NATIONAL ACADEMIES *Sciences Engineering Medicine*

Charting a Path in a Shifting Technical and Geopolitical Landscape:

Post-Exascale Computing for the National Nuclear Security Administration

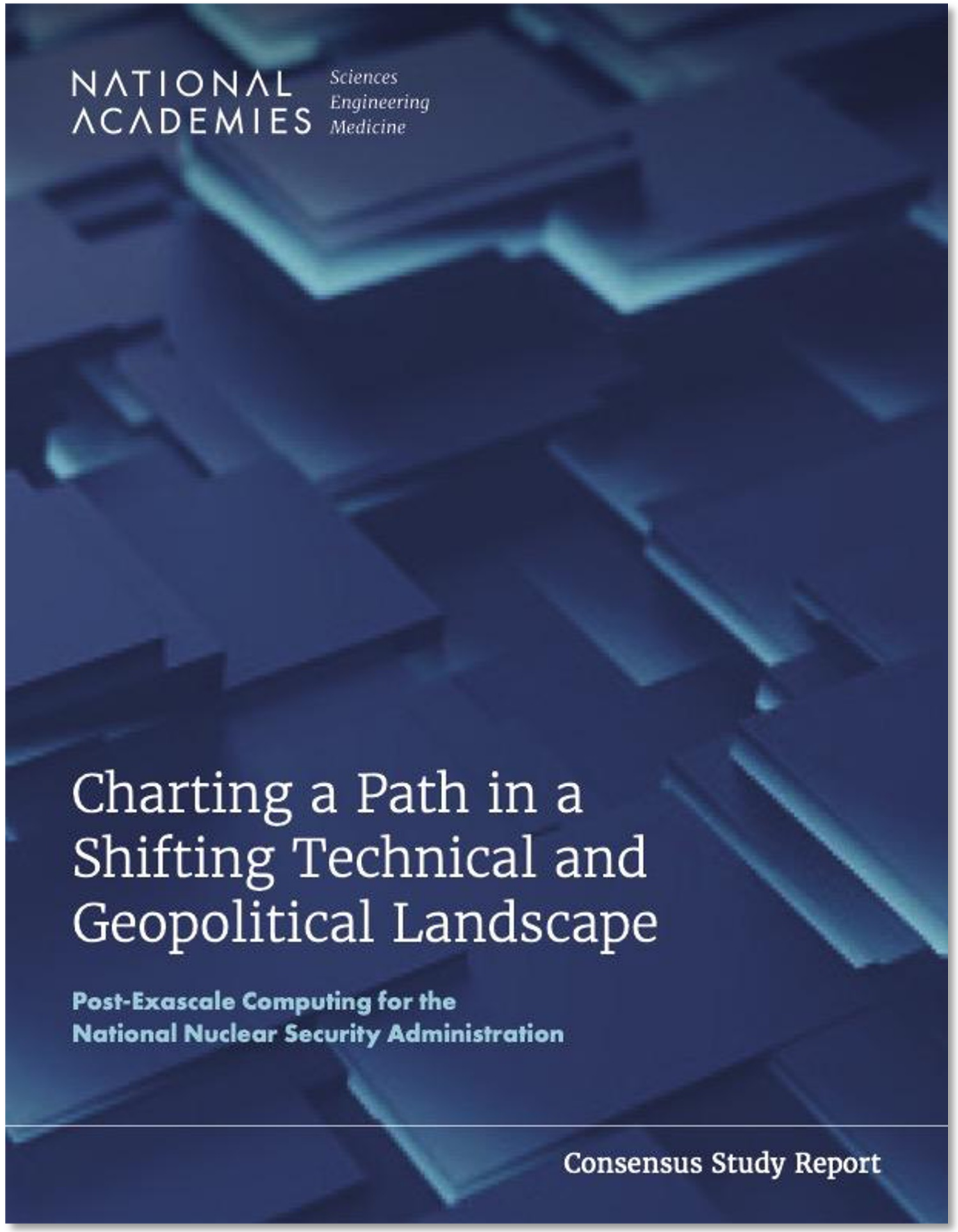
Committee on Post-Exascale Computing for the National Nuclear Security Administration

Computer Science and Telecommunications Board

JUNE 12, 2023 – ASCAC BRIEFING

Study Origin

Section 3172 of the FY2021 NDAA: “Review future of computing beyond exascale computing to meet national security needs at the National Nuclear Security Administration.”



