A NEW VINTAGE OF COMPUTING CUG 2013

Napa Valley, California • May 6–9

Measuring GPU Utilization on the Cray XK7

20 Years of Excellence in Computational Science

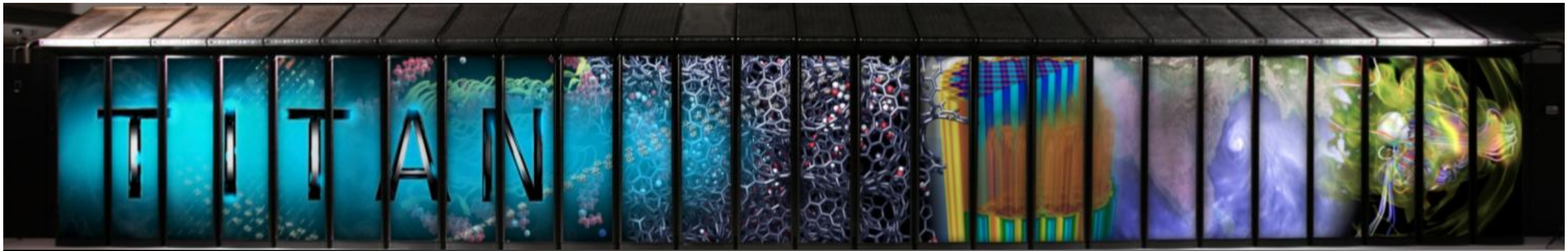
OLCF

Oak Ridge Leadership Computing Facility

1992–2012

Jim Rogers
Director of Operations
National Center for Computational Sciences
Oak Ridge National Laboratory

May 9, 2013



U.S. DEPARTMENT OF ENERGY | Office of Science

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Motivation: Transition from the Cray XT5 *Jaguar* to the XK7 *Titan* Heterogeneous Compute Nodes: CPU+GPU

- Implementation
  - Phase 1 [Complete 02/2012]
    - Cabinet Upgrades
    - XT5->XK Compute Blades
    - AMD 6274 Opteron (16-core)
    - 32GB/node DDR3 DRAM upgrade
    - Gemini Interconnect
  - Phase 2 [Complete 05/2013]
    - Power System Upgrades
    - NVIDIA Kepler K20x

- Schedule
  - ✓ 01/2009. CD-0 (Mission Need)
  - ✓ 01/2010. CD-1 (Alternative Selection / Cost Range)
  - ✓ 02/2011. CD-3a (Performance Baseline / Permission to Issue Solicitation)
  - ✓ 11/2011. CD-2/3b (Permission to Issue Subcontract)
  - 12/2013. CD-4 (Project Closeout)

Motivation: OLCF's Long Term Commitment to Hybrid Computing

- Titan is expected to remain in production through 2017
- Given a 60-month production life, it is even more important that we maximize the productivity of this hybrid architecture
- DOE Sponsor interest
  - How is OLCF effectively managing this resource for its user community?
- We need the complementary tools to understand GPU use:
  - How effectively are the users able to use the hybrid architecture?
  - How many delivered node-hours are GPU-enabled?
  - How can/should we adapt operational policies
    - allocation,
    - scheduling

- *The OLCF-3 Titan will provide the computational capability to accomplish breakthrough science for DOE, industry, and the nation*
  - *Transforming the nation's energy system and secure U.S. leadership in clean energy technologies.*
  - *Maintain a vibrant U.S. effort in science and engineering*

- Qualifying Risk
  - Significant investment:
    - Phase 1 subcontract ($60M)
    - Phase 2 subcontract ($40M)
  - Significant Architectural Change
    - Hybrid CPU+GPU node
  - Significant Software Challenges
    - OPENACC
    - CUDA

Interim GPU Utilization Measurement on Titan using ALTD

- ORNL examines, on a per-job basis, when jobs use accelerator-equipped nodes.
- Leverages the ORNL-developed Automatic Library Tracking Database (ALTD)
  - At link time, a list of libraries linked against is stored in a database
  - When the resulting program is executed via aprun, a new ALTD record is written that contains the specific executable, to be run, the batch job id, and other info
- Batch jobs are compared against the ALTD to see if they were linked against an accelerator-specific library
  - libacc*, libOpenCL*, libmagma*, libhmpp*, libcuda*, libcupti*, libcula*, libcublas*
  - Jobs whose executables are linked against one of the above are deemed to have used the accelerator
- Outliers
  - Job run outside of the batch system
    - ALTD knows about them, but we can't tie them to usage because there's no job record
  - ALTD is enabled by default, but if it's disabled we won't capture link/run info
    - We don't advertise how to disable it
    - Happens with debug sessions-debuggers can't handle the wrapped aprun
  - Codes compiled with nvcc aren't captured due to how it links
  - Codes using Open MPI (do not use aprun)

