# IBM Power Systems HPC solutions

*Faster time to insight with the high-performance, comprehensive portfolio designed for your workflows*

## Highlights

- IBM Power Systems HPC solutions are comprehensive clusters built for faster time to insight
- IBM POWER8 offers the performance, cache and memory bandwidth to drive the best results from high performance computing and high performance data analytics applications
- IBM HPC software is designed to capitalize on the technical features of IBM Power Systems clusters

Architecting superior high performance computing (HPC) clusters requires a holistic approach that responds to performance at every level of the deployment.

IBM high performance computing solutions, built with IBM® Power Systems™, IBM® Spectrum™ Computing, IBM Spectrum Storage™, and IBM Software technologies, provide an integrated platform to optimize your HPC workflows, resulting in faster time to insights and value.

## The industry's most comprehensive, data-centric HPC solutions

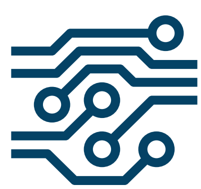
Only IBM provides a total HPC solution, including optimized, best-of-breed components at all levels of the system stack. Comprehensive solutions ensure:

- Rapid deployment
- Clusters that deliver value immediately after acceptance

IBM HPC solutions are built for data-centric computing, and delivered with integration expertise targeting performance optimization at the workflow level. Data-centric design minimizes data motion, enables compute capabilities across the system stack, and provides a modular, scalable architecture that is optimized for HPC.

### Data-centric HPC and CORAL

**Data-centric design was a primary reason the Department of Energy selected IBM for the CORAL deployment. Summit (Oak Ridge National Laboratory) and Sierra (Lawrence Livermore National Laboratory) will become some of the largest, most groundbreaking, and most utilized installations in the world. Bring that same data-centric design to your HPC cluster by partnering with IBM.**



## A total HPC solution

IBM HPC solutions offer industry-leading innovation within and across the system stack. From servers, accelerators, network fabric and storage, to compilers and development tools, cluster management software and cloud integration points, solution components are designed for superior integration and total workflow performance optimization. This comprehensive scope is unique among competitive technology providers and reflects IBM's deep expertise in data-centric system design and integration. Only IBM can deliver a data-centric system optimized for your workflows, realizing the fastest time to insight and value.

## Beyond the server: Superior data management and storage

A pillar of data-centric system innovation, IBM Spectrum Scale™ software-defined storage offers scalable, high-performance, and reliable unified storage for files and data objects. It does so with parallel performance for HPC users.

Implementing the unique advantages of IBM Spectrum Scale (formerly GPFS), IBM Elastic Storage Server is a storage solution that provides persistent performance at any scale. It ensures fast access and availability of the right data, at the right time, across clusters. Built in management and administration tools ensure ease of deployment and continual optimization.

