



Accelerating Research

An off the shelf 10U Mini-Supercomputer

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SCIENTIFIC COMPUTING EXPERT
JUNE 2013

GENE CENTER MUNICH AT LMU



- ▶ Established 1984 by Ernst Ludwig Winnacker
 - Now 15 Labs, over 300 people from over 20 countries
 - Huge growth under current director Patrick Cramer
- ▶ Research focus areas
 - Structural Biochemistry, Genome Maintenance, Regulation of Gene Expression
- ▶ High-profile publications
 - Science, Nature, Cell
- ▶ Research Techniques
 - Cryo-Electron Microscopy, X-Ray Crystallography, Next Generation Sequencing, Computational Biology

DIVERSE COMPUTATIONAL NEEDS



► High End Instruments

- Cryo-EM: FEI Titan Krios (4M€)
- Sequencing: Illumina GA II
- High Throughput Robot: Beckman Coulter
- Mass Spec: Thermo Scientific Orbitrap Elite

► 3D Reconstruction from Cryo-EM

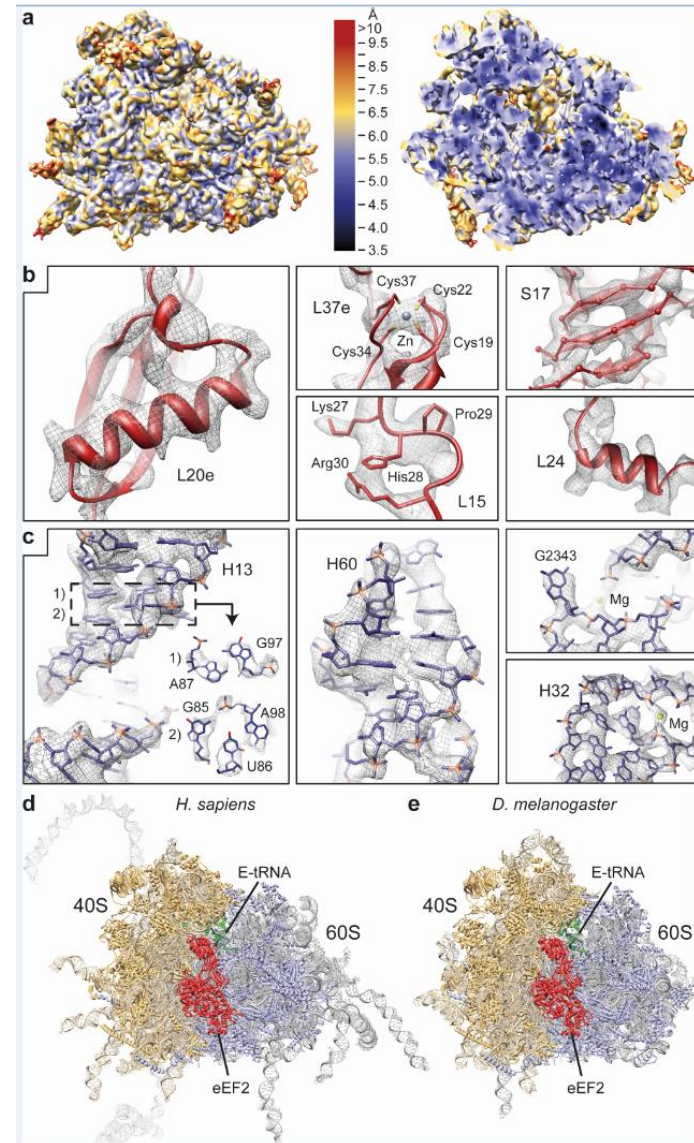
- 10k Raw Micrograph: $4096 \times 4096 \times 16 = 32\text{MB}$
- Up to 1M $\sim 256 \times 256 \times 32$ 2D particle images
- Resolution of 3D mass density down to 4\AA

► Software Packages

- SPIDER supports MPI (Frank, 1978)
- Relion needs MPI (Scheres, 2012)

“Structures of the human and Drosophila 80S ribosome.”
Anger AM, Armache JP et al., Nature, 2013

3D Ribosome Model



INTEGRATED SUPERCOMPUTERS ARE GREAT BUT ...