Study Tasks

1. **NNSA's computing needs** over the **next 20 years** that exascale computing will not support;
2. **Future computing technologies** for meeting those needs including quantum computing and other novel hardware, computer architecture, and software;
3. The likely **trajectory of promising hardware and software technologies and obstacles** to their development and their deployment by NNSA; and
4. The ability of the **U.S. industrial base**, including personnel and microelectronics capabilities, to meet NNSA's needs.

(full statement of task is available in the report or at www.cstb.org)

Study Committee

Kathy Yelick, NAE (Chair)	UC Berkeley and LBNL
John Bell, NAS	LBNL
Bill Carlson	IDA
Fred Chong	U of Chicago and Coldquanta
Dona Crawford	LLNL (retired)
Jack Dongarra, NAE	UT Knoxville
Mark Dean, NAE	UT Knoxville
Ian Foster	U of Chicago and ANL
Charlie McMillan	LANL (retired)
Dan Meiron	Caltech
Daniel Reed	U of Utah
Karen Willcox, NAE	UT Austin

Presentations to the Committee

NNSA HQ and Labs

3 SC Labs

White House OSTP

Hyperion Research

RIKEN

Teratec

Asian Tech. Info. Program (ATIP)

ARM

AMD

NVIDIA

HPE

IBM

Intel

Reviewers

William Gropp, NAE	UIUC
Susan Graham, NAE	UC Berkeley
Randal Bryant, NAE	CMU
David Culler, NAE	Google
William Dally, NAE	NVIDIA
Alan Edelman	MIT
Dennis Gannon	U of Indiana
Mark Horowitz	Stanford
Daniel Katz	UIUC
Cherry Murray	NAS/NAE
Jim Rathkopf	LANL, LLNL (retired)
Robert Rosner	U. of Chicago
Valerie Taylor	ANL

Study Scope

- The committee assessed and reported on:
  - NNSA mission needs for computing
  - Technology and market landscape and trends
  - Disruptions: cloud computing, specialized hardware, AI/ML, and quantum
- The report contains recommendations for a path forward:
  - NNSA did not present a specific roadmap for evaluation
  - The report does not contain a detailed roadmap
  - Recommends one be developed
- The committee received classified briefings from the NNSA Labs but determined that a classified annex to the report was not needed

Context: How did we get here?

- **Computing demands** continue to grow
- **Computing technology** has hit several “walls”
- The **computing industry** has changed dramatically
- The benefits of more **weak scaling** are limited
- **AI methods** are having huge impacts elsewhere
- **Quantum computing** has unknown potential
- **Cloud computing** is dominating the computing industry
- The **geopolitical landscape** presents mission uncertainties

The NNSA needs a new strategy for post-exascale computing

Findings and Recommendations

(paraphrased from report)

Overarching Finding

The combination of **increasing demands** for computing with the **technology and market challenges** in HPC requires an **intentional and thorough reevaluation of ASC's approach** to algorithms, software development, system design, computing platform acquisition, and workforce development.

Business-as-usual will not be adequate.

Finding 1: The demands for advanced computing continue to grow and will exceed the capabilities of planned upgrades across the NNSA labs.

- **Future mission challenges will increase the importance of computation** at and beyond the exascale.
- While HPC has traditionally played an important role, some emerging **challenges will require new approaches** to mathematics, algorithms, software, and system design.
- Assessments of **margins and uncertainties** will require additional computational capability beyond exascale; and enhanced computational capability will also be required should there emerge **requirements for new military capabilities.**
- The rapidly **evolving geopolitical situation reinforces the need for computing leadership**.