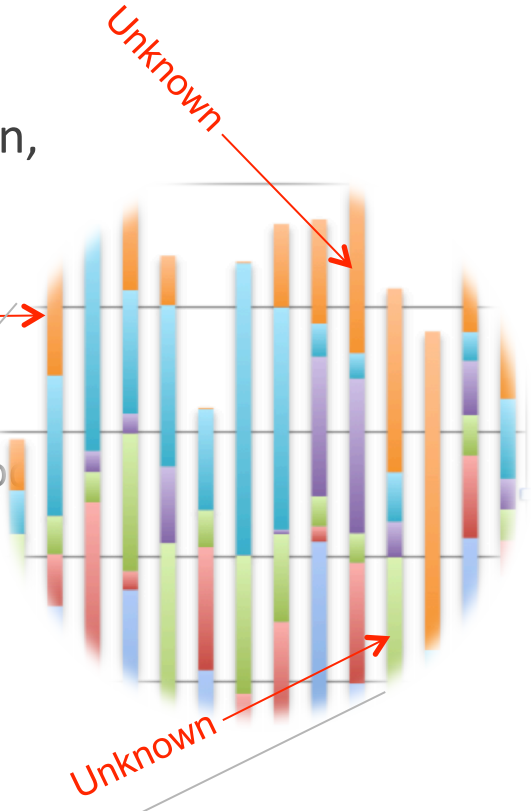
Making sense of an link statement

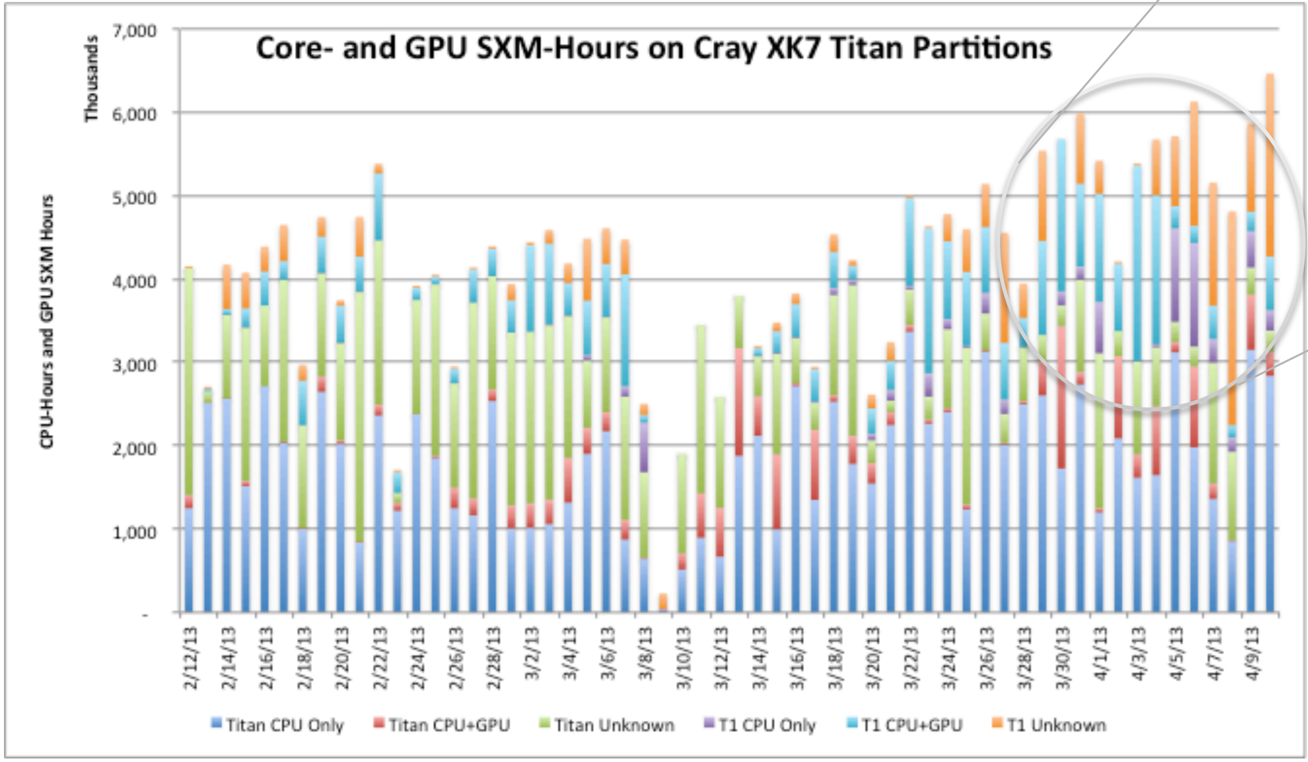
```
% lsms /usr/lib/../lib64/crt1.o /usr/lib/../lib64/crti.o
/opt/gcc/4.7.0/snos/lib/gcc/x86_64-suse-linux/4.7.0/crtbegin.o
libLSMS.aSystemParameters.o libLSMS.aread_input.o libLSMS.aPotentialIO.o
libLSMS.abuildLIZandCommLists.o libLSMS.aenergyContourIntegration.o
libLSMS.asolveSingleScatterers.o libLSMS.acalculateDensities.o
libLSMS.acalculateChemPot.o
/lustre/widow0/scratch/larkin/lsms3-trunk/lua/lib/liblua.a
/lustre/widow0/scratch/larkin/lsms3-trunk/lib/libLSMSLua.a
/lustre/widow0/scratch/larkin/lsms3-trunk/lib/libCommunication.a
…
-lcublas /opt/nvidia/cudatoolkit/5.0.28.101/lib64/libcublas.so -lcupti
/opt/nvidia/cudatoolkit/5.0.28.101/extras/CUPTI/lib64/libcupti.so -lcudart
/opt/nvidia/cudatoolkit/5.0.28.101/lib64/libcudart.so -lcuda
/opt/cray/nvidia/default/lib64/libcuda.so
/opt/cray/atp/1.4.4/lib//libAtpSigHCommData.a -lAtpSigHandler
/opt/cray/atp/1.4.4/lib//libAtpSigHandler.so -lgfortran
/opt/gcc/4.7.0/snos/lib/gcc/x86_64-suse-linux/4.7.0/../../../../lib64/
libgfortran.so -lhdf5_hl_cpp_gnu
/opt/cray/hdf5/1.8.8/gnu/47/lib/libhdf5_hl_cpp_gnu.so -lhdf5_hl_gnu
/opt/cray/hdf5/1.8.8/gnu/47/lib/libhdf5_hl_gnu.so -lhdf5_cpp_gnu
/opt/cray/hdf5/1.8.8/gnu/47/lib/libhdf5_cpp_gnu.so -lhdf5_gnu
/opt/cray/hdf5/1.8.8/gnu/47/lib/libhdf5_gnu.so -lz
/usr/lib/../lib64/libz.so -lscicpp_gnu
/opt/xt-libsci/11.1.00/gnu/47/interlagos/lib/libscicpp_gnu.so -lsci_gnu_mp
/opt/xt-libsci/11.1.00/gnu/47/interlagos/lib/libsci_gnu_mp.so -lgfortran
/opt/gcc/4.7.0/snos/lib/gcc/x86_64-suse-linux/4.7.0/../../../../lib64/
libgfortran.so -lmpichcxx_gnu_47
…
/opt/cray/pmi/3.0.1-1.0000.9101.2.26.gem/lib64/libpmi.so -lalpslli
/usr/lib/alps/libalpslli.so -lalpsutil /usr/lib/alps/libalpsutil.so
/lib64/libpthread.so.0 -lstdc++
/lib64/ld-linux-x86-64.so.2 -lgcc_s
/opt/gcc/4.7.0/snos/lib/gcc/x86_64-suse-linux/4.7.0/../../../../lib64/
libgcc_s.so /opt/gcc/4.7.0/snos/lib/gcc/x86_64-suse-linux/4.7.0/crtend.o
/usr/lib/../lib64/crtn.o
```

Summary Results of the ALTD Method

- Sample size reflect two partitions of Titan- one in production, and one reserved for internal software testing and development.
- Outliers (Unknowns) Continue to Dominate
  - The intermediate method using ALTD is not wholly effective, with ~34% of the delivered hours uncategorized by this method

Unknown





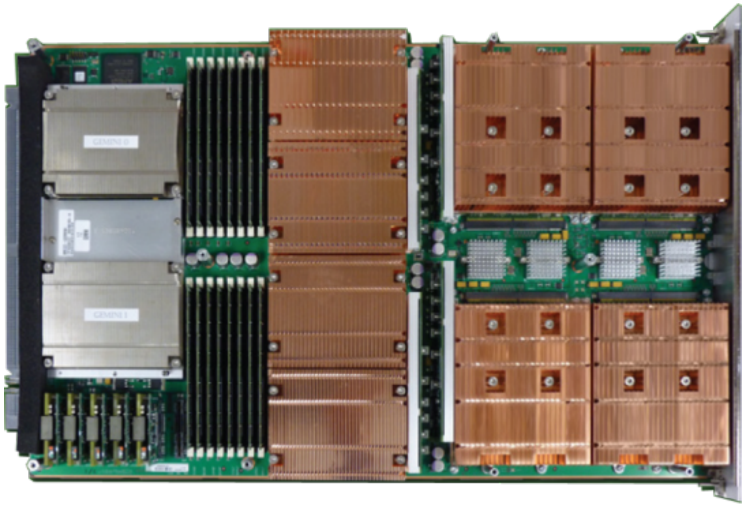
Uncaptured Edge Cases

- Nvcc
- Open MPI
  - Recently identified a workaround
- Anything outside of aprun
- Dedicated time
- Others? (still digging)

Titan: Cray XK7 System – Addressing the Scale of the GPU Utilization Requirement

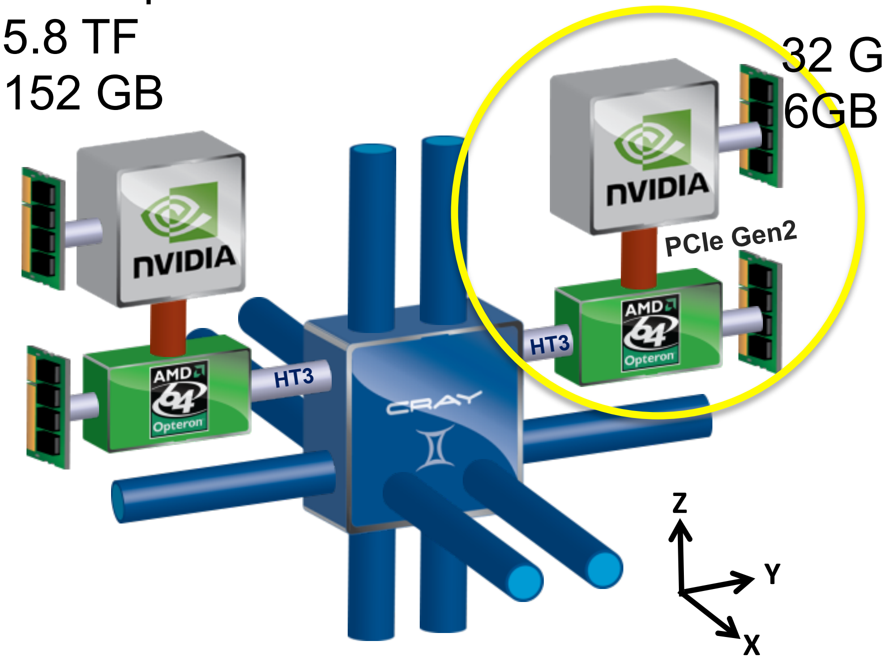
System:
200 Cabinets
18,688 Nodes
27 PF
710 TB