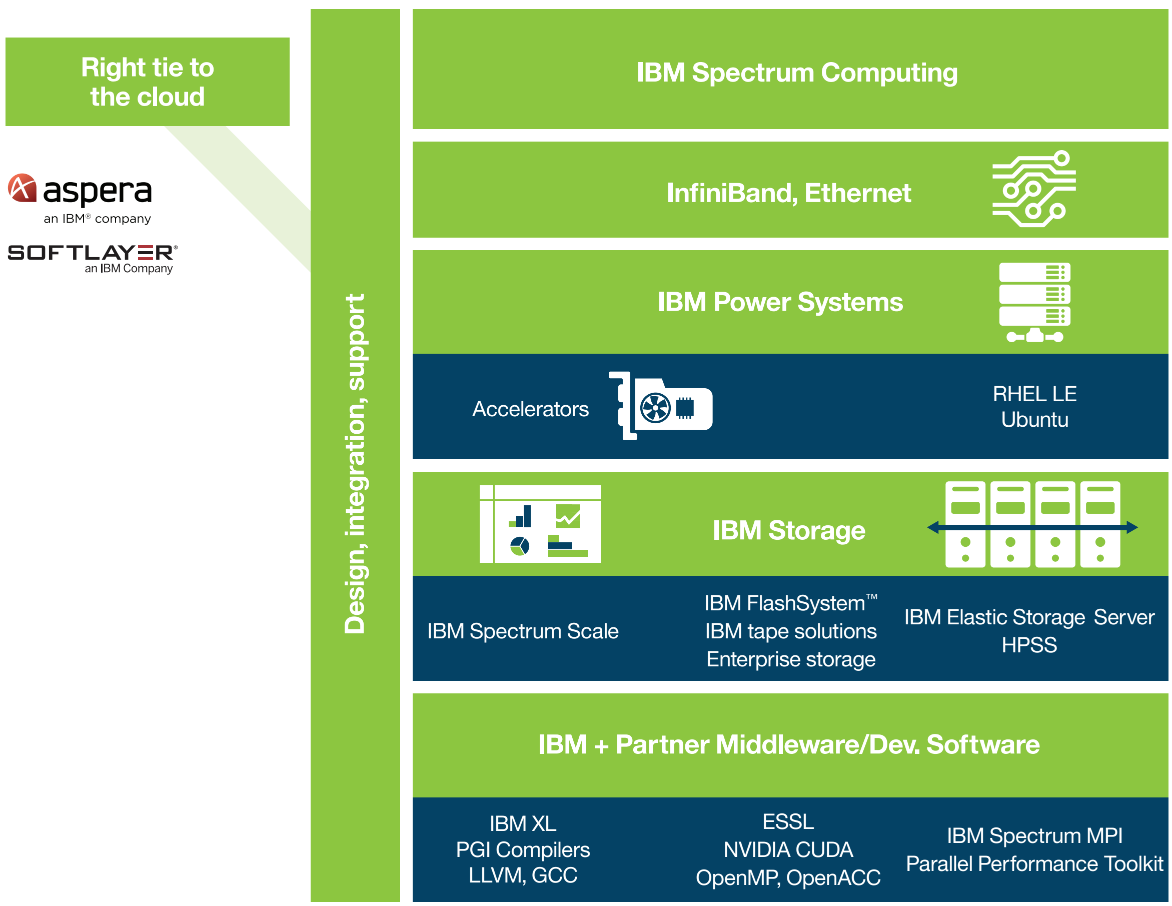



*Figure 1*: IBM HPC portfolio

## IBM POWER8: Designed for the intersection of high performance computing and high performance data analytics

The IBM POWER8® processor delivers industry-leading performance for HPC and high performance data analytics (HPDA) applications, with multi-threading designed for fast execution of analytics algorithms (eight threads per core), multi-level cache for continuous data load and fast response (including an L4 cache), and a large, high-bandwidth memory workspace to maximize throughput for data-intensive applications.

## New IBM Power Systems LC nodes for HPC and HPDA

The IBM Power Systems LC servers are designed for HPC workloads. They allow you to:

- Realize incredible speedups in application performance with accelerators
- Deploy a processor architecture designed for HPC performance
- Benefit from ecosystem innovation from the OpenPOWER Foundation

| System | Processor | Memory | Storage | Acceleration | HPC use cases |
|---|---|---|---|---|---|
| IBM Power Systems S822LC for High Performance Computing | 2x POWER8 with NVLink CPUs<br>10 cores each, 2.86-3.25Ghz | Up to 1TB<br>230 GB/s bandwidth | 2x 2.5” drives<br>(HDD or SSD)<br>NVMe for ultra-fast I/O | 4x NVIDIA Tesla P100 with NVLink GPU accelerators | Built for the next wave of GPU acceleration |
| IBM Power Systems S822LC | 2x POWER8 CPUs 10 cores each, 2.9-3.3 GHz | Up to 1 TB<br>230 GB/s bandwidth | 2x 2.5” drives (HDD or SSD)<br>NVMe for ultra-fast I/O | Optional CAPI-attached accelerators<br>Optional Tesla K80 | Built for CPU performance |
| IBM Power Systems S812LC | 1x POWER8 CPU, 10 cores each, 2.9-3.3 GHz | Up to 1 TB<br>115 GB/s bandwidth | 14x 3.5” drives (84TB, HDD, SSD) | Optional CAPI-attached accelerators | Optimized for Hadoop, Spark |

