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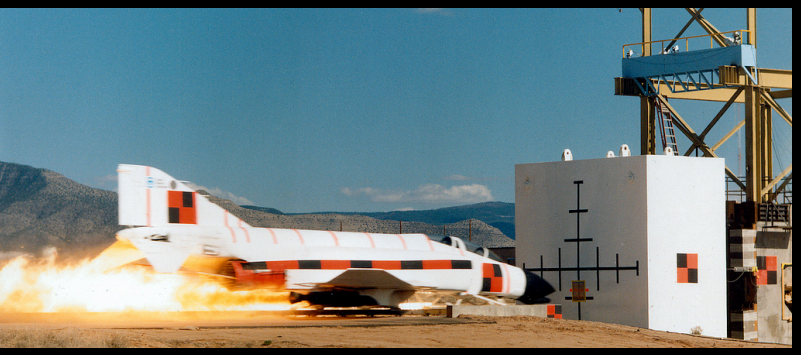
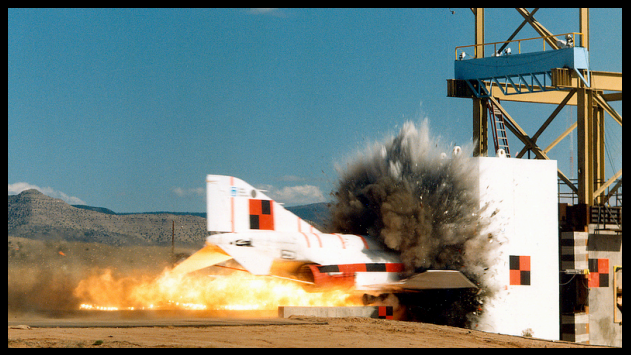


Oh, $#*@! Exascale!

The effect of emerging architectures on scientific discovery

Ultrascale Visualization Workshop, November 12, 2012

Kenneth Moreland, Sandia National Laboratories

DOE SDAV

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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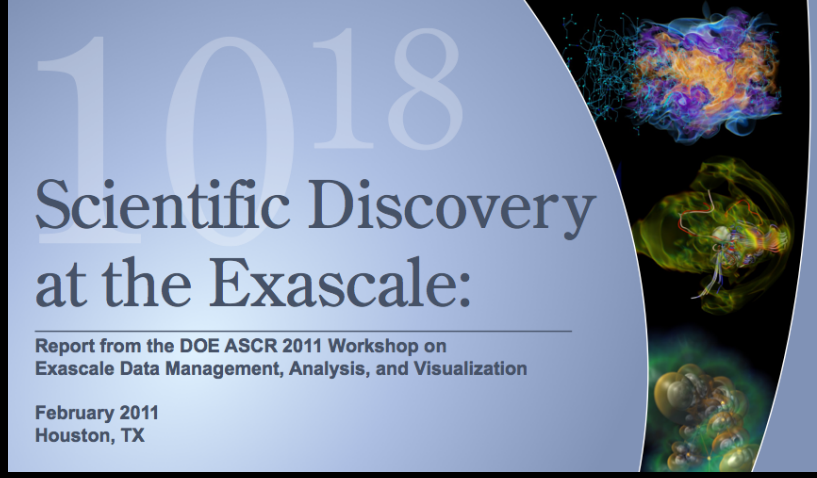
Slide of Doom



System Parameter	2011	"2018"		Factor Change
System Peak	2 PetaFLOPS	1 ExaFLOP		500
Power	6 MW	≤ 20 MW		3
System Memory	0.3 PB	32 – 64 PB		100 – 200
Total Concurrency	225K	1B × 10	1B × 100	40,000 – 400,000
Node Performance	125 GF	1 TF	10 TF	8 – 80
Node Concurrency	12	1,000	10,000	83 – 830
Network BW	1.5 KB/s	100 GB/s	1000 GB/s	66 – 660
System Size (nodes)	18,700	1,000,000	100,000	50 – 500
I/O Capacity	15 PB	300 – 1000 PB		20 – 67
I/O BW	0.2 TB/s	20 – 60 TB/s		10 – 30

