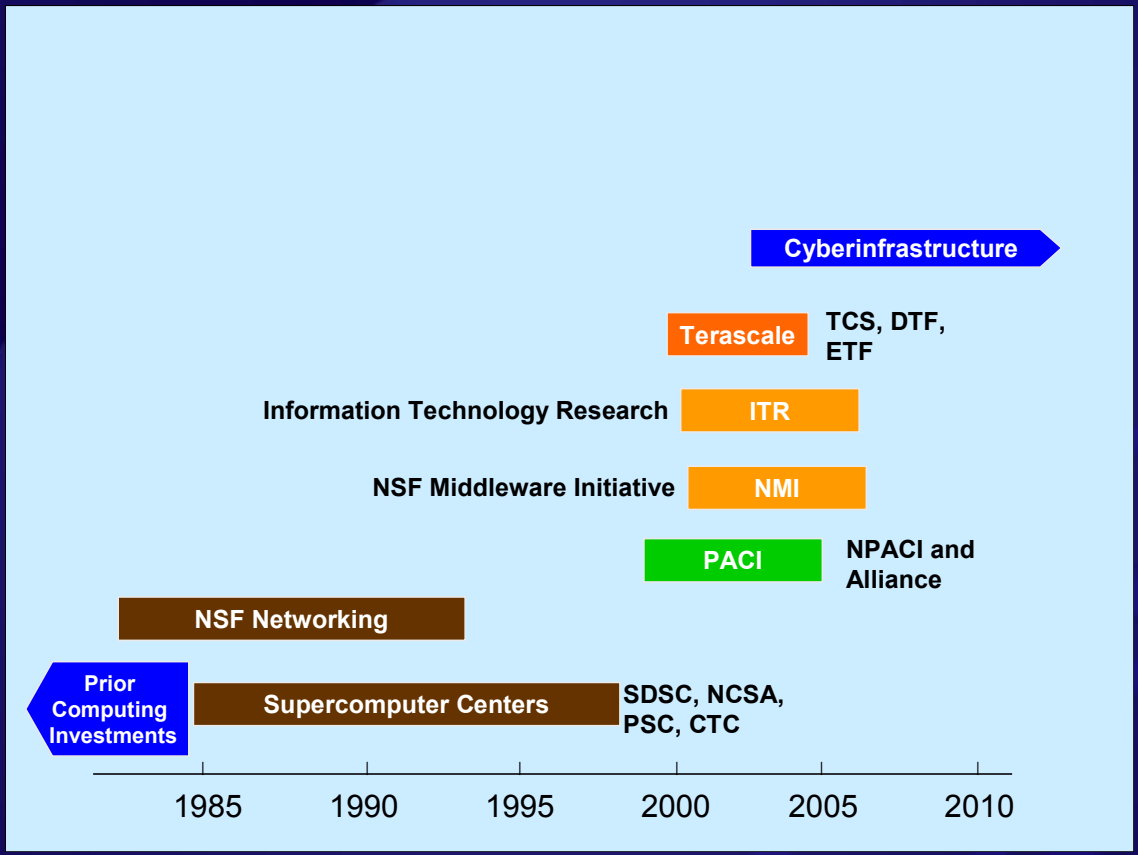
Topics Covered Today

- Guiding Principles for Shared Cyber-infrastructure at NSF
- Enabling role of Cyberinfrastructure:
  - *Molecular Architecture as a New Frontier*
  - *Computational Steering as a New Capability*
- Looking to the Future
  - *Tipping Point: Information flow reversal*

Guiding Principles for SCI at NSF

- Serve all of science & engineering
- Firm and continuing commitment to providing the most advanced cyberinfrastructure (CI), with high-end computing (HEC) at the core
- Encourage emerging CI while maintaining and transitioning extant CI
- Provide balance in CI equipment
- Strong links to ongoing fundamental research to create future generations of CI

History of NSF CI Investments



Looking to the Future

- Science frontiers as the drivers
- Balance capability *and* capacity:
  - the Extensible Terascale Facility (ETF)
- Emerging CPU-intensive and data-intensive paradigms for molecular architecture as an illustrative example
- The next wave