*Table 1*: Technical details for three Power Systems offerings

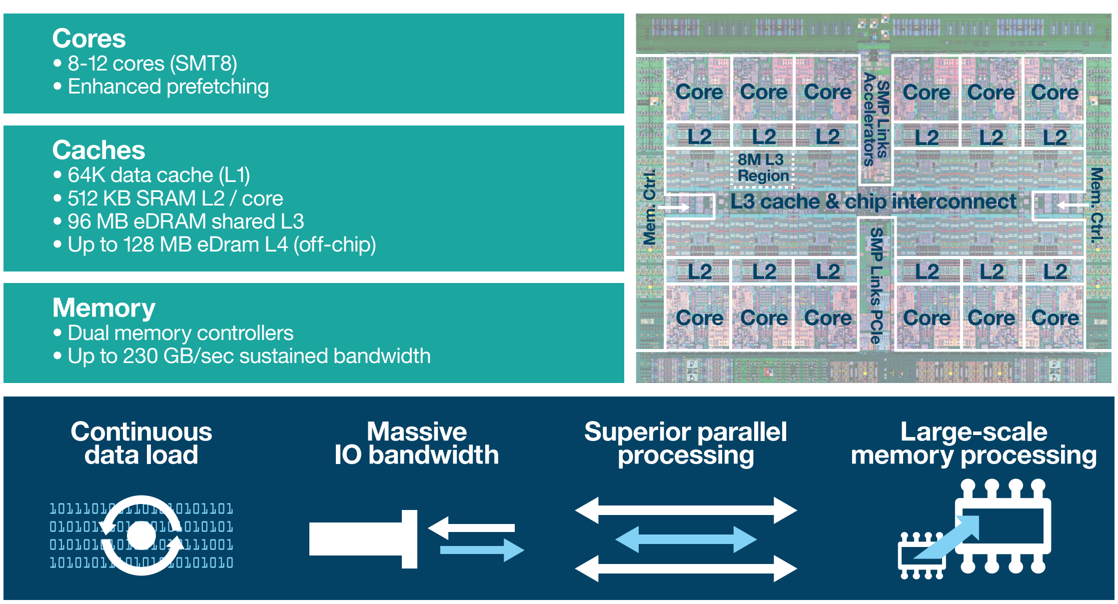


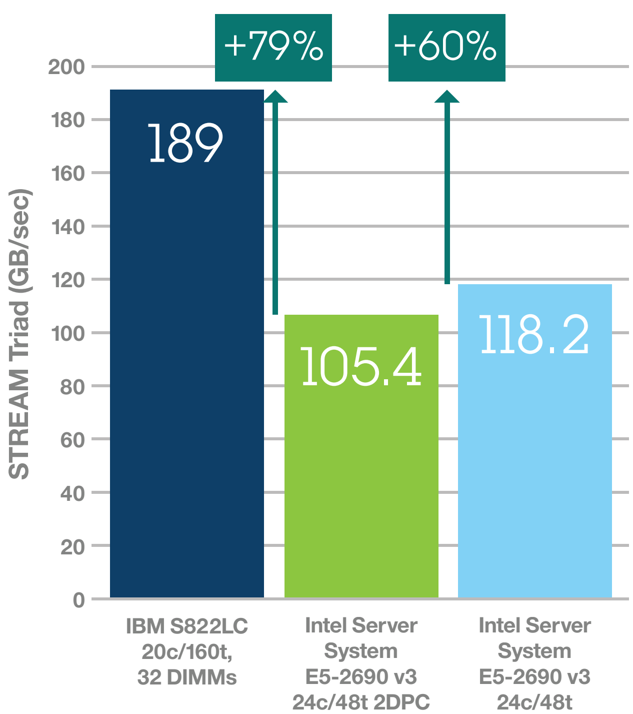

*Figure 2*: The POWER8 processor

## Leadership in HPC application performance

IBM HPC solutions are built for better HPC. They allow you to analyze faster, simulate better and process more through these attributes:

### Architectural advantages matched to HPC applications, such as memory bandwidth:

- 60-79 percent greater memory bandwidth compared to competing servers

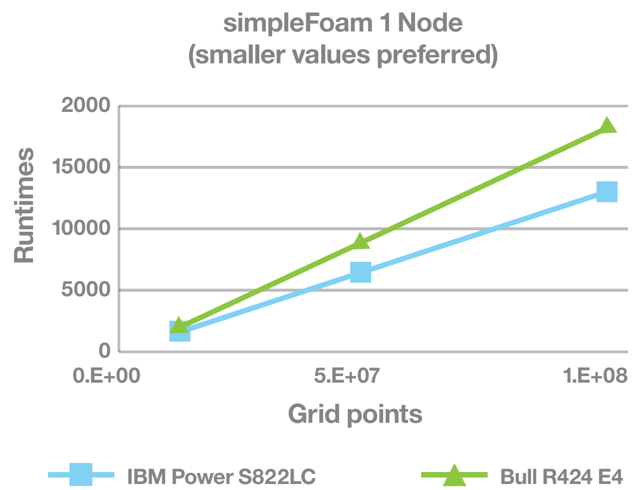



- IBM Power Systems S822LC results are based on IBM internal measurements of STREAM Triad; 20 cores / 20 of 160 threads active. POWER8; 3.5GHz, up to 1TB memory.
- Intel Xeon data is based on published data of Intel Server Systems R2208WTTYS running STREAM Triad; 24 cores / 24 of 48 threads active, E5-2690 v3; 2.3GHz