The Cray XC30™ Supercomputer Series Scalability Across the Performance Spectrum!



... can we have that in half a Rack within budget?

“OFF THE SHELF” INTEGRATED MINI-SUPERCOMPUTER: AMD’S SEAMICRO



AMD SeaMicro SM-15000

- ▶ Standard requirements
 - 4-6 normal power cables
 - No special cooling
 - 128 nodes productive within 48h

- ▶ High computational density at low power
 - 3.5KW per 10U
 - 3 SMs + file servers in a Rack < 12KW
 - 2048 cores per Rack possible

- ▶ Near linear MPI scaling for our needs
 - 8 Gbit/s per low power CPU
 - Amazing bandwidth per Instruction

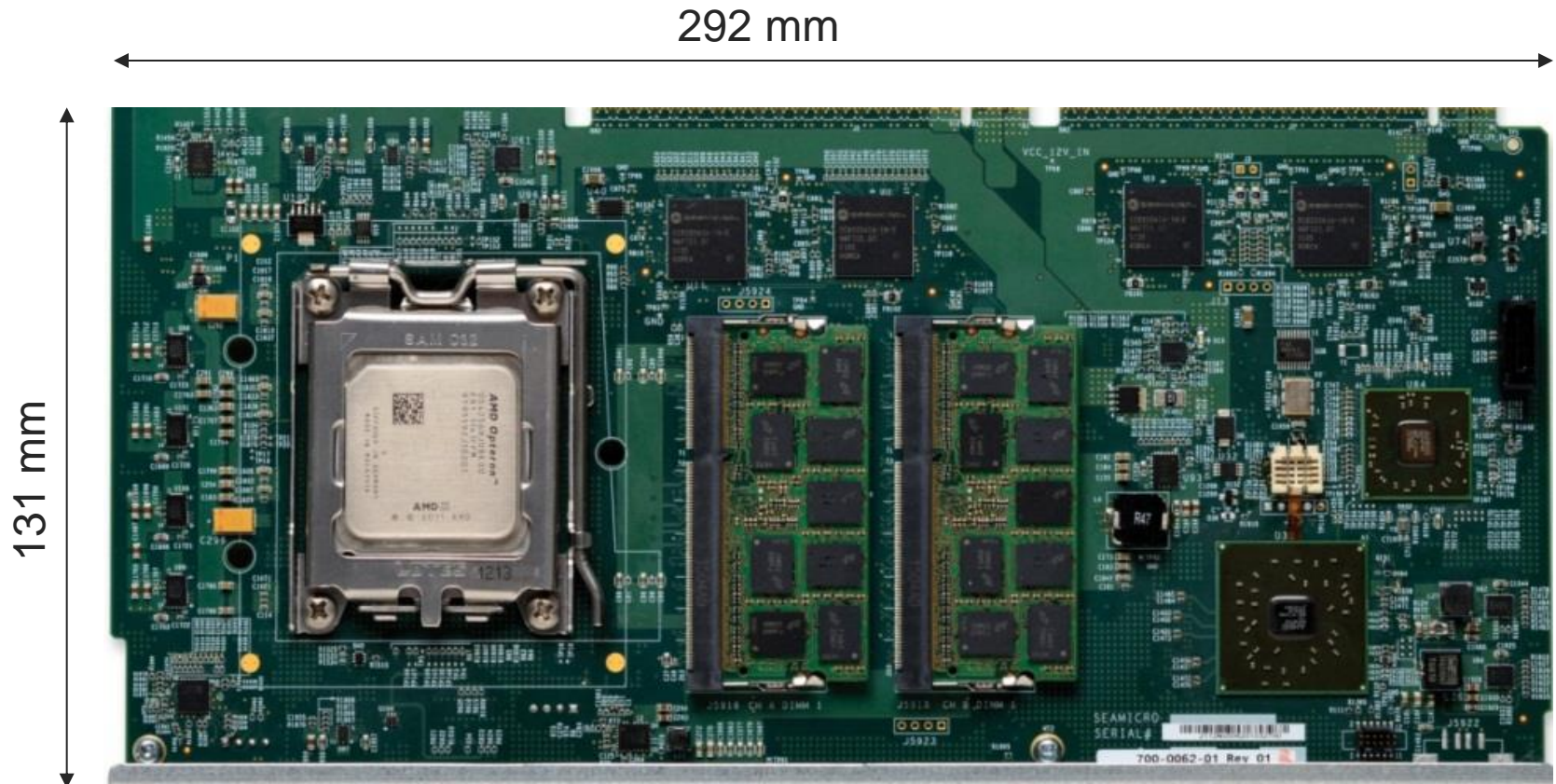
- ▶ Significant reduction in strain on budget
 - Total Cost of Ownership
 - Entry price
 - Personnel
 - FLOPs per Watt
 - Interconnect