Runtime of “hero” calculations (all 3D)

Lab resolution/fidelity	Number of Nodes	Memory Footprint	Wall-Clock Time
LANL moderate/moderate	2400 (Trinity)	~300–400 TB	6 months
LANL high/moderate	4990 (Trinity)	~600 TB	3–4 months
LLNL moderate/high	288 (CTS-1, ~25%)	~20 TB	1 month
LLNL high/moderate	3250 (Sierra, ~75%)	104 TB	5.8 days
LLNL very high/moderate	512 (Sierra, 12%)	32.8 TB	2 months

Subset of Application Challenges Beyond Exascale

- Reentry
- Complex geometry
- Combustion
- Extreme Environments

Reentry flight simulation example

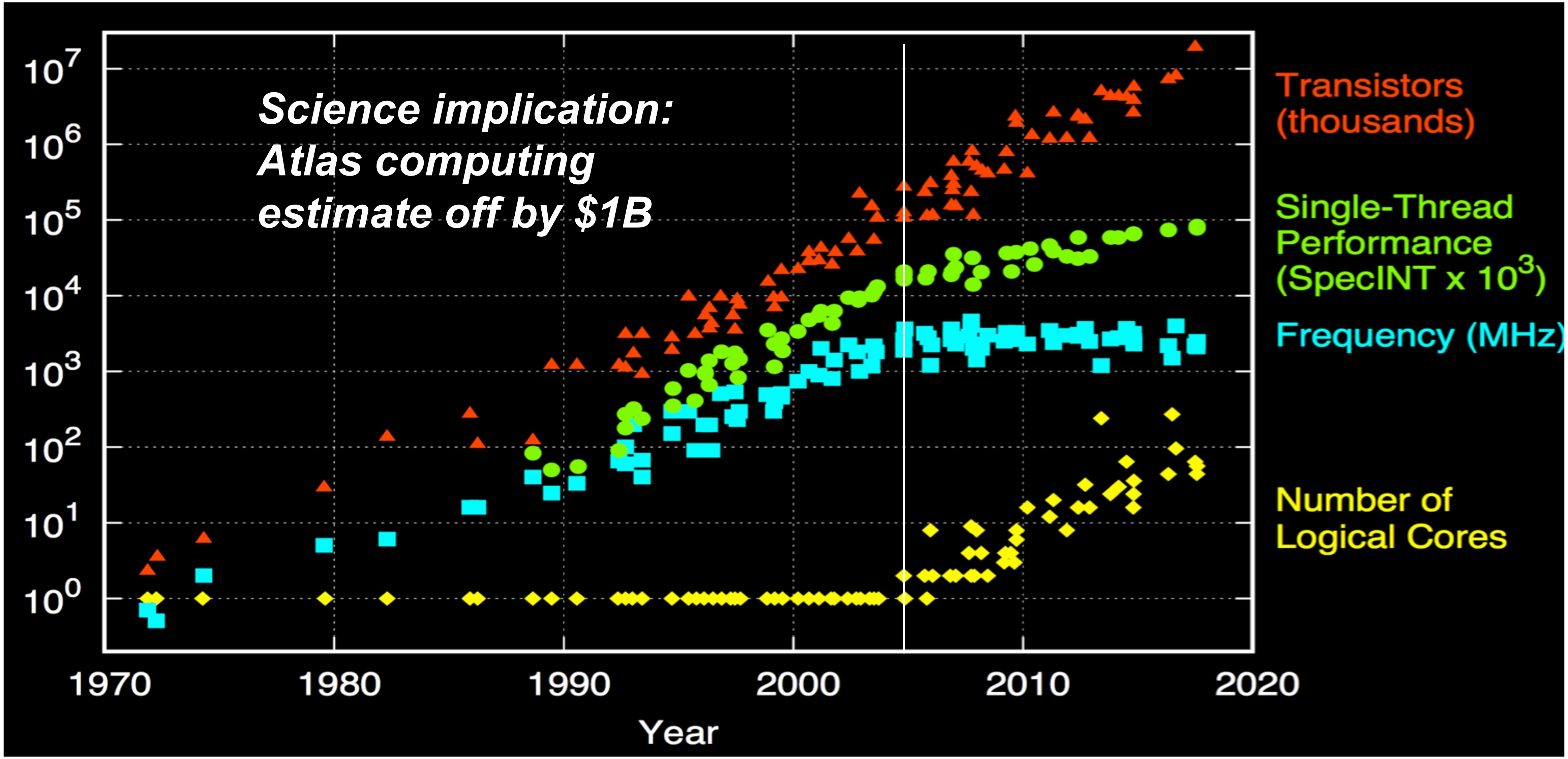
(Lower fidelity) ⟷ Fidelity based on customer/program requirements ⟷ (Higher fidelity)

