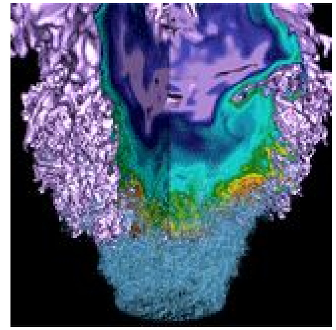
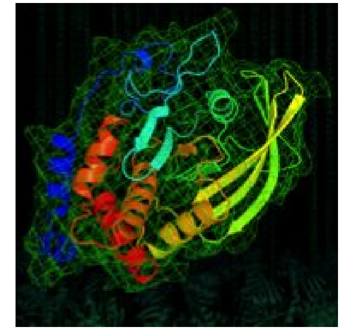
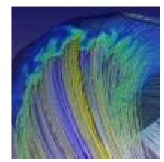
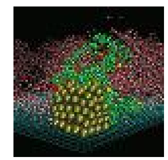
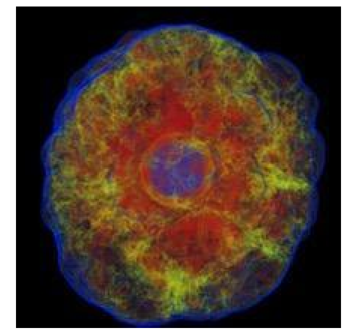
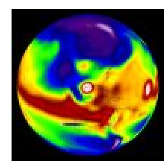
Cori Phase 1 Burst Buffer


NERSC 40 YEARS at the FOREFRONT

Debbie Bard, Wahid Bhimji, Dave Paul, et. al.

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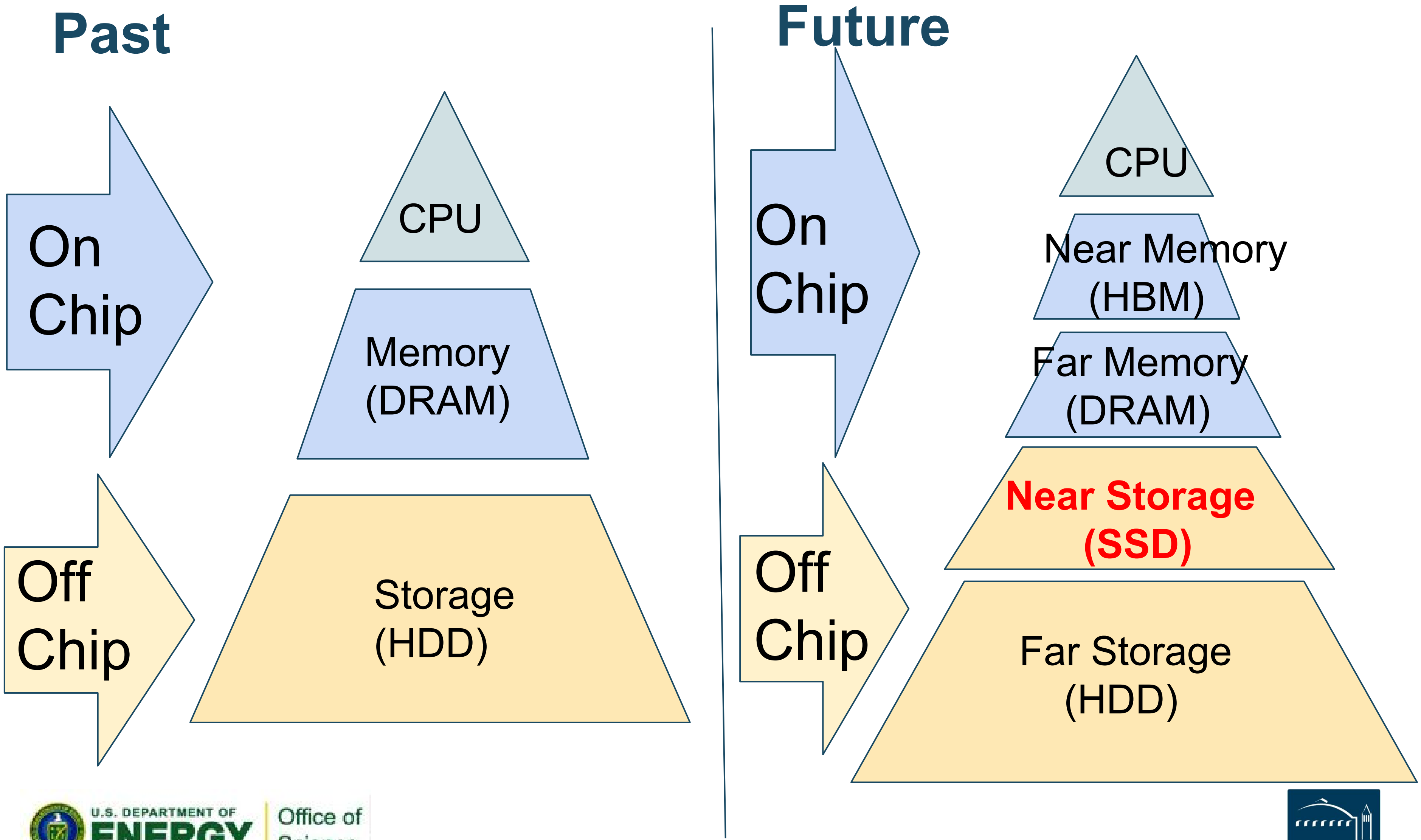
HPC memory hierarchy is changing