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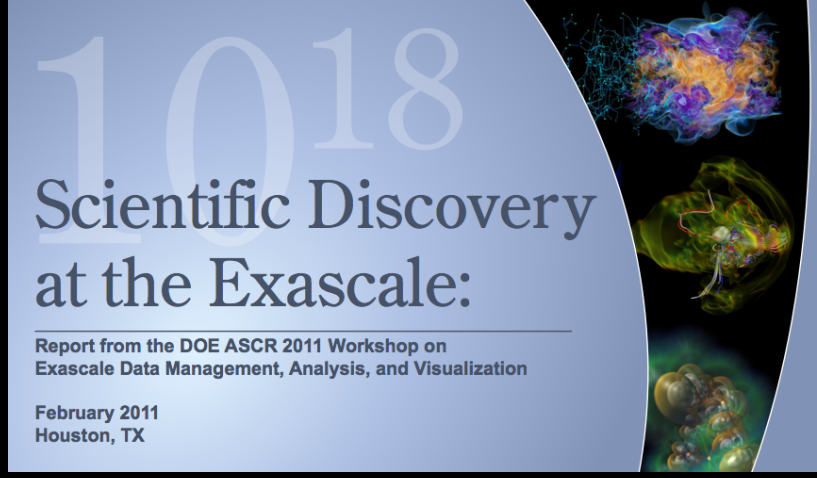

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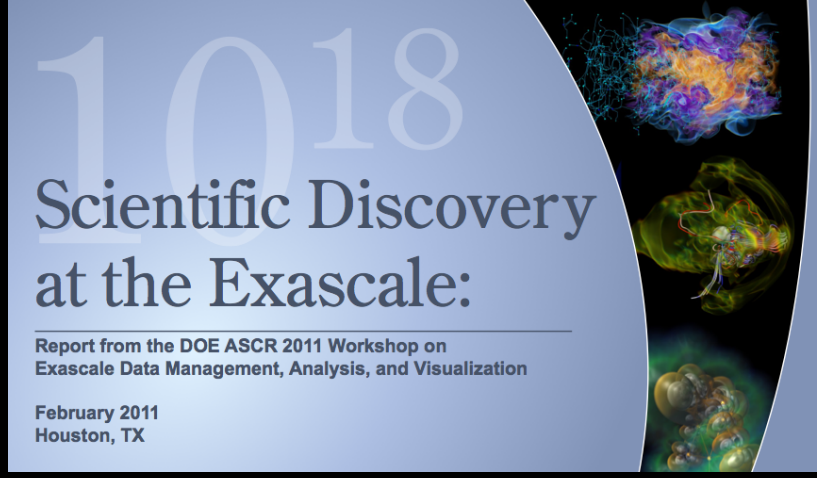

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Exascale Projection

	Jaguar – XT5	Exascale*	Increase
Memory	300 Terabytes	32 – 64 Petabytes	100 – 200×
Concurrency	224,256 way	10 – 100 billion way	Up to 400,000×

MPI Only?

- Vis object code + state: 20MB
- On Jaguar: 20MB × 200,000 processes = 4TB
- On Exascale: 20MB × 100 billion processes = 2EB !

*Source: Scientific Discovery at the Exascale, Ahern, Shoshani, Ma, et al.

Exascale Projection

	Jaguar – XT5	Exascale*	Increase
Memory	300 Terabytes	32 – 64 Petabytes	100 – 200×
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Visualization pipeline too heavyweight?

- On Jaguar: 1 trillion cells → 5 million cells/thread
- On Exascale: 100 trillion cells → 1000 cells/thread

*Source: Scientific Discovery at the Exascale, Ahern, Shoshani, Ma, et al.

Exascale Projection

	Jaguar – XT5	Exascale*	Increase
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Overhead of ghost/halo cells?