	RANS snapshots	HRLES snapshots	Time accurate HRLES	WRLES
Size & Quantity	▪ ~100-500 M cells ▪ >10 TB RAM ▪ 10000's of snapshots	▪ ~5-25 B cells ▪ >500 TB RAM ▪ 100's of snapshots	▪ ~5-25 B cells ▪ >500 TB RAM ▪ 5 full simulations	▪ ~50-100 B cells ▪ >2 PB RAM ▪ 1 or 2 time windows
Numerical Methods	▪ Implicit, steady-state ▪ 2^{nd}-order hybrid FV scheme ▪ Continuation solvers ▪ Tridiag solver & GMRES/Multigrid solver		▪ Implicit or IMEX, time accurate ▪ High-res, low-order FV scheme -or- high-order entropy-stable FD/FE ▪ Jacobi & SGS solvers & GMRES/ILU(0)	▪ IMEX or explicit, time accurate ▪ HR, LO FV scheme -or- high-order ES FD/FE ▪ Jacobi & SGS
Coupling & Analysis	▪ Ablation/structural coupling ▪ 6 DOF trajectory coupling ▪ Mesh refinement ▪ Parameter UQ		▪ Ablation/structural coupling ▪ 6 DOF trajectory coupling ▪ Mesh refinement ▪ Parameter UQ & In-situ viz	▪ Mesh refinement ▪ In-situ viz
Critical Components	▪ Scalable solvers ▪ Performance portability ▪ Embedded analysis (meshing, sensitivities, viz) ▪ V&V		▪ Scalable solvers ▪ Performance portability ▪ Embedded analysis ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V	▪ Performance portability ▪ Discretizations ▪ AMT & DataWarehouse ▪ V&V