Cabinet:
24 Blades
96 Nodes
139 TF
3.6 TB

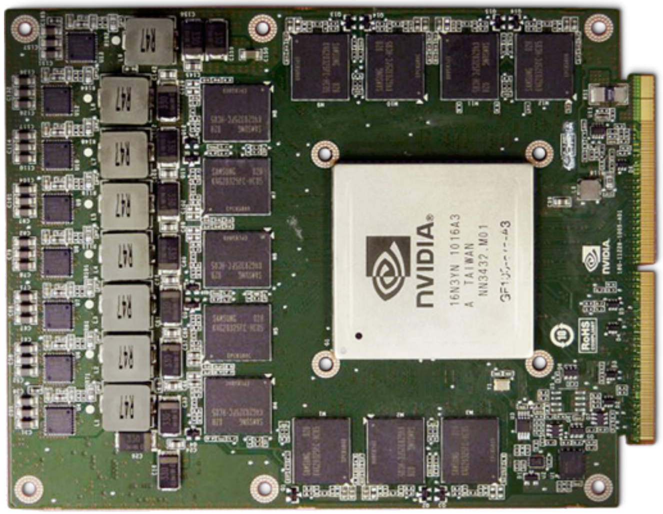


Board:
4 Compute Nodes
5.8 TF
152 GB

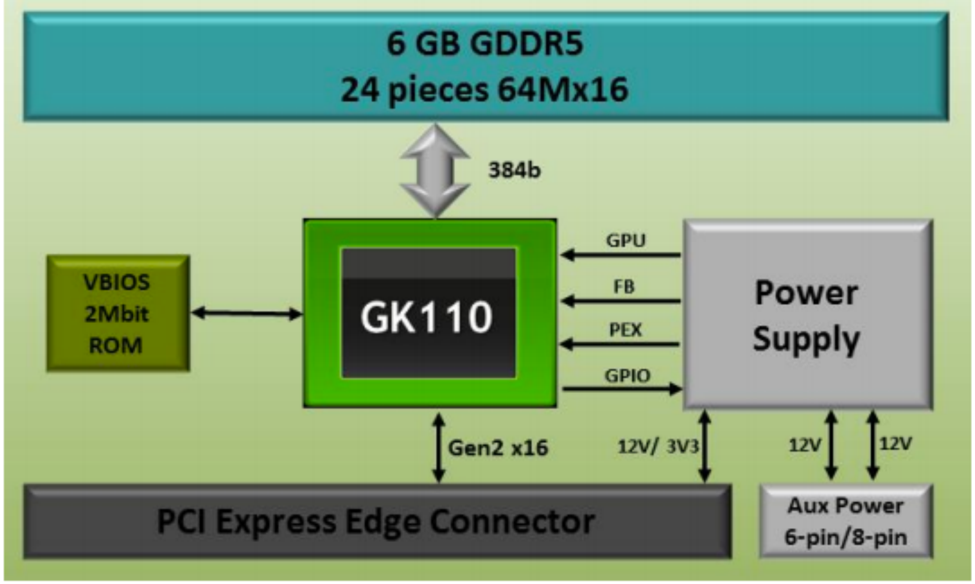
A Cray XK7 Heterogeneous Compute Node:
1.45 TF
32 GB DDR3
6GB GDDR5



NVIDIA Kepler K20x Block Diagram



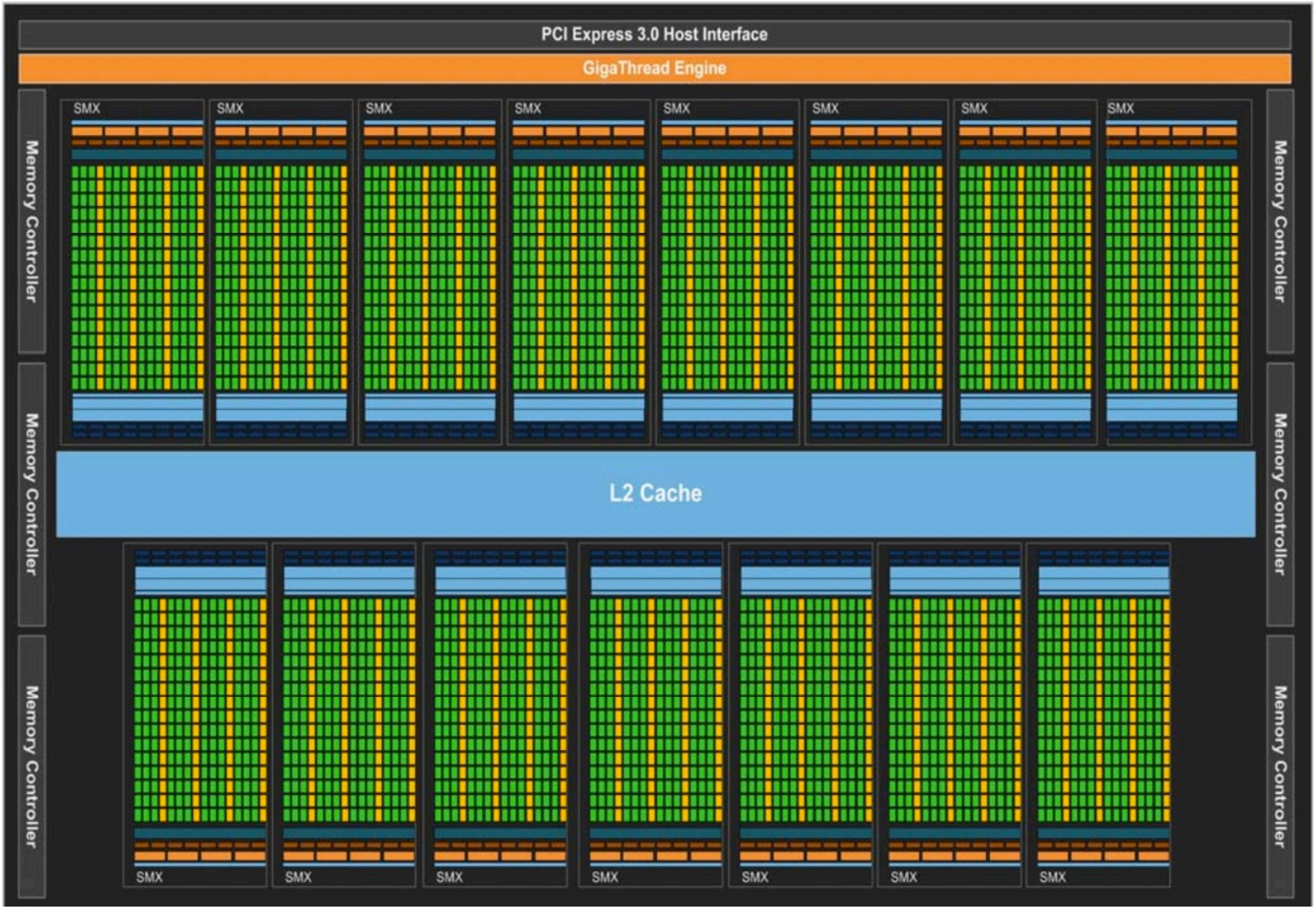
- The K20X is a single FRU based on the NVIDIA GK110 GPU



Images courtesy NVIDIA Corporation

Specifications	**Tesla K20X**
Chip	GK110
Package Size	GPU 45 mm × 45 mm 2397-pin S-FCBGA
Processor Clock	732 MHz
Memory Clock	2.6GHz
Memory Size	6GB
Memory I/O	384-bit GDDR5
Board Power	235W (225W power cap on Titan)
Idle Power	~25W
Thermal Cooling Solution	Passive Heat Sink

Kepler GK110 Full Chip Block Diagram



The NVIDIA GK110 in Titan

- (From previous slide), the NVIDIA GK110 product family contains 14 or 15 SMXs. The Titan product has 14.
- For each SMX: 192 single-precision CUDAcores, 64 double-precision units, 32 special function units(SFU), and 32 load/store units (LD/ST).
- For each SMX: four warp schedulers and eight instruction dispatch units, allowing four 32-thread warps to be issued and executed concurrently.

