cuNumeric.jl : Automating Distributed Numerical Computing

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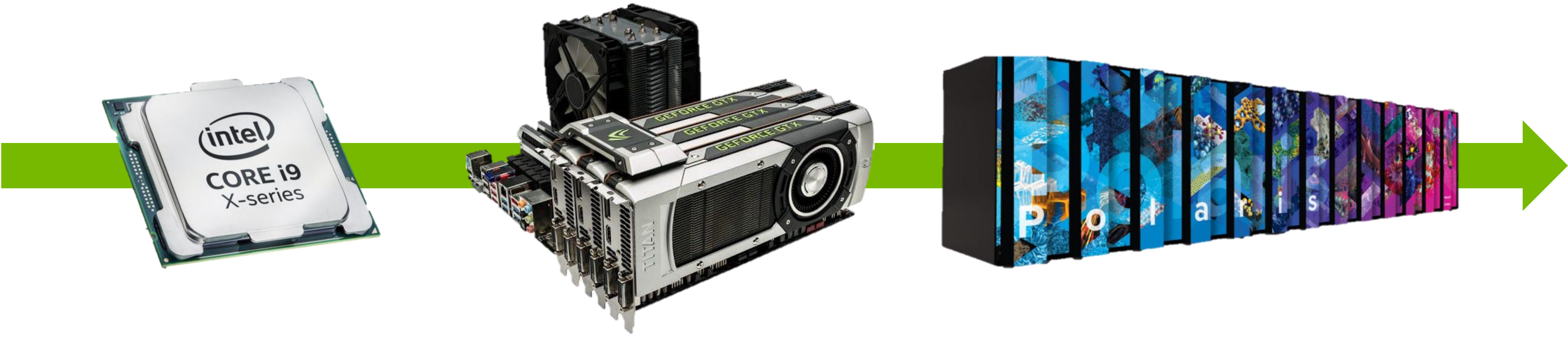
The Goal: Scale with Zero Code Changes

- "Easy" to implement the correct physics in a high-level language like Python, Julia, or MATLAB
- Time consuming to modify code to scale across multiple CPUs/GPUs
  - Need to learn and debug new technologies like OpenMPI, CUDA etc.



Code that runs on a single CPU core should also be able to run on multiple cores, multiple GPUs and across multiple nodes

cuNumeric.jl: Distributed Code with Minimal Effort

- Core Type: **NDArray**
  - Drop-in replacement for Base.Array but can represent data across multiple devices
  - Key Differences: Operations are broadcast by default, slices are always views, avoid scalar indexing

```
(3.8.0) (base) david@dubliner:~/julia-con/slides-examples/diff$ cat diff_grayscott.txt
1,2d0
< using cuNumeric
<
81,84c79,82
<     u = cuNumeric.ones(dims)
<     v = cuNumeric.zeros(dims)
<     u_new = cuNumeric.zeros(dims)
<     v_new = cuNumeric.zeros(dims)
---
>     u = ones(dims)
>     v = zeros(dims)
>     u_new = zeros(dims)
>     v_new = zeros(dims)
86,87c84,85
<     u[1:150, 1:150] = cuNumeric.random(FT, (150, 150))
<     v[1:150, 1:150] = cuNumeric.random(FT, (150, 150))
---
>     u[1:150, 1:150] = random(FT, (150, 150))
>     v[1:150, 1:150] = random(FT, (150, 150))
(3.8.0) (base) david@dubliner:~/julia-con/slides-examples/diff$
```

7 LOC changed for 2D Gray Scott Reaction-Diffusion simulation

Legate Enables Composable and Distributed Libraries

By providing data and task management abstractions, this enables the efficient implementation of complex library APIs.

NumPy | SciPy | pandas | scikit learn | dmlc XGBoost | HDF | . . .

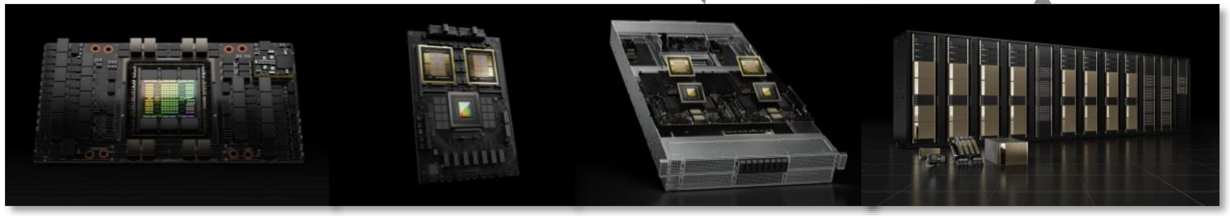
cuPyNumeric	Legate Sparse	Legate Dataframe	Legate RAFT	Legate Boost	Legate IO

Legate Framework

Legate Core - Productivity & Composability Layer

Legion - Implicit Parallelism Layer

Realm - Runtime for Scalable and Portable Execution



Single GPU | Mixed CPU/GPU | Single-Node Multi-GPU | Multi-Node Multi-GPU Cloud & Supercomputer

Wouldn't this be great in Julia?

