

## INCORPORATING NVM INTO DATA-INTENSIVE SCIENTIFIC COMPUTING



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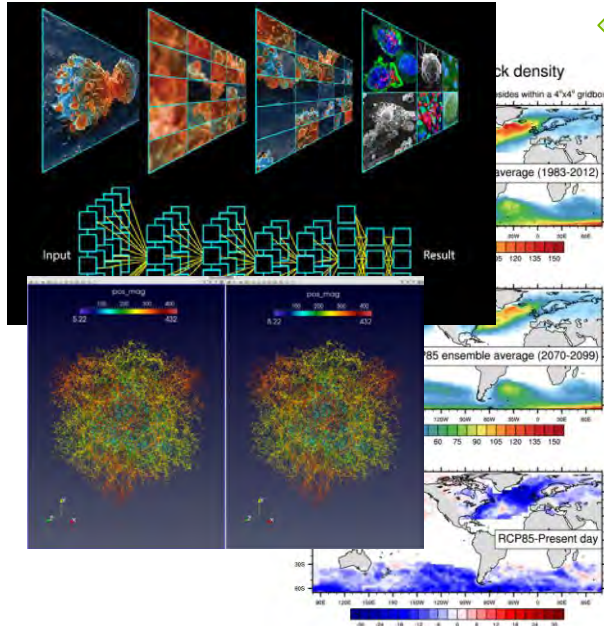
Argonne Leadership Computing Facility

IBM Blue Gene/Q (Mira)  
Cray XC40 (Theta)

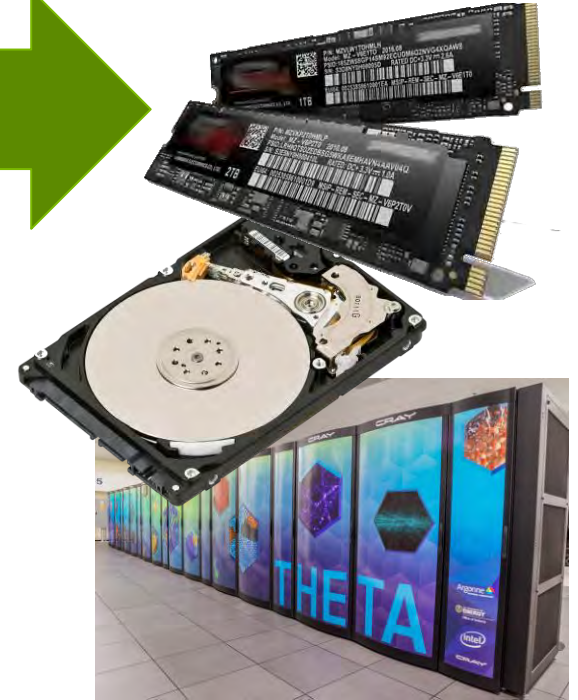
(Under construction:  
A21 exascale system)

# THE ROLE OF ANL/MCS DATA-INTENSIVE SCIENCE RESEARCH

(one perspective)



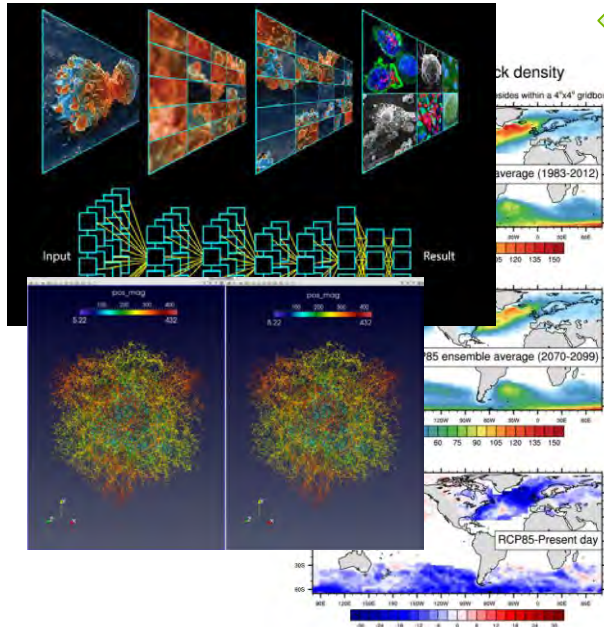
Techniques, algorithms, and software to bridge the “last mile” between scientific applications and storage systems