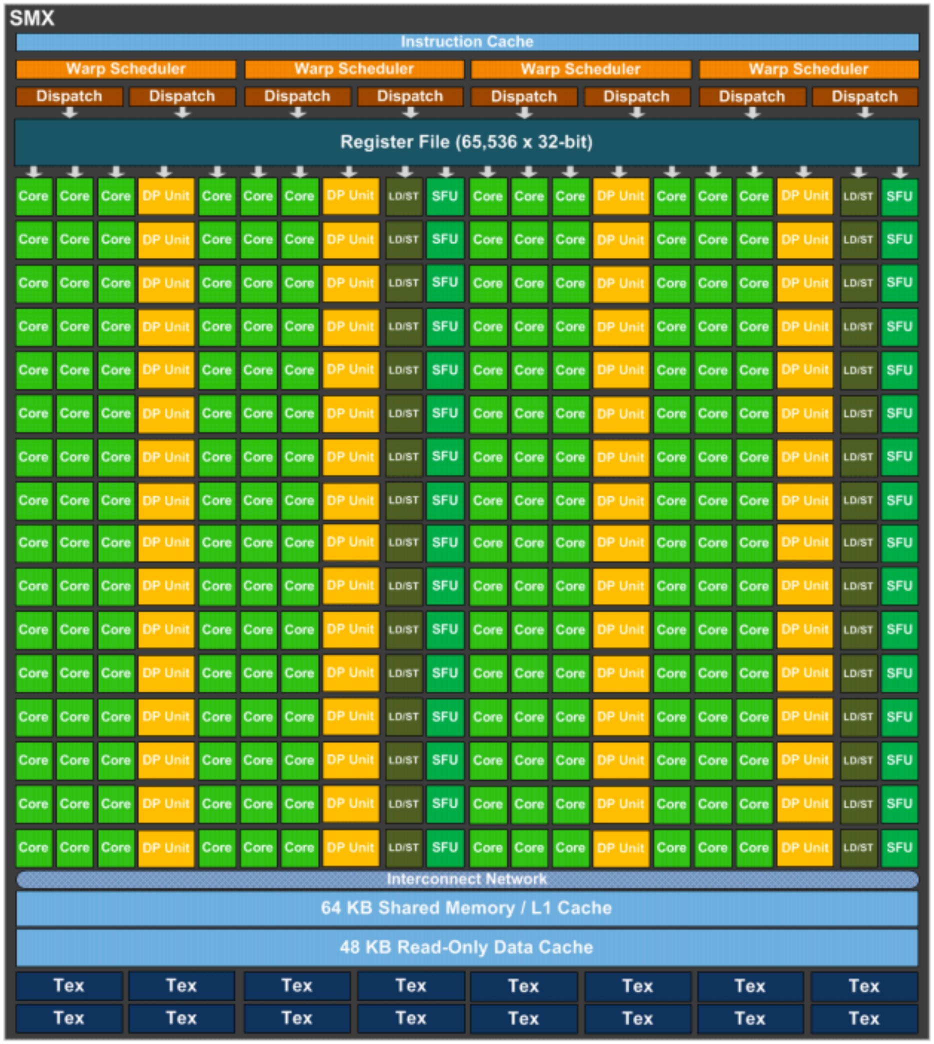
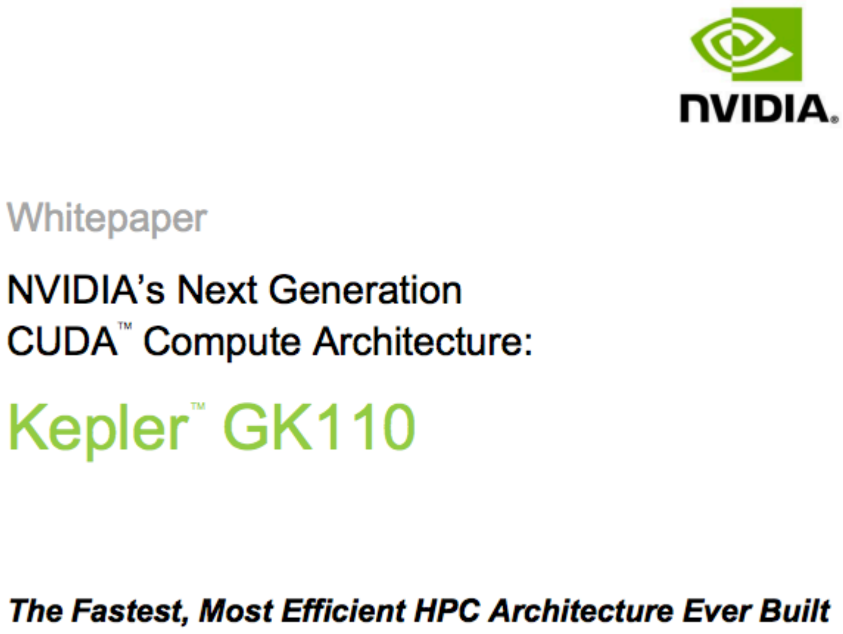


Image courtesy NVIDIA Corporation

The NVIDIA GK110 Deep Dive

For more information on Kepler that includes all of the hardware deep dive, including the significant feature improvements from Fermi to Kepler:

Dynamic Parallelism,
Hyper-Q,
the Grid Management Unit,
and GPU Direct),



Whitepaper

NVIDIA's Next Generation
CUDA™ Compute Architecture:

Kepler™ GK110

The Fastest, Most Efficient HPC Architecture Ever Built

Reference:

NVIDIA's Next Generation CUDA™
Compute Architecture: Kepler TM GK110

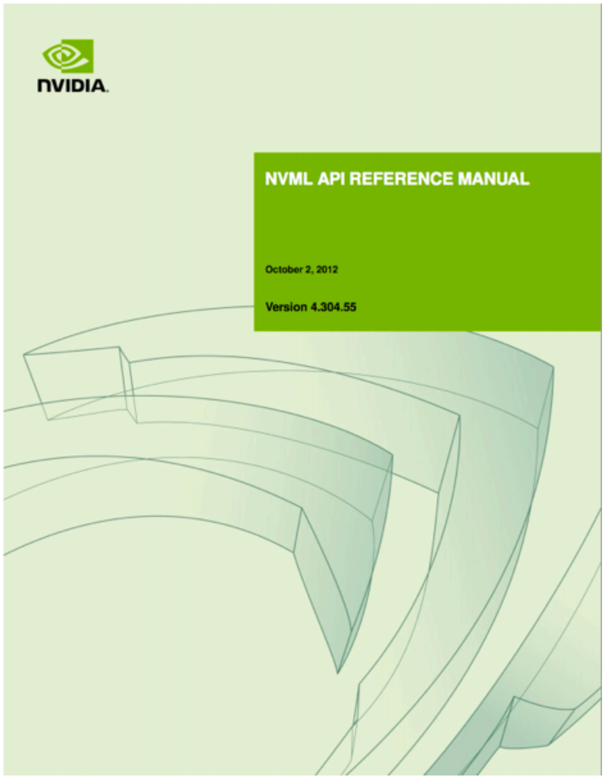
http://www.nvidia.com/content/PDF/kepler/NVIDIA-Kepler-GK110-Architecture-Whitepaper.pdf

The System-Level Interface to the GK110
- the NVIDIA Management Library (NVML)

- NVML is a C-based API for monitoring and managing various states of the NVIDIA GPU devices. The runtime version of NVML ships with the NVIDIA display driver, and the SDK provides the appropriate header, stub libraries and sample applications. Each new version of NVML is backwards compatible and is intended to be a platform for building 3rd party applications.

- States that may be queried include:
  - ECC error counts: Both correctable single bit and detectable double bit errors are reported. Error counts are provided for both the current boot cycle and for the lifetime of the GPU.
  - **GPU utilization: Current utilization rates are reported for both the compute resources of the GPU and the memory interface.**
  - Active compute process: The list of active processes running on the GPU is reported, along with the corresponding process name/id and allocated GPU memory.
  - Clocks and PState: Max and current clock rates are reported for several important clock domains, as well as the current GPU performance state.
  - Temperature and fan speed: The current core GPU temperature is reported, along with fan speeds for non-passive products.
  - Power management: For supported products, the current board power draw and power limits are reported.
  - Identification: Various dynamic and static information is reported, including board serial numbers, PCI device ids, VBIOS/Inforom version numbers and product names.