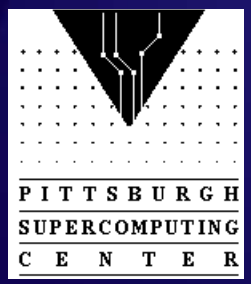
TeraGrid Partners

National Center for Supercomputing Applications

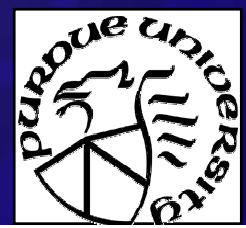
Center for Advanced Computing Research

Argonne National Laboratory

Indiana University



Texas Advanced Computing Center

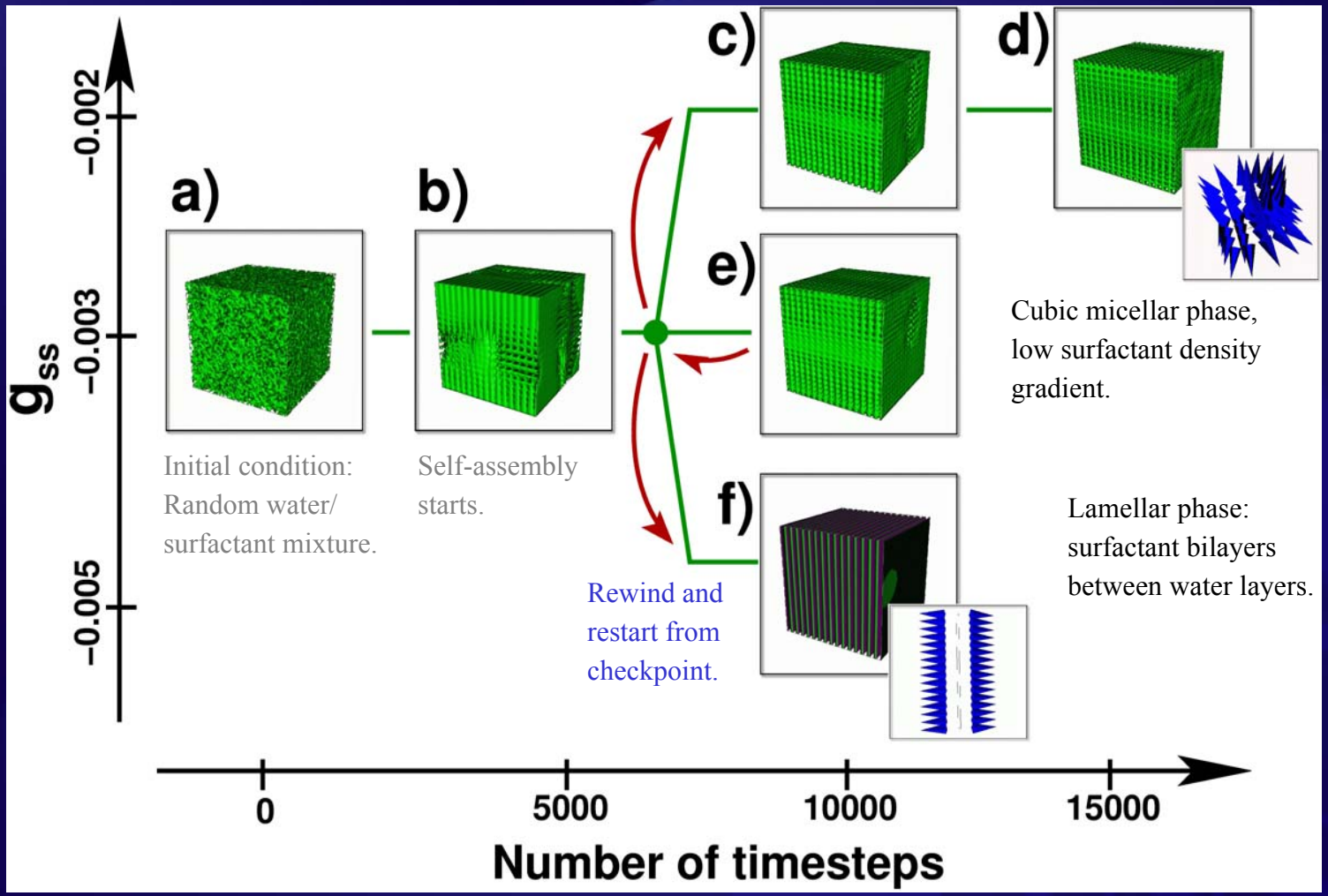


Purdue University

TeraGyroids Project

- Amphiphiles: hydrophobic tails and hydrophilic heads, dispersed in solvents or oil/water mixtures, self assemble into complex shapes; gyroids are of particular interest in biology
- Shapes from a parameters space:
  - Abundance, initial distribution of each component
  - strength of the surfactant-surfactant coupling,
- Desired structures simulated only in very large systems
- Project goal is to study defect pathways and dynamics in gyroid self-assembly

Exploring parameter space through computational steering



Cyberinfrastructure: the future consists of …

- Computational engines (supercomputers, clusters, workstations – capability and capacity)
- Mass storage (disk drives, tapes, …) and persistence
- Networking (including optical, wireless, ubiquitous)
- Digital libraries/data bases
- Sensors/effectors
- Software (operating systems, middleware, domain specific tools/platforms for building applications)
- Services (education, training, consulting, user assistance)

All working together in an integrated fashion.

