

Julia and JACC.jl for easy CPU/GPU programming

William F Godoy, Pedro Valero-Lara, Het Mankad, **Keita Teranishi**, and
Jeffery Vetter

Computer Science and Mathematics Division
Advanced Computing Systems Research Section

July 30th 2024,

Contents

- Julia's value proposition for science: LLVM + Coordinated Ecosystem
- Update: Efforts in HPC
- JACC: Julia for Accelerators
- Resources: where to get started?
- Acknowledgments

Contents

- **Julia's value proposition for science: LLVM + Coordinated Ecosystem**

Update: Efforts in HPC

JACC: Julia for Accelerators

Resources: where to get started?

Acknowledgments

Landscape of computing: The Tower of Babel

- Scientific software:
 - Performance languages: C, C++, Fortran
 - High-level productivity languages: Python, Matlab, R
- Plethora of programming models for heterogeneous computing . Standard, vendor-specific, third party
- Major shift: vendor compiler convergence around LLVM
- Slowdown in Moore's Law cadence puts more focus on massively parallel, vectorized computing: ARM, NVIDIA/AMD GPU, Intel's Xeon, KNL, Sapphire Rapids, AVX-512
- AI/ML + traditional HPC requires powerful reproducible programming abstractions for computation, communication and data
- Choosing a programming model is not always a technical decision

1
oneAPI

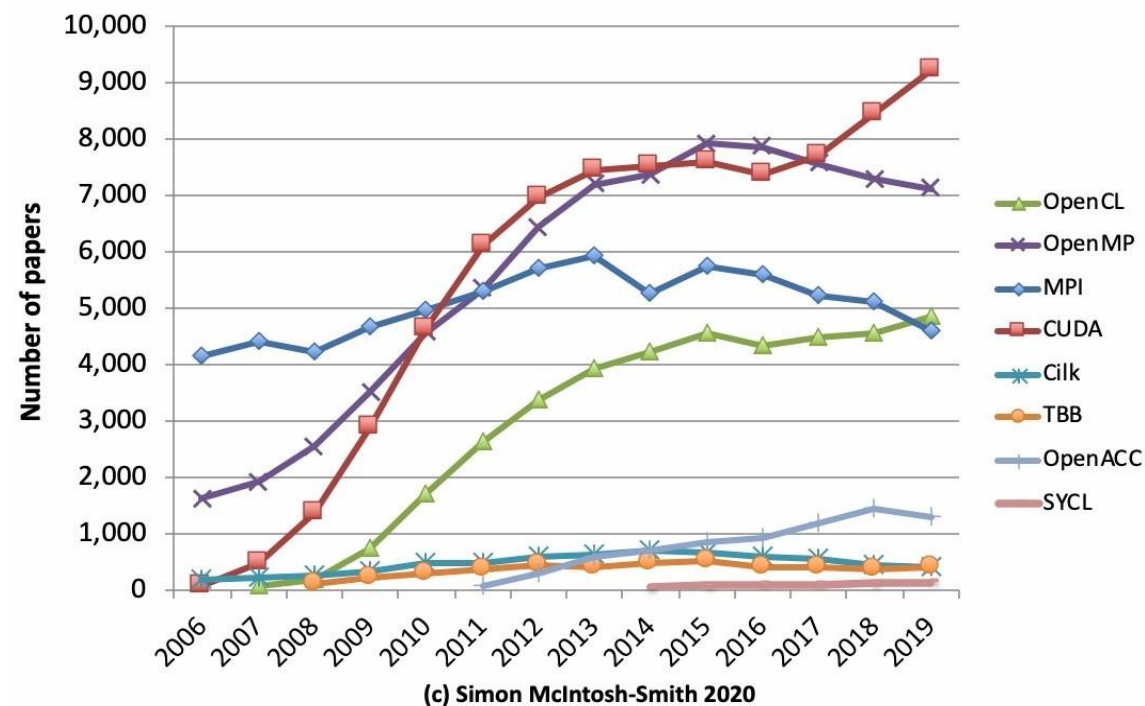


OpenACC
Directives for Accelerators

OpenMP

AMD
ROCm

kokkos

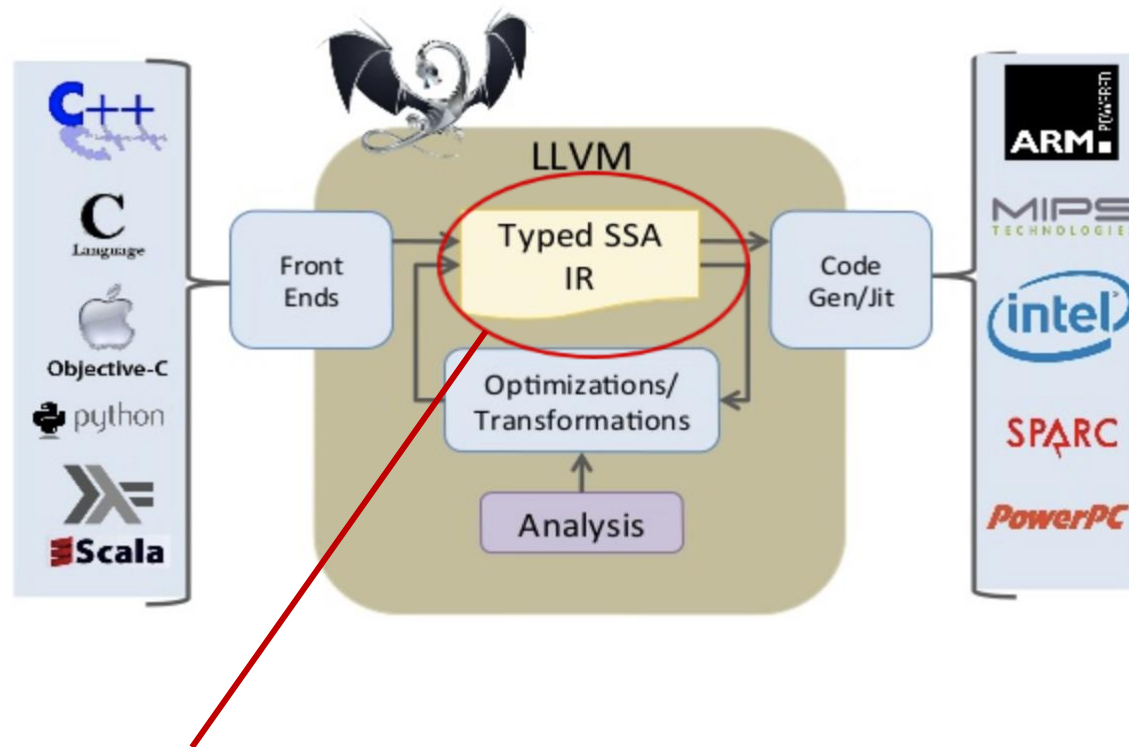


LLVM: a game changer <https://llvm.org/>

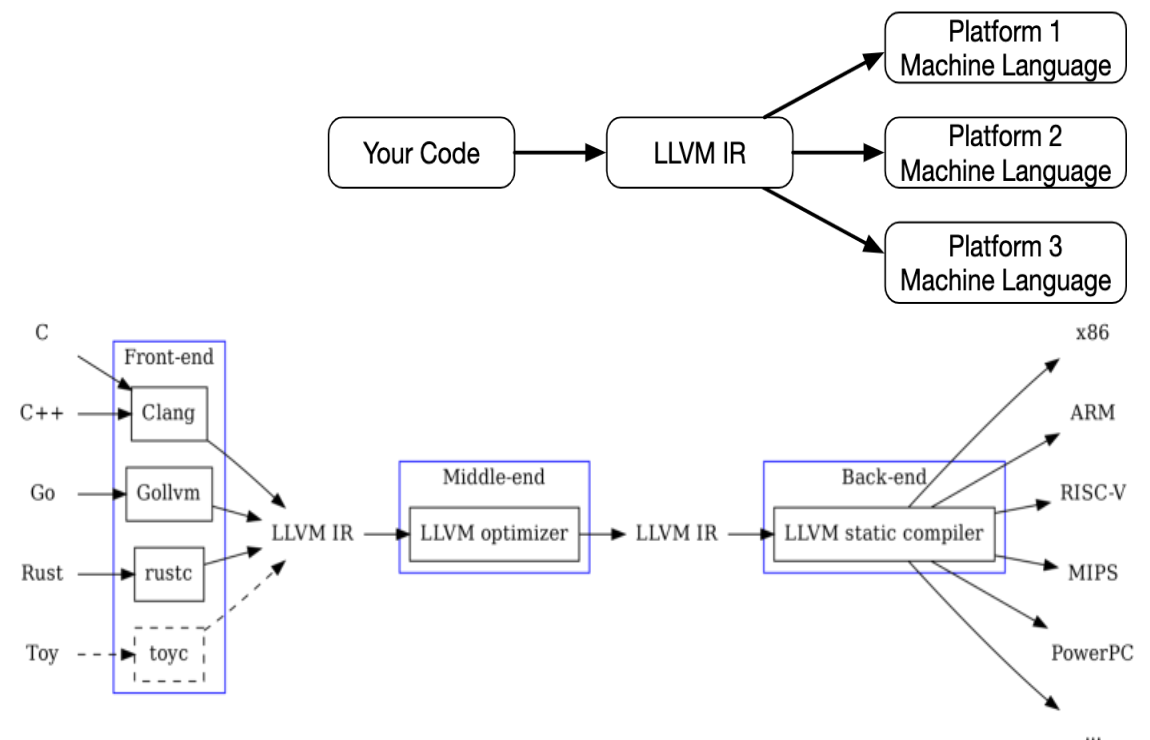
<http://www.aosabook.org/en/llvm.html>

LLVM Compiler Infrastructure

[Lattner et al.]



C. Lattner and V. Adve, "LLVM: a compilation framework for lifelong program analysis & transformation," *International Symposium on Code Generation and Optimization, 2004. CGO 2004.*, 2004, pp. 75-86, <https://doi.org/10.1109/CGO.2004.1281665>.



LLVM Typed Static Single Assignment (SSA) Intermediate Representation (IR) aka LLVM-IR: <https://patshaughnessy.net/2022/2/19/llvm-ir-the-esperanto-of-computer-languages>

LLVM: Vendor and programming model adoption



Intel

Developer ▾ / Tools ▾ / oneAPI ▾ / Components ▾ / Intel® oneAPI DPC++/C++ Compiler / Intel® Compilers Adopt LLVM

Intel C/C++ compilers complete adoption of LLVM

1
oneAPI



The next generation Intel C/C++ compilers are even better because they use the LLVM open source infrastructure.

<https://www.ornl.gov/project/proteas-tune>

OpenACC
Directives for Accelerators

<https://csmd.ornl.gov/project/clacc>

ARM

ARM Compiler Builds on Open Source LLVM Technology

April 08, 2014

Velocity of open source Clang and LLVM combined with the stability of commercial products improve code quality, performance and power efficiency on ARM processors



OpenMP

<https://openmp.llvm.org>

NVIDIA

NVIDIA CUDA 4.1 Compiler Now Built on LLVM

By Chris Lattner
Dec 19, 2011

CUDA LLVM Compiler



LLVM Commits

NVIDIA's CUDA Compiler (NVCC) is based on the widely used LLVM open source compiler infrastructure. Developers can create or extend programming languages with support for GPU acceleration using the NVIDIA Compiler SDK.