"Given that the OCP disaggregated server concept is not even in the market yet, AMD deserves respect for their forward thinking."

Forbes, Apr 2013

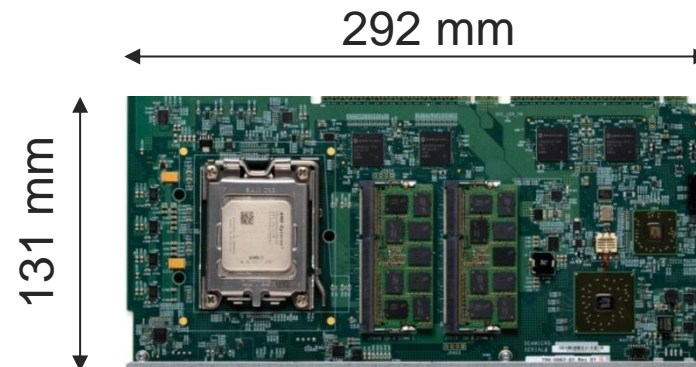
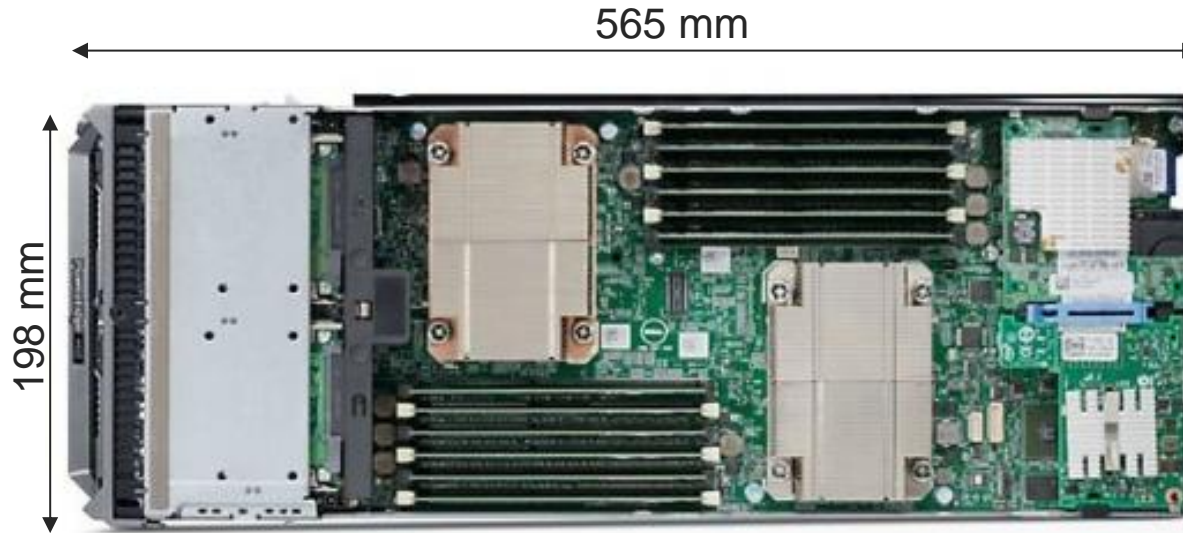
A SEAMICRO NODE IS BASICALLY JUST A PCI-E CARD