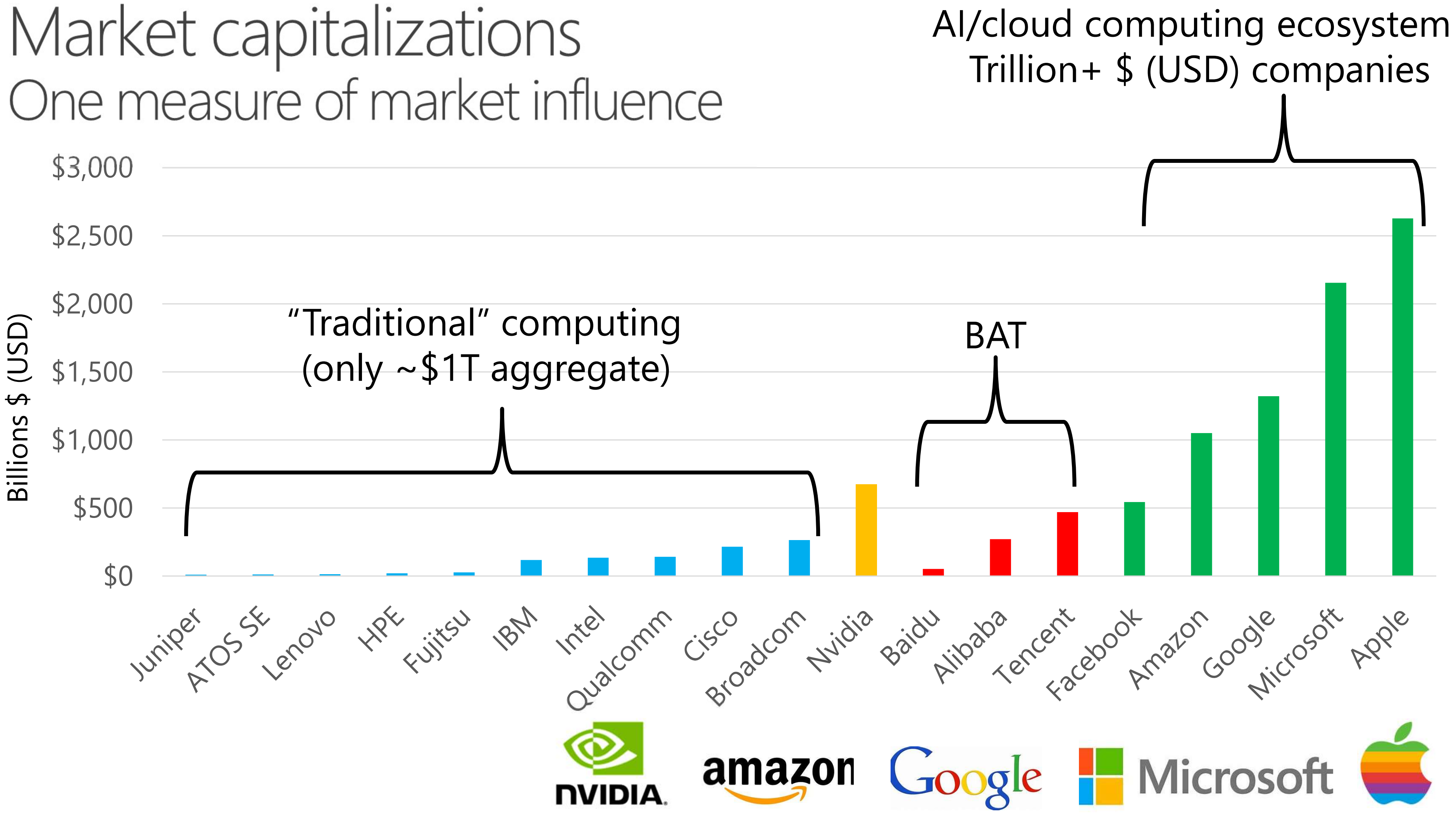
Finding 2: The **computing technology and commercial landscapes are shifting rapidly**, requiring a change in NNSA's computing system procurement and deployment models.

- **Semiconductor manufacturing** is largely offshore;
- All U.S. exascale systems are being produced by a **single integrator**.
- The joint **Exascale Computing Project created a software stack** for systems software and applications, but **there is no plan to sustain it**.
- **Cloud providers are engaged in hardware and software innovations** and will have more market influence in **technology and talent** but are **not aligned with NNSA** requirements.

Dennard Scaling is Dead; Moore's Law Will Follow



Cloud "Hyperscalars" dominate computing



Cloud computing opportunities

Conventional public cloud access is not recommended for NNSA

- Security concerns, cost competitiveness, and architectural mismatch

However, NNSA should carefully consider their relationship to the Cloud

- Join them
  - Hyperscalers are designing their own hardware (not for sale)
  - Research on AI hardware (including, but not exclusively for AI methods)
  - Novel partnership models to be explored
- Beat them at their own game
  - Design NNSA-relevant hardware
  - More Co-Design at the Labs (hardware, OS, compilers…)
  - Recognize significant costs and consider other government partners

Recommendation 1: **NNSA should develop and pursue new and aggressive comprehensive design, acquisition, and deployment strategies** to yield computing systems matched to future mission needs.

NNSA should document this computing roadmap and have it **reviewed by a blue-ribbon panel** within a year after publication of this report and updated periodically thereafter.

- The roadmap should lay out the case for **future application goals** and associated computing requirements for both open and classified problems;
- include **research activities** and how outcomes might affect the roadmap;
- be explicit about **traditional and nontraditional partnerships**, including cloud providers, academia, government laboratories, and cross-government coordination to ensure the necessary influence and resources;
- identify **key government and laboratory leadership** to develop and execute a unified organizational strategy.