Apple

Fast and powerful

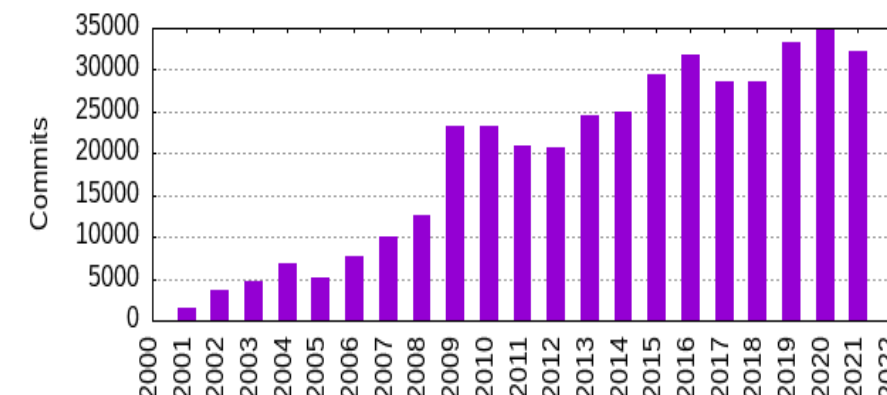
From its earliest conception, Swift was built to be fast. Using the incredibly high-performance LLVM compiler technology, Swift code is transformed into optimized machine code that gets

AMD Updates ROCm™ For Heterogenous Software Support

Community support continues to grow for AMD Radeon Open eCcosystem (ROCm™), AMD's open source foundation for heterogenous compute. Major development milestones in the latest update include:

- The HIP-Clang compiler is now up-streamed and reviewed by the LLVM™ community, providing a better open source experience for the developer,

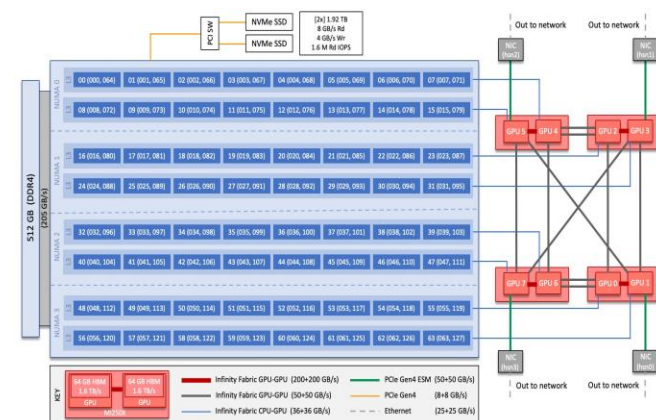
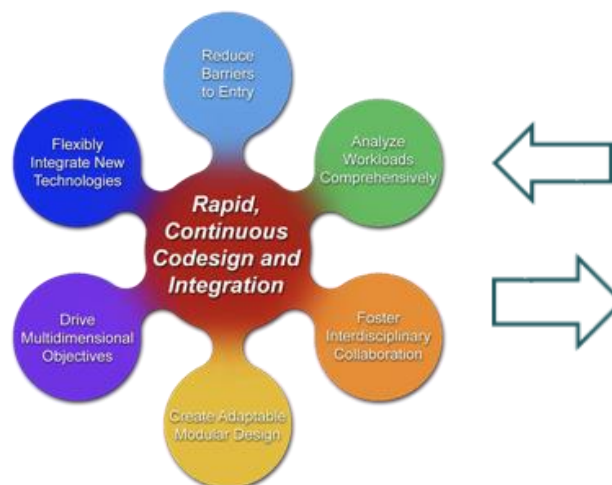
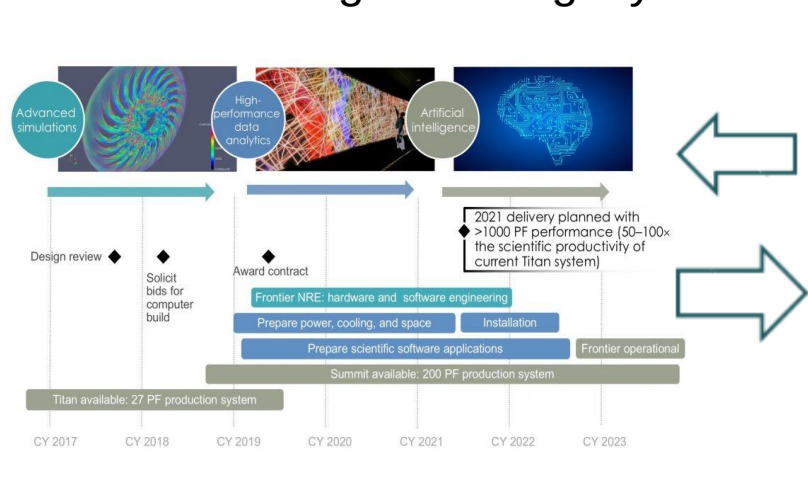
AMD
ROCm



Rethink how we do Computing

- Scientific programming is HARD (specially on our Leadership Computing Facilities, LCFs)
- Software is our “specialized science equipment” for science
- There is still a lot of plumbing to be done
- Programming productivity is always a challenge
- Barrier to entry from idea to portable performance
- AI/ML+HPC is a multidisciplinary co-design challenge
- How to leverage ECP legacy?

*“Can a machine translate a sufficiently rich mathematical language into a sufficiently economical program at a sufficiently low cost to make the whole affair feasible?”-----
----- Backus on Fortran (1980)*



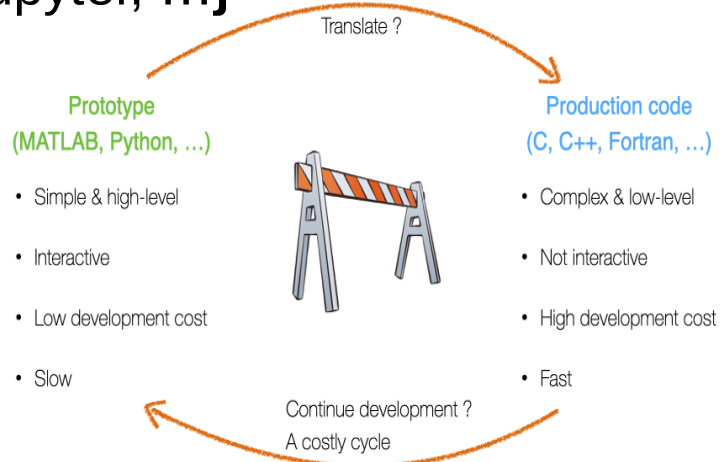
Key question: “What novel approaches to software design and implementation can be developed to provide performance portability for applications across radically diverse computing architectures?” from Reimagining Codesign for Advanced Scientific Computing: Unlocking Transformational Opportunities for Future Computing Systems for Science. DOE Report <https://doi.org/10.2172/1822198>

Julia's value proposition for HPC

- Designed for “scientific computing” (Fortran-like) and “data science” (Python-like) with **performant kernel code via LLVM compilation**
- Lightweight **interoperability with existing Fortran and C libraries**
- Julia is a **unifying workflow language** with a **coordinated ecosystem**

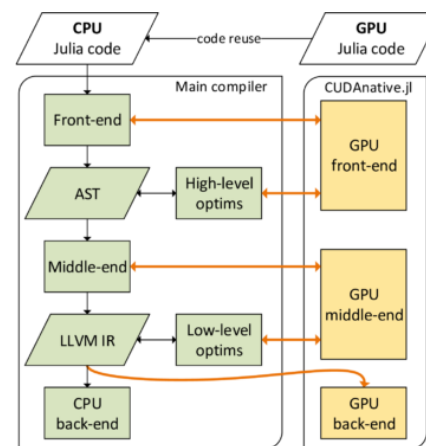
“Julia **does not** replace Python, but the costly workflow process around **Fortran+Python+X**, **C+X**, **Python+X** or **Fortran+X** (e.g. GPUs)”

where **X** = { conda, pip, pybind11, cython, Python, C, Fortran, C++, OpenMP, OpenACC, CUDA, HIP, CMake, numpy, scipy, matplotlib, Jupyter, ... }

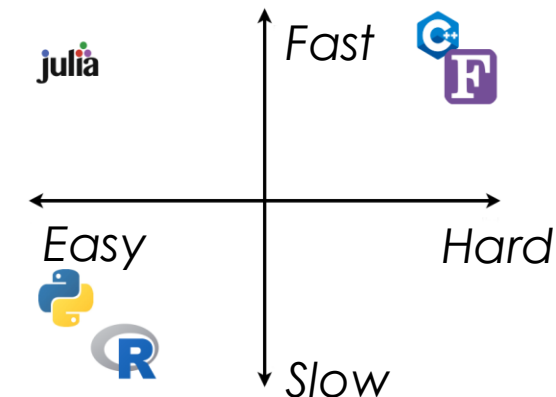


<https://pde-on-gpu.vaw.ethz.ch/lecture7>

LLVM



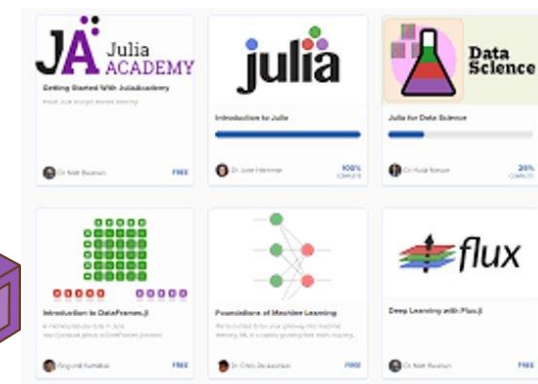
<https://developer.nvidia.com/blog/gpu-computing-julia-programming-language/>