COMPARISON TO A BLADE SERVER



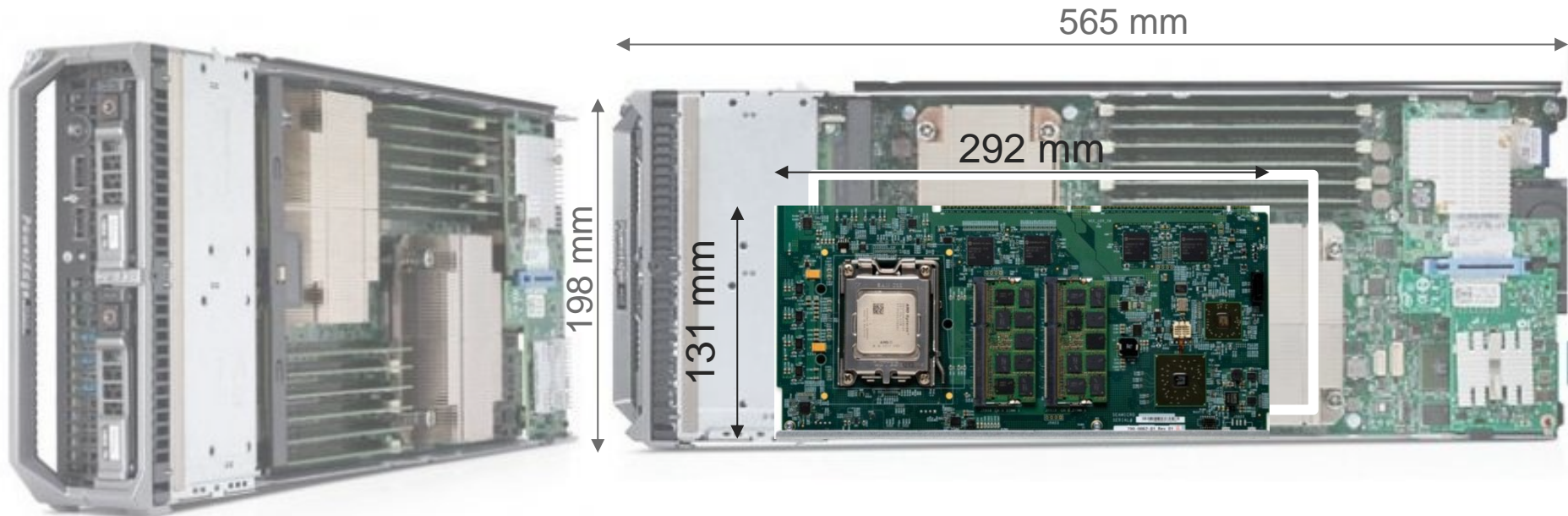
Option 1



COMPARISON TO A BLADE SERVER



Option 2



COMPARISON OF SM15000 TO A BLADE CENTER



**AMD's SeaMicro
SM15000-Opteron**



**AMD's SeaMicro
SM15000-Xeon**



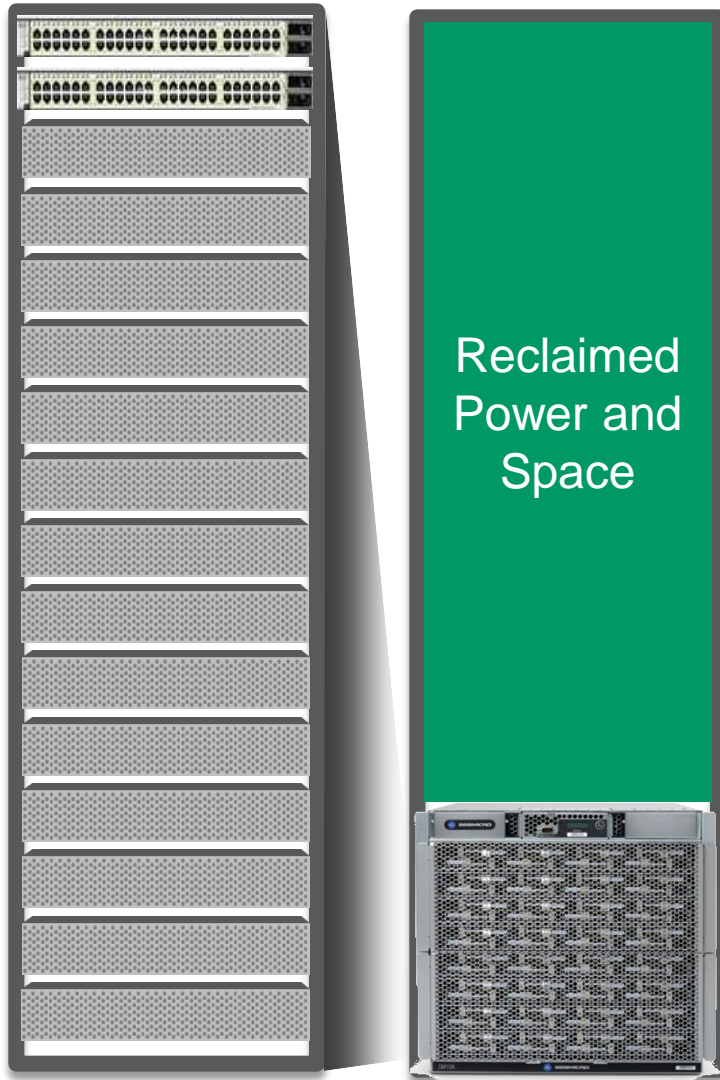
Blade Center



Comparison	SM15000-OP AMD Opteron 4365 EE (Measured)	SM15000-XN Intel Xeon E3-1265Lv2 (Measured)	Blade Center Intel Xeon E5-2470 (estimated)
Nodes	64	64	16
Number of Cores	512	256	256
GHz	2000	2500	2300
Network GBit/s per core	1.0	2.0	0.6
HPL Performance (TFLOP/s) Efficiency (estimated %)	2867 70%	3584 70%	3300 70%
Power HPL (kW)	5.82	4.54	6.10
MFLOPS/W	639	785	548
CPU Price per Core	?€	65€	150€