HPC memory hierarchy is changing

Past

On Chip

CPU

Memory (DRAM)

Off Chip

Storage (HDD)

Future

On

CPU

Chip

Far Storage (HDD)

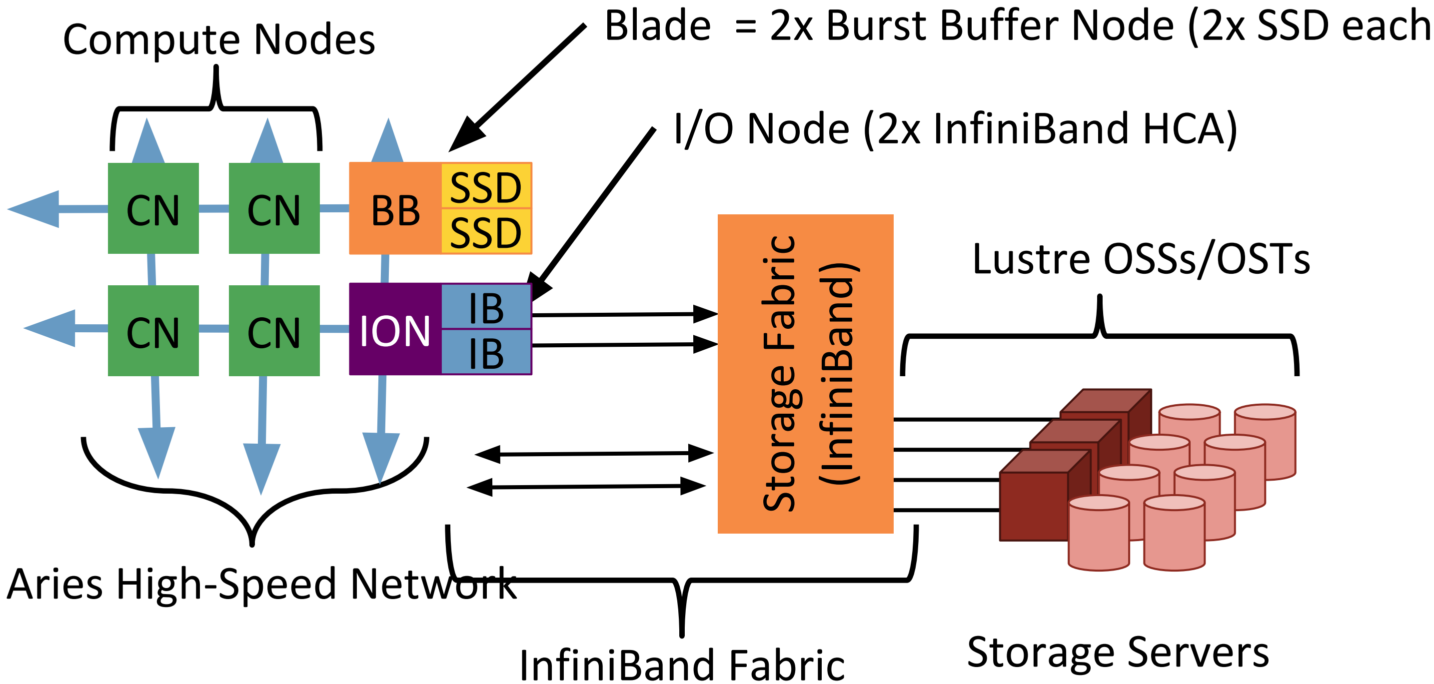
Why a Burst Buffer?