<https://juliadatascience.io/>



Rich data science ecosystem

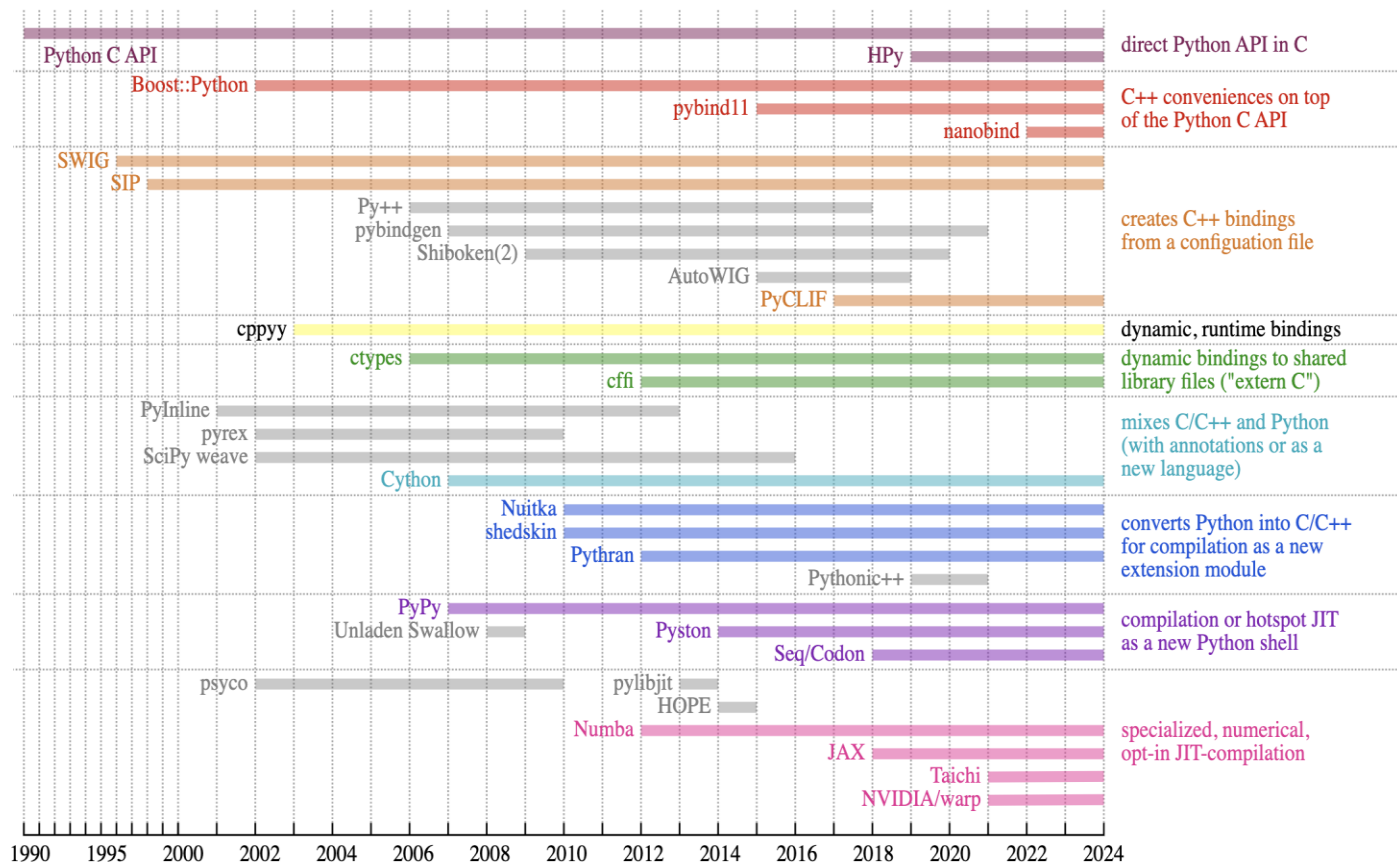


<https://quantumzeitgeist.com/learning-the-julia-programming-language-for-free/>

Python is not enough...and is a fragmented world

<https://pyreadiness.org/3.12/>

Make Python faster



<https://raw.githubusercontent.com/jpivarski-talks/2023-05-01-hsf-india-tutorial/main/img/history-of-bindings-2.svg>

Python 3.12 Readiness

Python 3.12 support graph for the 360 most popular Python packages!

What is this about?

Python 3.12 is a [currently supported version of Python](#). This site shows Python 3.12 support for the 360 most downloaded packages on PyPI:

1. 209 **green** packages (58.1%) support Python 3.12;
2. 151 **white** packages (41.9%) don't explicitly support Python 3.12 yet.

Package 'x' is white. What can I do?

There can be many reasons a package is not explicitly supporting Python 3.12:

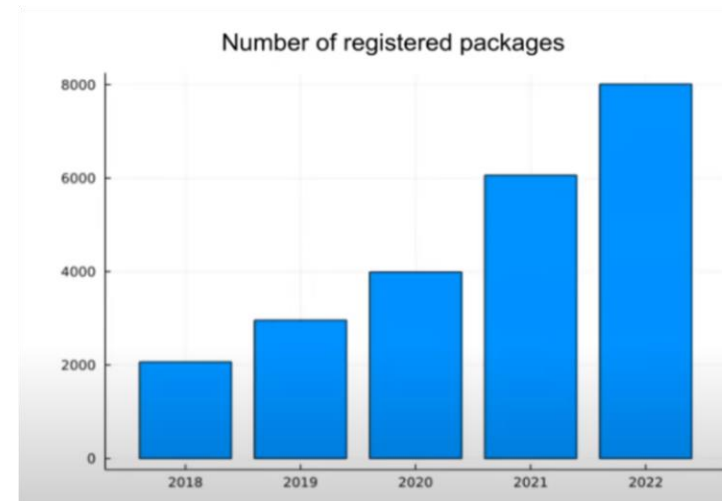
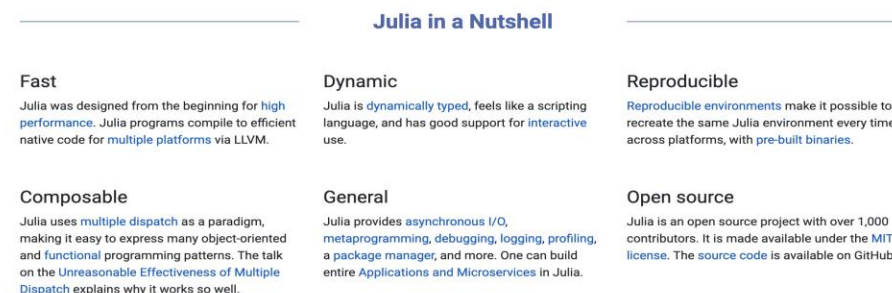
- If you are package maintainer, it's time to start supporting Python 3.12. If you are not able to give the time needed, please seek for help from the community.
- If you are user of the package, send a friendly note to the package maintainer. Or fork it, and send a pull request to help move the project towards Python 3.12 support, by adding the classifier and ensuring the project is tested against Python 3.12.



Julia Brief Walkthrough



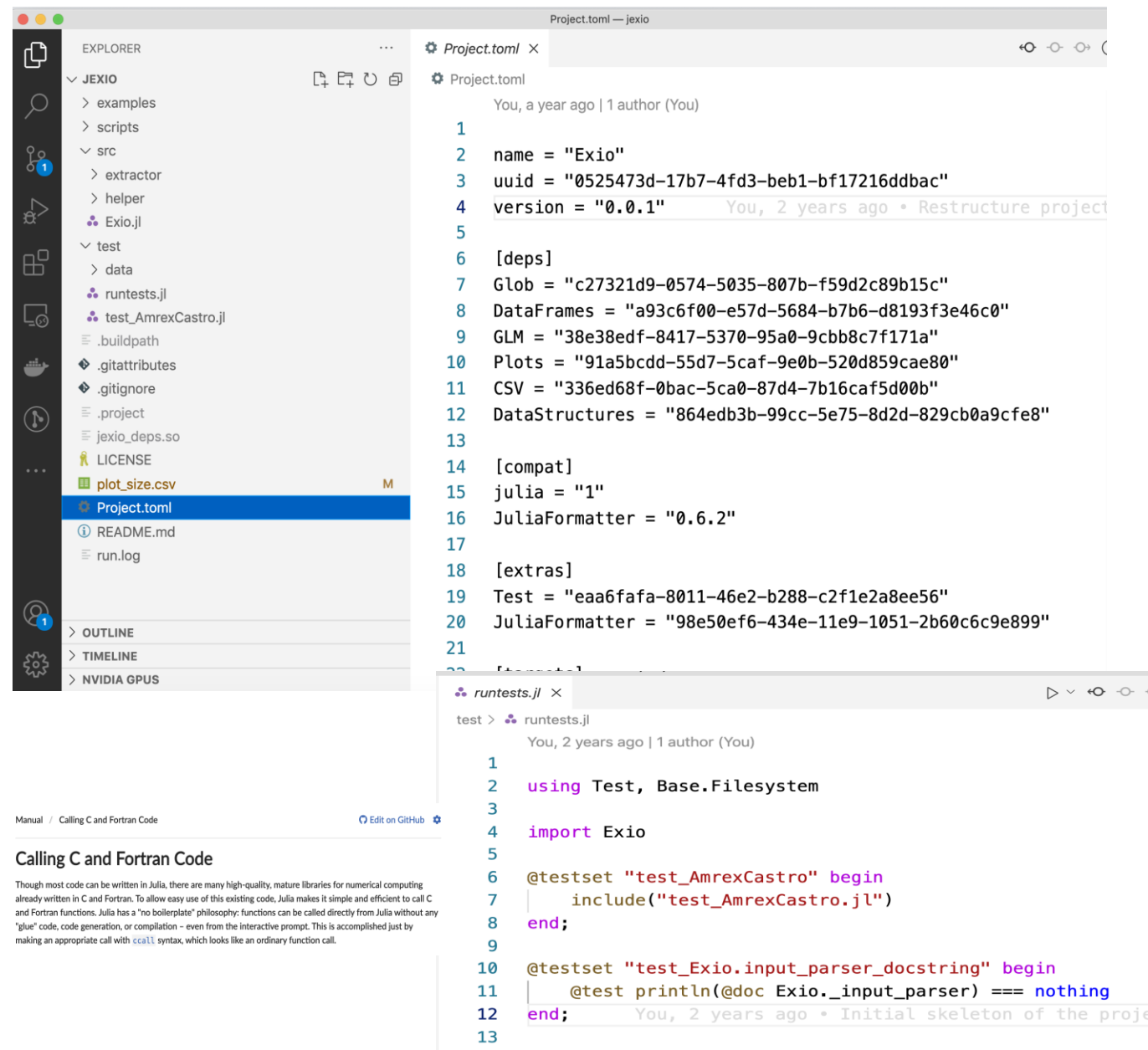
- ❑ History: started at MIT in the early 2010s (predates Python Numba)
<https://julialang.org/blog/2022/02/10years/>
- ❑ JuliaHub (formely Julia Computing) and MIT are major contributors:
<https://juliacomputing.com/case-studies>
- ❑ First stable release v1.0 in 2018, **v1.10 as of 2024**
<https://julialang.org/>
- ❑ Open-source GitHub-hosted packages and ecosystem with MIT permissive license:
<https://github.com/JuliaLang/julia>
- ❑ Community: annual JuliaCon summer conference:
<https://juliacon.org/2024/>



95% of Julia packages in the registry had some form of CI
(youtube.com/watch?v=9YWwiFbaRx8)

Julia Brief Walkthrough

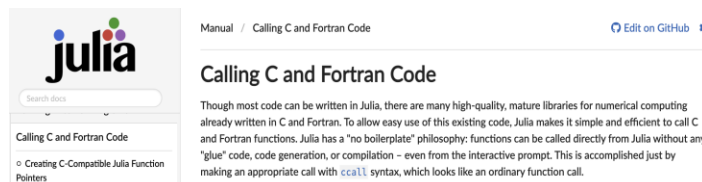
- ❑ Reproducibility is in the core of the language:
 - Interactive: Jupyter, [Pluto.jl](#)
 - Packaging [Pkg.jl](#)
 - Environment [Project.toml](#)
 - Testing [Test.jl](#)
- ❑ Just-in-time or Ahead-of-time compilation with [PackageCompiler.jl](#)
- ❑ Powerful metaprogramming for code instrumentation: `@profile`, `@time`, `@testset`, `@test`, `@code_llvm`, `@code_native`, `@inbounds`,
- ❑ Interoperability is key: `@ccall`, `@cxx`, [PyCall](#), [CxxWrap.jl](#)



