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Sandia National Laboratories

Chapel and Grafiki Integration

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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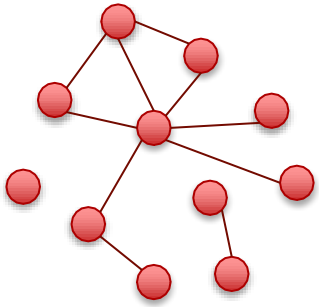
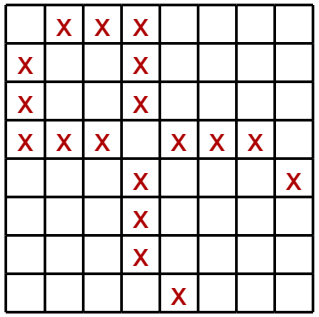
Chapel and Grafiki integration: using the right tool for every job



Chapel's PGAS enables analysts to easily manipulate parallel graph data (e.g., extract largest connected component via label propagation)



Grafiki's linear-algebra-based parallel graph algorithms enable efficient parallel graph analysis (e.g., vertex hitting times)

Composing tools is challenging

- Different parallel paradigms: PGAS in Chapel vs MPI in Grafiki
- Different data formats: Edge lists in Chapel vs matrix in Grafiki
- Huge graphs prohibit copying/reformatting data in memory

Three new approaches to integrate Chapel graph manipulation with Grafiki graph analysis ***without requiring additional copy of graph***

- ***Direct calls*** from Chapel to Grafiki using Chapel's C interface
- Separate Chapel & Grafiki processes access ***shared mmap memory***
- Chapel and ***Containerized*** Grafiki access shared mmap memory

Requirement to not copy data allows ability to solve larger problems

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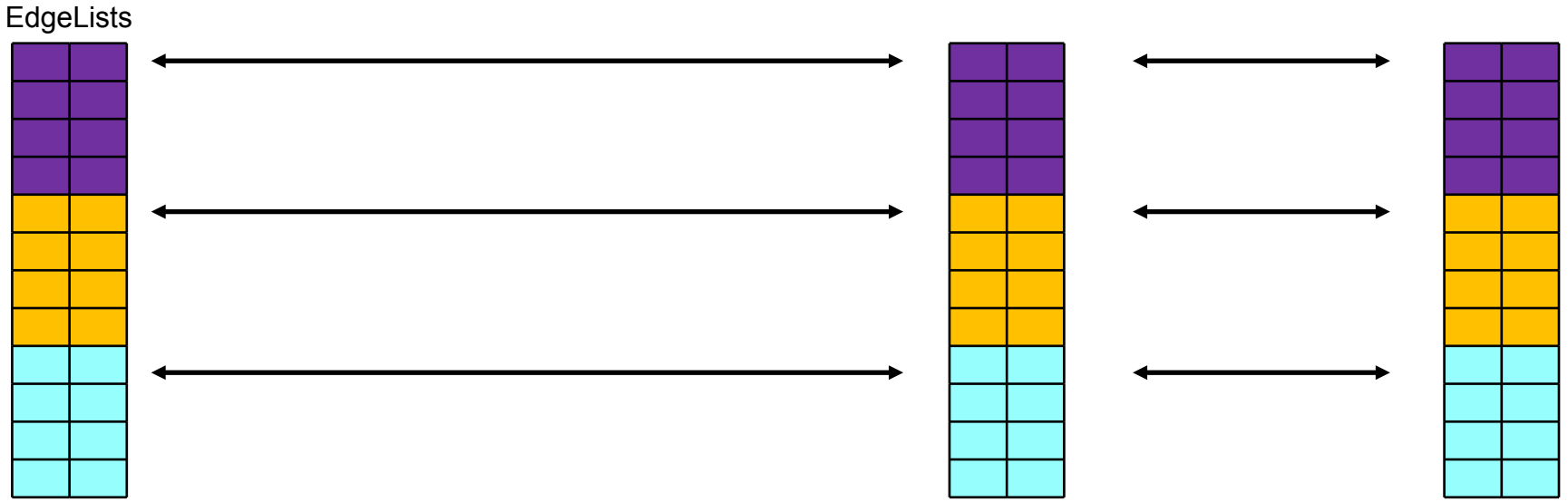
- **Share data with files is not scalable**
  - Chapel reads data, modifies it, and writes results to a new file
  - C++ program reads new file and performs some analysis with it
- **Sharing data with native data structures requires copies that use extra memory**
  - Chapel reads data, modifies it, and shares it with C++ program
  - C++ program rearranges data, which creates a copy, and performs some analysis with it