- On Jaguar: 1 trillion cells → 5 million cells/thread
  - Partition into ~171^3 blocks
  - $6 \times 171^2 \approx 175K$ ghost/block → 35 billion ghost total
  - Ghost cells **~3.5% size of original data**
- On Exascale: 100 trillion cells → 1000 cells/thread
  - Partition into 10^3 blocks
  - $6 \times 10^2 \approx 600$ ghost/block → 60 trillion ghost total
  - Ghost cells **60% size of original data**

*Source: Scientific Discovery at the Exascale, Ahern, Shoshani, Ma, et al.

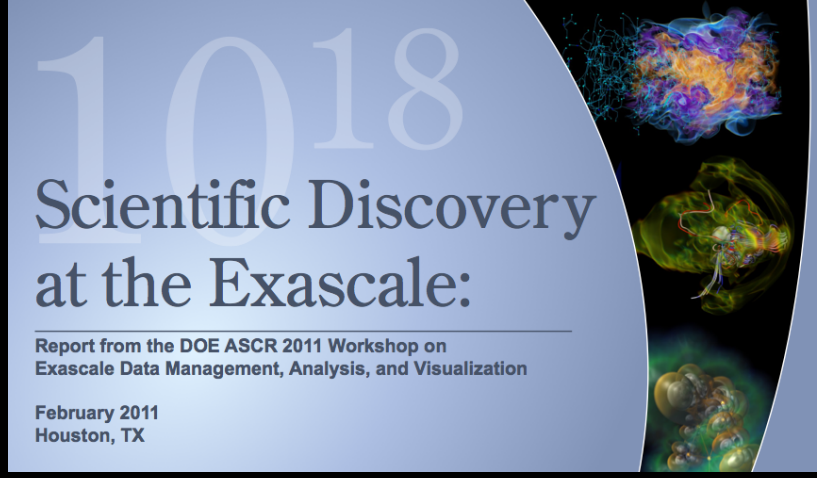
Exascale Programming Challenges

- At some point, domain decomposition fails
  - Too many halo cells, too much communication
- Possible new architectures and programming models
  - GPU accelerators hate decomposition
- Threaded (OpenMP) programming is easier than distributed (MPI) programming.

LIES!!!

  - Threading needs careful planning for memory affinity (inherent in distributed)
  - Sharing memory locations invites read/write collisions (explicit in distributed)
  - PGAS will save us? I'm skeptical.
- Best practice approach: Encapsulated Multithreaded Operations
  - Multiple DOE projects underway: Dax (ASCR), PISTON (ASC), EAVL (LDRD)
  - If successful, minimal impact on applications
  - Might be some changes in scope of what can be done

Slide of Doom



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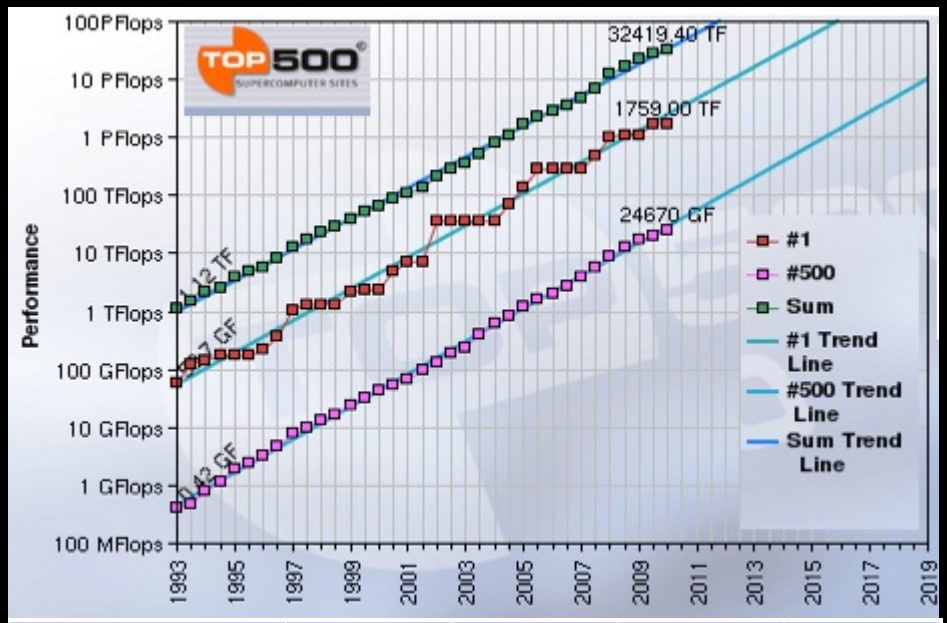
Extreme scale computing