The screenshot shows a VS Code editor with two files open. The top file is `Project.toml` for a project named "jexio". It contains fields for `name`, `uuid`, `version`, `[deps]` (listing various scientific computing packages), `[compat]` (specifying Julia 1), and `[extras]` (listing test sets). The bottom file is `runtests.jl`, which uses the `Test` module and `Base.Filesystem` to run tests. It includes a test set for `test_AmrexCastro` and another for `test_Exio` that checks for the presence of `Exio._input_parser`.

```
Project.toml — jexio
Project.toml
You, a year ago | 1 author (You)
1
2 name = "Exio"
3 uuid = "0525473d-17b7-4fd3-beb1-bf17216ddb1c"
4 version = "0.0.1"
5
6 [deps]
7 Glob = "c27321d9-0574-5035-807b-f59d2c89b15c"
8 DataFrames = "a93c6f00-e57d-5684-b7b6-d8193f3e46c0"
9 GLM = "38e38edf-8417-5370-95a0-9cbb8c7f171a"
10 Plots = "91a5bcdd-55d7-5caf-9e0b-520d859cae80"
11 CSV = "336ed68f-0bac-5ca0-87d4-7b16caf5d00b"
12 DataStructures = "864ed3b3-99cc-5e75-8d2d-829cb0a9cfe8"
13
14 [compat]
15 julia = "1"
16 JuliaFormatter = "0.6.2"
17
18 [extras]
19 Test = "eaa6fafa-8011-46e2-b288-c2f1e2a8ee56"
20 JuliaFormatter = "98e50ef6-434e-11e9-1051-2b60c6c9e899"
21
22 [test]
23

runtests.jl
test > runtests.jl
You, 2 years ago | 1 author (You)
1
2 using Test, Base.Filesystem
3
4 import Exio
5
6 @testset "test_AmrexCastro" begin
7     include("test_AmrexCastro.jl")
8 end;
9
10 @testset "test_Exio.input_parser_docstring" begin
11     @test println(@doc Exio._input_parser) == nothing
12 end;
13
```



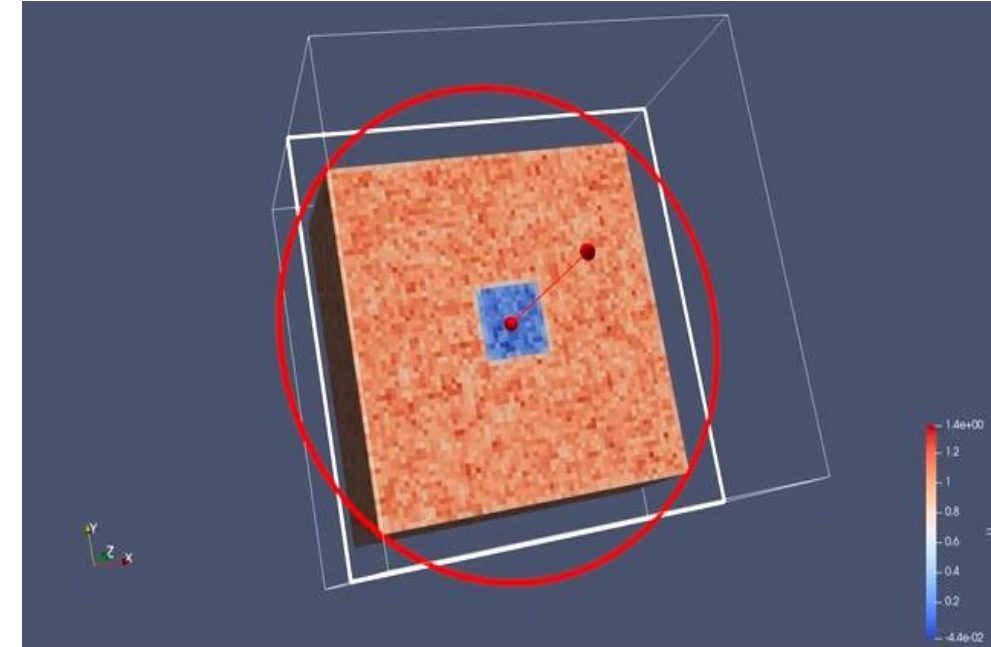
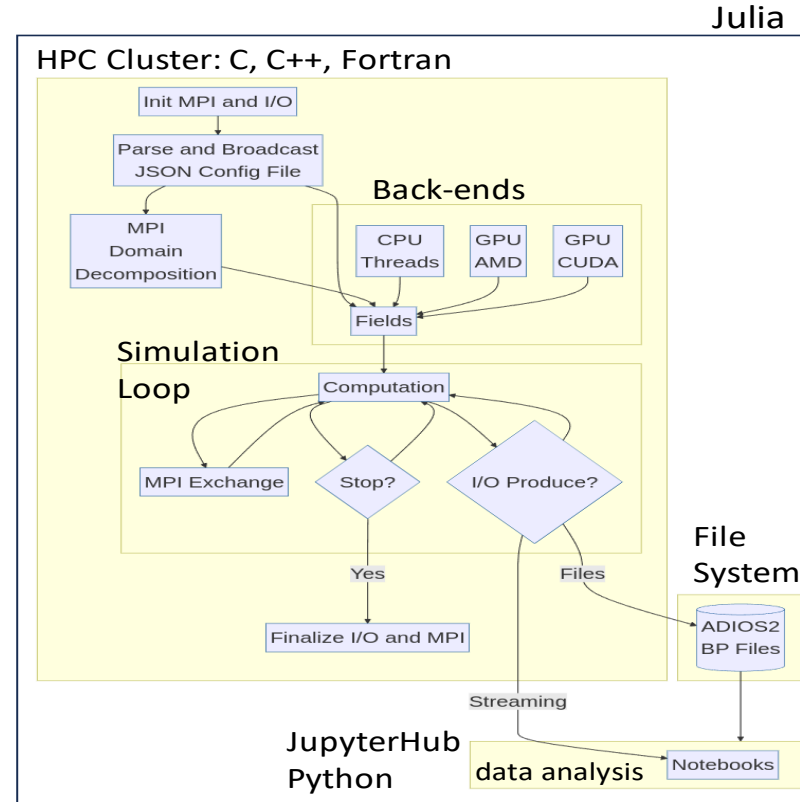
Contents

- Julia's value proposition for science: LLVM + Coordinated Ecosystem
- **Efforts in HPC**
- JACC: Julia for Accelerators
- Resources: where to get started?
- Acknowledgments

Gray-Scott miniapp: <https://github.com/JuliaORNL/GrayScott.jl>

Simple 3D 2-variable diffusion-reaction solver

- CPU Threads, CUDA.jl and **AMDGPU.jl** backends using multiple dispatch
- Parallel I/O ADIOS2, can be visualized with ParaView
- MPI.jl for communication
- Configuration and job scripts for Frontier, Crusher and Summit under ./scripts/
- Data analysis on JupyterHub



Best paper at SC23 WORKS

RESEARCH-ARTICLE 🐦 in 🌐 f ✉
Julia as a unifying end-to-end workflow language on the Frontier exascale system

Authors: William F. Godoy, Pedro Valero-Lara, Calira Anderson, Katrina W. Lee, Ana Gainaru, Rafael Ferreira Da Silva, Jeffrey S. Vetter [Authors Info & Claims](#)

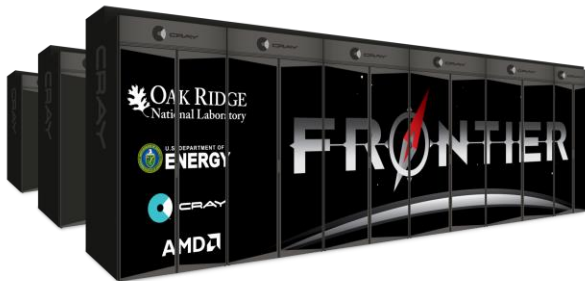
SC-W '23: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis • November 2023 • Pages 1989–1999 • <https://doi.org/10.1145/3624062.3624278>

$$\frac{\partial U}{\partial t} = D_U \nabla^2 U - UV^2 + F(1 - U) + nr \quad (1a)$$

$$\frac{\partial V}{\partial t} = D_V \nabla^2 V + UV^2 + -(F + k)V \quad (1b)$$

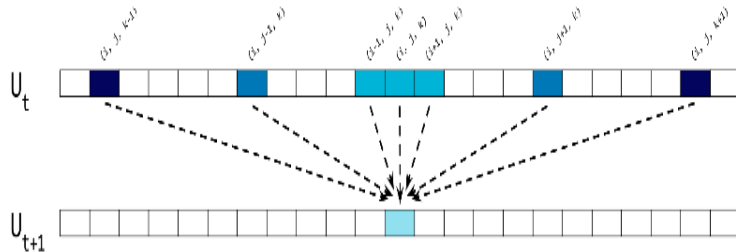
Research question: Can I write an entire HPC workflow in Julia?

<https://doi.org/10.1145/3624062.3624278>



Frontier on-node scalability using AMDGPU.jl

7-point stencil



$$fetch_size_{effective} = [L^3 - 8 - 12(L - 2)] \cdot sizeof(T) \quad (4a)$$

$$write_size_{effective} = (L - 2)^3 \cdot sizeof(T) \quad (4b)$$

$$bandwidth_{effective} = \frac{(fetch_size + write_size)_{effective}}{kernel_time} \quad (5a)$$

$$bandwidth_{total} = \frac{(FETCH_SIZE + WRITE_SIZE)_{rocp}}{kernel_time} \quad (5b)$$

Table 2: Average bandwidth comparison of different stencil implementations on a single GPU.

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	

Table 3: rocp outputs for HIP 1-variable and Julia GrayScott.jl implementations

kernel metric	HIP 1-var	GrayScott.jl	
		1-variable no random	2-variable (application)
wgr	256	512	512
lds	0	29,184	29,184
scr	0	8,192	8,192
FETCH_SIZE (GB)	25.08	25.40	50.80
WRITE_SIZE (GB)	8.35	8.38	16.78
TCC_HIT (M)	9.14	10.80	24.60
TCC_MISS (M)	8.36	8.69	17.19
Avg Duration (ms)	28.74	54.03	111.07

Listing 2: Julia AMDGPU.jl Gray-Scott kernel

```

using AMDGPU
using Distributions

function _laplacian(i, j, k, var)
    l = var[i - 1, j, k] + var[i + 1, j, k]
      + var[i, j - 1, k] + var[i, j + 1, k]
      + var[i, j, k - 1] + var[i, j, k + 1]
      - 6.0 * var[i, j, k]
    return l / 6.0
end

function _kernel_amdgpu!(u, v, u_temp, v_temp,
                        sizes, Du, Dv, F, K,
                        noise, dt)

    k = (workgroupIdx().x - 1) * workgroupDim().x
      + workitemIdx().x
    j = (workgroupIdx().y - 1) * workgroupDim().y
      + workitemIdx().y
    i = (workgroupIdx().z - 1) * workgroupDim().z
      + workitemIdx().z

    if k == 1 || k >= sizes[3] ||
        j == 1 || j >= sizes[2] ||
        i == 1 || i >= sizes[1]
        return
    end

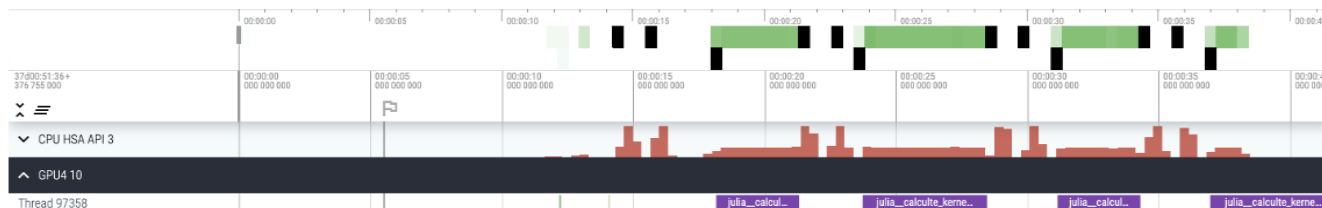
    @inbounds begin
        u_ijk = u[i, j, k]
        v_ijk = v[i, j, k]

        du = Du * _laplacian(i, j, k, u)
              - u_ijk * v_ijk^2 + F * (1.0 - u_ijk)
              + noise * rand(Uniform(-1, 1))

        dv = Dv * _laplacian(i, j, k, v)
              + u_ijk * v_ijk^2 - (F + K) * v_ijk

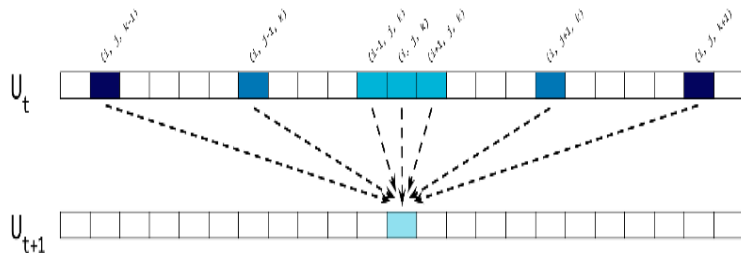
        u_temp[i, j, k] = u_ijk + du * dt
        v_temp[i, j, k] = v_ijk + dv * dt
    end

    return nothing
end
    
```



Frontier on-node scalability using AMDGPU.jl

7-point stencil



$$fetch_size_{effective} = [L^3 - 8 - 12(L - 2)] \cdot sizeof(T) \quad (4a)$$

$$write_size_{effective} = (L - 2)^3 \cdot sizeof(T) \quad (4b)$$

$$bandwidth_{effective} = \frac{(fetch_size + write_size)_{effective}}{kernel_time} \quad (5a)$$

$$bandwidth_{total} = \frac{(FETCH_SIZE + WRITE_SIZE)_{rocprof}}{kernel_time} \quad (5b)$$

Table 2: Average bandwidth comparison of different stencil implementations on a single GPU.