*Figure 3*: STREAM Triad

### Compelling application performance versus competing server architectures:

- CFD results 40 percent faster on OpenFOAM on IBM Power System S822LC compared to competing servers

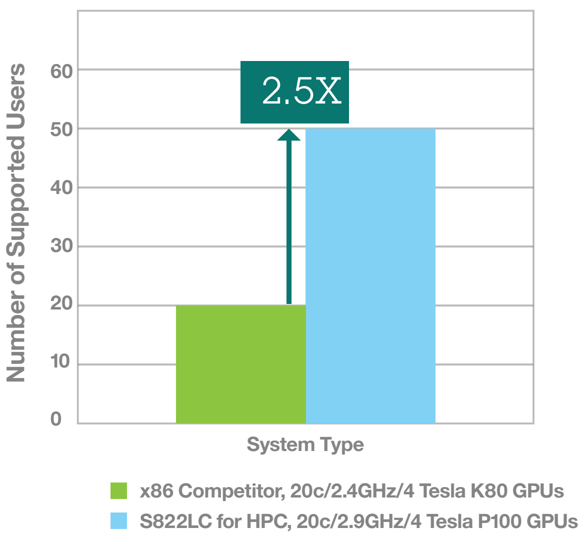



- Results are based on IBM internal testing of systems running OpenFOAM version 2.3.0 code benchmarked on POWER8 systems. Individual results will vary depending on individual workloads, configurations and conditions.
- IBM Power Systems S822LC, POWER8, 3.5 GHz, 512 GB memory, 2x 10 core processors/4 threads per core. Job size 128GB memory per socket.
- BULL R424-E4, Intel Xeon E5-2680v3, 2.3 GHz, 256 GB memory, 2x 10 core processors/1 thread per core. Job size 128GB memory per socket.

*Figure 4*: OpenFOAM simpleFoam 1 node

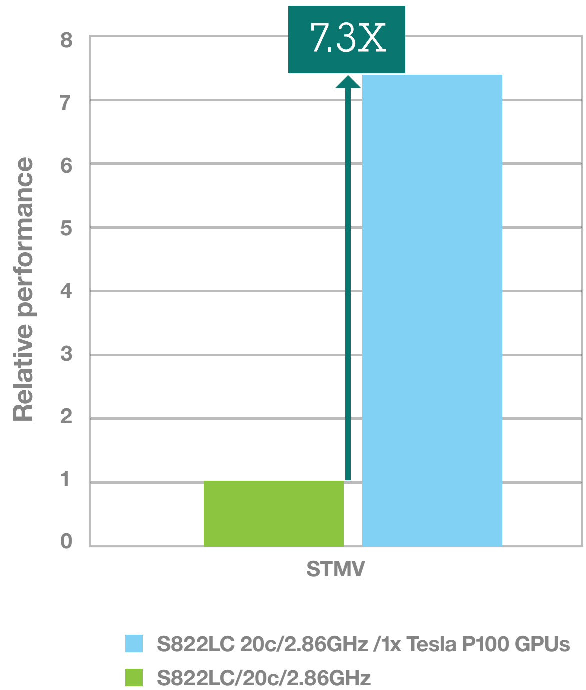
### Compelling throughput on GPU computing applications and workloads:

- Up to a 7.3X improvement in NAMD performance by adding NVIDIA Tesla P100 GPUs
- Up to a 2.5X increase in number of supported Kinetica Filter-by-Location queries (<1 sec reponse) through POWER8, Tesla P100, and NVIDIA NVLink
- Up to 2.91X the bandwidth of x86 servers featuring PCI-E x16 3.0 interfaces, unlocking the power of custom code



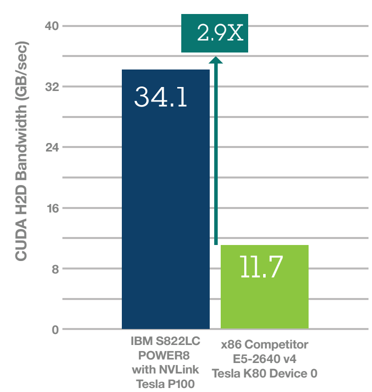

- Results are based on IBM internal testing of Kinetica Filter-by-Location query with 280,000,000 records
  Individual results will vary depending on individual workloads, configurations and conditions.
- IBM Power Systems S822LC; 20 cores / 160 threads, POWER8 with NVLink, 2.86GHz, 256GB memory, 4 Tesla P100 GPUs
- x86 Competitor, 20 cores / 40 threads, Xeon E5-2640 v4; 2.4GHz, 256GB memory, 4 Tesla K80 GPUs