Benchmark measurements and estimates by AMD/Seamicro

COMPARED TO A STANDARD BEOWULF CLUSTER



SeaMicro SM15000

- ▶ About half the power
- ▶ About half the space

512 Cores
COMPUTE



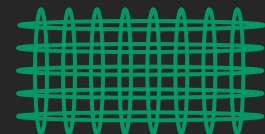
16 X 10 GIG
UPLINKS



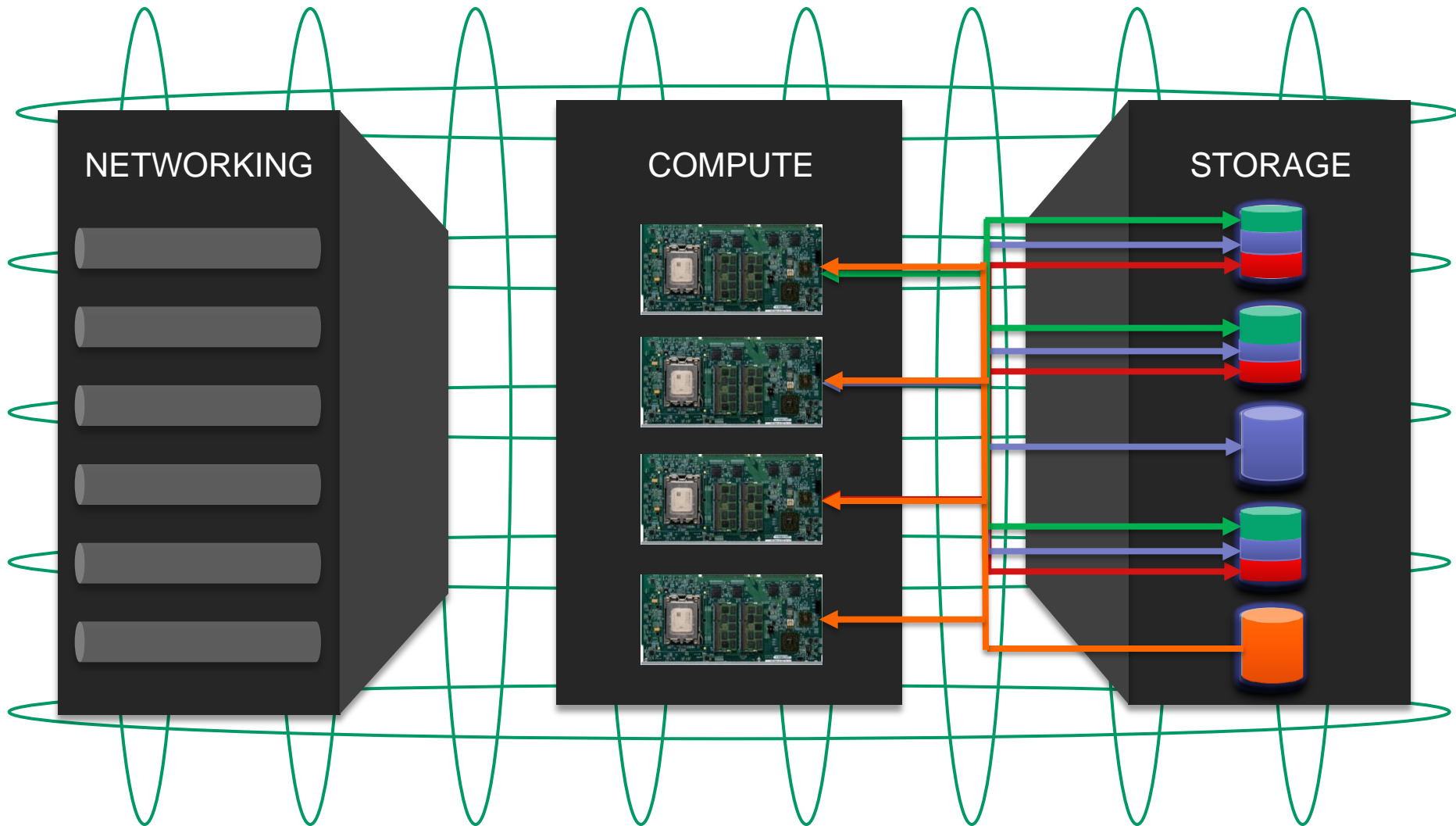
64TB-5PB
STORAGE



1.28 Tbps
FREEDOM FABRIC

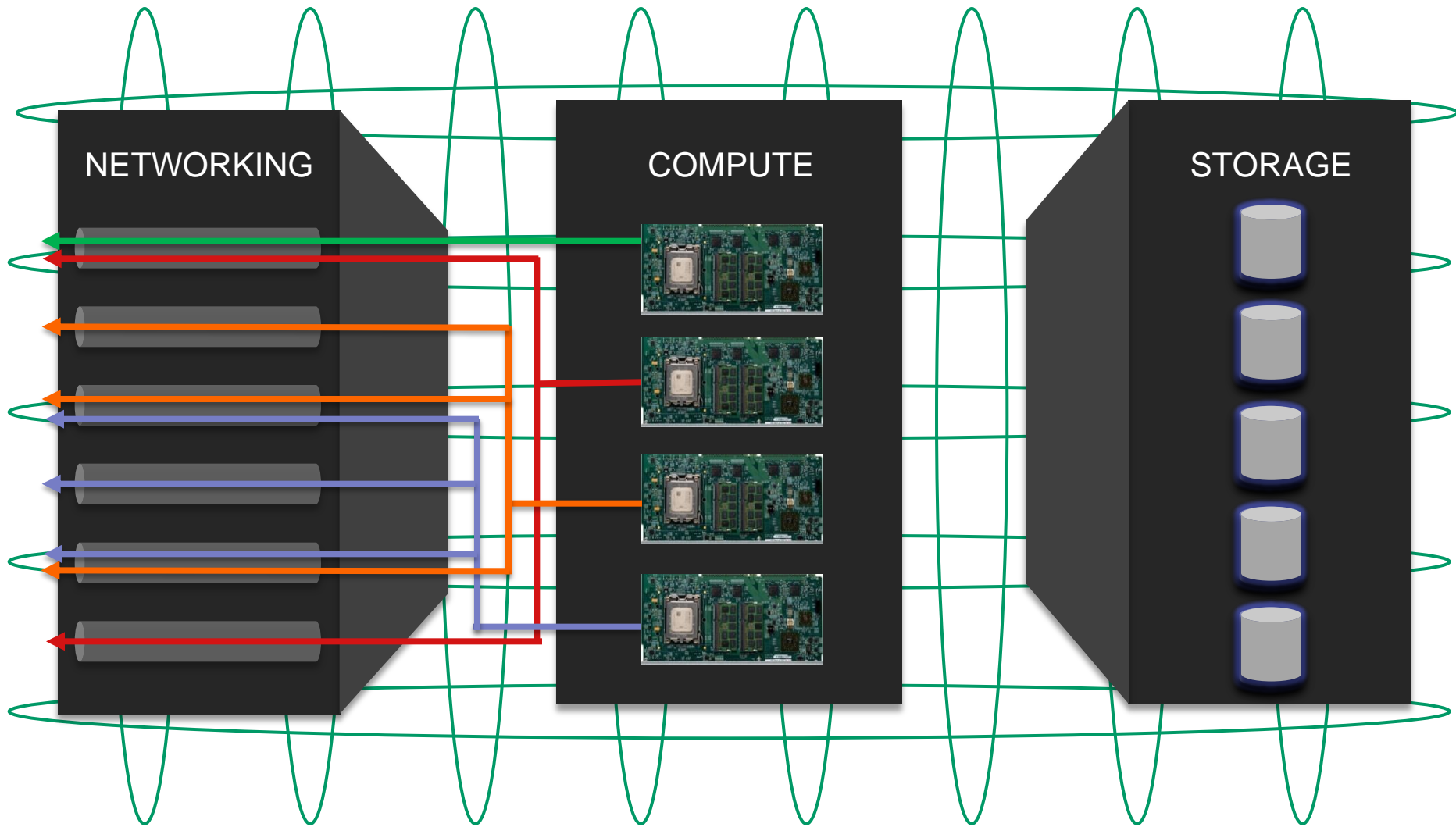


FABRIC INTERCONNECT PROVIDES ANY SERVER TO ANY DISK DRIVE CONNECTIVITY AT 10 GBPS



1.28 Tbps, 3-D Torus FREEDOM FABRIC

NETWORK I/O IS SHARED TO MINIMIZE NIC COSTS AND AVOID UNDERUTILIZATION OR CONGESTION—NO INFINIBAND



1.28 Tbps, 3-D Torus FREEDOM FABRIC

MINI-SUPERCOMPUTER IN A BOX



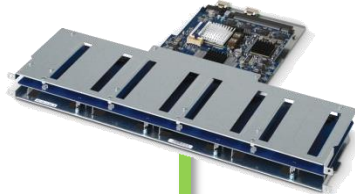
64 HDDs/SDDs

- Share drives across all servers
- Assign one server to one or more drives as needed
- In service upgrades as needed



64 Industry standard x86 servers

- Opteron, Xeon, Atom
- Energy efficient processor
- 20 Gbps per socket, 16X traditional servers



5 Petabytes Fabric Storage

- Extends supercompute fabric to external storage
- 1,344 LFF/SFF drives
- Map to any CPU—same as internal drives

160 Gbps Network I/O

- Share network I/O across all servers
- Eliminate TOR switch
- Minimize cabling
- In service upgrades as needed





Thanks

- ▶ Prof. Dr. Roland Beckmann, GCM
- ▶ Dr. Andreas Anger, GCM
- ▶ Young-Sae Song, AMD/Seamicro
- ▶ Joshua Mora, AMD/Seamicro

Questions