- ***nvidia-smi*** is an existing application that uses the nvml API. An example follows-



NVIDIA

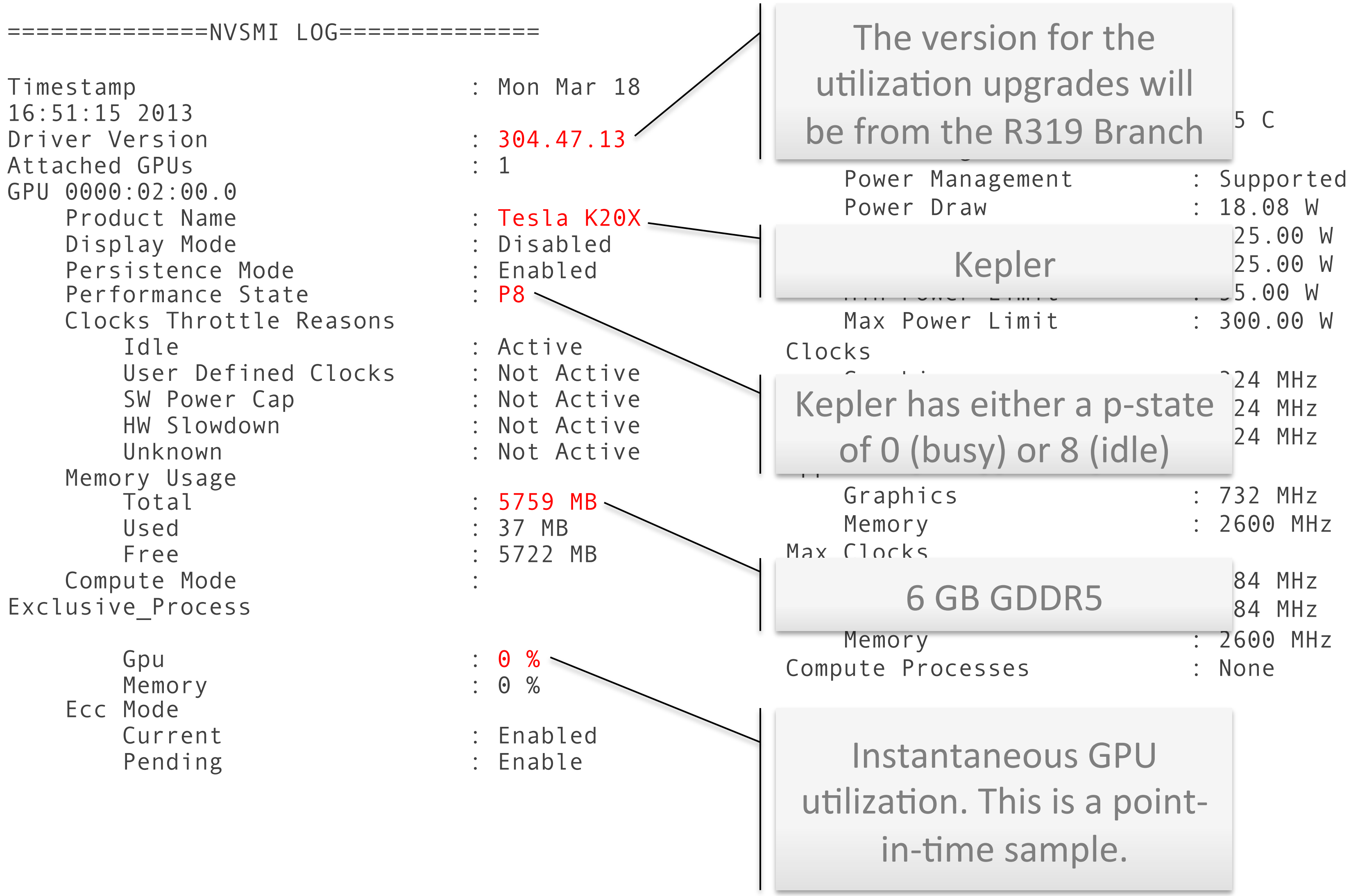
NVML API REFERENCE MANUAL

October 2, 2012

Version 4.304.55

NVML API Reference: https://developer.nvidia.com/sites/default/files/akamai/cuda/files/CUDADownloads/NVML_cuda5/nvml.4.304.55.pdf

nvml-smi Output (truncated) from a single Titan Kepler GPU



```
==============NVSMI LOG==============

Timestamp                           : Mon Mar 18
16:51:15 2013
Driver Version                      : 304.47.13
Attached GPUs                       : 1
GPU 0000:02:00.0
    Product Name                    : Tesla K20X
    Display Mode                    : Disabled
    Persistence Mode                : Enabled
    Performance State               : P8
    Clocks Throttle Reasons
        Idle                        : Active
        User Defined Clocks         : Not Active
        SW Power Cap                : Not Active
        HW Slowdown                 : Not Active
        Unknown                     : Not Active
    Memory Usage
        Total                       : 5759 MB
        Used                        : 37 MB
        Free                        : 5722 MB
    Compute Mode                    :
Exclusive_Process

        Gpu                         : 0 %
        Memory                      : 0 %
    Ecc Mode
        Current                     : Enabled
        Pending                     : Enable
```

```
                                          5 C

    Power Management          : Supported
    Power Draw                : 18.08 W
                               25.00 W
                               25.00 W
                               5.00 W
    Max Power Limit           : 300.00 W
Clocks
                               24 MHz
                               24 MHz
                               24 MHz

    Graphics                  : 732 MHz
    Memory                    : 2600 MHz
Max Clocks
                               84 MHz
                               84 MHz
    Memory                    : 2600 MHz
Compute Processes             : None
```

The version for the utilization upgrades will be from the R319 Branch

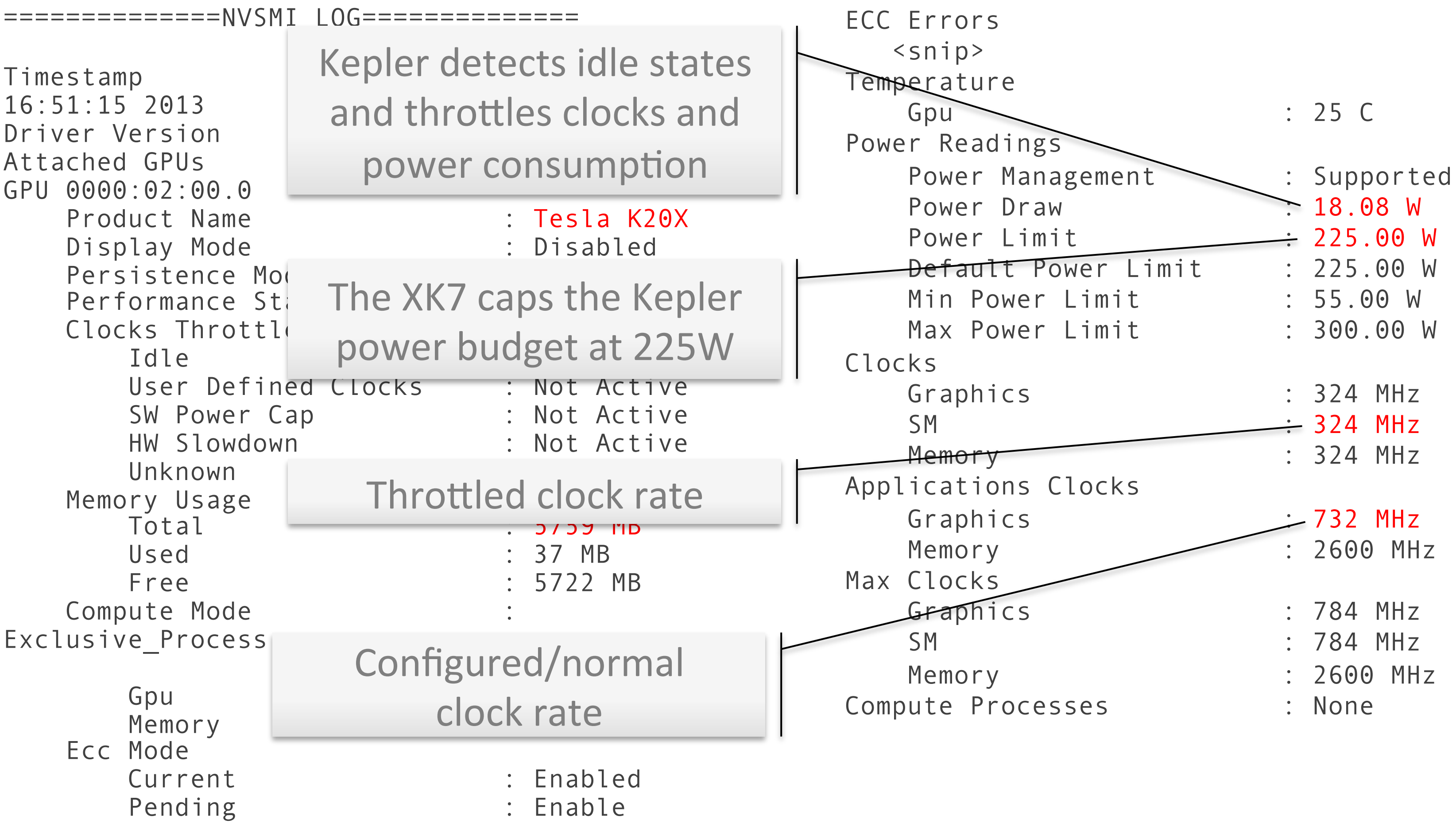
Kepler

Kepler has either a p-state of 0 (busy) or 8 (idle)

6 GB GDDR5

Instantaneous GPU utilization. This is a point-in-time sample.