*Figure 5*: Kinetica accelerated database performance




- Results are based on IBM internal testing of systems running NAMD version 2.11 STMV code benchmarked on POWER8 systems with NVIDIA Tesla P100 GPUs
  Individual results will vary depending on individual workloads, configurations and conditions.
- IBM Power Systems S822LC; 20 cores / 160 threads, POWER8 with NVLink; 2.86GHz, 256GB memory
- IBM Power Systems S822LC; 20 cores / 160 threads,

*Figure 6*: NAMD performance




- IBM Power Systems S822LC results are based on IBM internal measurements of CUDA H2D BW Test; 20 cores / POWER8 with NVLink; 2.86GHz, up to 256GB memory, 1 Tesla P100
- Intel Xeon data is based on IBM internal testing ; 20 cores / 40 threads active, Xeon E5-2640 v4 2.4GHz, Tesla K80 GPU Device 0.
  Test executed measures bandwidth solely to Device 0 (of devices 0, 1).

*Figure 7*: CUDA H2D bandwidth for developers

## Workflow-based design with software defined infrastructure

Software defined infrastructure (SDI) provides a complete HPC software solution customizable based on your needs. Incorporating both community and IBM-supported software solutions—IBM Spectrum Computing workload and infrastructure management, IBM Spectrum Scale storage, and optimized HPC libraries—SDI delivers a flexible solution for all cluster sizes, accommodating changing needs.

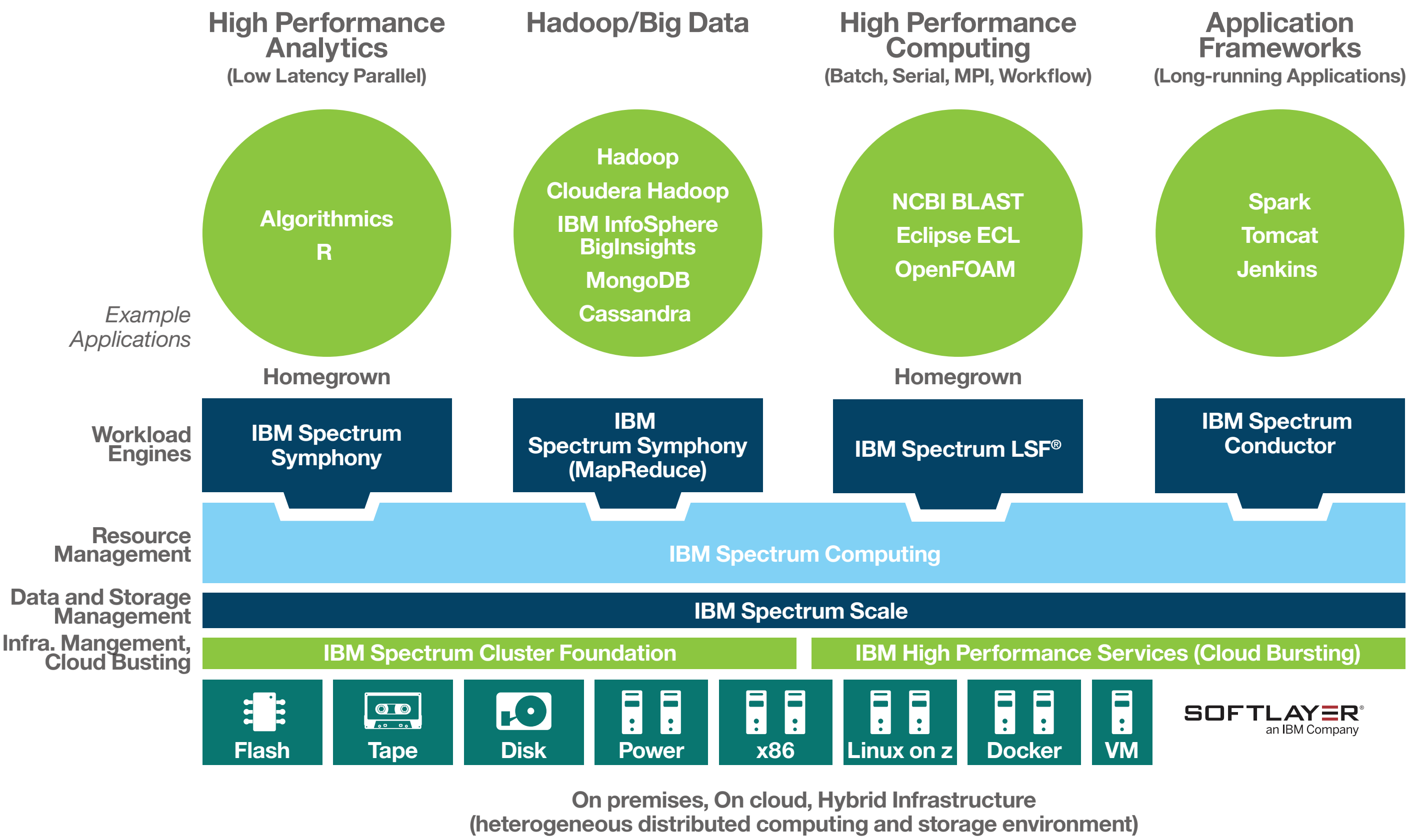



*Figure 8*: Investments in software defined infrastructure: Indicative of workflow-based design