# THE ROLE OF ANL/MCS DATA-INTENSIVE SCIENCE RESEARCH

(one perspective)



This entails:

- Characterizing access
- Modeling architectures
- Optimizing data services
- **Incorporating new technology such as NVM**



# DATA-INTENSIVE SCIENTIFIC COMPUTING

## Constraints on NVM integration from an end-user perspective

- Efficiency
  - CPU hours (and storage) are a scarce commodity
  - This has a direct impact on scientific time to solution
- Portability
  - Applications must execute on multiple platforms
  - The science itself will outlive all of those platforms
- Ease of use
  - Scientists would like to focus on their problem domain
  - Not the mysterious ways of `vendor_api_write_foo()`

# DATA-INTENSIVE SCIENTIFIC COMPUTING

## Potential solutions in the storage design space

- Efficiency
  - Portability
  - Ease of use
1. A global parallel file system
    - POSIX is portable and easy to use (or at least well understood)
    - Re-engineering needed to address latency shifting by orders of magnitude
    - Semantics and API make this challenging
  2. “Here are some NVM devices: have fun!”
    - Dedicated developers will always be able to maximize efficiency with this approach
    - Not enough ninja programmers for this to be a viable long term option
  3. Specialized data services
    - *There are challenges and opportunities*
    - ***NVM APIs*** can help

# WHAT DO WE MEAN BY SPECIALIZED DATA SERVICES?



# SPECIALIZED DATA SERVICES

- Semantics and capabilities tailored to a problem domain
- Provisioned and instantiated on-demand
- Abstracting storage technology from the application
- Target more than just checkpointing
- *A way to leverage NVM characteristics by bypassing conventional storage software infrastructure*

Examples are already common in HPC!



# AN ECOSYSTEM OF DATA SERVICES

## Science Workflow

**Executables  
and  
Libraries**

SPINDLE

**Checkpoints**

SCR

FTI

**Input and  
Intermediate  
Data  
Products**

DataSpaces

MDHIM

Kelpie

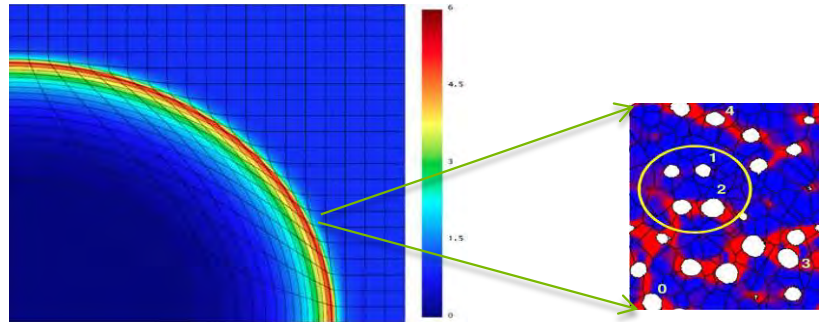
**Performance  
Data**

Darshan

LMT

*There is an opportunity to extend this concept to domain-specific scientific data models as well.*

# A SCIENTIFIC DATA MODEL EXAMPLE: MULTI-SCALE SIMULATION



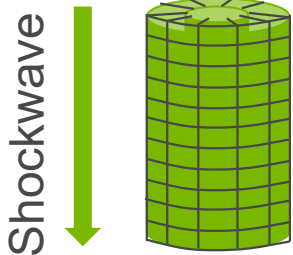
Coarse-scale model

Fine-scale model

Multi-scale models simulate across multiple time and length scales.