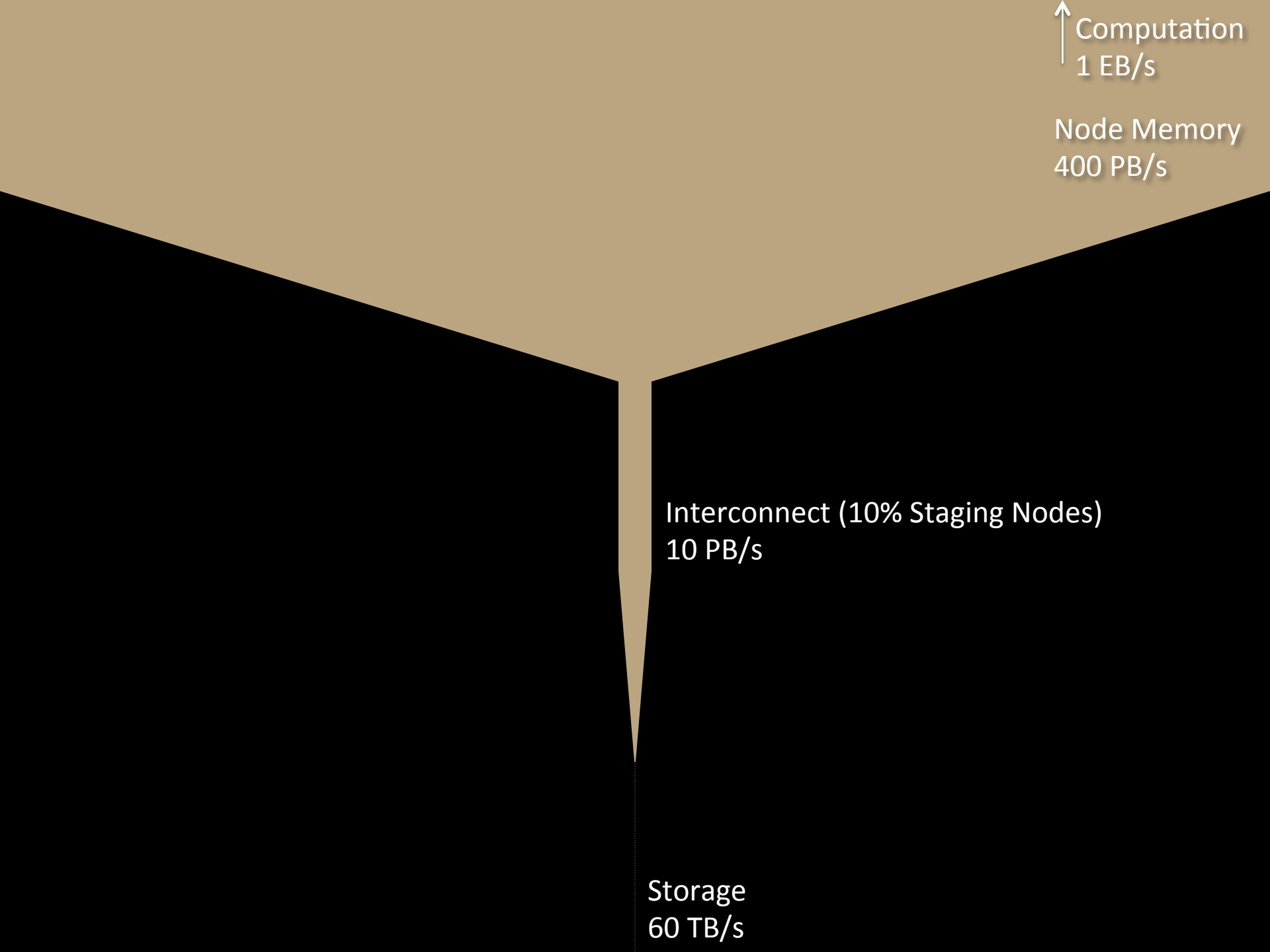
- Trends
  - More FLOPS
  - More concurrency
  - Comparatively less storage, I/O bandwidth
- ASCI purple (49 TB/140 GB/s) – JaguarPF (300 TB/ 200 GB/s)
  - Most people get < 5 GB/sec at scale