## IBM HPC software optimized for Power Systems

IBM HPC software is designed to seamlessly exploit and deliver optimal performance of IBM Power Systems HPC clusters.

Libraries and development tools ensure you can easily reap the performance benefits of specialized hardware and data-centric system design, including support for CUDA-aware-MPI with IBM Spectrum MPI, drop-in acceleration of OpenMP applications on CPU or Tesla GPU with IBM PESSL, and IBM XL C++/Fortran compilers for parallel development.

Then, put your performance optimized applications to work with maximum efficiency with IBM Spectrum workload management tools. Supply them with data through IBM Spectrum Scale: a scalable, reliable, high-performance parallel file system.

| | Products | Client benefits |
|---|---|---|
| Systems management | IBM Spectrum Cluster Manager<br>xCAT | • Ease of use: web portal<br>• Customizable: admin productivity<br>• Faster time to system productivity<br>• Robust monitoring |
| Application runtime | IBM MPI runtime<br>ESSL/PESSL<br>CUDA runtime | • Optimize parallel runtime<br>• Optimized LAPACK and ScaLPACK libraries<br>• User-controlled workflow support |
| Development productivity | Parallel Performance Toolkit<br>IBM XL Compiler Suite<br>Rogue Wave TotalView debugger | • Modern application development environment using Eclipse<br>• Performance analysis tools to help analyze applications<br>• Optimized complier for IBM Power Systems |
| Workload management | IBM Spectrum LSF | • Optimize utilization of resources<br>• Policy-aware and resource-aware scheduling |
| Data management | IBM Spectrum Scale<br>HPSS<br>IBM Spectrum Protect | • Scalable/reliable storage for parallel filesystem (Elastic Storage Server solution also available)<br>• ILM for transparent migration of data from storage to tape and back<br>• Enhance availability with RAID-based ESS and tape |
| Application environment | IBM Spectrum Conductor | • Simplify job submission for repeatable workload<br>• Customizable<br>• Faster time to system productivity |