Finding 3: **Bold and sustained research and development** investments in hardware, software, and algorithms—including higher-risk research activities to explore new approaches—are critical if NNSA is to meet its future mission needs.

- Physics-based simulators will remain essential but **novel mathematical and computational science approaches** will be needed.
- **VVUQ will become increasingly important** for simulation of complex systems with models of different fidelity, including data-driven approaches.
- An end to transistor scaling will drive **novel computer architectures** ill suited to current methods, software libraries, and programming models.
- They will require **early involvement of applied mathematicians and computational scientists**.
- Technology and market trends will **shift co-design effort to the laboratories**.

Finding 3: **Bold and sustained research and development** investments in hardware, software, and algorithms—including higher-risk research activities to explore new approaches—are critical if NNSA is to meet its future mission needs.

- Advances in **applied mathematics and computational science** have potential impact beyond traditional simulation, e.g., on experimental data.
- **AI methods** may continue to benefit NNSA, but will likely **complement rather than replace** physics-based simulations in the post-exascale era.
- **Quantum technology** has the potential to improve the fundamental understanding of material properties needed by NNSA.
- However, **breakthroughs in quantum algorithms and systems are needed** to make quantum computing practical for multiphysics stockpile modeling. Quantum computing is more likely to serve as a **special-purpose accelerator** than to replace leading-edge computing.

Recommendation 2: NNSA should foster and pursue high-risk, high-reward research in applied mathematics, computer science, and computational science to cultivate radical innovation and ensure future intellectual leadership needed for its mission.

- NNSA should strengthen efforts in **applied mathematics and computational science** R&D.
- NNSA should strengthen efforts in **computer science** R&D to build a substantial, sustained, and broad-based intramural research program.
- NNSA should **expand research in AI** to explore the use of these methods both for predictive science and for emerging applications.
- NNSA should continue to **invest in and track quantum computing** R&D for future integration into its computational toolkit.

AI opportunities

AI can neither be dismissed as irrelevant to NNSA **nor embraced** as a replacement for physics-based simulation at this time.

- NNSA needs to invest in R&D and consider **how this affects its roadmap**; they may have missed opportunities.
- NNSA could **drive R&D in AI** for physics-based problems, improving high confidence, etc.
- AI may **reduce computational costs** of some simulation problems (e.g., surrogates);
- But the Labs have estimated **large increased costs** for others.
- **AI hardware is continuing to improve**, and there may be opportunities to influence it.

Finding 4: The NNSA laboratories face s**ignificant challenges in recruiting and retaining the highly creative workforce** that NNSA needs, owing to competition from industry, a shrinking talent pipeline, and challenges in hiring diverse and international talent.

- The ASC program currently faces a **challenge maintaining a competitive workforce; and this challenge will continue to grow**.
- The U.S. national security enterprise has benefited enormously from **inclusion of global talent**.
- Addressing the challenges laid out in this report will require a nurturing environment that **reduces distractions, funding uncertainty, and administrative burdens**, while providing employees the **time and flexibility for the creative thinking** required to solve these problems.

Recommendation 3: NNSA should develop an aggressive national strategy through partnership across agencies and academia to address its workforce challenge.

- NNSA should make concerted efforts to nurture and retain existing staff; more aggressively **grow the pipeline**; create an **efficient and modern, yet secure environment**; grow existing **workforce programs**; and **collaborate with other federal agencies** to support ambitious talent development.
- NNSA should also develop a **deliberate strategy to attract an international workforce** and to provide them with a welcoming environment while thoughtfully managing the **attendant national security risks**.

Key takeaways

- The NNSA is positioned to take advantage of exascale computing, but **computing demand will continue to grow** beyond exascale.
- **Technical and market factors** will create challenges for computing performance growth.
- A **bold roadmap that deviates from business-as-usual should** consider purpose-built hardware, novel algorithms to address weak scaling, AI methods, new partnerships, and alternative acquisition models.
- **An advanced workforce and visionary leadership will be needed** to shepherd the changes required for NNSA's post-exascale mission goals.

Thank you!

The report is available for download from National Academies Press at https://nap.edu/26916