Exploring Julia as a unifying end-to-end workflow language for HPC on Frontier

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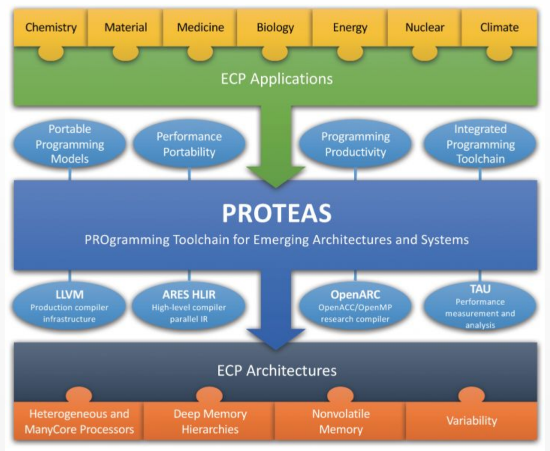


Abstract

- Objective: Explore the performance and scaling of Julia as an alternative language for high-performance computing (HPC) workflow component development on Frontier.
- Approach: We evaluated a 7-point stencil reaction-diffusion solver, GrayScott.jl using Julia's HPC stack: MPI.jl, AMDGPU.jl, and ADIOS2.jl.

Background

- Two-language problem: Scientists prototype solvers for various problems in high-productivity languages (e.g., Python), but need a solver in a traditional HPC language (e.g., C++, Fortran) for larger computations and speed.
- Julia: Meant to solve the two language problem by combining features of high-productivity languages with HPC capabilities.
  - High-productivity: Scientific/mathematical syntax, packaging environment, mathematical libraries, interactive, flexible
  - High-performance: MPI.jl, GPU programming model packages

Simulation

- Reaction-diffusion Gray-Scott 2-variable model:
  - *U, V* output concentrations of reacting and diffusing chemicals.

System of Equations	Discretization of Laplacian Term
$\frac{\partial U}{\partial t} = D_U \nabla^2 U - UV^2 + F(1-U) + nr$ $\frac{\partial V}{\partial t} = D_V \nabla^2 V + UV^2 + -(F+k)V$	$\nabla^2 U^t_{i,j,k} = -U^t_{i,j,k} + \frac{1}{6}\left[U^t_{i-1,j,k} + U^t_{i+1,j,k} + U^t_{i,j-1,k} + U^t_{i,j+1,k} + U^t_{i,j,k-1} + U^t_{i,j,k+1}\right]$

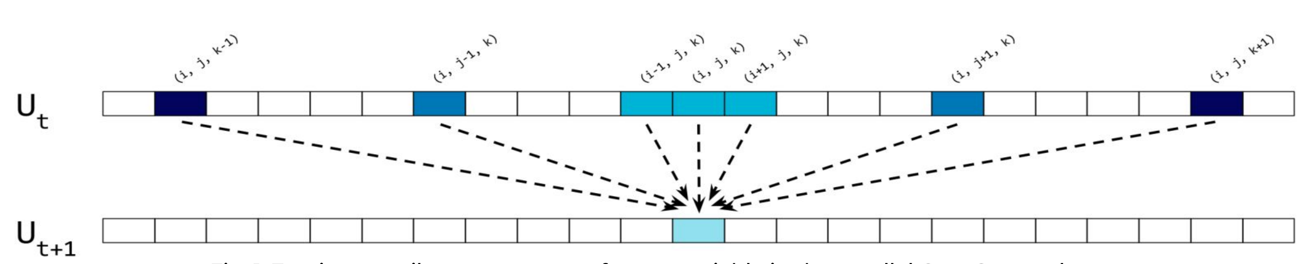


Fig. 1: 7-point stencil memory access for one variable in the parallel Gray-Scott solver.

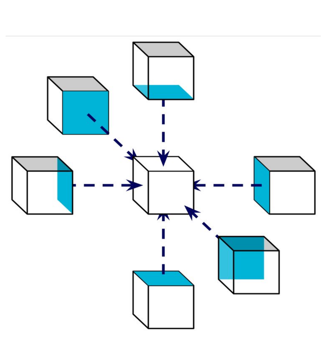


Fig. 2: MPI_Send/Recv memory patterns in Cartesian communicator decomposition used in simulation.