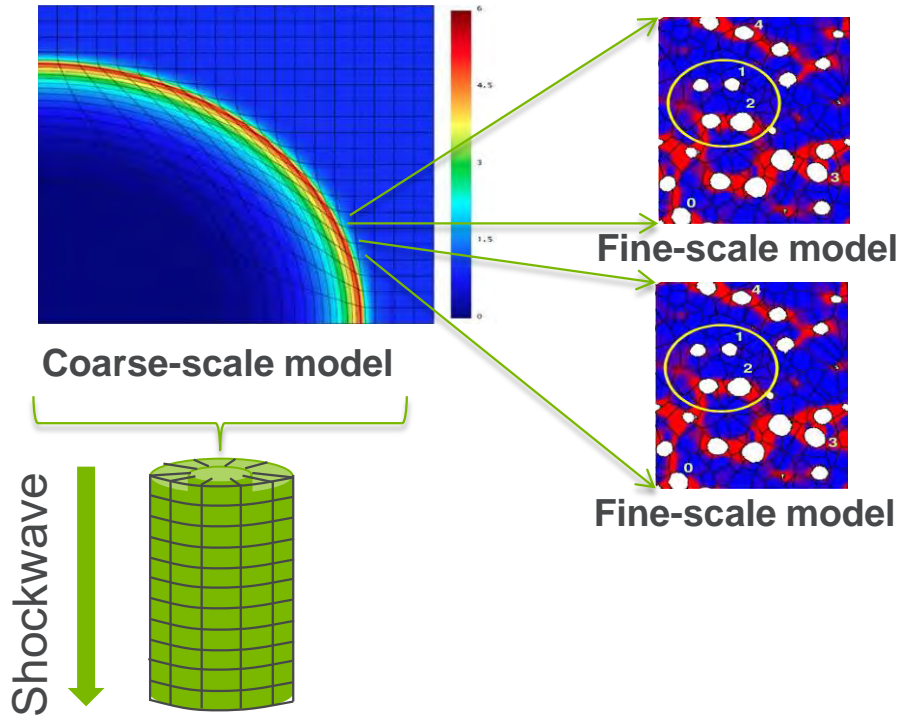
This example is a hydrodynamics unstructured mesh with an FFT-based PDE solver.

We will use it to illustrate a motif that occurs in other problem domains as well and highlights the need for reusable building blocks.



R. Lebensohn et al, Modeling void growth in polycrystalline materials, *Acta Materialia*, <http://dx.doi.org/10.1016/j.actamat.2013.08.004>.