C++ program needs to have general abstractions to use data in any format

- **Grafiki relies on Trilinos for linear algebra classes and linear/eigen solvers**
- **Replaced Grafiki's use of concrete CrsMatrix class with abstract RowMatrix**
  - RowMatrix user provides implementation of key operations (SpMV, norms, etc.)
- **New Chapel-based RowMatrix uses edge lists directly from Chapel to perform matrix operations – *no data copy***

Approach 1: Chapel program calls Grafiki through Chapel's C interface



Chapel creates EdgeList in BlockDomain arrays

Each **Chapel** locale directly calls C function (in *coforall*) with pointer to its local data

C function instantiates RowMatrix from EdgeList pointers

C function calls Grafiki

Grafiki computes using RowMatrix

Pro: Simple proof-of-concept for data sharing

Con: Intrusive to user: needs to link with Trilinos and Grafiki

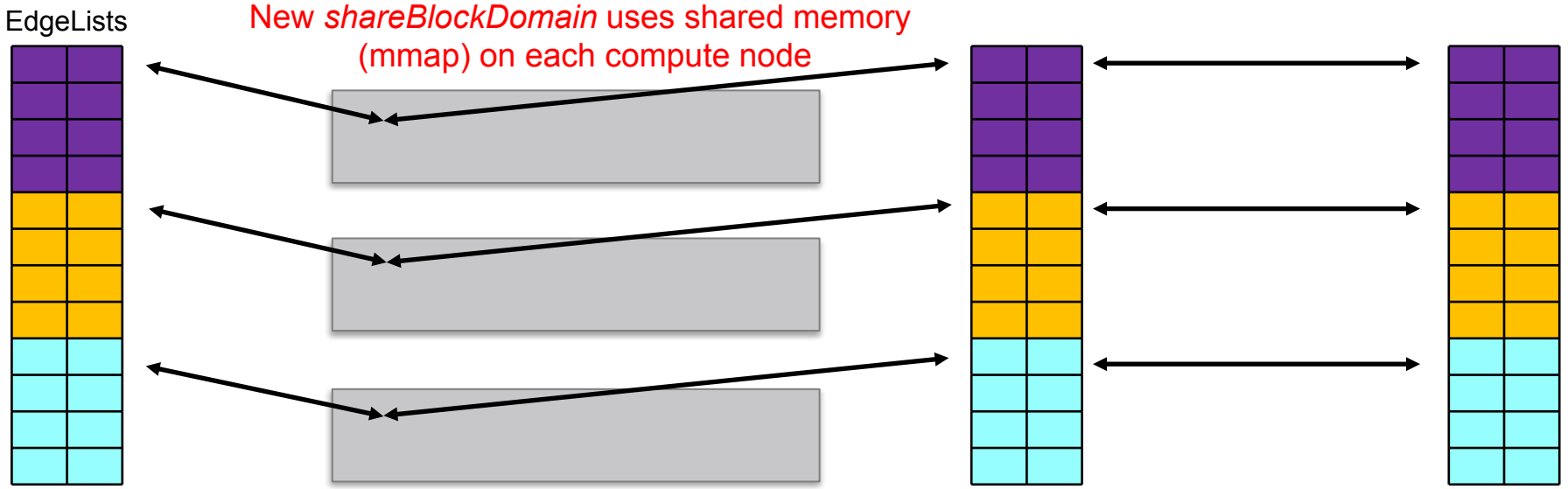
Approach 1 details: Coordinating Chapel locales and MPI ranks

- **Numbers of Chapel locales and MPI ranks are equal**
- **Calls from Chapel to Grafiki must be made from each locale in parallel**
  - All locales must enter Grafiki together to avoid hanging in Grafiki's MPI collective communication
  - Chapel coforall launches one task per locale
- **Locales provide pointers to local edge list arrays**

```
coforall loc in Locales {
    on loc {
        var subdom = edgelist.localSubdomain();
        call_C_function(c_ptrTo(edgelist[subdom.low]), ...);
    }
}
```

Image is Unclassified

Approach 2: Separate Chapel and Grafiki processes share data in mapped memory



Chapel creates EdgeList in *new shareBlockDomain* arrays that *use mmap memory*

Chapel program signals (via POSIX semaphore) external C process to begin

C process instantiates RowMatrix from EdgeList pointers in *mmap'ed memory*

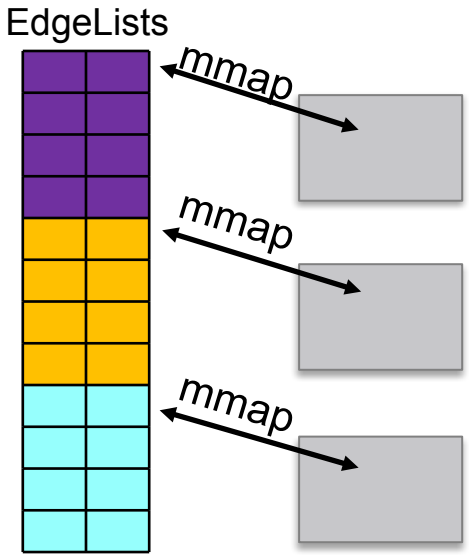
C process calls Grafiki, signals Chapel when done