https://developer.nvidia.com/legate
https://legion.stanford.edu/

How Legate Works

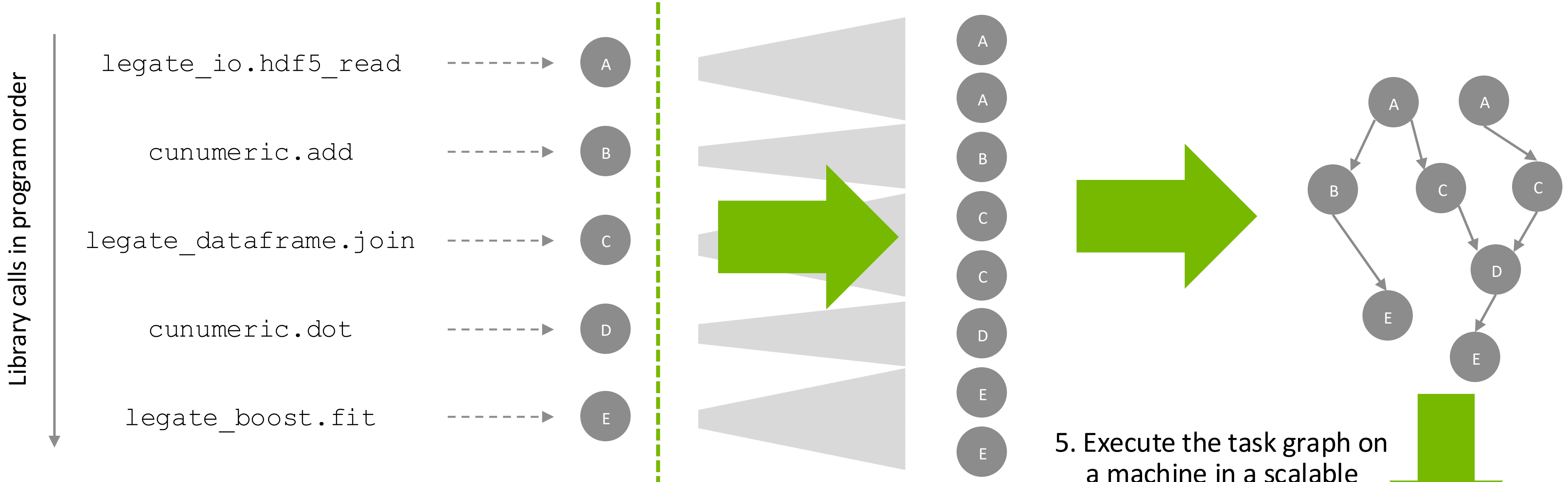
Implicit parallelism via “scale-free” tasking

1. Legate program makes API calls

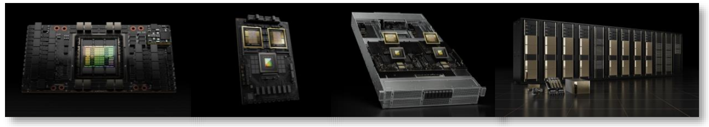
2. Legate libraries issue **“scale-free” tasks**

3. Convert each scale-free task to parallel tasks

4. Analyze data dependencies and constructs a task graph



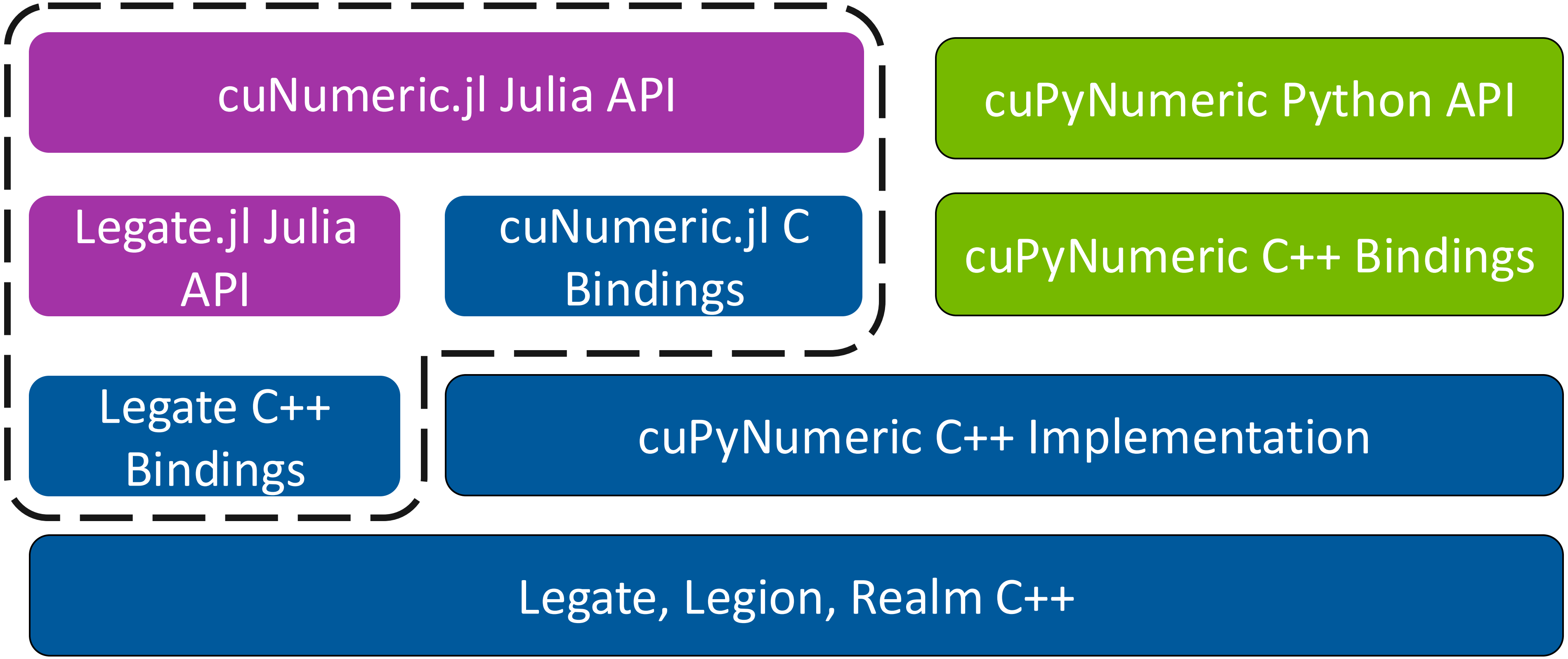
5. Execute the task graph on a machine in a scalable manner



Legate Framework

Legate libraries are **free of any explicit parallelization or synchronization/data movement**, making them **composable and transparently scalable** by construction