# A SCIENTIFIC DATA MODEL EXAMPLE: MULTI-SCALE SIMULATION

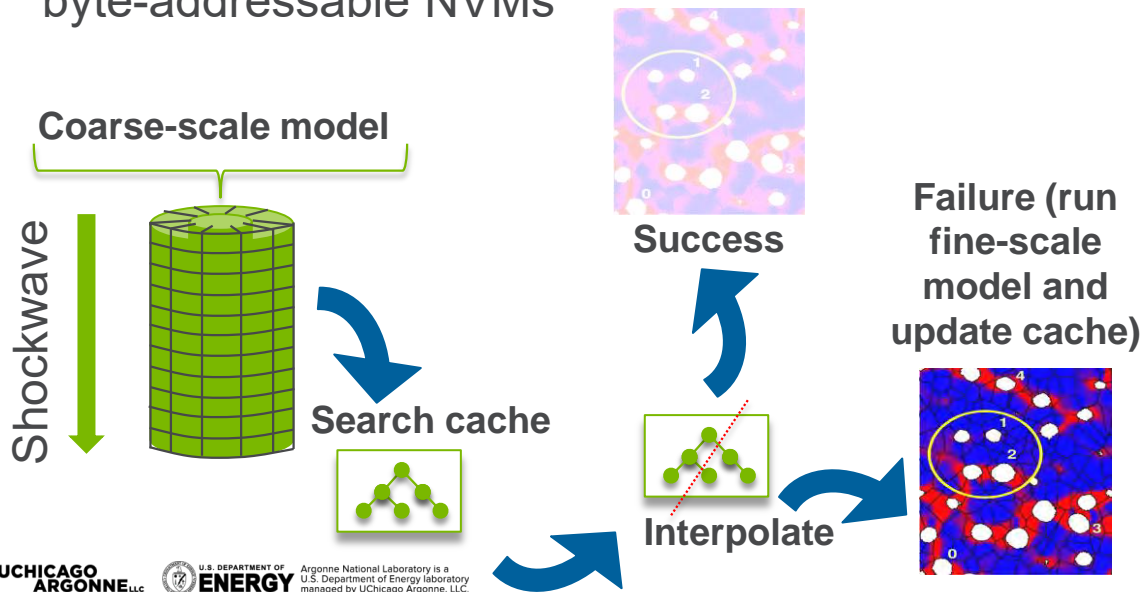


- Phenomena such as shock waves propagate through coarse-scale model
- This sometimes requires recomputation of similar (or identical) fine-scale models

If the fine-scale model is expensive, then we should cache fine-scale results for later use.

# COMPUTATIONAL CACHING AS A SPECIALIZED DATA SERVICE

- Search cache for nearest neighbors in parameter space, interpolate, and check error bounds
- Could be a distributed data service that leverages low latency, byte-addressable NVMs



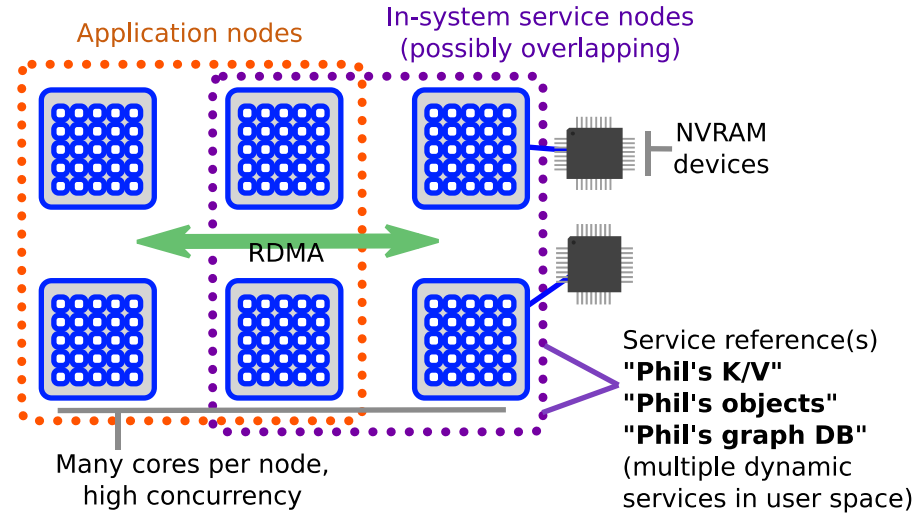
This isn't a standard file system or database.

NVM APIs:

- Give us building blocks for new data models
- Let us differentiate classes of memory

# TECHNICAL CHALLENGES FOR SPECIALIZED DATA SERVICES IN HPC

- Where is the NVM?
  - Local to compute nodes, remote access, or remote access via fabric?
- Integration with custom HPC networks
  - Dragonfly, torus, fat tree, exotic APIs
- Concurrency
  - Applications with > 100 thousand processes
- Access mode
  - User-space access helps to enable dynamic services on time-shared systems