- **Handle spikes in IO bandwidth requirements without increasing size of PFS**
  - Reduce job wallclock time
  - Compute resources idle during IO bursts
- **Disk-based PFS bandwidth is expensive**
  - Capacity is relatively cheap
- **SSD bandwidth is relatively cheap**
- **-> Separate bandwidth and spinning disk**
  - Provide high BW without wasting PFS capacity
  - Leverage Cray Aries network speed

Burst Buffer implementation

- **High BW SSDs in service nodes, directly attached to Aries network**
- **Software creates pool of available memory**
  - DataWarp service daemons
  - DataWarp file system (using DVS, LVM, XFS)
  - Integrated with SLURM
- **Allocation portions of this pool to users per-job, or in a persistent reservation**
- **Users see a POSIX-compatible FS**
- **Can stage data in and out from BB to PFS**
  - Before/after compute job starts - *saves compute time*
  - Asynchronously during compute job

Burst Buffer Architecture



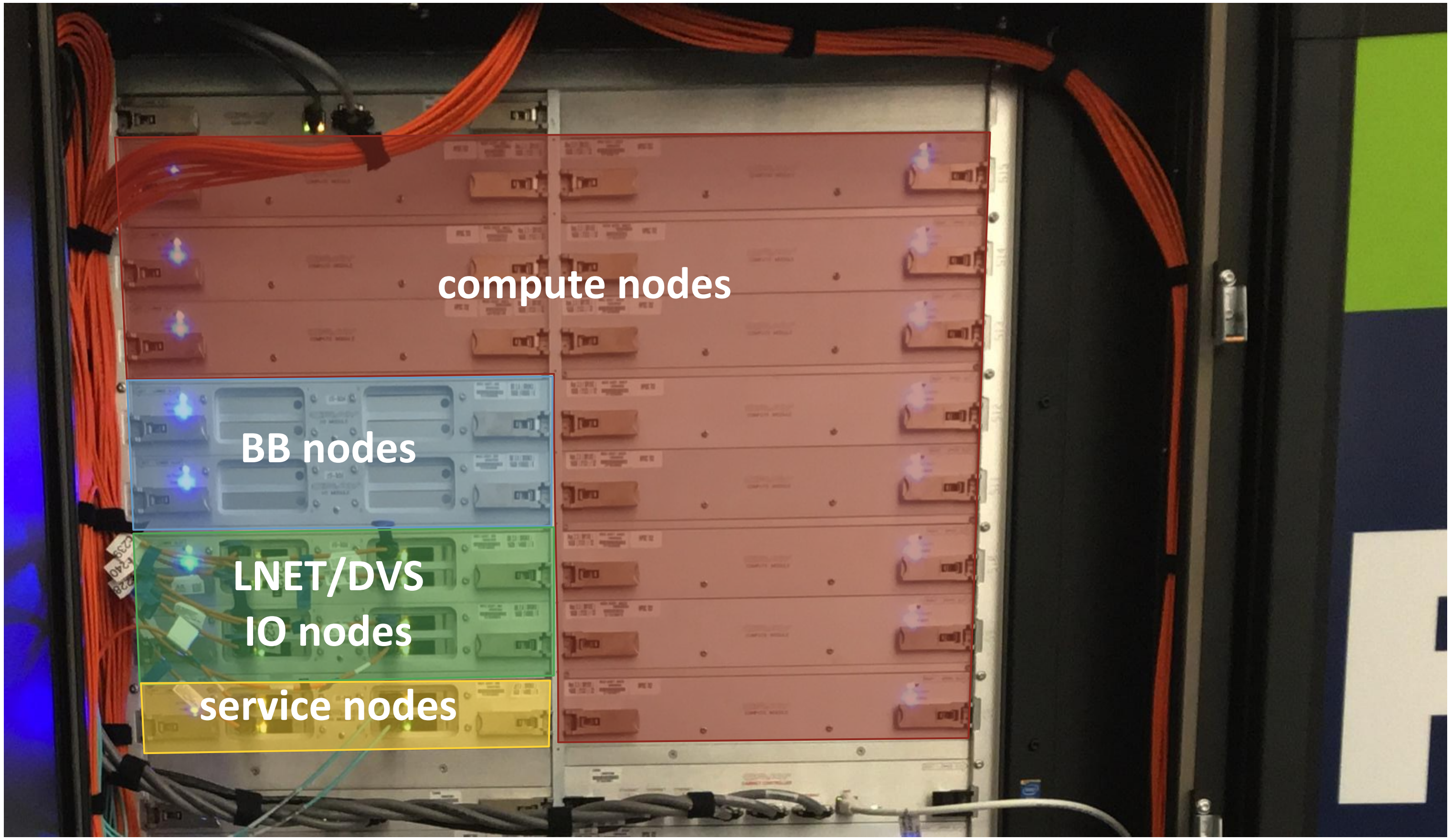
- **Cori Stage 1 configuration: 920TB on 144 BB nodes (288 x 3.2 GB SSDs)**
- **>1.5 PB total coming with Cori Phase 2**
- **Lustre: 30PB PFS**