*Table 2*: Benefits of IBM and partner technologies for various use cases

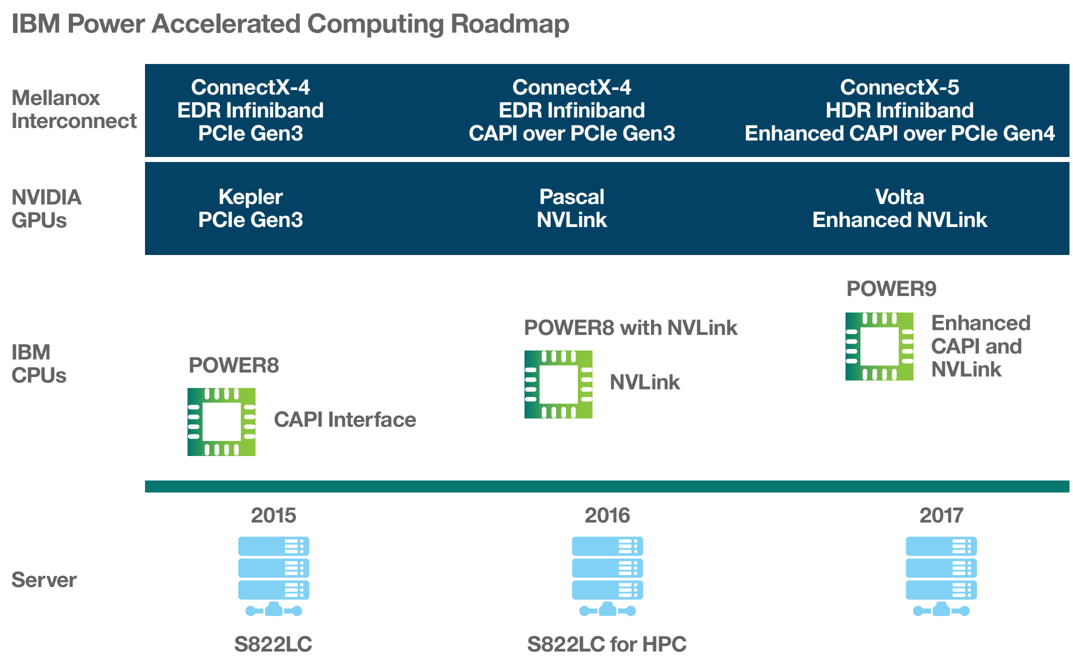



*Figure 9*: IBM Power Accelerated Computing Roadmap

## Differentiated acceleration

Acceleration is critical to building leading HPC clusters. IBM Power Systems offers choice and flexibility for hardware acceleration of HPC and HPDA workloads. Two different options for differentiated acceleration are available:

- *CAPI (Coherent Accelerator Processor Interface):* Memory and cache coherency, treating the accelerator as a peer-processor with virtual addressing. For select network, compute, and storage accelerators.
- *NVIDIA NVLink:* A broader, fatter pipe to NVIDIA GPUs than ever before, enabling the faster host-device, device-device communication many HPC applications require.

## POWER8 with NVLink

Available now in the Power Systems S822LC for HPC, POWER8 with NVLink delivers a 2.5X faster CPU-to-GPU interface than PCI-E x16 3.0, enabling ultra-fast memory access between CPU and GPU when combined with Unified Memory and NVIDIA Page Migration Engine. The platform also provides improved GPU-to- GPU link bandwidth.

Previous barriers related to difficulty of data movement, memory capacity and the burden of custom coding for data management can now make way for GPU acceleration, opening up new application classes to accelerated computing.

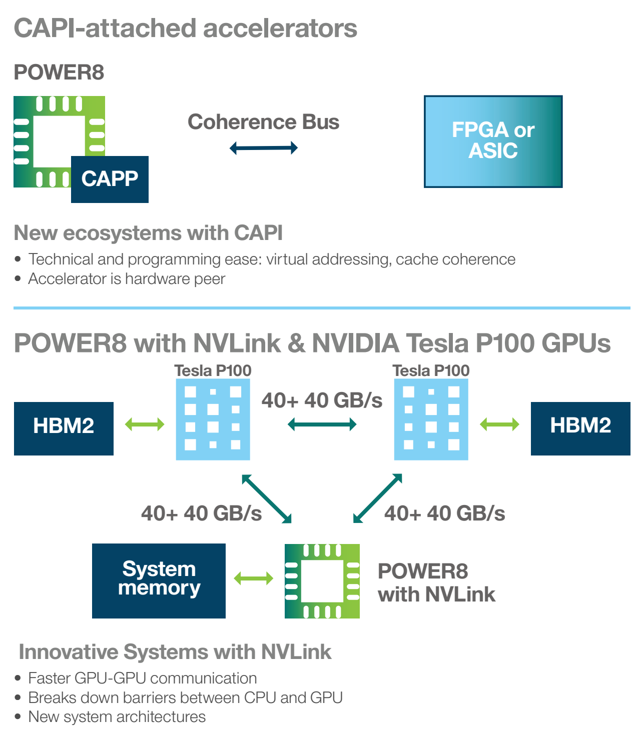



*Figure 10*: Differentiated accelerator interfaces: CAPI and NVLink


*Figure 11*: Revolutionizing computing through open innovation

## Revolutionizing computing through open innovation

As a founding member of the OpenPOWER Foundation with NVIDIA, Google, and others, IBM has broadened access to the Power architecture with accelerators.

This brings the leading processor together with the best of our partners and end users across the ecosystem—from HPC and HPDA, to hyperscale data centers, to system designers worldwide. Learn more about the ecosystem at www.openpowerfoundation.org.

## Delivering accelerated application performance for HPC

Your applications run on the POWER8 platform, often with far superior performance and accelerated computing support. A sampling of HPC applications suited for IBM Power Systems HPC servers:

Power Systems OpenPOWER™

**GPU Supported. Talk to your IBM salesperson for the latest version of the IBM HPC Applications Summary (ibm.biz/hpcapplications)*

*Hundreds of thousands of packages, including non-HPC applications, are offered in ppcle Linux distributions. Explore at ibm.biz/ospat-tool*