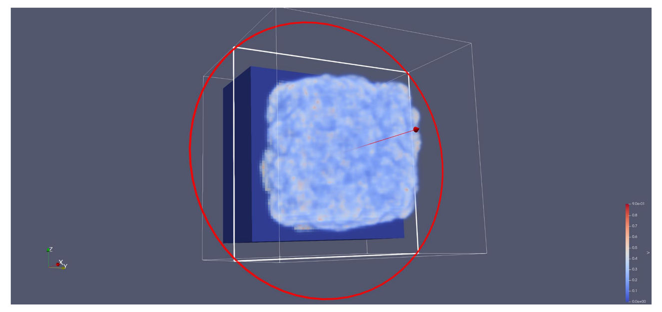
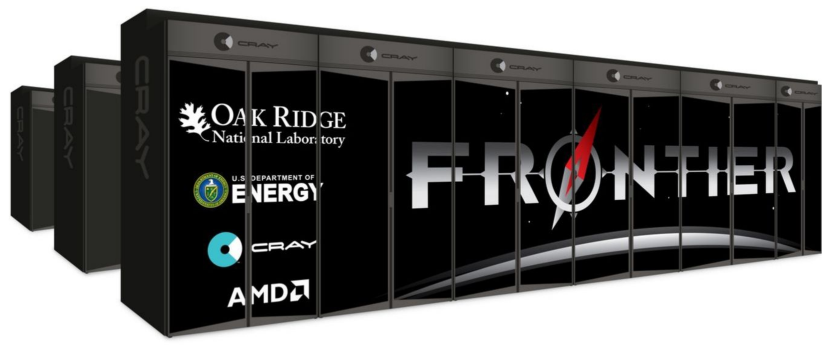


Fig. 3: *V* diffusing at t=109.

Frontier Exascale System

Frontier Characteristics	
Nodes	9,408
—GPU Architecture—	
GPU	4×AMD MI250X 8×GCDs
Memory Bandwidth	HBM2E 64 GB 1,600 GB/s per GCD



Implementation

- Running GrayScott.jl simulation in Julia on Frontier:

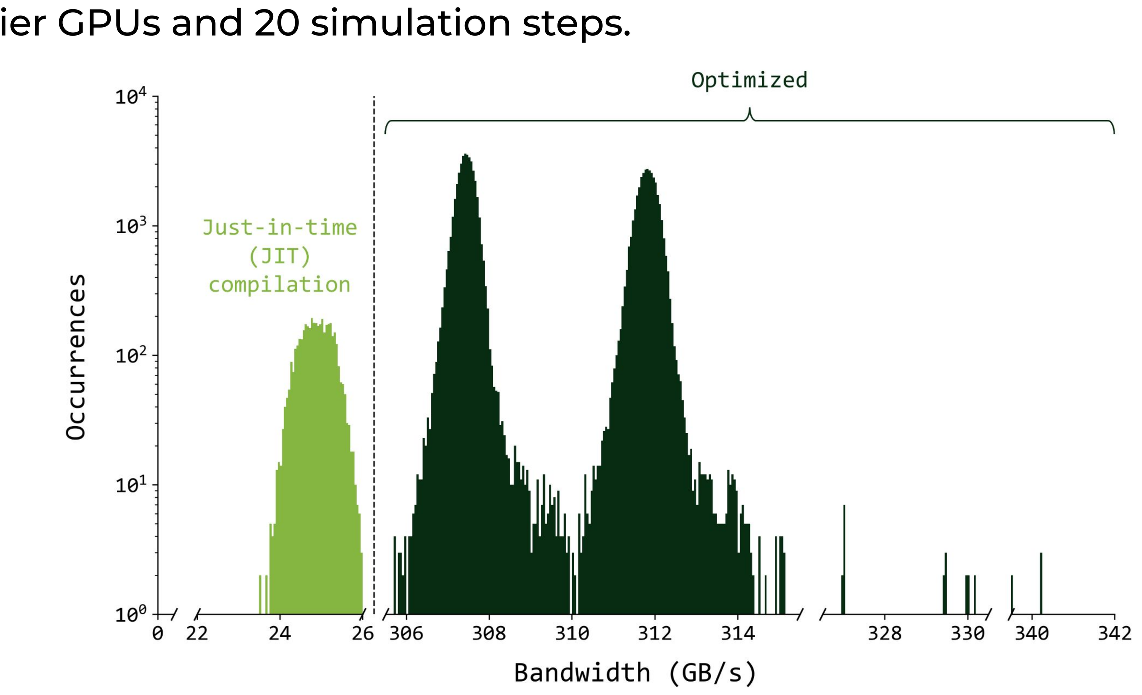
```
#1 Configure Frontier environment by loading modules.
#2 Set MPI backend; Tell MPIPreferences to use Cray's MPICH.
julia --project=$GS_DIR -e 'using Pkg; Pkg.add("MPIPreferences")'
julia --project=$GS_DIR -e 'using MPIPreferences; MPIPreferences.use_system_binary(;
library_names=["libmpi_cray"], mpiexec="srun")'
### Adds a custom branch in case the development version is needed (for devs to test new
features)
julia --project=$GS_DIR -e 'using Pkg;
Pkg.add(url="https://github.com/utkarsh530/AMDGPU.jl.git", rev="u/random")'
#3 Instantiate the project by installing packages listed in Project.toml.
julia --project=$GS_DIR -e 'using Pkg; Pkg.instantiate()'
### Verify the packages are installed correctly.
julia --project=$GS_DIR -e 'using Pkg; Pkg.build()'
julia --project=$GS_DIR -e 'using Pkg; Pkg.precompile()'
#4 Select number of MPI processes per number of GPU's when running the simulation.
srun -n 8 --ntasks-per-node=8 --gpus-per-node=8 --gpu-bind=closest julia --project=$GS_DIR
$GS_DIR/gray-scott.jl settings-files.json
    # Select GPU programming model (AMDGPU for Frontier) in settings-files.json.
    ###snippet from settings-files.json
     {
       "L": 2048,
        "output": "gs-8MPI-8GPU-2048L-F64.bp",
        "precision": "Float64",
       "backend": "AMDGPU"
     }
```