Burst Buffer Architecture Reality

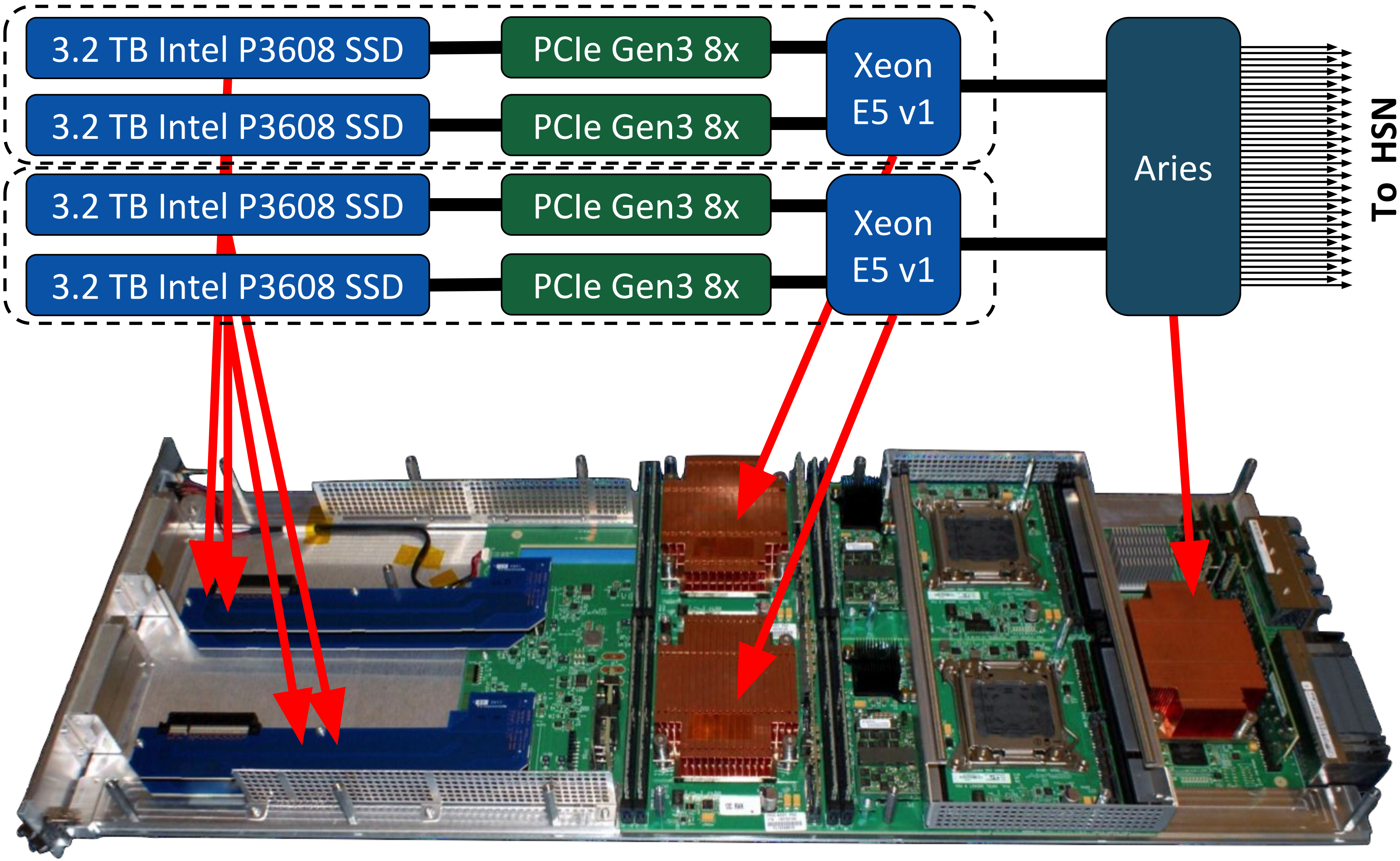
Photo from Glenn Lockwood

BB nodes scattered throughout HSN fabric

2 BB blades/chassis (12 nodes/cabinet) in Phase I



Burst Buffer Blade = 2xNodes



Burst Buffer Feature Timeline

NERSC

Stage 3

In-transit processing and filtering

Stage 2

Transparent caching mode

we are here

Stage 1

Striping, "bad" I/O pattern remediation, per-job and persistent allocations

API will provide means to
- set cache size
- set read-ahead window size
- force consistency point (flush)

Stage 0

Static mapping of compute to BB node, manual data migration

3Q14 → 4Q14 → 1Q15 → 2Q15 → 3Q15 → 4Q15 → 1Q16 → 2Q16 → 3Q16

Burst Buffer Early User Program

- Aug 10th: solicited proposals for BB Early Users program.
  - Award of exclusive early use of BB on Cori P1, plus help of NERSC experts to optimise application for BB.
- Selection criteria include:
  - Scientific merit;Computational challenges; Cover range of BB data features; Cover range of DoE Science Offices.
- Great interest from the community, 29 proposals received.
- Decided to support more applications than we'd originally anticipated
  - some applications already had LDRD funding at LBNL, and existing support from NERSC staff.
- ~20 applications not supported by NERSC staff, but do have early access to Cori P1 and the BB.

Burst Buffer Early Users