The Mochi Project  
ANL, LANL, CMU, HDFG

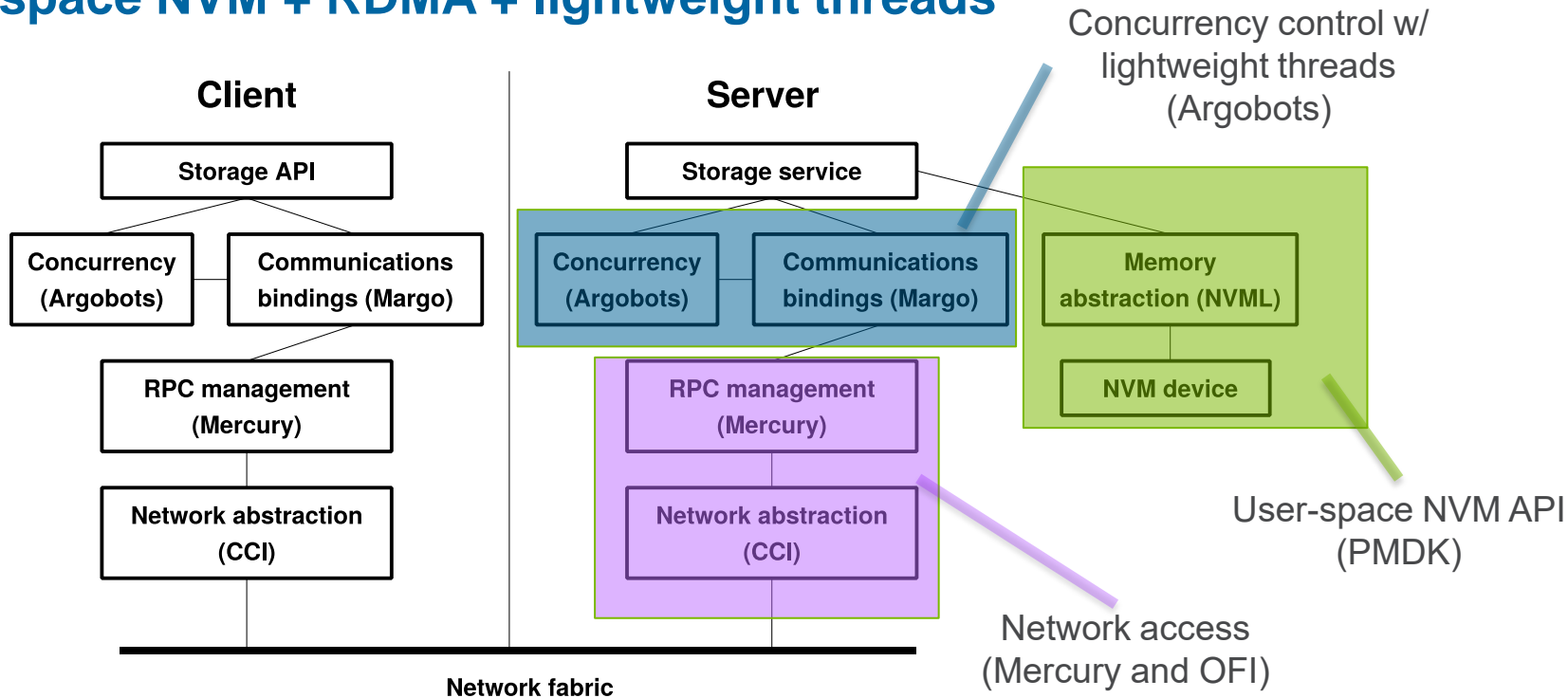
<https://www.mcs.anl.gov/research/projects/mochi>