Grafiki computes using RowMatrix

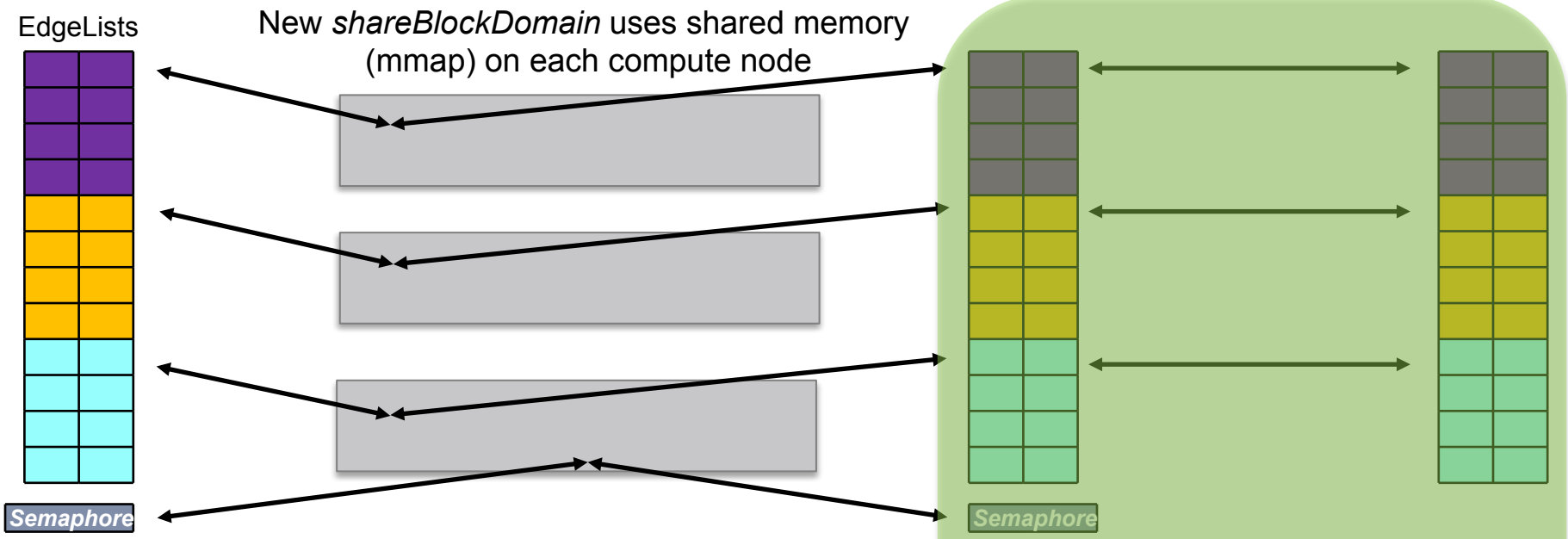
Less intrusive: user uses Chapel as usual, only substituting *shareBlockDomain* for *BlockDomain* for shared data

Approach 2 details: new *shareBlockDomain*

- **Chapel Domains**
  - describe distribution of data across locales (processors)
  - manage global address space indexing
- **Chapel's Block Domain assigns contiguous chunks of global arrays to locales**
  - Each locale's local array is a separate allocation
- **New *shareBlock Domain* replaces the local array allocation with mmap regions in shared memory**
  - Separate mmap backing file for each shared array
  - Backing file names are shared between processes through tiny meta-data file
  - Chapel users simply substitute *shareBlock* for *Block* in their code



Approach 3: Chapel and Containerized Grafiki further simplify user experience



Chapel creates EdgeList in *new shareBlockDomain* arrays that use mmap memory

Chapel program signals external C process to begin *via pseudo-semaphore (mmap int)*

Container image provides pre-built C process and Grafiki libraries that run as in Approach 2.