Burst Buffer User Case	Active Early Users
IO Bandwidth: Writes (checkpointing)	• Nyx/BoxLib astro simulations • VPIC IO
IO Bandwidth: Reads	• Electron Cryo-microscopy image analysis
"Bad" IO pattern, eg. high IOPs	• Spark analytics framework • ALS TomoPy
Workflow coupling and visualization	• Climate simulation, analysis and visualization
in transit / in-situ analysis	• ChomboCrunch / VisIt carbon sequestration simulation
Staging intermediate data	• Phoenix3D radiation transport simulation • ALICE data analysis (HEP)

~40 active Burst Buffer Users

Challenges ...

- **Initial instabilities resolved in early patches**
  - Early Users are the best testers of a new system!
  - New issues cropping up as use patterns are extended
- **Minor usability issues being addressed by Cray**
  - Syntax sensitivities, informative error codes, improved documentation...
- **Work is on-going, in collaboration with Cray, to understand user application IO patterns and performance**
  - optimising configuration of hardware/software for widely varying use cases is an interesting challenge
  - e.g. balance of performance in writing large vs small files

Performance testing ongoing

- **Burst Buffer is exceeding (nearly all) benchmark performance targets**
  – Work on-going to improve MPIO shared file write
  – IOPs particularly impressive
  – Out-performs Lustre (Lustre also exceeds requirements)