Software Stack



Generates parallel tasks

Determines data dependencies and orders task execution

Executes tasks on target hardware

New Contributions

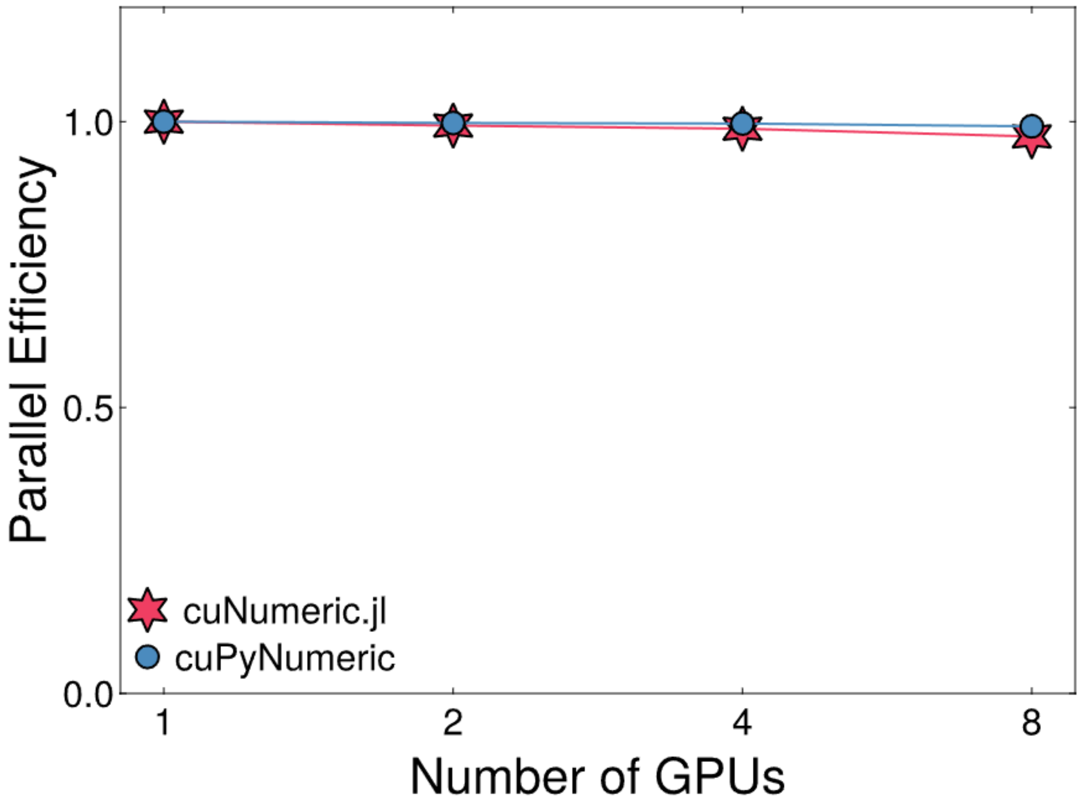
Monte Carlo Integration

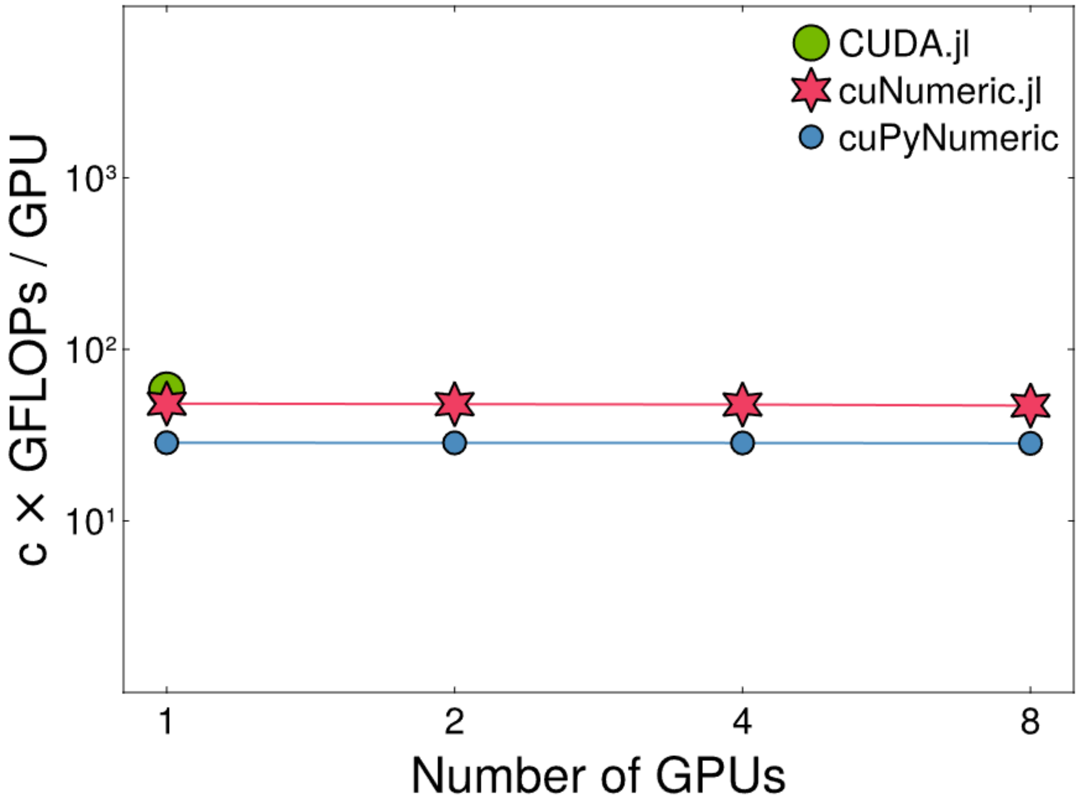
- Embarrassingly Parallel → Should scale perfectly
- cuNumeric.jl directly calls C++, cuPyNumeric passes through several layers of Python before C++

Syntax:

```
integrand = (x) -> exp(-square(x))
N = 1_000_000
x_max = 5.0
domain = [-x_max, x_max]
Ω = domain[2] - domain[1]
samples = Ω*cuNumeric.rand(NDArray, N) - x_max
estimate = (Ω/N) * sum(integrand(samples))
```

Benchmark (8x A100):