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

Table 3: rocprof outputs for HIP 1-variable and Julia Gray-Scott.jl implementations

kernel metric	HIP 1-var	GrayScott.jl	
		1-variable no random	2-variable (application)
wgr	256	512	512
lds	0	29,184	29,184
scr	0	8,192	8,192
FETCH_SIZE (GB)	25.08	25.40	50.80
WRITE_SIZE (GB)	8.35	8.38	16.78
TCC_HIT (M)	9.14	10.80	24.60
TCC_MISS (M)	8.36	8.69	17.19
Avg Duration (ms)	28.74	54.03	111.07

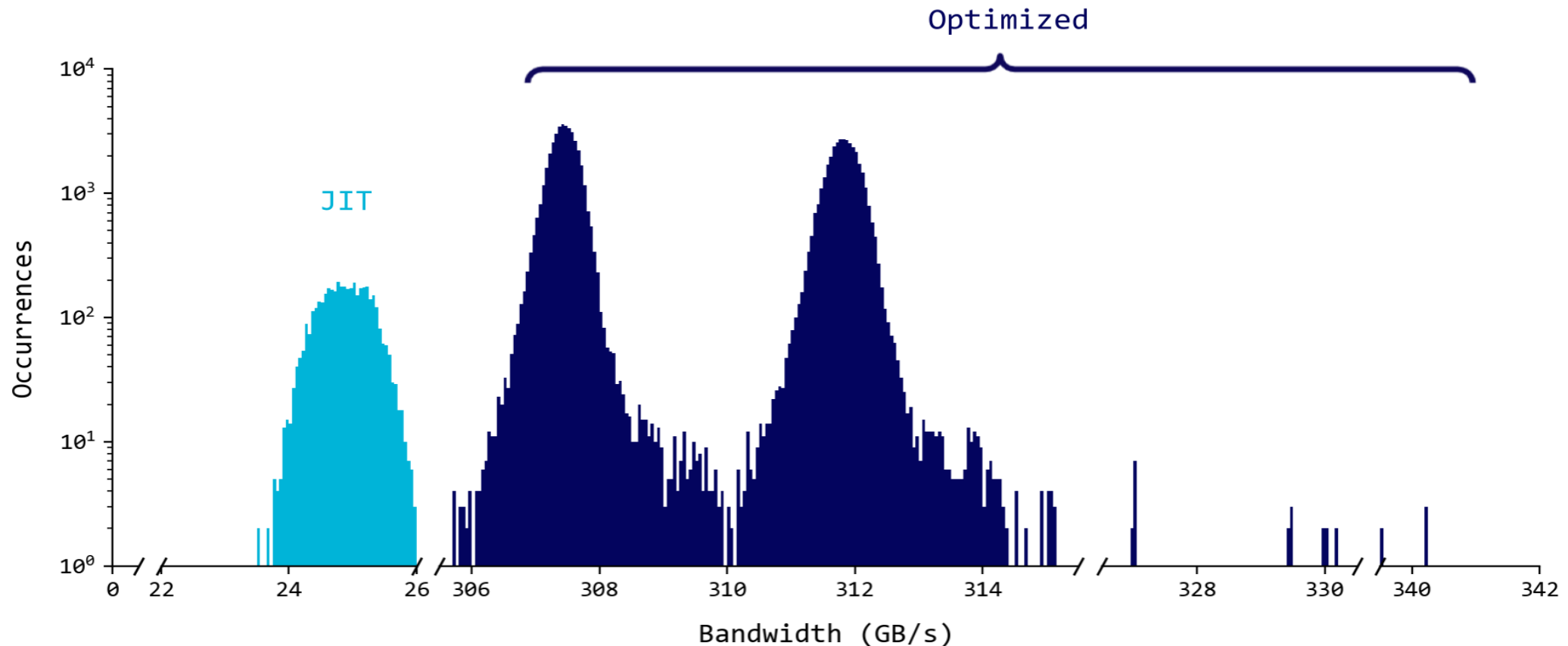
Listing 4: GrayScott.jl application kernel unique memory loads (14) and store (2) in LLVM-IR

```
%94 = load double, double addrspace(1)* %93, align 8
%103 = load double, double addrspace(1)* %102, align 8
%107 = load double, double addrspace(1)* %106, align 8
%110 = load double, double addrspace(1)* %109, align 8
%114 = load double, double addrspace(1)* %113, align 8
%117 = load double, double addrspace(1)* %116, align 8
%122 = load double, double addrspace(1)* %121, align 8
%126 = load double, double addrspace(1)* %125, align 8
%312 = load double, double addrspace(1)* %311, align 8
%315 = load double, double addrspace(1)* %314, align 8
%318 = load double, double addrspace(1)* %317, align 8
%321 = load double, double addrspace(1)* %320, align 8
%325 = load double, double addrspace(1)* %324, align 8
%329 = load double, double addrspace(1)* %328, align 8
...
store double %345, double addrspace(1)* %353, align 8
store double %355, double addrspace(1)* %363, align 8
```

Julia AMDGPU.jl reaches ~50% bandwidth (performance) of HIP
 No surprises on: FETCH/WRITE SIZE, LLVM-IR
 rocprof reports more activity “lds” on Julia

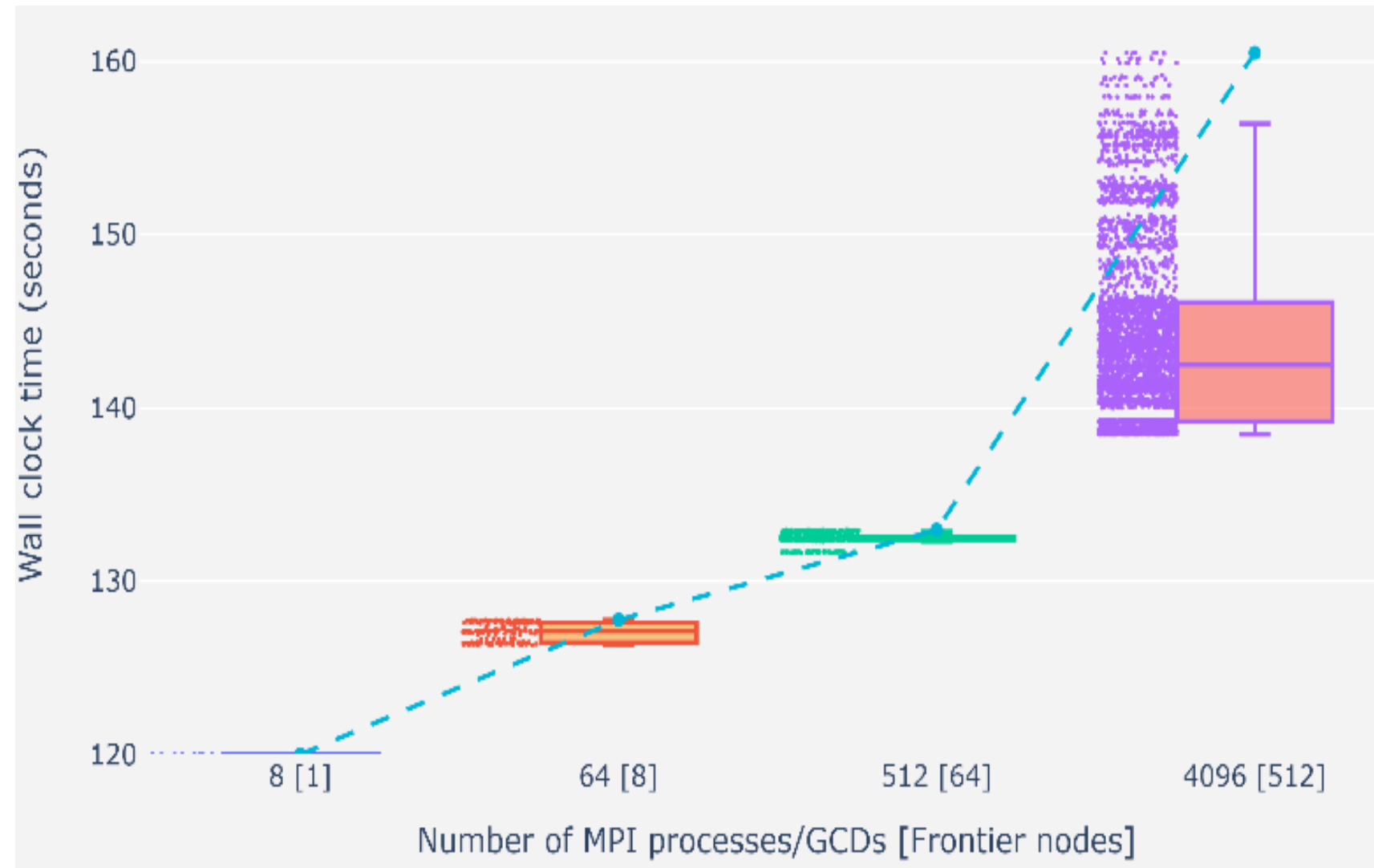
Frontier on-node scalability using AMDGPU.jl for several GPUs

Bandwidth distribution for 4,096 GCD (GPUs) and 20 timesteps. HIP ~ 600 GB/s (800 GB/s claimed on MI250x), Theoretical Peak on MI250x = 1,600 GB/s