	140 Burst Buffer Nodes : 1120 Compute Nodes ; 4 processes/node					
	IOR Posix FPP		IOR MPIO Shared File		IOPS	
	Read	Write	Read	Write	Read	Write
Required (GB/s) or IOPS	820	820	656	656	7200000	7200000
Best Measured	905	873	803	351	12591978	12527427
Lustre (peak SOW)	708	751	573	223	-	-

*Bandwidth tests: *8 GB block-size 1MB transfers IOPS tests: 1M blocks 4k transfer*

Example application (preliminary)

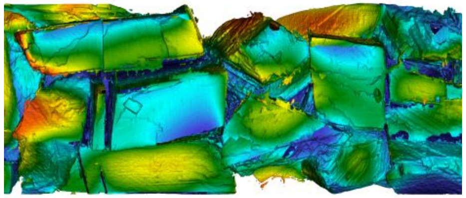
ChomboCrunch

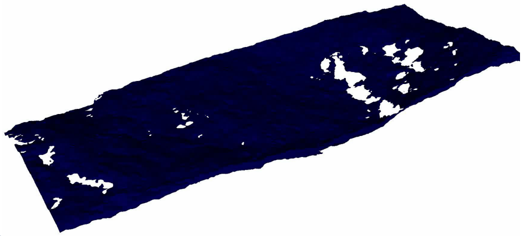
Andrey Ovsyannikov, LBL

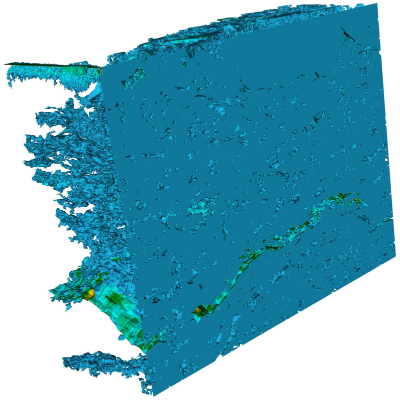
Simulates pore-scale reactive transport processes associated with carbon sequestration

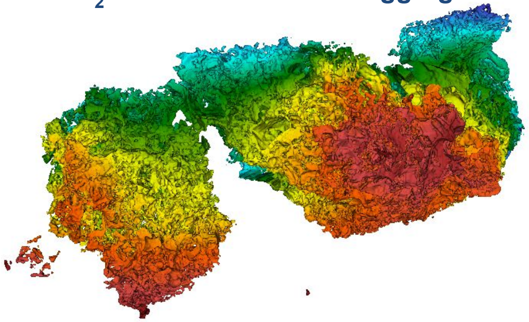
- Applied to other subsurface science areas:
  - Hydrofracturing (aka “fracking”)
  - Disposing of used fuel
- Extended to engineering applications
  - Lithium ion battery electrodes
  - Paper manufacturing (hpc4mfg)

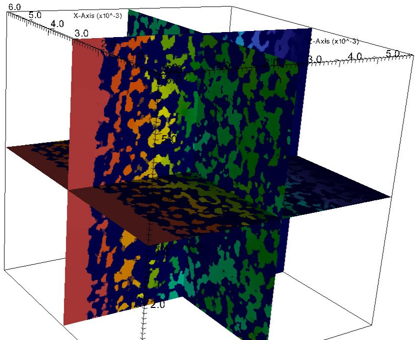
- *Common feature: ability to perform direct numerical simulation from image data of arbitrary heterogeneous, porous materials*