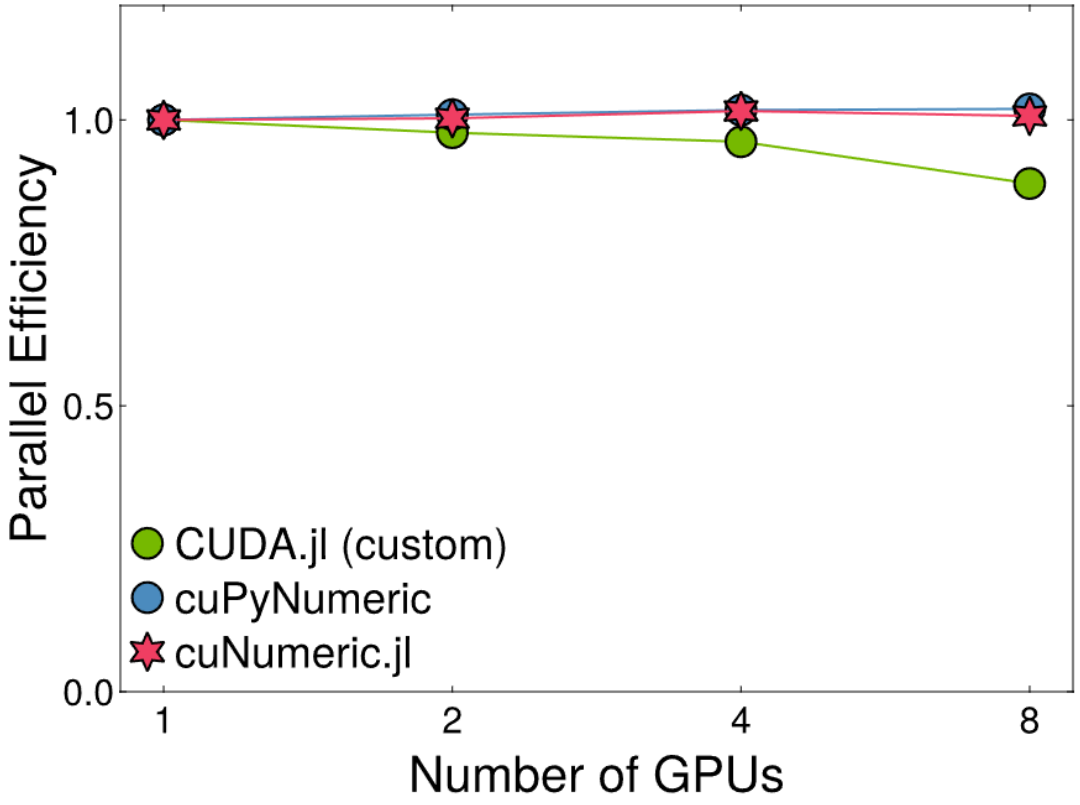
*Actual FLOPs unknown, off by constant factor (c < 1.0)

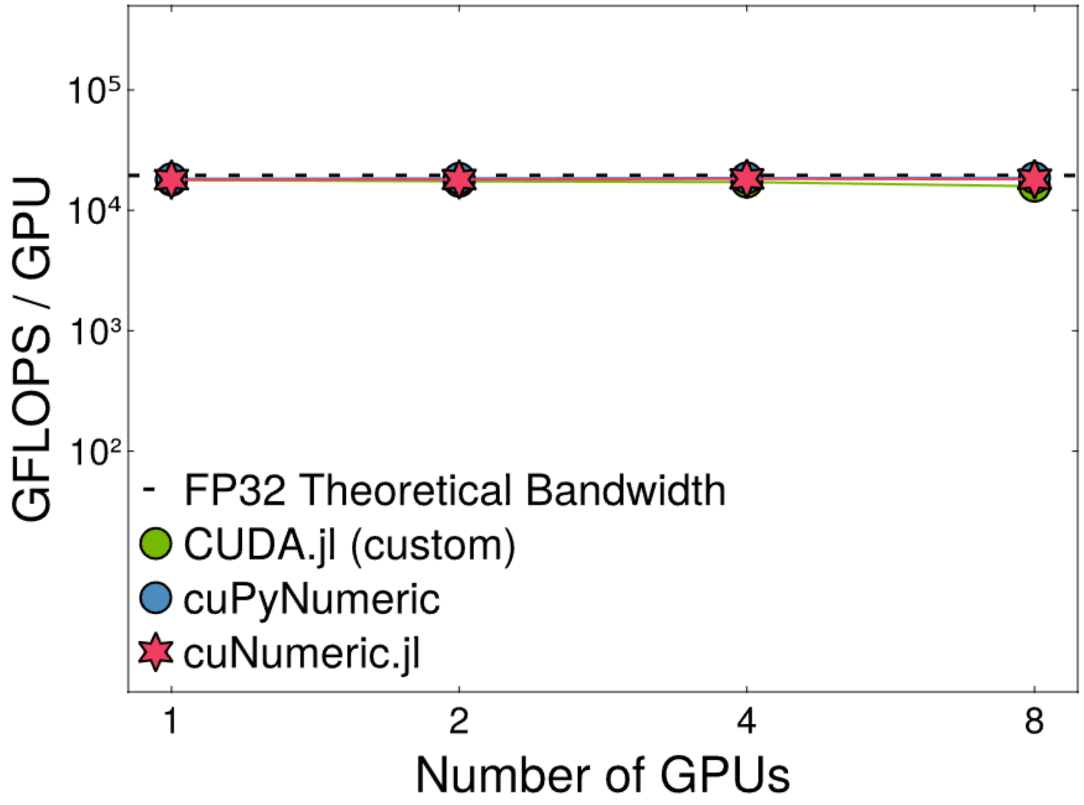
Matrix Multiplication

Syntax*:

```
N = 10
A = cuNumeric.rand(Float32, N, N)
B = cuNumeric.rand(Float32, N, N)
C = cuNumeric.zeros(Float32, N, N)
mul!(C, A, B)
```

Benchmark (8x A100):