nvml-smi Output (truncated) from a single Titan Kepler GPU



```
==============NVSMI LOG==============

Timestamp
16:51:15 2013
Driver Version
Attached GPUs
GPU 0000:02:00.0
    Product Name                    : Tesla K20X
    Display Mode                    : Disabled
    Persistence Mo
    Performance St
    Clocks Throttl
        Idle
        User Defined Clocks         : Not Active
        SW Power Cap                : Not Active
        HW Slowdown                 : Not Active
        Unknown
    Memory Usage
        Total                       : 5759 MB
        Used                        : 37 MB
        Free                        : 5722 MB
    Compute Mode                    :
Exclusive_Process

        Gpu
        Memory
    Ecc Mode
        Current                     : Enabled
        Pending                     : Enable
```

```
ECC Errors
   <snip>
Temperature
    Gpu                            : 25 C
Power Readings
    Power Management               : Supported
    Power Draw                     : 18.08 W
    Power Limit                    : 225.00 W
    Default Power Limit            : 225.00 W
    Min Power Limit                : 55.00 W
    Max Power Limit                : 300.00 W
Clocks
    Graphics                       : 324 MHz
    SM                             : 324 MHz
    Memory                         : 324 MHz
Applications Clocks
    Graphics                       : 732 MHz
    Memory                         : 2600 MHz
Max Clocks
    Graphics                       : 784 MHz
    SM                             : 784 MHz
    Memory                         : 2600 MHz
Compute Processes                  : None
```

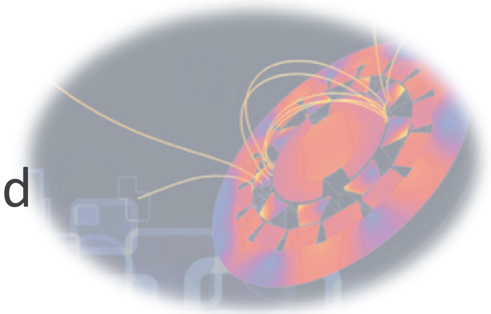
Kepler detects idle states and throttles clocks and power consumption

The XK7 caps the Kepler power budget at 225W

Throttled clock rate

Configured/normal clock rate

Requirements Gathering as a Community



- In early 2012, we identified a critical need to understand “GPU utilization” in a broader context.
- At a CUG 2012 BOF, the XK community initiated a discussion about what types of data would be appropriate or helpful. That initial list described items including:
  - Number of GPU contexts opened
    - how many times is cuInit() called?
  - Number of GPU kernels run
    - This self-destructed, since dynamic parallelism added the capability to spawn kernels on the GPU, from the GPU, and eliminated the ability to map this from the CPU-side.
  - Amount of time (GPU-seconds) accrued
    - the amount of time that a job has a GPU context open. This is ***not*** the amount of time that a kernel is running on the GPU, and is an indicator of one of the design points of the implemented solution
  - High water mark of memory used – how much of the 6GB of GDDR5 were allocated?
- By Q4 2012, we reached a decision point where we could proceed, defining both method and definition for Measuring NVIDIA GPU Utilization

NVIDIA's Response to the Need for Utilization Data
- Driver Changes and API Extensions

- ORNL, NVIDIA, and Cray discussed mechanisms for making information on GPU utilization available from any single Kepler, and mechanisms from the Cray perspective on aggregating all of the math so that the utilization of the GPUs could be defined and reported on a per-job basis. The underlying mechanism is an NVIDIA API that includes the function:

*nvmlDeviceGetAccountingStats (nvmlDevice_t device, unsigned int pid, nvmlAccountingStats_t *stats)*

- This extension is available for Tesla ™and Quadro ®products from the Kepler family. The function queries a process's accounting statistics, capturing GPU utilization across the lifetime of a process. Accounting stats can be queried during life time of the process and after its termination. Accounting stats are kept in a circular buffer; newly created processes overwrite information about old processes.

nvmlAccountingStats_t struct

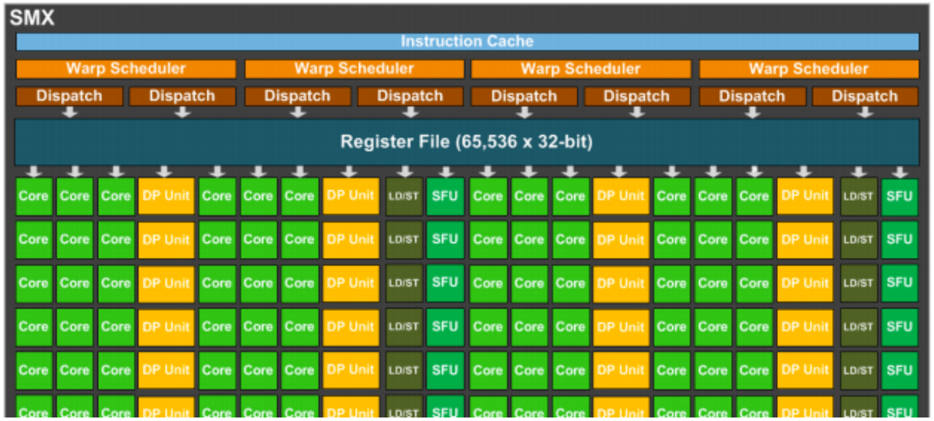
unsigned int gpuUtilization	*Percent of time over the process's lifetime during which one or more kernels was executing on the GPU. Utilization stats just like that returned by nvmlDeviceGetUtilizationRates but for the life time (to date) of a process (not just the last second).*
unsigned int memoryUtilization	*Percent of time over the process's lifetime during which global (device) memory was being read or written.*
unsigned long long maxMemoryUsage	*Maximum total memory in bytes that was ever allocated by the process.*
unsigned int startTimeStamp	*Timestamp of the moment process allocated GPU (TODO) define how to map timestamp to system time.*
unsigned int endTimeStamp	Timestamp of the process termination.

Defining GPU Utilization for Kepler

- What (exactly) is meant by GPU Utilization?
  - GPU utilization is an assessment of whether work is scheduled.

Is work active on ANY of the 14 SMs?

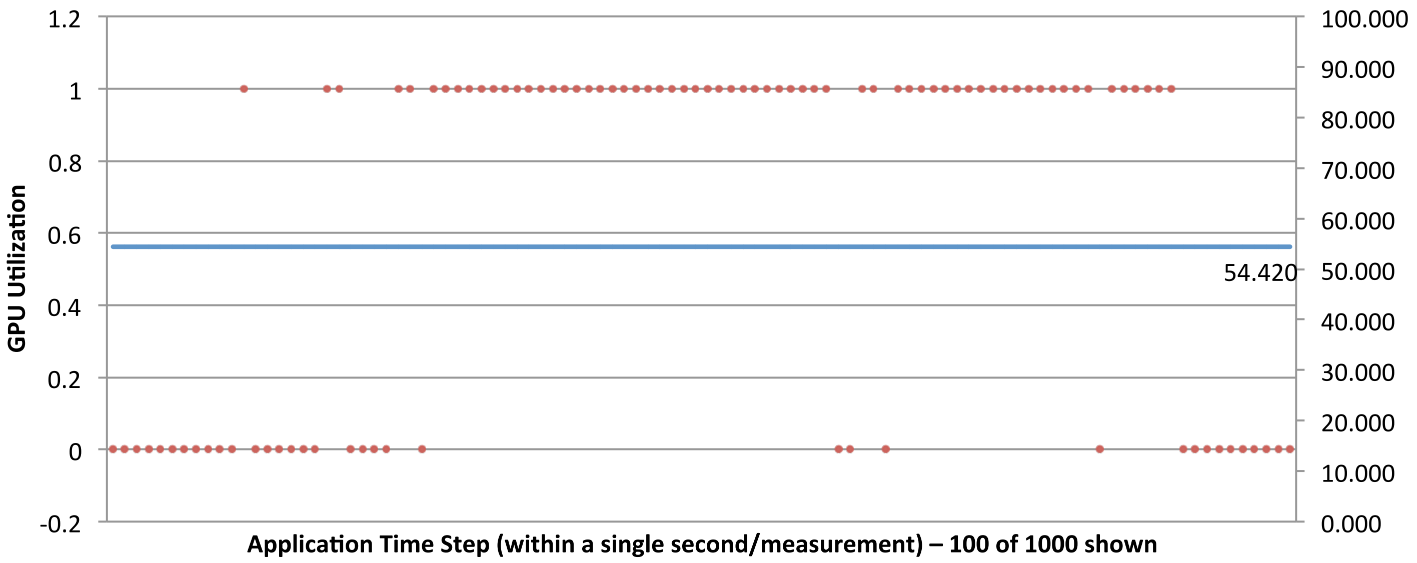
- This assessment is made O(1000) times per second already. By taking advantage of an existing mechanism, there is no additional overhead required.
- These transient values are not retained.
- At the end of a one second interval, these samples are aggregated and averaged, and the 1-second value is saved as a data point.
- At the end of an application run, each of the 1-second values are aggregated and averaged, and the n-second value is saved in to the 128-deep pid/GPU_utilization buffer.