# BUILDING SPECIALIZED DATA SERVICES WITH NVM

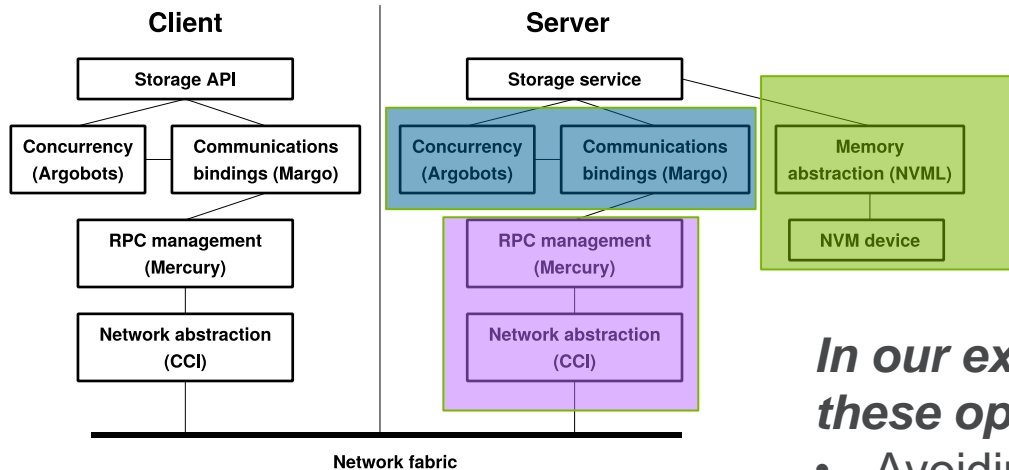
# ARCHITECTING AN NVM-BACKED DATA SERVICE

## User space NVM + RDMA + lightweight threads



# ARCHITECTING AN NVM-BACKED DATA SERVICE

## User space NVM + RDMA + lightweight threads



Modularity helps with extensibility, portability, and reuse, but is this too many layers/components?

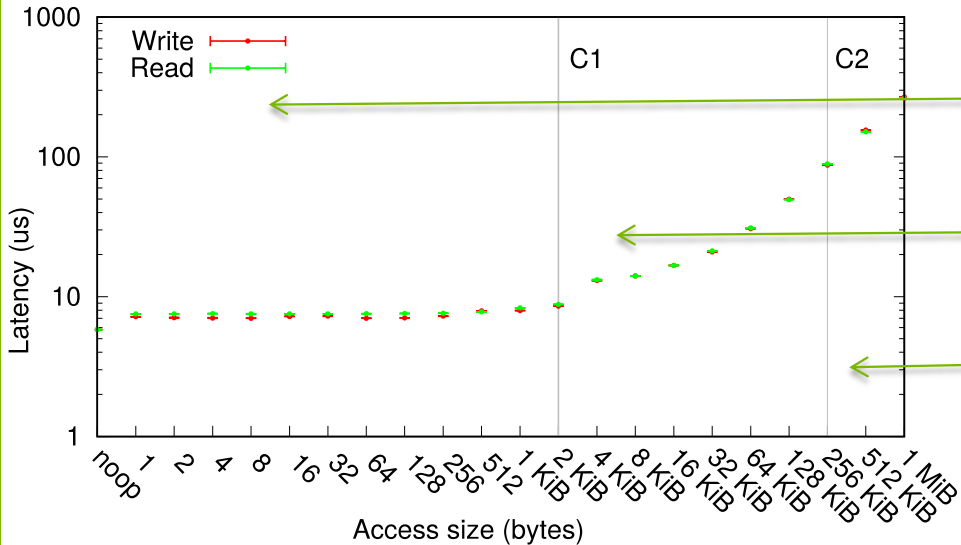
***In our experience, no. We prioritize these optimizations instead:***

- Avoiding privileged mode transitions
- Avoiding context switches in general
- Avoiding memory copies
- Reducing CPU load

# ACCESS LATENCY

How much latency do those software layers add?