*Float32 random number generation not supported yet, requires type cast

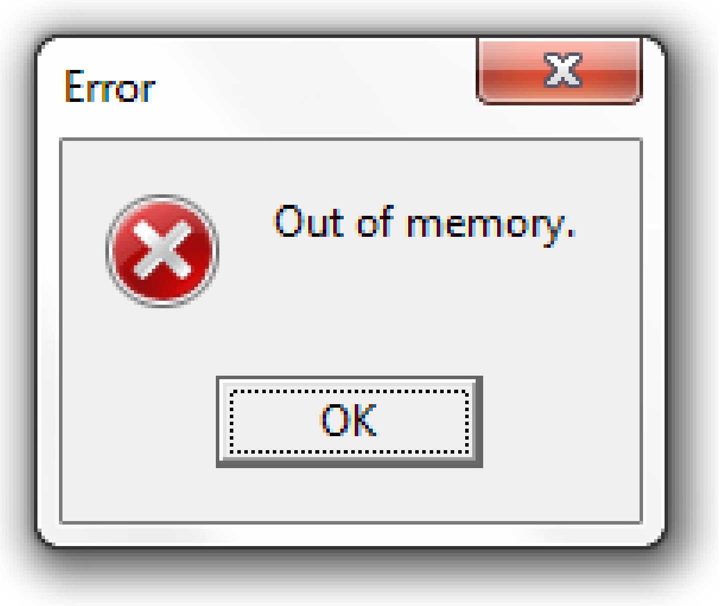
Gray Scott Reaction Diffusion (2D)

Syntax:

```julia
N = 100
u = cuNumeric.ones((N, N))
v = cuNumeric.ones((N, N))
for i in iters
    F_u = ((u[2:(end - 1), 2:(end - 1)] .* (v[2:(end - 1), 2:(end - 1)]
        .* v[2:(end - 1), 2:(end - 1)])) - (f+k)*v[2:(end - 1), 2:(end - 1)])
    #.... more physics
    #.... update u and v
    GC.gc()
end
```

Manual GC allows Gray Scott to run

Benchmark (8x A100):



Each object, including slices, are treated as a temporary and remain uncollected.
Why are they not collected before OOM?

Foreign Memory is not automatically garbage collected

- GC sees foreign memory as a pointer → 8 bytes
- GC relies on the heap size (of Julia objects) to decide when GC is invoked

```julia
using CUDA, Profile

arr = CUDA.ones(Float32, 10_000_000)
Profile.take_heap_snapshot()
Base.summarysize(arr)
```

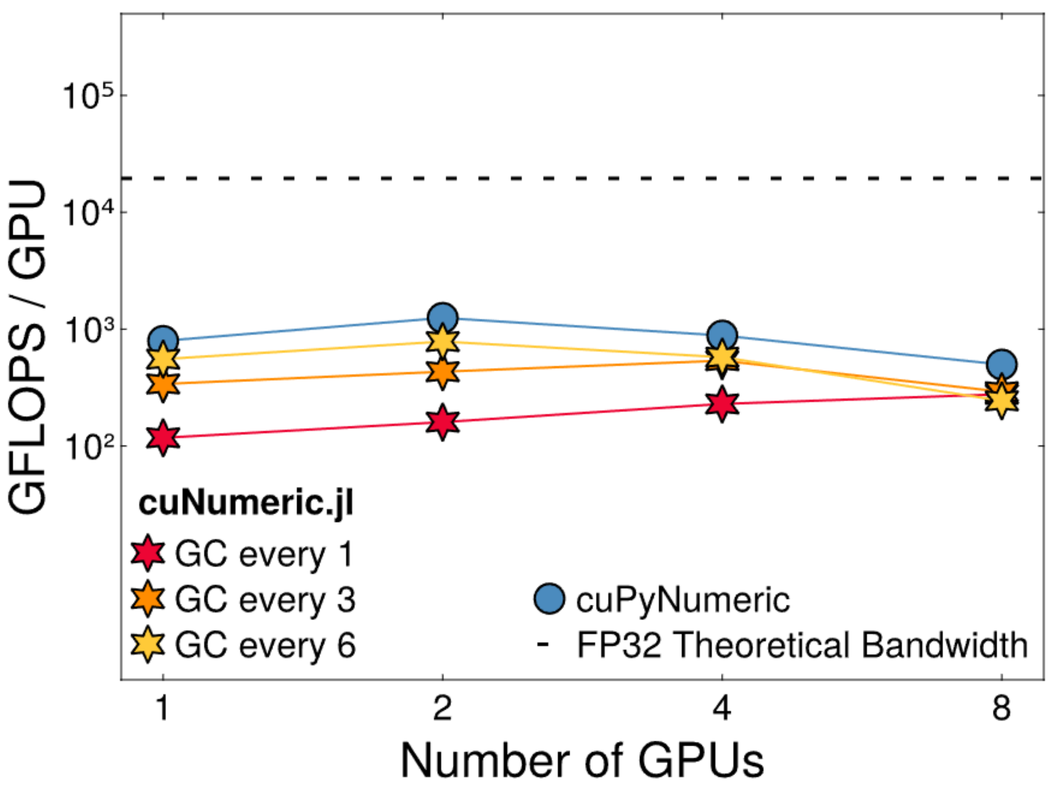
~40MB

Julia sees GPU data as 184 bytes

Constructor	Retained Size
▼ CUDA.CuArray{Float32, 1, CUDA.Devi	0.2 kB
▼ data :: GPUArrays.DataRef{CUDA.M	0.1 kB
▼ rc :: GPUArrays.RefCounted{CUD	0.1 kB
▼ obj :: CUDA.Managed{CUDA.Dev	0.1 kB
stream :: CUDA.CuStream @4	0.0 kB
count :: Base.Threads.Atomic	0.0 kB
finalizer :: typeof(CUDA.poo	0.0 kB