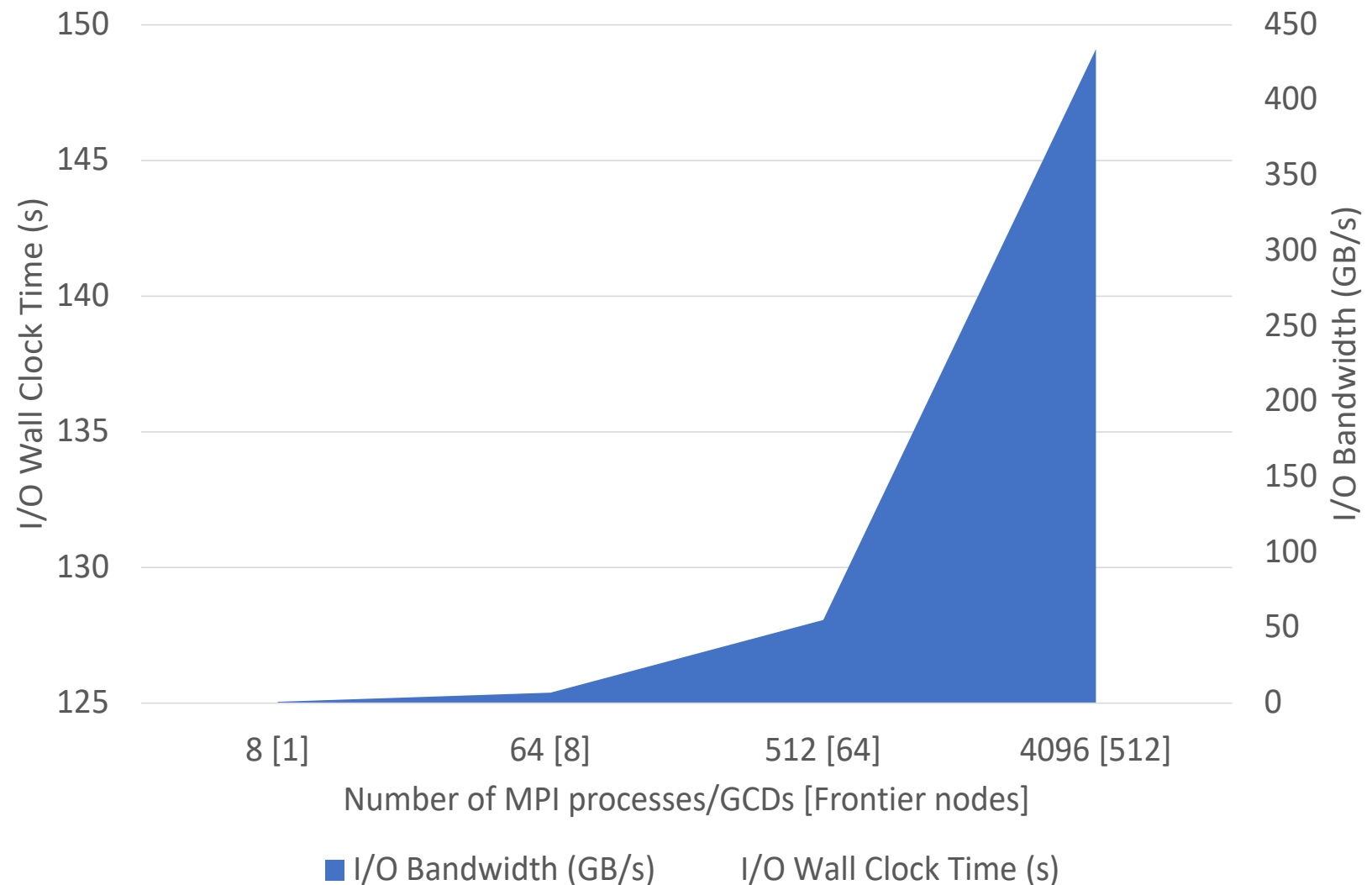
GrayScott.jl Weak Scaling on Frontier

- Tested successfully up to 512 nodes (5% of Frontier) 1 GCD/MPI proc using MPI.jl
- Tried 4K nodes (50% of Frontier) resulted in a libfabric error
- 2-3% variability up to 64 nodes
- 12-15% variability at 512 nodes



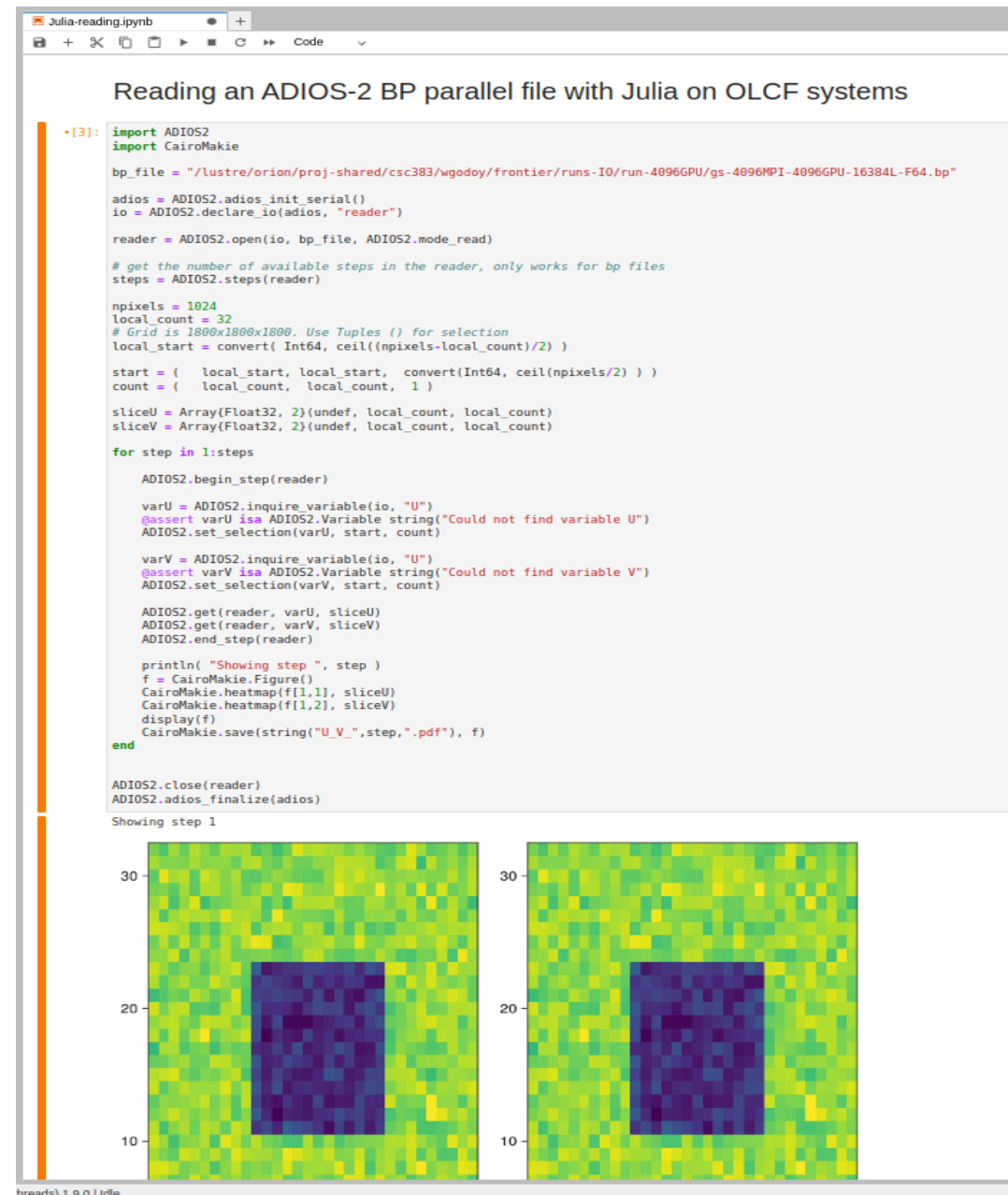
GrayScott.jl Parallel I/O Weak Scaling on Frontier file system

- We tested parallel I/O using Julia via the [ADIOS2.jl](#) Julia bindings
- ADIOS2 is a high-performance data I/O library funded by the US Department of Energy SC ASCR
- Results are shown for the Orion file system
- ADIOS2.jl shows negligible overhead wrt ADIOS2



Data analysis on JupyterHub at OLCF

- <https://jupyter.olcf.ornl.gov/>
- We launched a Julia kernel on JupyterHub to read and analyze data
- We read with ADIOS2.jl and visualize with Makie.jl
- JIT and TTFX (time to first plot) can be a nuance
- Pluto.jl?



Julia on Frontier

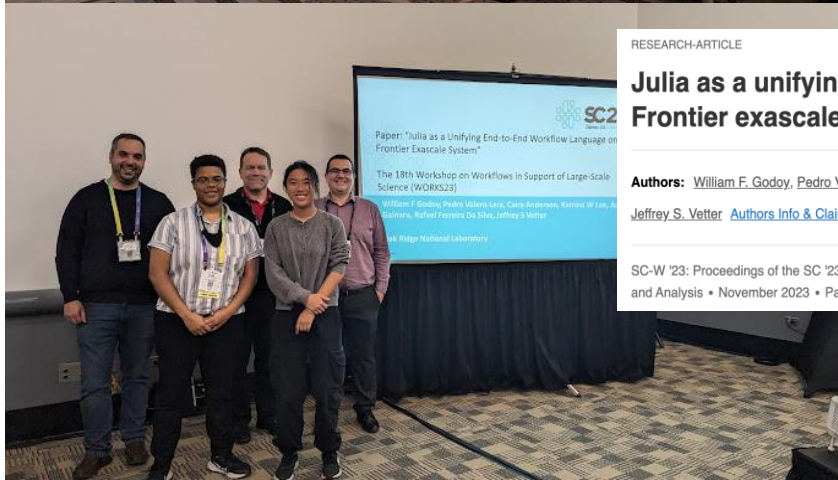
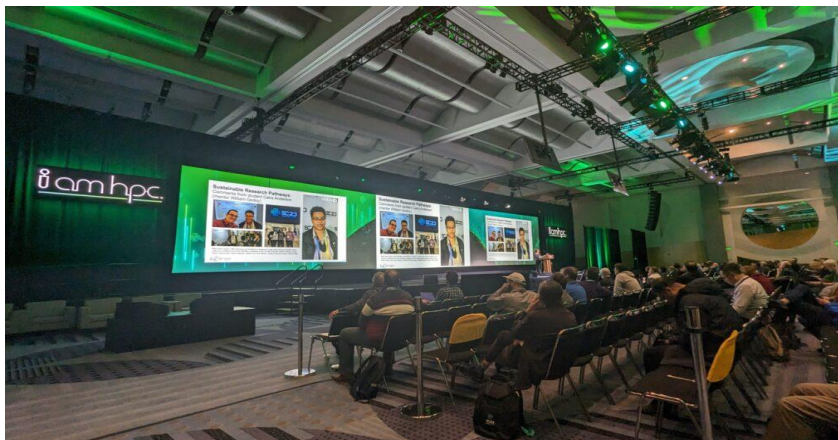
- Recent efforts:
 - Investigate new approaches in the post-ECP landscape: Julia for HPC, LLMs for HPC
 - Recent interest in the high-productivity + high-performance space
 - Enabled me to mentor in our internship program for the last 3 years
 - Build a “Julia for HPC” community
<https://juliaparallel.org/resources/>

Evaluation of OpenAI Codex for HPC parallel programming models kernel generation

William F. Godoy, Pedro Valero-Lara, Keita Teranishi, Prasanna Balaprakash, and Jeffrey S. Vetter
Oak Ridge National Laboratory
Oak Ridge, TN, USA
{godoywf},{valerolarap},{teranishik},{pbalapra},{vetter}@ornl.gov

Evaluating performance and portability of high-level programming models: Julia, Python/Numba, and Kokkos on exascale nodes