- RAM in place of pmem
- No busy polling
- Each access is at least 1 network round trip, 1 libpmem access, and 1 new thread



Protocol modes:

- Eager mode, data is packed into RPC msg
- Data is copied to/from pre-registered RDMA buffers
- RDMA “in place” by registering memory on demand

Crossover points would be different depending on transport

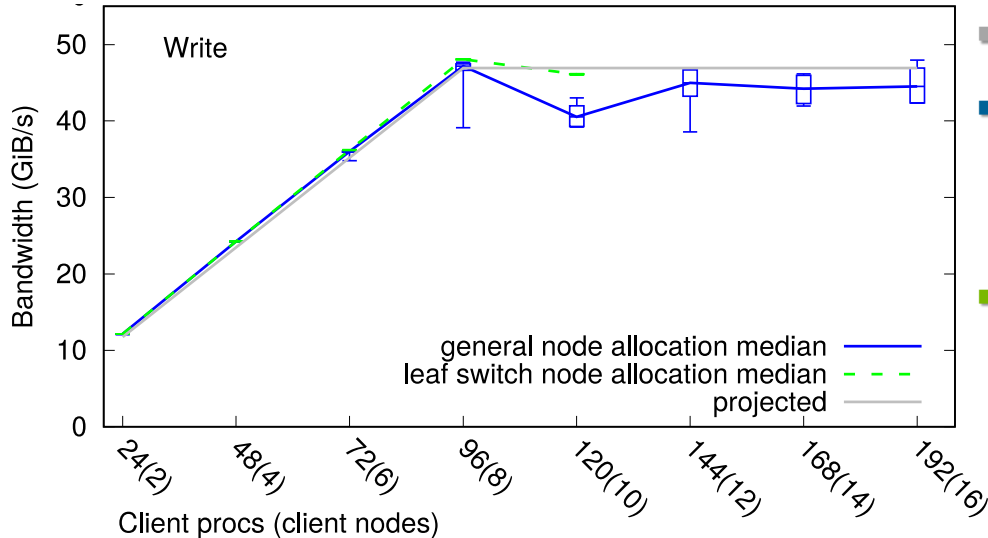
# ACCESS LATENCY

## Observations and questions

- Single digit microsecond access latencies: could it be tuned further?
  - Consider adaptive polling
  - Optimize memory allocation
  - OFI providers (and others) are improving rapidly
- What about the long tail?
  - Previous slide shows confidence interval for 10,000 samples at each point, and the intervals are quite narrow
  - But there are outliers: worst noop sample was  $> 70$  microseconds
  - This leads to the dreaded jitter problem in HPC
- The cost of memory copy vs. registration is a key factor in optimization



# AGGREGATE BANDWIDTH



- **Grey line** is projected maximum
- **Blue line** is a normal allocation
  - Whiskers (min and max) show significant variance
- **Green line** is an allocation with all nodes on one leaf switch
  - Whiskers (min and max) show very little variance

- Same system as in previous example
- 8 servers (1 per node)
- Up to 192 application processes (12 per node)

# AGGREGATE BANDWIDTH

## Observations and questions

- New problems arise when storage latency isn't the longest pole in the tent:
  - E.g., network topology (In this example, internal switch routing)
  - Consider dynamic routing and congestion-avoidance algorithms?
  - Better internal service instrumentation?
  - Make the storage system topology-aware?
- The service can saturate aggregate bandwidth relatively easily
- PMDK atomics help avoid serialization
  - Especially when creating and destroying objects
- How does this software architecture hold up at larger scales?

# COMMENTARY ON THE ROLE OF NVM APIS IN SCIENTIFIC COMPUTING

- We surely appreciate faster file systems and databases, but there are many other possibilities to consider
- NVM is easier to integrate into HPC if it gets along with our other technologies
  - RDMA networks, user-space provisioning, lightweight concurrency
- Bottlenecks aren't where they used to be
- Some degree of standardization is helpful
  - Minimize burden on developers for portability
- What is the role of PMoF?
  - Important technology, but not a full solution for concurrency and flow control
- Right now focus is on “get it to work, fast!”, but focus will shift over time: characterization, elasticity, multi-objective optimization, and more

**THANK YOU!**

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