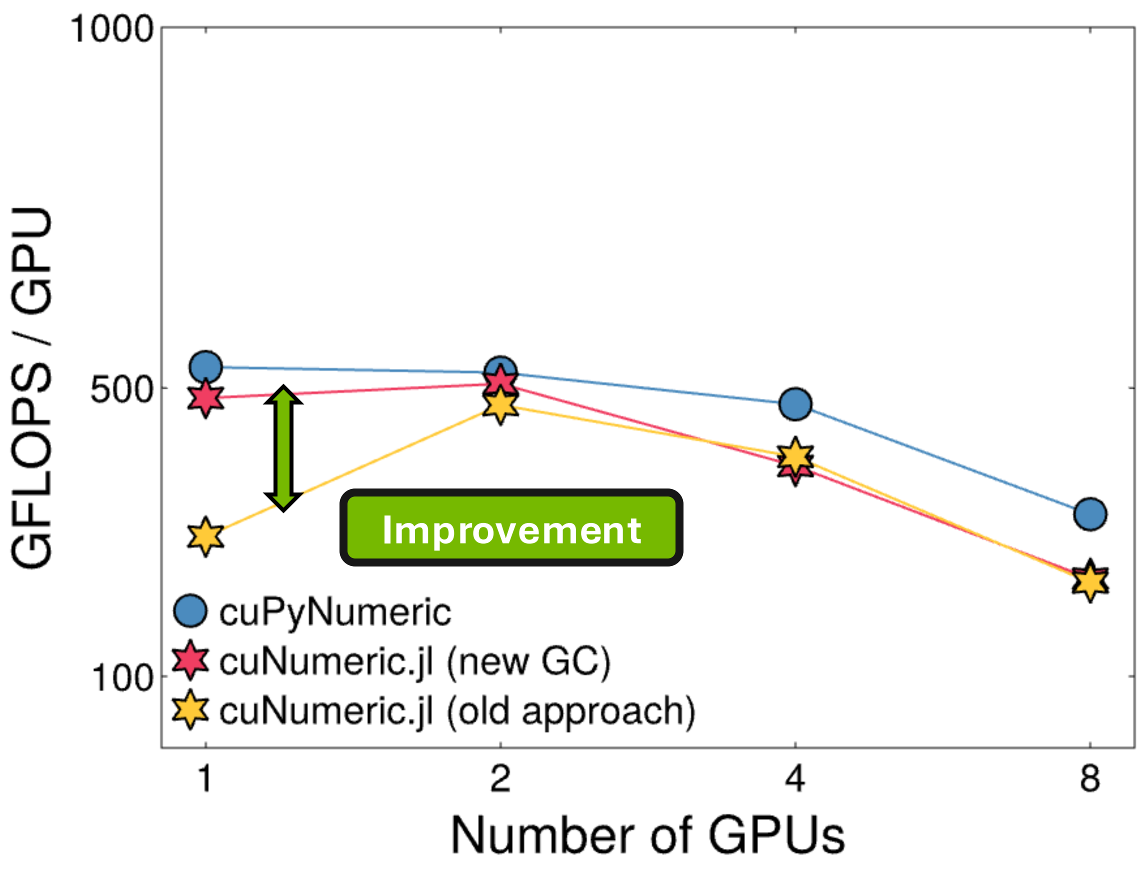
184 bytes in heap snapshot too

Garbage Collection heavily impacts performance



- All existing GPU backends in Julia:
  - Calculate array memory footprint in the constructor
  - Track GPU memory allocations
  - Manually calls GC based on a memory pressure heuristic
  - try-catch on allocation to avoid OOM
- NDArray Properties:
  - Deferred execution model conceals Julia object's physical size at creation
  - Runtime cannot recover from failed mapping allocation

Custom heuristic GC improves performance




```
N = 100
u = cuNumeric.ones((N, N))
v = cuNumeric.ones((N, N))
for i in iters
    F_u = ((u[2:(end - 1), 2:(end - 1)] .* (v[2:(end - 1), 2:(end - 1)]
        .* v[2:(end - 1), 2:(end - 1)])) - (f+k)*v[2:(end - 1), 2:(end - 1)])
    #.... more physics
    #.... update u and v
end
```

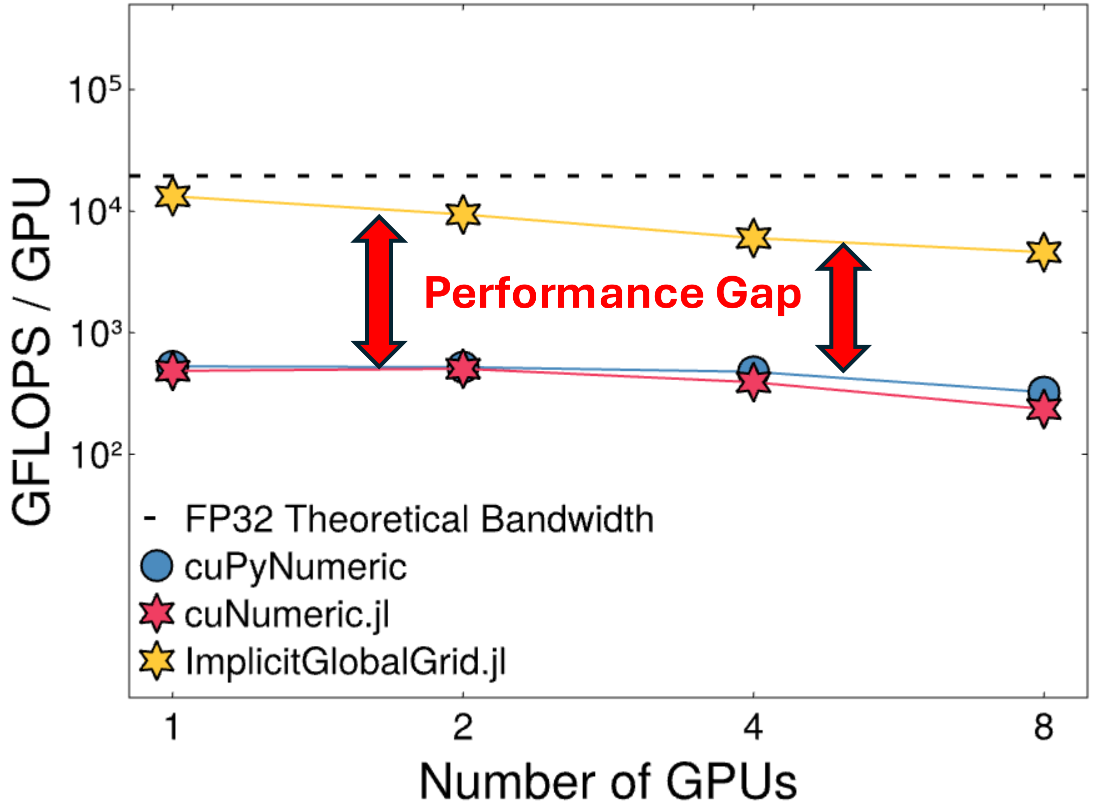
Automatic GC allows Gray Scott to run

- We are still exploring solutions to achieve better scalability

Unfused Operations Bottleneck Performance

ImplicitGlobalGrid.jl:

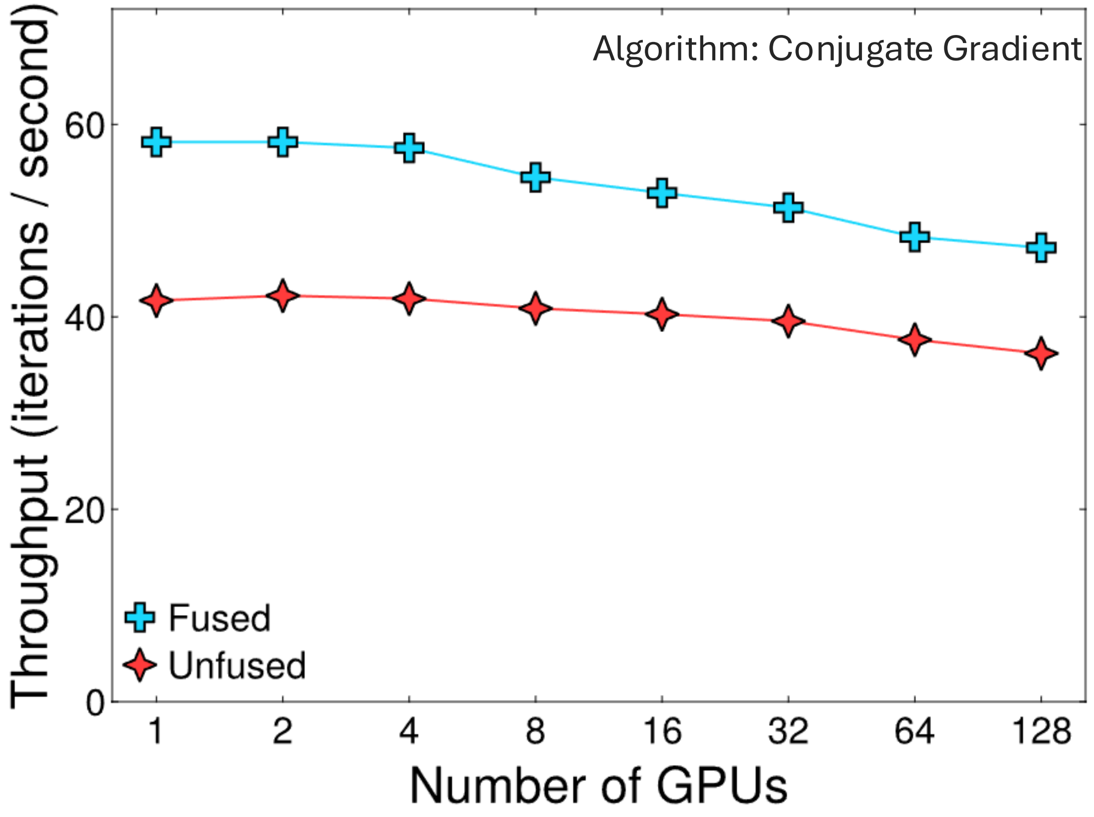
- Stencil-based PDE solver
- Multi-node CPU and GPU (NVIDIA & AMD)
- Minimal code changes



Räss, L., Omlin, S., & Podladchikov, Y. Y. *JuliaCon* 2019.

Kernel Fusion:

- Under development in cuPyNumeric, but shown to provide 2x speed-up on average and up to 10x
- With CUDA.jl and Legate.jl we propose to generate fused, distributed kernels



Rohan Yadav, https://doi.org/10.1145/3669940.3707216, *ASPLOS* 2025

Multi-GPU CUDA Kernels with cuNumeric.jl

- To enable kernel fusion, we need to be able to run CUDA.jl kernels through Legate.jl

```julia
using cuNumeric
using CUDA

function kernel_add(a, b, c, N)
    i = (blockIdx().x - 1i32) * blockDim().x + threadIdx().x
    if i <= N
        @inbounds c[i] = a[i] + b[i]
    end
    return nothing
end


N = 1024
threads = 256
blocks = cld(N, threads)

a = cuNumeric.full(N, 1.0f0)
b = cuNumeric.full(N, 2.0f0)
c = cuNumeric.ones(Float32, N)

task = cuNumeric.@cuda_task kernel_add(a, b, c, UInt32(1))

cuNumeric.@launch task=task threads=threads blocks=blocks \
                  inputs=(a, b) outputs=c scalars=UInt32(N)
```