William F. Godoy, Pedro Valero-Lara, T. Elise Dettling, Christian Trefftz, Ian Jorquera, Thomas Sheehy, Ross G. Miller, Marc Gonzalez-Tallada, Jeffrey S. Vetter
Oak Ridge National Laboratory
{godoywf},{valerolarap},{dettlingte},{trefftzci},{jorqueraid},{sheehytb},{rgmiller},{gonzalezalm},{vetter}@ornl.gov
Valentin Churavy
Massachusetts Institute of Technology
vchuravy@mit.edu



RESEARCH-ARTICLE



Julia as a unifying end-to-end workflow language on the Frontier exascale system

Authors: William F. Godoy, Pedro Valero-Lara, Caira Anderson, Katrina W. Lee, Ana Gainaru, Rafael Ferreira Da Silva,

Jeffrey S. Vetter [Authors Info & Claims](#)

SC-W '23: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis • November 2023 • Pages 1989–1999 • <https://doi.org/10.1145/3624062.3624278>

Highlights:

<https://shinstitute.org/srp-mentor-spotlight>

- Building Julia for HPC **research** and **community** activities: tutorials, papers, SC BoFs 2022/2023
- 2023 IPDPS HIPS workshop paper
- 2023 ICPP P2S2 paper on generative AI for HPC kernels
- Best Paper** at the SC23 WORKS workshop
- D-HPC Workshop at SC23

Julia HPC Efforts

- Projects:
- External Engagements with Julia HPC
 - Monthly meetings with stakeholders
 - [JuliaCon 2022/2023 HPC minisymposium](#)
 - Julia HPC Position paper in the works
 - [ECP BoF Session on Rapid Prototyping for HPC using Julia, Python Numba, Flang](#)
 - [SC22/23 BoF "Julia for HPC"](#)
- Internal Engagements
 - Tutorials at ORNL Software and Data Expo
 - [Julia Workshop for ORNL Science](#)
 - [OLCF User Call: Julia for HPC](#)

Bridging HPC Communities through the Julia Programming Language

Journal Title
XX(X):1–18
©The Author(s) 2022
Reprints and permission:
sagepub.co.uk/journalsPermissions.nav
DOI: 10.1177/ToBeAssigned
www.sagepub.com/

SAGE

Valentin Churavy¹, William F Godoy², Carsten Bauer³, Hendrik Ranocha⁴, Michael Schlottke-Lakemper⁵, Ludovic Räss^{6,7}, Johannes Blaschke⁸, Mosè Giordano⁹, Erik Schnetter^{10,11,12}, Samuel Omlin¹³, Jeffrey S. Vetter², Alan Edelman¹

¹ Massachusetts Institute of Technology, USA

² Oak Ridge National Laboratory, USA

³ Paderborn Center for Parallel Computing, Paderborn University, Germany

⁴ Department of Mathematics, University of Hamburg, Germany

⁵ High-Performance Computing Center Stuttgart (HLRS), University of Stuttgart, Germany

⁶ Laboratory of Hydraulics, Hydrology and Glaciology (VAW), ETH Zurich, Switzerland

⁷ Swiss Federal Institute for Forest, Snow and Landscape Research (WSL), Birmensdorf, Switzerland

⁸ National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

⁹ Centre for Advanced Research Computing, University College London, Gower Street, London, WC1E 6BT, United Kingdom

¹⁰ Perimeter Institute, 31 Caroline St. N., Waterloo, ON, Canada N2L 2Y5

¹¹ Department of Physics and Astronomy, University of Waterloo, 200 University Avenue West, Waterloo, Ontario, Canada N2L 3G1

¹² Center for Computation & Technology, Louisiana State University, Baton Rouge, LA 70803, USA

¹³ Swiss National Supercomputing Centre (CSCS), ETH Zurich, Switzerland



JULIA FOR HPC
JuliaCon 2022 Minisymposium



🔥 Live Talks! 🔥

Register

About

Join Discord

Schedule

Sponsors

Julia for High-Performance Computing

👤 Carsten Bauer, Michael Schlottke-Lakemper, Hendrik Ranocha, Johannes Blaschke, Jeffrey Vetter

🕒 07/26/2022, 10:00 AM — 1:00 PM EDT

🟢 Green

Abstract:

The "Julia for HPC" minisymposium aims to gather current and prospective Julia practitioners in the field of high-performance computing (HPC) from multidisciplinary applications. We invite participation from industry, academia, and government institutions interested in Julia's capabilities for supercomputing. The goal is to provide a venue for Julia enthusiasts to share best practices, discuss current limitations, and identify future developments in the scientific HPC community.

Community Efforts in HPC

- Leverage HPC “backends”:

- [AMDGPU.jl](#)
- [CUDA.jl](#)
- [KernelAbstractions.jl](#)
- [MPI.jl](#)
- [Threads](#) (part of Base)
- [ADIOS2](#) , [HDF5](#)

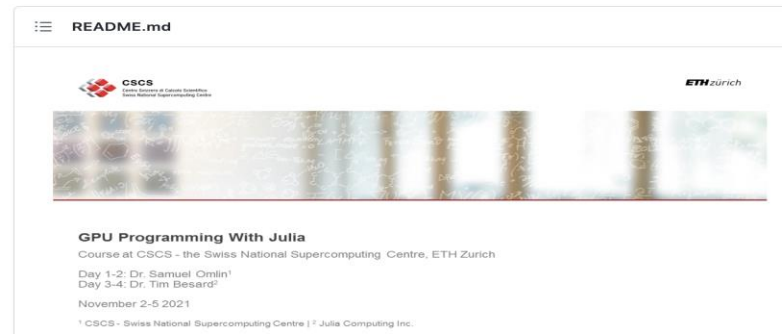
- [Monthly HPC Call](#) (Valentin Churavy, MIT)

- [Porting miniWeather App to Julia](#) (Youngsung Kim, Hyun Kang, and Sarat Sreepathi, CSED)

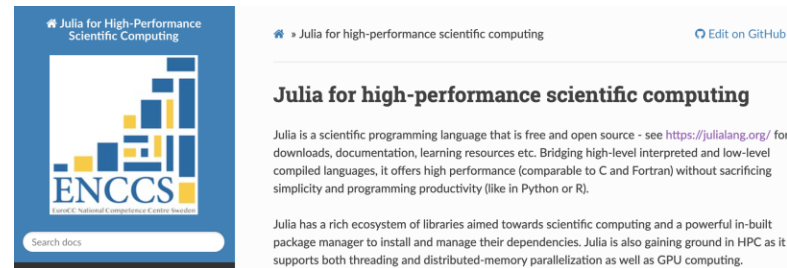
- <https://ptsolvers.github.io/GPU4GEO/software/>

- <https://arxiv.org/abs/2207.03711>

<https://github.com/omlins/julia-gpu-course>



<https://enccs.github.io/Julia-for-HPC>



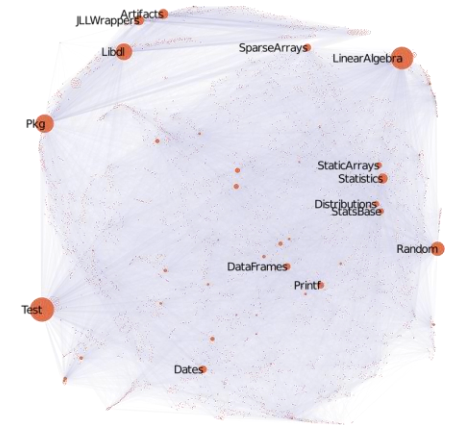
<https://docs.dftk.org/stable>



<https://juliaastro.github.io/dev>

<https://github.com/JuliaParallel>

[Top15 most popular packages](#)



[ECP ExaSDG on Summit](#)

Research | July 06, 2022

Rapid Prototyping with Julia: From Mathematics to Fast Code

By Michel Schanen, Valentin Churavy, Youngdae Kim, and Mihai Anitescu

Software development—a dominant expenditure for scientific projects—is often limited by technical programming challenges, not mathematical insight. Here we share our experience with the Julia programming language in the context of the U.S. Department of Energy's Exascale Computing Project (ECP) as part of ExaSDG, a power grid optimization application. Julia is a free and open-source language that has the potential for C-like performance

SIAG/OPT Views and News

A Forum for the SIAM Activity Group on Optimization

Volume 29 Number 1

December 2021

Contents

Articles
Targeting Exascale with Julia on GPUs for multiperiod optimization with scenario constraints
M Anitescu, K Kim, Y Kim, A Maldonado, F Pacaud, V Rao, M Schanen, S Shin, A Subramanyam 1
Conic optimization for solving convex quadratic optimization with indicators
A Gómez 15

Articles

Targeting Exascale with Julia on GPUs for multiperiod optimization with scenario constraints

Mihai Anitescu, Kibaek Kim, Youngdae Kim, Adrian Maldonado, François Pacaud, Vishwas Rao, Michel Schanen, Sungsho Shin, Anirudh Subramanyam¹

Quantum Physics

(Submitted on 8 Jul 2022)

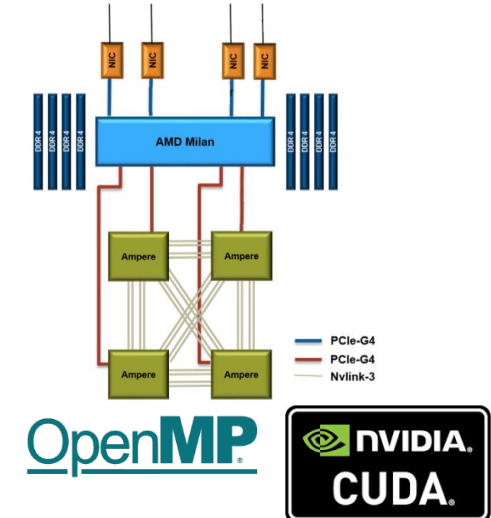
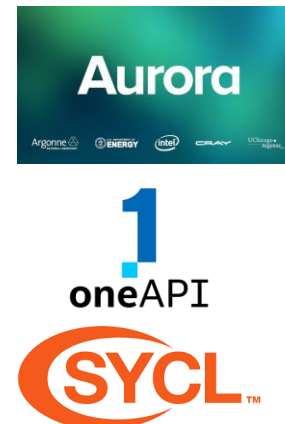
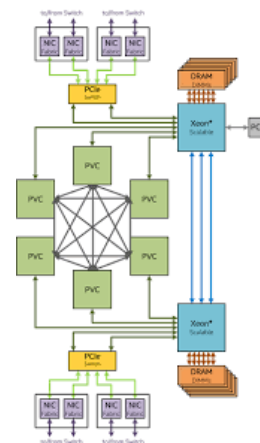
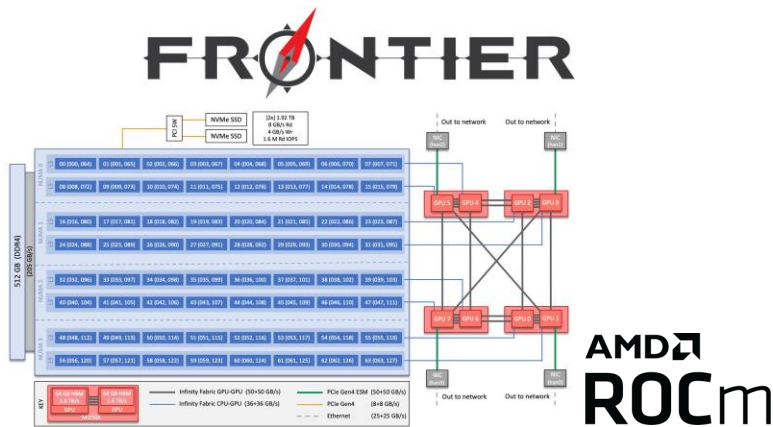
Large-Scale Simulation of Quantum Computational Chemistry on a New Sunway Supercomputer

Honghui Shang, Li Shen, Yifan Fan, Zhiqian Xu, Chu Guo, Jie Liu, Wenhao Zhou, Huan Ma, Rongfen Lin, Yuling Yang, Fang Li, Zhuoya Wang, Yunquan Zhang, Zhenyu Li

Quantum computational chemistry (QCC) is the use of quantum computers to solve problems in computational quantum chemistry. We develop a high performance variational quantum eigensolver (VQE) simulator for simulating quantum computational chemistry problems on a new Sunway supercomputer. The major innovations include: (1) a Matrix Product State (MPS) based VQE simulator to reduce the amount of memory needed and increase the simulation efficiency; (2) a combination of the Density Matrix Embedding Theory with the MPS-based VQE simulator to further extend the simulation range; (3) A three-level parallelization scheme to scale up to 20 million cores; (4) Usage of the Julia script language as the main programming language, which both makes the programming easier and enables cutting edge performance as native C or Fortran; (5) Study of real chemistry systems based on the VQE simulator, achieving nearly linearly strong and weak scaling. Our simulation demonstrates the power of VQE for large quantum chemistry systems, thus paves the way for large-scale VQE experiments on near-term quantum computers.