Results

- We compared the speed of accessing the GPU allocated arrays u and v for 7 read (fetch/load) and 1 write operations of our GrayScott.jl kernel in Julia with an AMD provided HIP implementation of a Laplacian kernel.

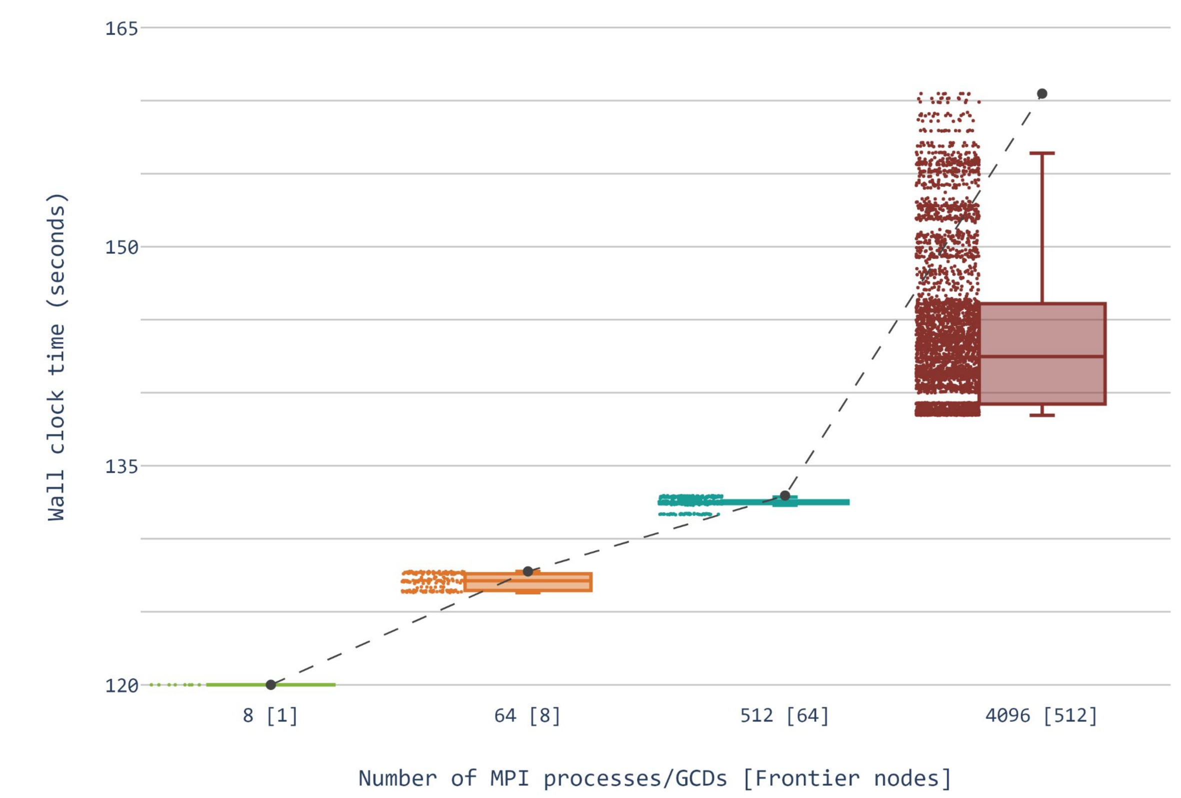
Kernel	Bandwidth (GB/s) Effective	Total
Julia GrayScott.jl		
- 2-variable (application)	312	570
- 1-variable no random	312	625
HIP single variable	599	1,163
Theoretical peak MI250x	1,600	