CUDA.jl kernel

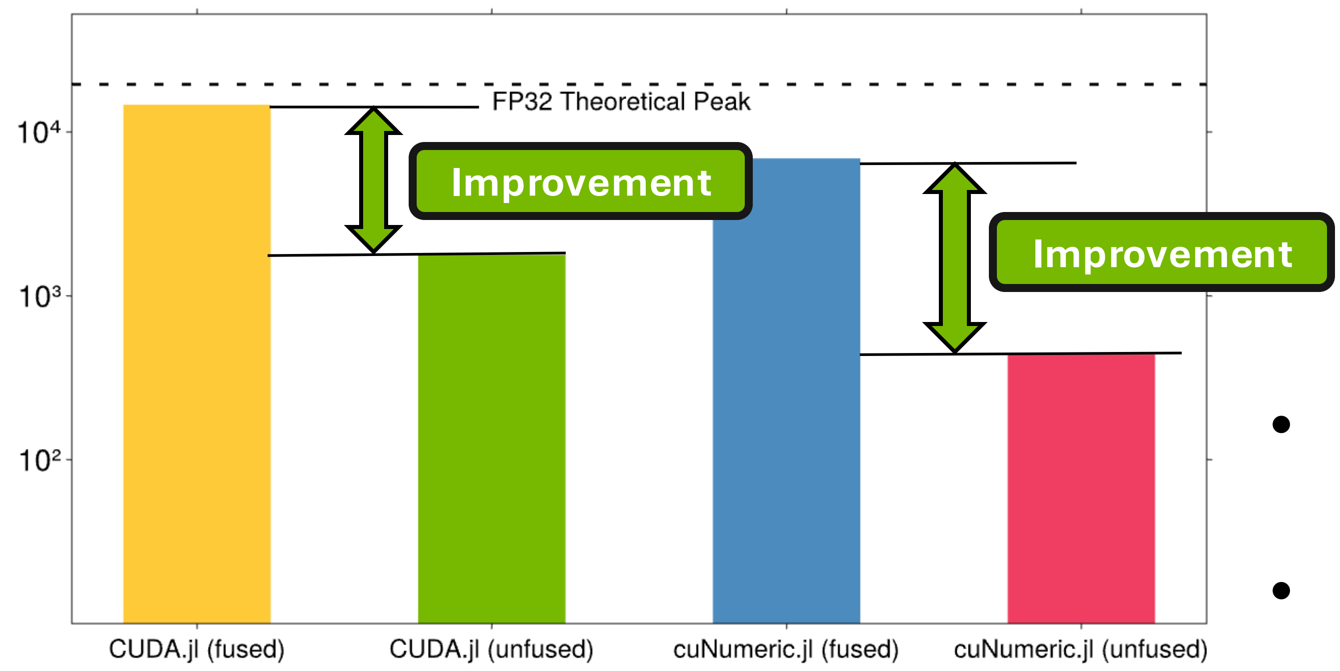
Initialize NDArrays

Compile

Launch

Gray Scott mini 1D with custom CUDA.jl kernels

Benchmark (1x A30x):



Syntax:

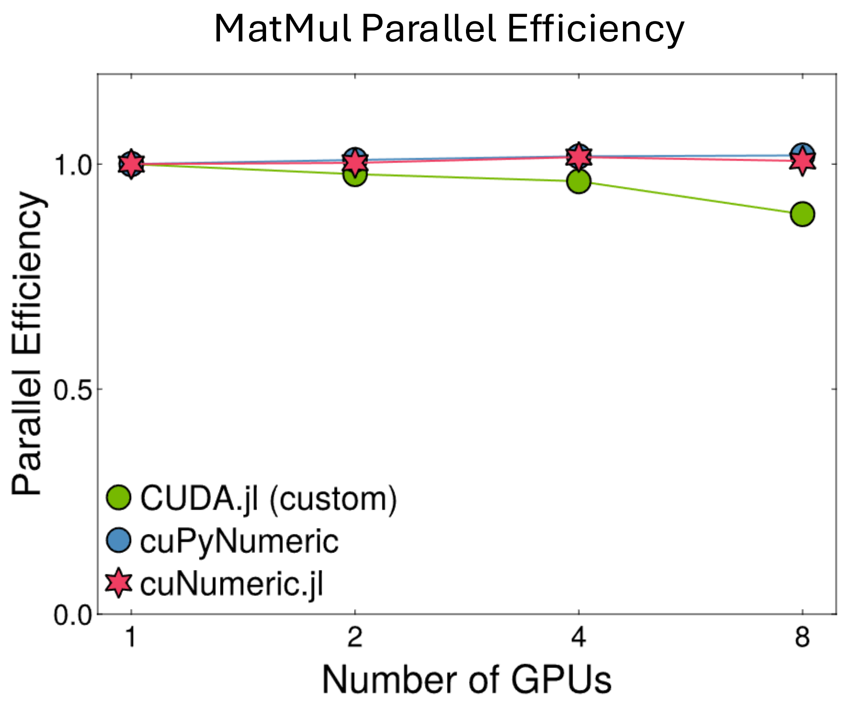
```
function fused_kernel(u, v, F_u, F_v, N::UInt32, f::Float32, k::Float32)
    i = (blockIdx().x - 1i32) * blockDim().x + threadIdx().x
    if i <= (N*N-2)
        @inbounds begin
            u_ij = u[i + 1]
            v_ij = v[i + 1]
            v_sq = v_ij * v_ij
            F_u[i] = (-u_ij * v_sq) + f*(1.0f0 - u_ij)
            F_v[i] = (u_ij * v_sq) - (f + k)*v_ij
        end
    end

    return nothing
end
```

- Operator invocation overhead limits performance scalability
- Ongoing backend enhancements for multi-dimensional workloads and multi-GPU execution
- Backend overhead is amortized as GPU count increases

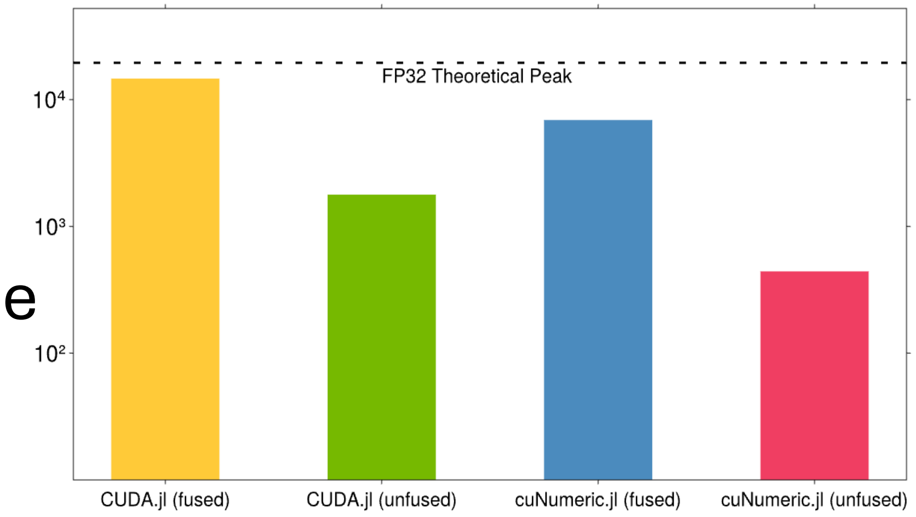
Conclusions and Future Work

- Minimal code changes for scaling across large heterogeneous distributed systems
- Good weak scaling efficiency on diverse applications
- Ability to register custom CUDA kernels



Next Steps

1. Support a wider range of custom CUDA kernels
2. Improve robustness and accessibility of package installation
3. Enhance integration with Julia Abstraction interface + Legate
4. Benchmark on multi-node systems
5. Better GC heuristics



Aiming for September* beta release

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Pat McCormick pat@lanl.gov

*this is an estimate; we will register the package upon beta launch

Check out our repo
https://github.com/JuliaLegate/cuNumeric.jl/

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