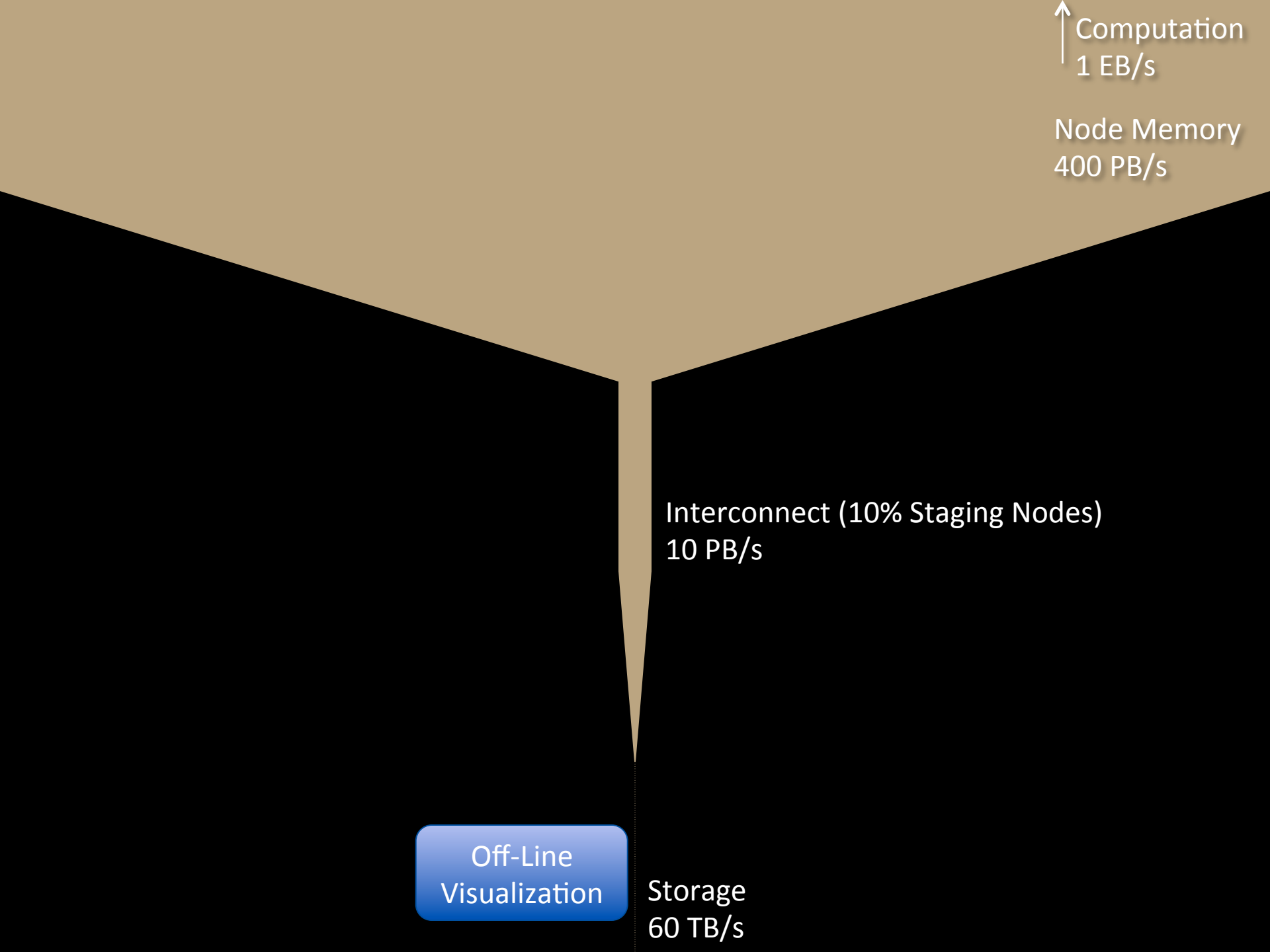


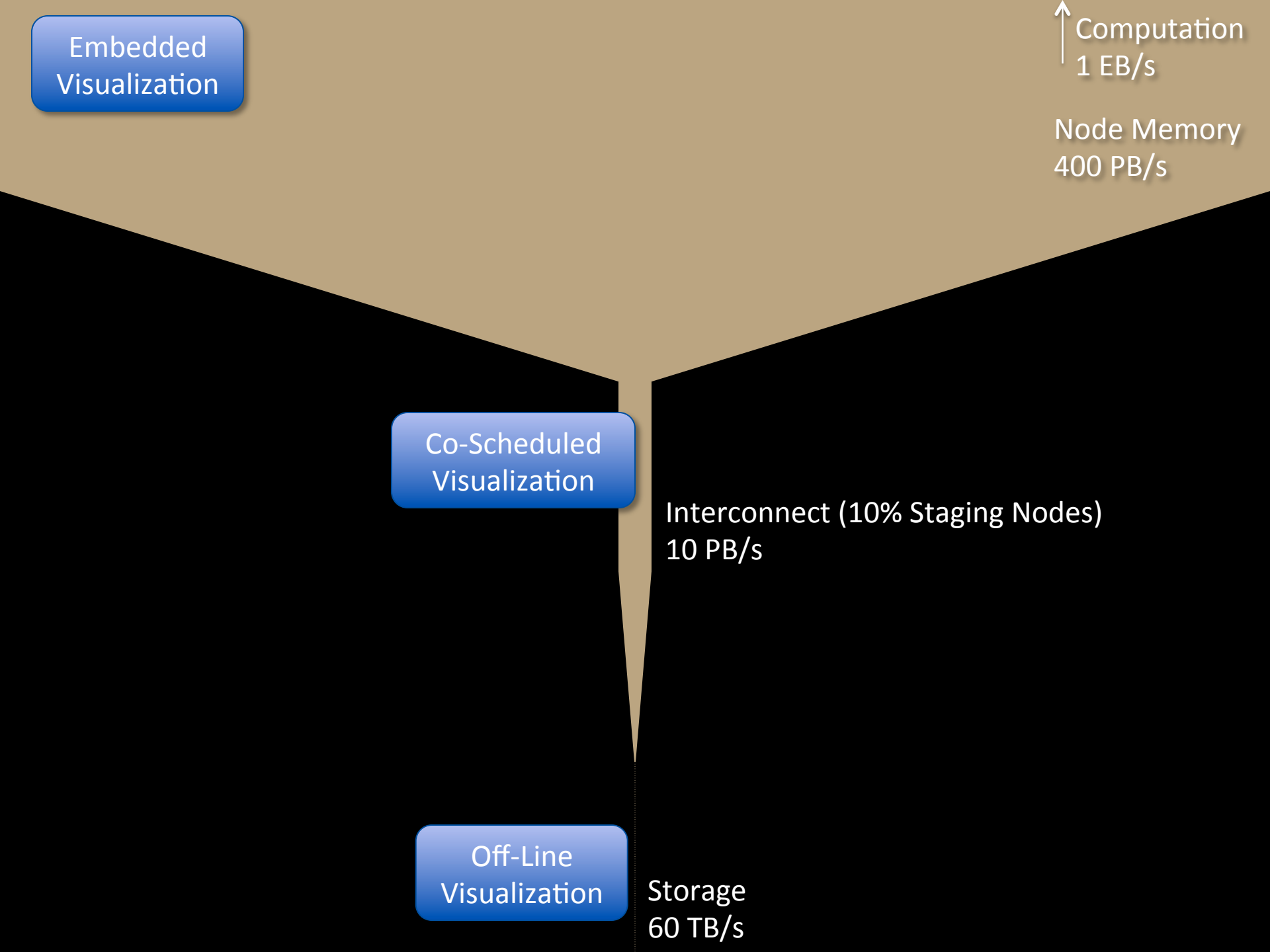
Systems	2009	2011	2015	2018
System Peak Flops/s	2 Peta	20 Peta	100-200 Peta	1 Exa
System Memory	0.3 PB	1 PB	5 PB	10 PB
Node Performance	125 GF	200 GF	400 GF	1-10 TF
Node Memory BW	25 GB/s	40 GB/s	100 GB/s	200-400 GB/s
Node Concurrency	12	32	O(100)	O(1000)
Interconnect BW	1.5 GB/s	10 GB/s	25 GB/s	50 GB/s
System Size (Nodes)	18,700	100,000	500,000	O(Million)
Total Concurrency	225,000	3 Million	50 Million	O(Billion)
Storage	15 PB	30 PB	150 PB	300 PB
I/O	0.2 TB/s	2 TB/s	10 TB/s	20 TB/s
MTTI	Days	Days	Days	O(1Day)
Power	6 MW	~10 MW	~10 MW	~20 MW