Cyberinfrastructure: Tipping Point

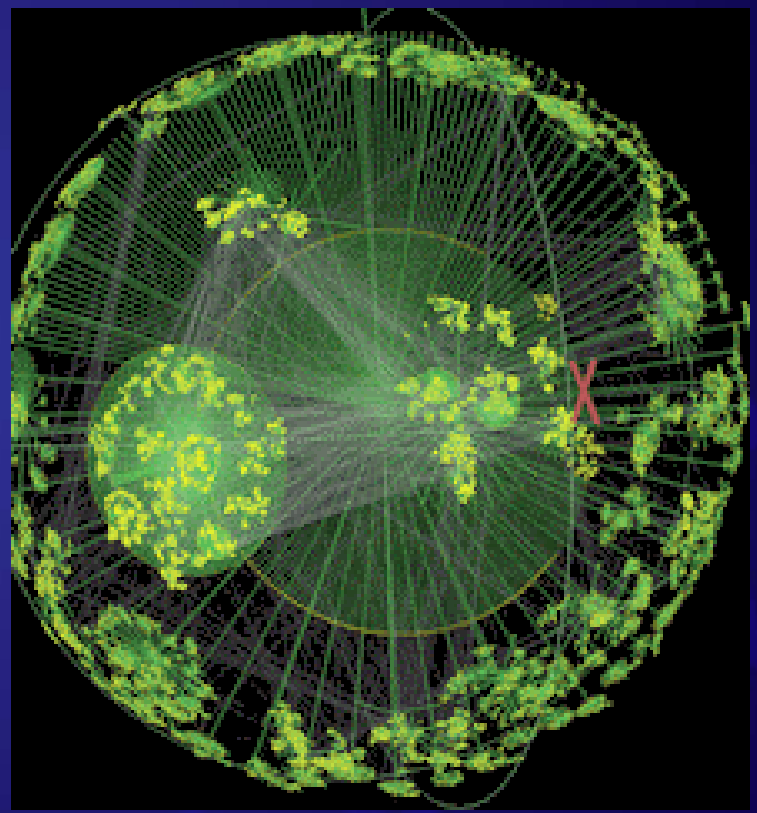
Information Flow Reversal

Internet Historical Roots

Create & Compute at the core; then broadcast to the periphery

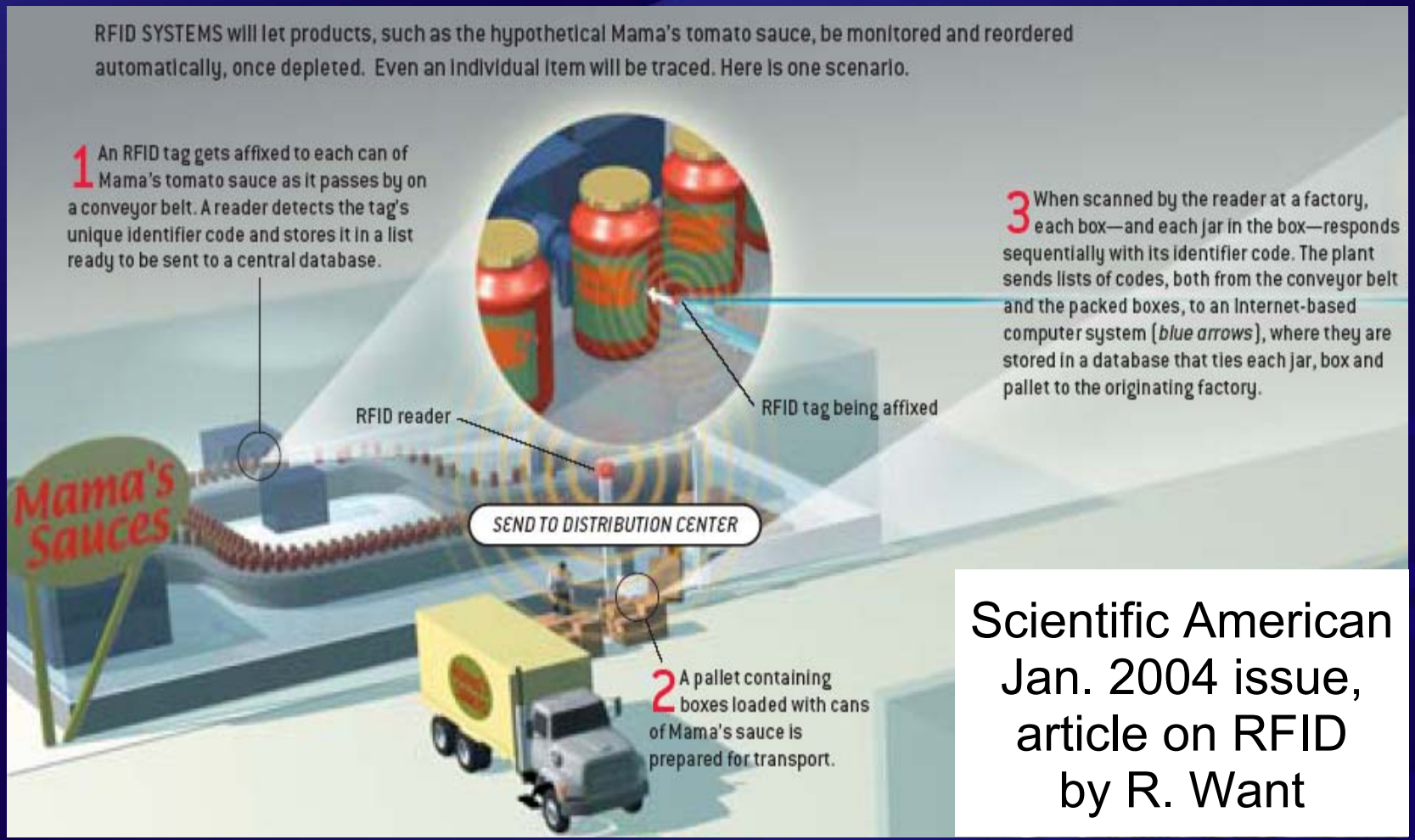
The Next Wave

Massive data generated at the periphery; novel systems & architectures; revitalized core of high-end computers



Topological view of the Internet

Sensor-Nets and the "new" Bar Code



Scientific American Jan. 2004 issue, article on RFID by R. Want

Closing Remarks

- Enabling role of CI for S&E Research is the same paradigm for the transformative power of the new wave of the "e" revolution: immediate economic and societal impact
- Massive data generation at the periphery, HEC at the core, and a new architecture linking the core to the periphery - these are the central elements of CI
- A strategy of a balanced and broad CI to serve all of science and engineering; transition from extant CI to the exciting possibilities of future CI