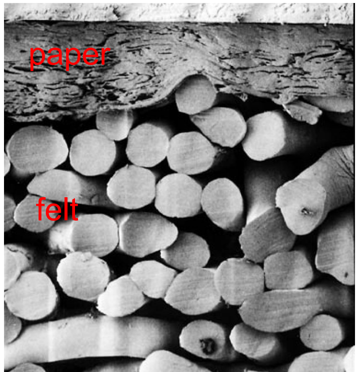

pH on crushed calcite in capillary tube


Transport in fractured dolomite


Flooding in fractured Marcellus shale


O_2 diffusion in Kansas aggregate soil

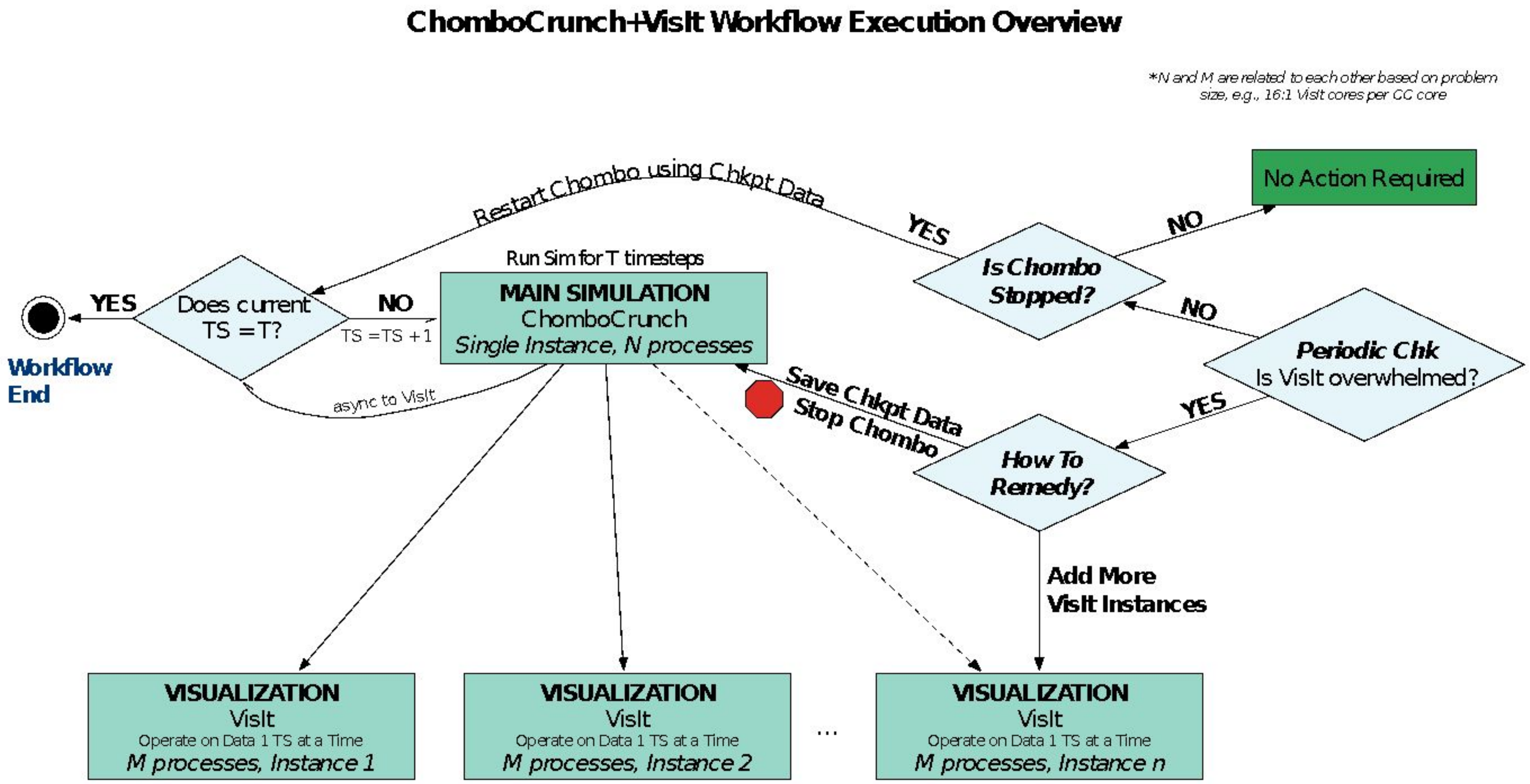

Electric potential in Li-ion electrode



Paper re-wetting

Example application (preliminary)

ChomboCrunch + VisIt workflow



Example application (preliminary)

- **Running more MPI processes gives higher-resolution simulations -> produces larger output plot files**
- Benchmark: reactive flow in a cylinder channel randomly packed by a set of spheres
  - Mesh resolution varies from 256^3 (512 MPI ranks) to 2048*512*512 (16384 MPI ranks)