- We evaluated the bandwidth distribution of a run of GrayScott.jl across 4,096 Frontier GPUs and 20 simulation steps.

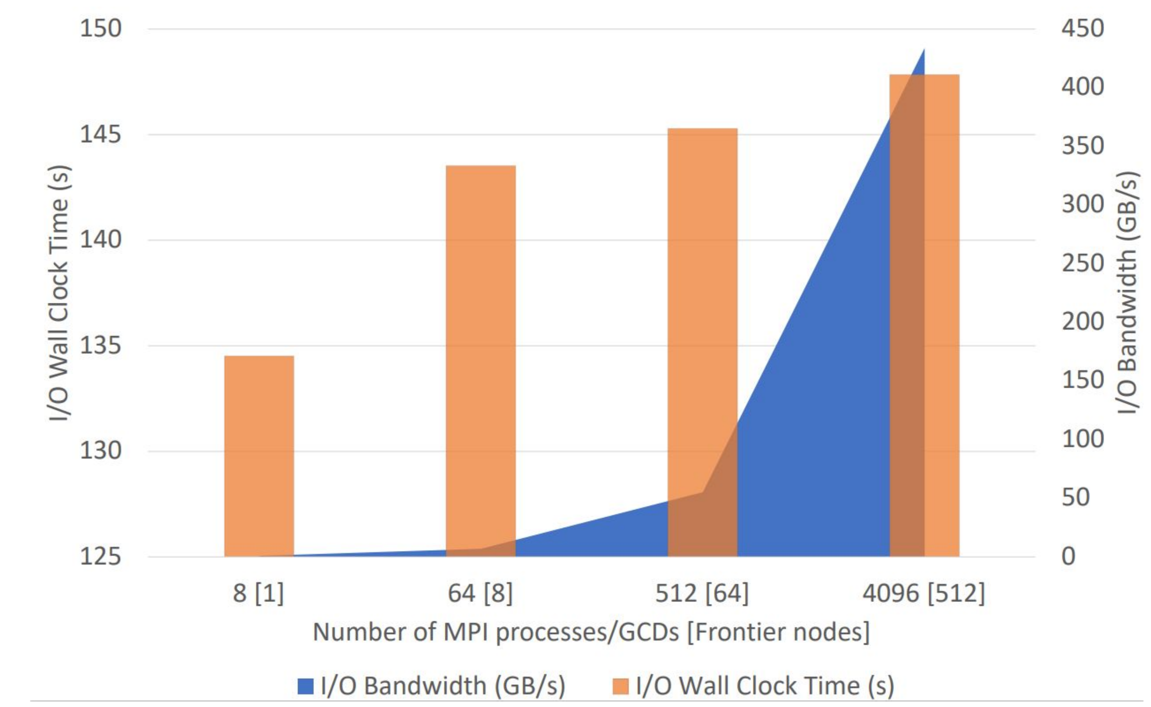


Results (cont.)

- We evaluated the weak scalability (without I/O) of the GrayScott.jl simulation on up to 4,096 GPUs or 512 nodes of Frontier.



- We evaluated the weak scalability of the parallel I/O component, ADIOS2.jl, saving only one output step.



Conclusion

- Julia achieved ~50% of the bandwidth of AMD's HIP implementation of a similar kernel.
- Julia's JIT causes performance to suffer initially.
- Weak scalability with and without I/O was somewhat linear, can indicate that Julia's bindings are lightweight layers on MPI, ADIOS2.
- Julia was able to complete simulation on up to ~50% of the Frontier System.
- Next Steps:
  - Further evaluate other metrics of performance: Strong scalability, compare with C++ version of GrayScott.jl.
  - Explore the capabilities of Julia's tools for data visualization and interactive computing with this HPC workload.

Acknowledgements

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