ILLUSTRATION: A. TOVEY

From J. Dongarra, "Impact of Architecture and Technology for Extreme Scale on Software and Algorithm Design," Cross-cutting Technologies for Computing at the Exascale, February 2-5, 2010.


Computation
1 EB/s
Node Memory
400 PB/s
Interconnect (10% Staging Nodes)
10 PB/s
Storage
60 TB/s


Computation
1 EB/s
Node Memory
400 PB/s
Interconnect (10% Staging Nodes)
10 PB/s
Off-Line
Visualization
Storage
60 TB/s


Embedded Visualization
Computation
1 EB/s
Node Memory
400 PB/s
Co-Scheduled Visualization
Interconnect (10% Staging Nodes)
10 PB/s
Off-Line Visualization
Storage
60 TB/s

Space of Solutions

	Capability	Coupling	Footprint	Transfer	Interactive
Tightly Integrated	Low	Tight	**Low**	**None**	No
Embedded	**High**	Tight	High	Possible memcpy	No
Hybrid	**High**	Tight	Medium	Subset Hi Speed Transfer	**Yes**
Co-Scheduled	**High**	**Loose**	~5% Extra Nodes	Hi Speed Transfer	**Yes**
Off-Line	**High**	**Loose**	**None**	Slow Persistent Storage Cost	**Yes**

Other Exascale Challenges

- Resilience
  - Mean time to failure
  - Robustness for in situ
  - Soft errors
  - Uncertainty
- Compression/extraction
  - Feature characterization
  - Lossy/lossless compression
- Provenance
  - Capture functions, algorithms, parameters
- Uncertainty Quantification

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  - The DOE Office of Science, Advanced Scientific Computing Research, under award number 10-014707, program manager Lucy Nowell
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  - Argonne National Laboratory: Venkatram Vishwanath, Mark Hereld, Michael E. Papka
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