# MPI ranks	File size	Requested BB capacity	**BB BW**	Lustre BW
512	7.4GB	1 BB node	**1.8GB/s**	0.44GB/s
2048	29.5GB	4 BB nodes	**4.7GB/s**	1.5GB/s
16384	236 GB	16 BB nodes	**34.2GB/s**	8.4GB/s

Burst Buffer enables high-resolution analysis of simulations

User Experience so far (tentative)

- **Writing large files (with large block I/O) is fast (checkpointing use case)**
- **Reading/Writing small files (or small I/O transfers) is problematic in some cases**
  - Generally in many cases our BB performance is worse than our Lustre filesystem (which is high-performance).
  - Client-side caching helps Lustre performance
- **Some jobs with many files fail at large scale on compute nodes**
- **Still some system instabilities**

Working to profile applications I/O and tune burst buffer stripe sizes and other configurables...

Expected performance improvements

1. DVS client-side caching

- Lustre has client-side caching, currently DVS does not
- Will help small R/W transfers on BB
- Can currently use "iobuf" library for user-side caching

2. Smaller granularity

- "Grain" is minimum amount of space allocated on each BB node, currently 213GB
  - E.g. request 500GB BB allocation - get 3x213GB "grains".

3. MPI-IO shared file performance

- Change underlying file striping on BB

We're working with Cray to improve BB performance

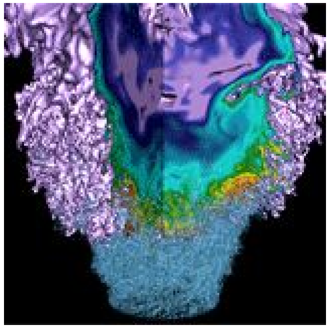
Timeline for Access

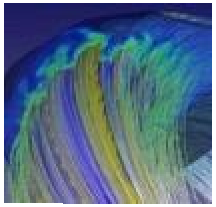
- **Currently only Early Users have access**
- **Plan to allow all users access shortly after we've accepted the BB**
  - Dependent on system being stable - i.e. no kernel panics that bring down compute nodes, major bugs fixed.

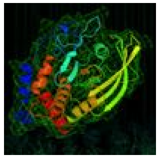
Summary

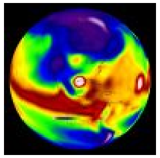
- **BB/DataWarp functional and meets most SOW performance targets**
  - out-performs Lustre in benchmarks
- **Variety of issues affecting user progress**
  - but these are being resolved and users making some progress
- **Some performance pay-off for real use-cases but not all.**
  - We are learning/tweaking configuration
  - Working with Cray to implement performance improvements
- **Profiling I/O patterns to optimise and starting to build whole workflows using the Burst Buffer.**

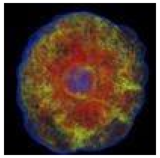
Thankyou

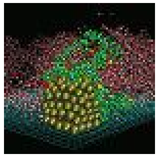












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Use Cases by BB feature

Application	I/O bandwidth: reads	I/O bandwidth: writes (checkpointing)	High IOPs	Workflow coupling	In-situ / in-transit analysis and visualization	Staging intermediate files/ pre-loading data
Nyx/Boxlib		X		X	X	
Phoenix 3D		X		X		X
Chomo/Crunch + Visit		X		X	X	
Sigma/UniFam/Sipros	X	X	X			X
XGC1	X	X				X
PSANA				X	X	X
ALICE	X					
Tractor			X	X		X
VPIC/IO					X	X
YODA			X			X
ALS SPOT/TomoPy	X			X	X	X
kitware				X	X	

Use Cases by BB feature

Application	I/O bandwidth: reads	I/O bandwidth: writes (checkpointing)	High IOPs	Workflow coupling	In-situ / in-transit analysis and visualization	Staging intermediate files/ pre-loading data
Electron cryo-microscopy						X
htslib						X
Falcon	X	X				
Ray/HipMer	X	X	X			X
CESM	X	X				
ACME/UV-CDAT					X	X
GVR		X				
XRootD				X		X
OpenSpeedShop	X	X				
DL-POLY		X				
CP2K		X				
ATLAS	X		X			X