### Astrophysics

| | | | | |
|---|---|---|---|---|
| GADGET | HACC | p-GADGET | Peasoup | PLUTO |

### Bio and Life Sciences **Genomics**

| | | | | | |
|---|---|---|---|---|---|
| ALLPATHS-LG | Bowtie 2 | FASTX-Toolkit | MrBayes | RSEM | Spades |
| BALSA | BWA | FastQC | MUSCLE | SAMtools | SplazerS |
| bamkit | cutadapt | FreeBayes | nose (Library) | salmon | SQLite |
| BarraCUDA | ELSA | GATK | Illumina (ISAAC) | samblaster | STAR-FUsion |
| bcftools | ESP | GenoomonFisher | PairHMM | scalpel | Tabix |
| BEDtools | chimerascan | HMMER | PHYLIP | scikit-bio | TASSEL |
| BEDOPS | Churchill | HTSeq | PICARD | seqtk | T-Coffee |
| BFAST | Cufflinks - 2.1.1 | HTSlib | Pindel | setuptools (Library) | TopHat |
| Bioconductor | Databiology | IGV | PLINK, plink-ng | SHRiMP | Trimmomatic |
| BLAST | DELLY2 | Kraken | Primer3 | SnpEff, SnpSift | Trinity |
| Boost (Supporting Library) | diamond | LoFreq | RAxML | SOAP3-dp | VCFtools |
| Bowtie | FASTA /Smith Waterman | LUMPY | R-EBSeq | SOAPaligner/SOAP2 | Velvet/Oases |
| | | Mothur | RNA-star | SOAPDenovo | Zlib |

### Bio and Life Sciences **Bioinformatics/Translational Medicine**

| | | | | | |
|---|---|---|---|---|---|
| ACUMI | Bio Builds | BioVelocity | Galaxy | LoFreq | Zato Analytics |
| | bioPython | | IGV | tranSMART Suite | |

### Bio and Life Sciences **Molecular Dynamics, Computational Chemistry**

| | | | | | |
|---|---|---|---|---|---|
| AMBER | CHARMM | GROMACS | NAMD | VMD | QMCPACK |
| CoMD | CPMD | MAFIA | Nest | Q-Box | Quantum Espresso |

### CFD/CAE

| | | | | | |
|---|---|---|---|---|---|
| AMG2013 | Culises | LBM D2Q37 (Lattice-Boltzmann) | LS-DYNA | Ludwig | OpenFOAM |
| ALYA | Code-Saturne | | MiniGhost | Nekbone | SU2 |
| AVUS | Lattice -Boltzmann | | | | |

### Chemistry and Physics

| | | | | | |
|---|---|---|---|---|---|
| B-CALM | GAMESS | KKRnano | Lulesh | LSQR | SNAP |
| DL-POLY | Heat3d | Lattice QCD, QUDA | LSMS | MCB | UMT2013 |
| | | | | | VASP |

### Databases

| | | | | | |
|---|---|---|---|---|---|
| Kinetica (formerly GPUdb) | MapD | | | | |

### Deep Learning

| | | | | | |
|---|---|---|---|---|---|
| Caffe | caffe-nv | CNTK | DIGITS | Theano | Torch |
| caffe-ibm | Chainer | TensorFlow | PowerAI | | |

### Finance and Math

| | | | | | |
|---|---|---|---|---|---|
| Altimesh Hybridizer | STAC-A2 | STAC-M3 | Julia | | |

### Libraries

| | | | | | |
|---|---|---|---|---|---|
| AmgX | cuBLAS | cuDNN | cuRAND | LIBLINEAR | NumPy |
| AMG2013 | CUDA Math Lib | cuFFT | cuSOLVER | OpenBLAS | NPP |
| Atlas | | | cuSPARSE | NCCL | Thrust |
| | | | FFTW (vectorized on Power) | | |

### Metadata

| | | | | | |
|---|---|---|---|---|---|
| DirectFlow | iRODS | MODS | Nirvana | OpenARC HOMP | PyReshaper |

### Geosciences, Oil and Gas

| | | | | | |
|---|---|---|---|---|---|
| Echelon | heat3d | RTM Kernel (IBM) | SeisSol | | |

### Programming Tools, Specialized Languages

| | | | | | |
|---|---|---|---|---|---|
| Allinea | Panasas DirectFlow | MODS | OpenARC | Python (Supporting Library) | R |
| GCC | XL C/C++ | XL Fortran | PGI Accelerator C/C++ | | R tidyverse, R cowplot |
| | | | | | PGI Fortran |

### Utilities, Workload Orchestration

| | | | | | |
|---|---|---|---|---|---|
| IBM ILOG® | LuaJIT | WSMP | Spectrum Cluster Manager | Spectrum LSF | Spectrum Conductor |

### Weather

| | | | | | |
|---|---|---|---|---|---|
| AROME | Cosmo SVN | HYCOM | MG2 | MPAS-A | RegCM |
| CamSE | JURASSIC | LES | Meso-NH | POPPerf | WRF |

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