Kepler GPU – Sampling Per Second

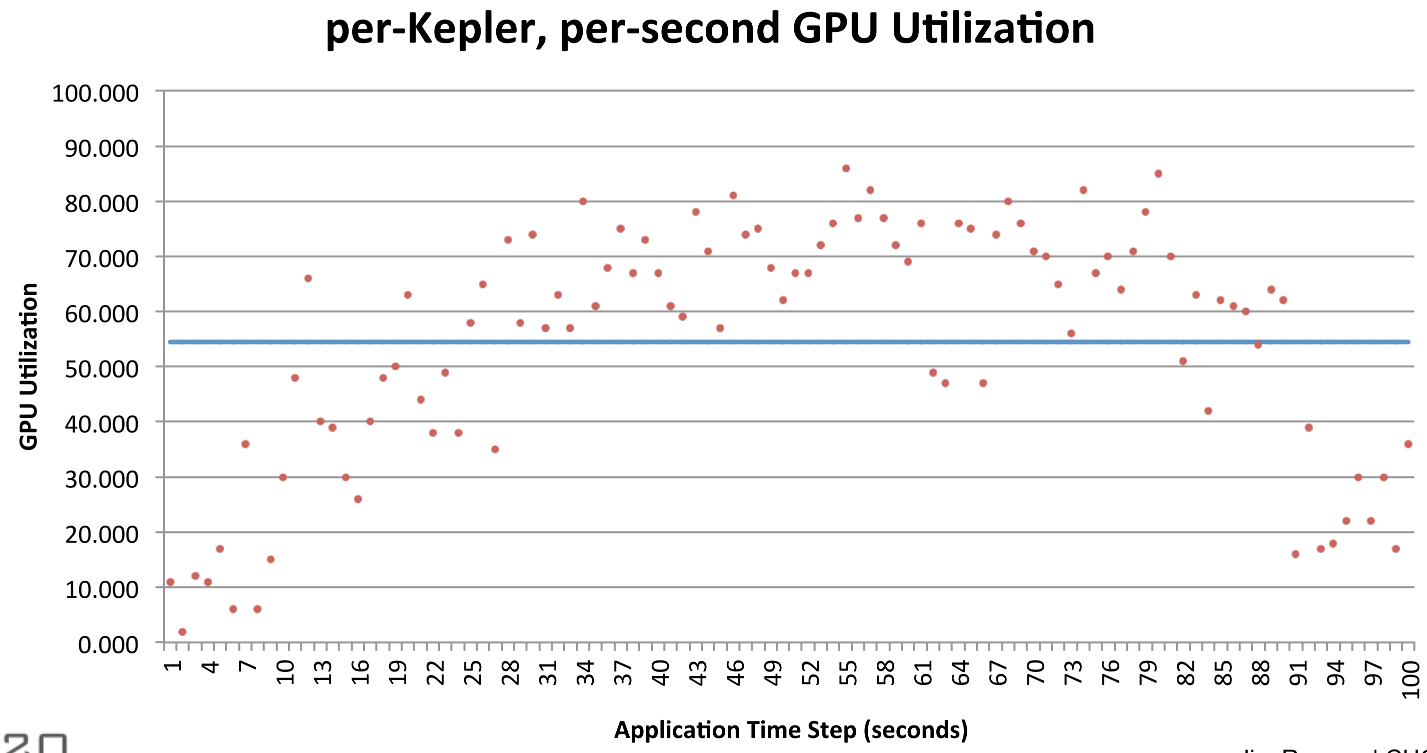
- During a single second, the GPU samples whether any of the 14 SMs are in use, and aggregates on the order of 1000 samples to determine the GPU utilization during that one second.
- Each of those samples is a binary result.
- If there is any instruction executing on any SM, a value of 1 is returned.
- At the end of the time interval (one second), the arithmetic mean for that interval is returned
- This per-second value that is then averaged over the term of the entire run and returned by the call to (API routine).

per-Kepler, single-second GPU Utilization (binary state, O(1000) samples per second)



Kepler GPU – Sampling Across the Lifetime of an Application

- For each Kepler, each of the samples that are available each second of the life of an application are tracked and aggregated. In addition, the Start and End Times are known, providing the capability to calculate the "rolling average" GPU utilization at any time that the routine *nvmlDeviceGetAccountingStats* is called.
- By calling this routine at the end of an application, the single-Kepler GPU utilization, expressed as a percentage between 0-100% is available.
- By then aggregating all of the single-Kepler GPU utilization results using the pid as the filter, Cray can report on the average GPU utilization across all Keplers associated with an application.



GPU Reporting and Accounting Update

- Current Status
  - Received GPU Accounting API in early January
  - Received Alpha driver from the CUDA 5.5/R319 Branch on February 15
  - Initial evaluation of the API is underway
  - Working open issues with NVIDIA
- NVIDIA is delivering production GPU-utilization in CUDA 5.5
  - R319 Branch Release candidate planned for early May
  - Target production release planned mid-July.
  - Cray will deliver CUDA 5.5 with CLE 4.2 UP02 on XK
- Resource Utilization Recording (RUR)
  - Cray moving to a more extensible accounting infrastructure
  - RUR targeted for CLE 4.2 UP02 and aligned with CUDA 5.5 release
  - RUR CUG paper dovetails with this presentation

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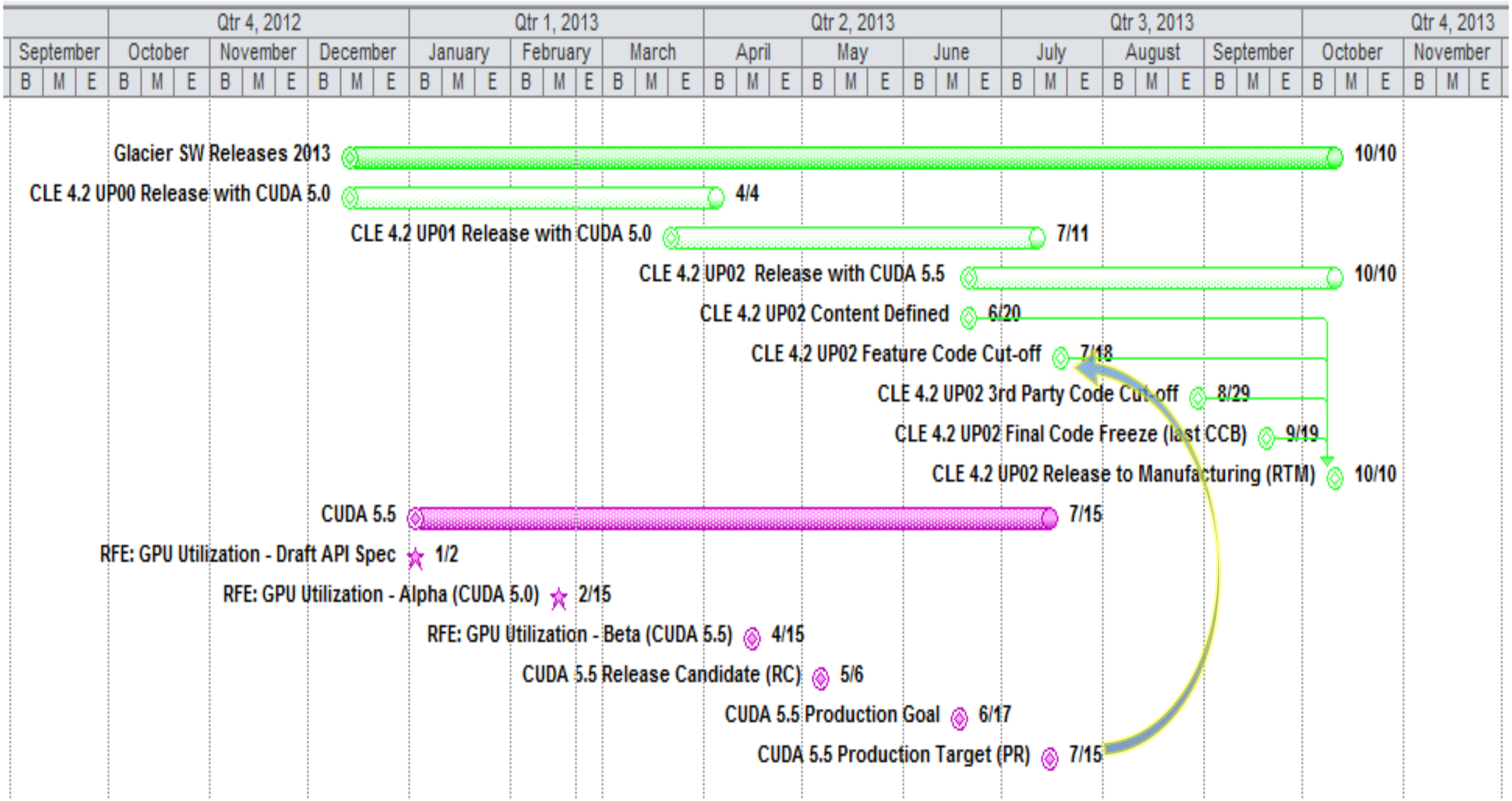
XK CLE 4.2 and CUDA 5.5 Release Milestones