Least intrusive: Container handles details of building and running C process and Grafiki

Demonstrations done with Chapel on MPI and SMP systems

- **MPI-enabled Chapel on Cray / Haswell (mutrino)**
  - Single locale / rank per node, multiple nodes
- **Shared-memory Chapel on Xeon (kahuna)**
  - Single node, multiple locales / ranks per node
  - Uses containerized Grafiki with Singularity
- **Compare**
  - approach One – Chapel's C interoperability
  - approach Two – separate processes
  - Look at Chapel label propagation and Grafiki hitting times

Using mmap memory shows no performance penalty against a Chapel's usual memory

Platform	Number of Locales	Chapel LabelPropagation Time per iteration (seconds) One	Chapel LabelPropagation Time per iteration (seconds) Two	Grafiki Hitting Times Time per iteration (seconds) One	Grafiki Hitting Times Time per iteration (seconds) Two
Kahuna	1	1.24	1.22	0.0285	0.0287
	2	NA	1.91	NA	0.0162
	4	NA	1.56	NA	0.0087
	8	NA	1.00	NA	0.0045
	16	NA	0.65	NA	0.0051
Mutrino	1	0.82	0.89	0.0215	0.0230
	2	0.65	0.77	0.0113	0.0120
	4	0.44	0.47	0.0058	0.0062
	8	0.22	0.29	0.0031	0.0033
	16	0.11	0.15	0.0018	0.0018

Bcsstk29.mtx
600k nonzeros
14k rows & columns

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Kahuna used chapel SMP 1.23, and we were unable to run approach 1 on more than one locale

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mmap memory performs equal to Chapel's usual memory when comparing approach One and Two

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	16	NA	3749	NA	188
Mutrino	4	OOM	10333	OOM	371
	16	1274	3079	103	105
	64	320	824	30	26

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Using mmap memory shows no performance penalty against a Chapel's usual memory

There is a noticeable loss of performance in the Chapel label propagation using mmap memory. We hypothesize that this is due to using Chapel 1.23's Block Domain as a template for share block.

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We still observe no performance penalty when using the mmap memory in the C++ program

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Future Work

- **Extend operability to different Chapel distributions**
  - Option for chapel to accept a user defined allocator
- **Analyze container performance**
- **Analyze Chapel and C++ integrated code against pure Chapel implementation**

Approach 3 details: Containerized Grafiki

Container software stack significantly different than Chapel requirements

Created container to include our software stack

- Alpine 3.12, GCC 9.3, MPICH 3.2, OpenBLAS, Trilinos (develop branch), and Grafiki
- Custom Grafiki-connector code

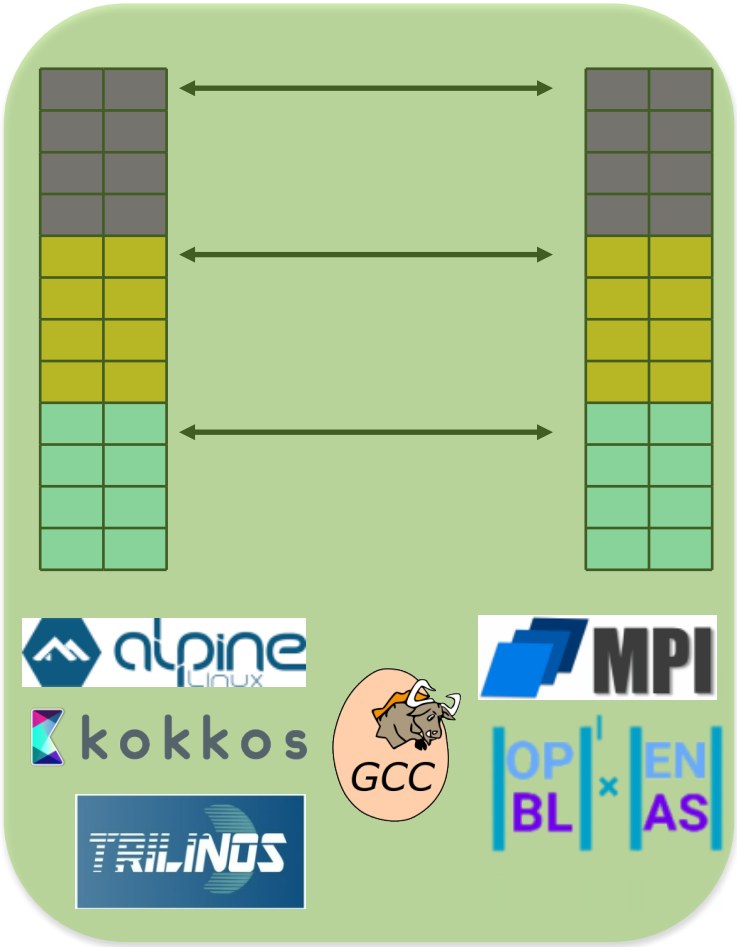
Built and tested as OCI (Docker) container

Converted to Singularity SIF on HPC clusters

Challenge: While `mmap` memory works across containers, POSIX Semaphores do not!

- Semaphores created on parent process stack, unusable in container after namespace creation
- Solution: Implement "pseudo-semaphore" signaling mechanism using a `mmap int`
- Tested and validated with MPI (Kahuna)

More refinement of container image to continue



Containers allow researchers to blend tailored software capabilities with user software requirements