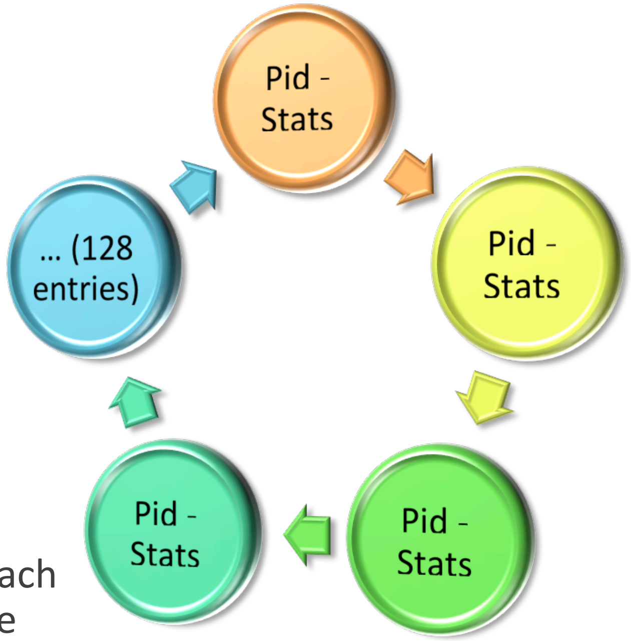


Glacier SW Releases 2013	10/10
CLE 4.2 UP00 Release with CUDA 5.0	4/4
CLE 4.2 UP01 Release with CUDA 5.0	7/11
CLE 4.2 UP02 Release with CUDA 5.5	10/10
CLE 4.2 UP02 Content Defined	6/20
CLE 4.2 UP02 Feature Code Cut-off	7/18
CLE 4.2 UP02 3rd Party Code Cut-off	8/29
CLE 4.2 UP02 Final Code Freeze (last CCB)	9/19
CLE 4.2 UP02 Release to Manufacturing (RTM)	10/10
CUDA 5.5	7/15
RFE: GPU Utilization - Draft API Spec	1/2
RFE: GPU Utilization - Alpha (CUDA 5.0)	2/15
RFE: GPU Utilization - Beta (CUDA 5.5)	4/15
CUDA 5.5 Release Candidate (RC)	5/6
CUDA 5.5 Production Goal	6/17
CUDA 5.5 Production Target (PR)	7/15

PRELIMINARY, Cray Confidential and Proprietary Information

Engineering Takeaways

- An elegant solution from an engineering perspective. The changes to the device driver, NVML libraries and API:
  - Take advantage of existing transient data
  - Minimize performance impact to the GPU (near zero impact)
  - Still provides both the pid list and util numbers on a per-Kepler perspective to the recipient
- Energy Efficiency
  - At p-state 0, the chip is operating at 732MHz and consuming somewhere between 160 and 225W.
  - At p-state 8, the chip is idle, and is operating at 324MHz, consuming as little as 20W or less.
- Saving State Information
  - The pid/statistics buffer is 128 deep, per Kepler, saving the pid and GPU utilization information in a round-robin fashion.
- Potential Future Work -
  - Currently, in a single second, there are ~1000 samples taken each second, per GK110. The assumption is that in each sample, the SMs are busy, or they are not.
  - Within the existing hardware, there is a capability to assess during that cycle how many SMs (0-14) are available, i.e. the granularity of the reporting could change from 0/1 (0%-100%) to 0-1 (0%-100%, step 7.14%).



Questions?

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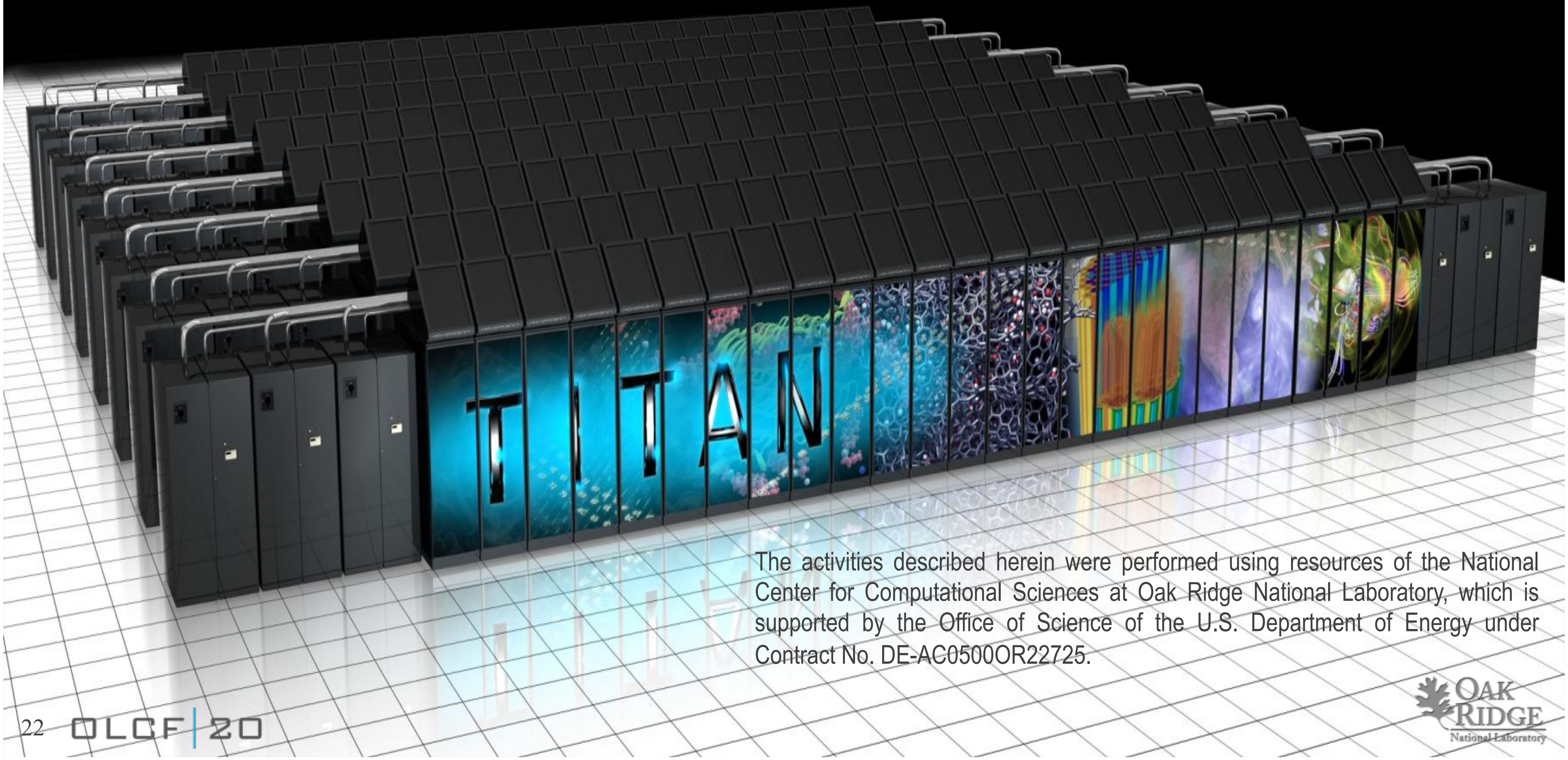

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