JACC: Performance Portability and Programming Productivity

- Performance portability is an important target for the DOE
- The DOE leadership computing facilities are GPU-accelerated systems
- Performant portable layers are a priority for DOE: e.g. Kokkos, Raja, OpenMP, OpenACC
- **Program “once” and deploy “everywhere”**

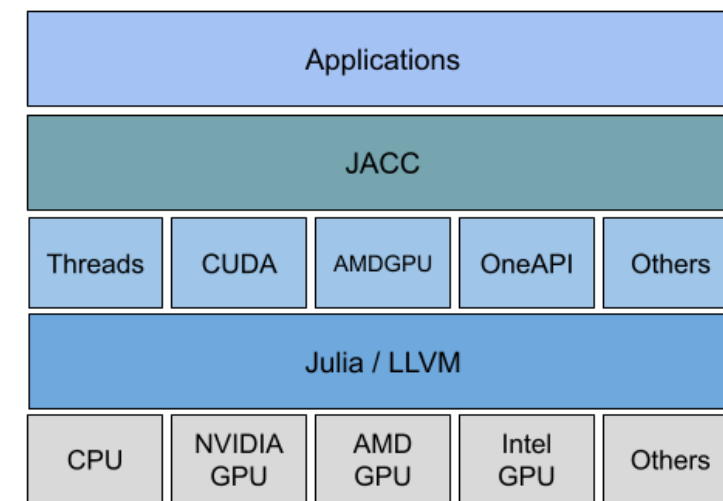


Contents

- Julia's value proposition for science: LLVM + Coordinated Ecosystem
- Efforts in HPC
- **JACC: Julia for Accelerators**
- Resources: where to get started?
- Acknowledgments

JACC (Julia ACCelerated), What is that??

- *Think in Kokkos, but now imagine that it is easy to use*
- The metaprogramming and performance portability model of Julia
 - One code running everywhere
- JACC is a unified Julia front-end in top of multiple backends
 - Threads (CPUs), CUDA (NVIDIA GPUs), AMDGPU (AMD GPUs), and OneAPI (Intel GPUs)
- Hide low-level and device specific implementation
 - Memory, granularity, etc.
- Improve programming productivity for Science and HPC
- A growing community (family)
 - BNL(NERSC), Argonne, MIT, ETHZ, FI/CCQ, ...
 - You are welcome to join (JACC meetings once a month)



JACC model, How to use it??

- **Descriptive, not prescriptive**
- Two main components
- JACC.Array
 - An alias to the corresponding backend memory management
- JACC.parallel_for and JACC.parallel_reduce
 - Kernel passed an argument
 - Uni-dimensional and bi-dimensional APIs
- JACC.ones or JACC.zeros
- JACC.shared
 - Exploit in-chip programable GPUs shared memory

```
# Unidimensional arrays
function axpy(i, alpha, x, y)
    x[i] += alpha * y[i]
end
function dot(i, x, y)
    return x[i] * y[i]
end
SIZE = 1_000_000
x = round.(rand(Float64, SIZE) * 100)
y = round.(rand(Float64, SIZE) * 100)
alpha = 2.5
dx = JACC.Array(x)
dy = JACC.Array(y)
JACC.parallel_for(SIZE, axpy, alpha, dx, dy)
res = JACC.parallel_reduce(SIZE, dot, dx, dy)

# Multidimensional arrays
function axpy(i, j, alpha, x, y)
    x[i,j] = x[i,j] + alpha * y[i,j]
end
function dot(i, j, x, y)
    return x[i,j] * y[i,j]
end
SIZE = 1_000
x = round.(rand(Float64, SIZE, SIZE) * 100)
y = round.(rand(Float64, SIZE, SIZE) * 100)
alpha = 2.5
dx = JACC.Array(x)
dy = JACC.Array(y)
JACC.parallel_for((SIZE, SIZE), axpy, alpha, dx, dy)
res = JACC.parallel_reduce((SIZE, SIZE), dot, dx, dy)
```

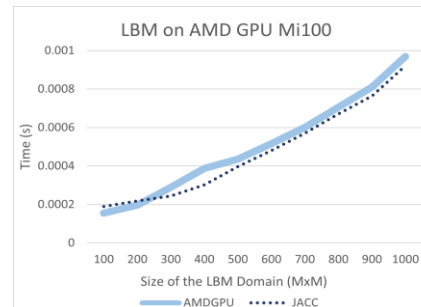
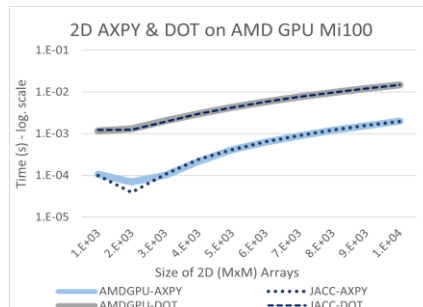
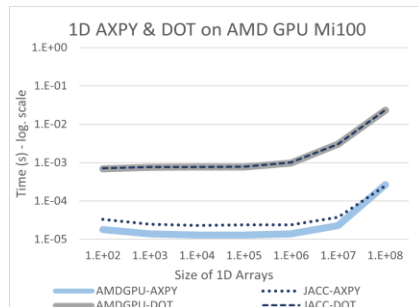
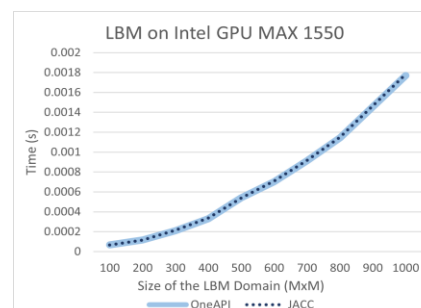
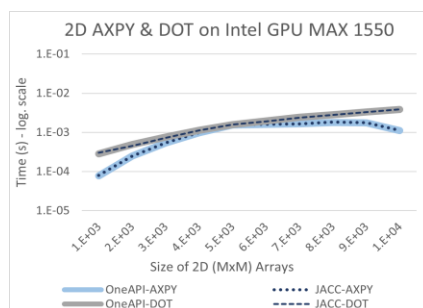
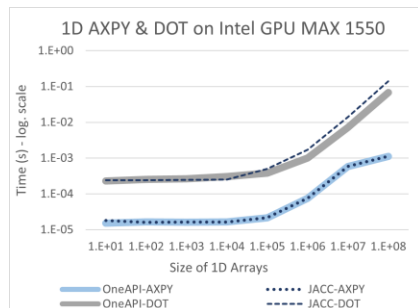
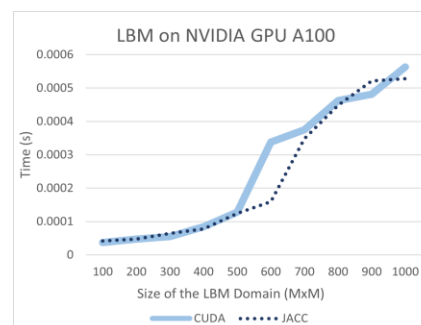
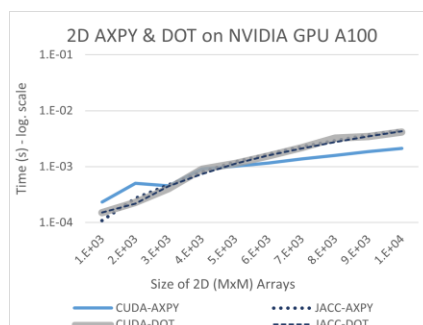
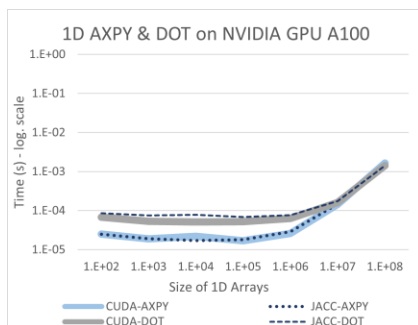
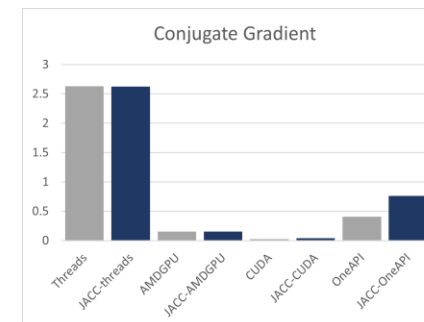
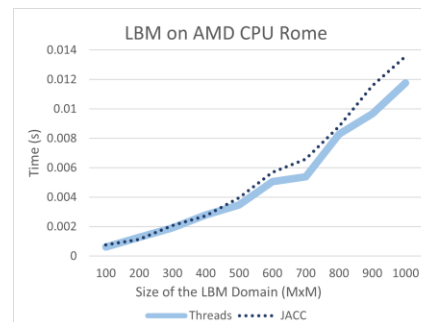
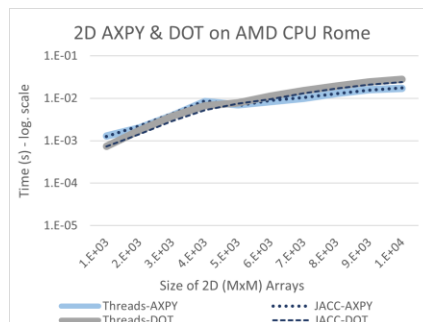
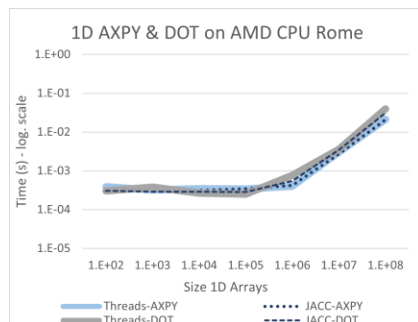
How is JACC implemented??

- *The simpler the better, use everything that Julia can provide*
- Every JACC front-end capability has to be implemented many times
 - One implementation per backend

```
#JACC.Array and JACC.parallel_for on top of
Threads
function __init__()
    const JACC.Array = Base.Array{T,N} where {T,N}
end
#Unidimensional
function parallel_for(N::I, f::F, x...) where {I<:
    Integer,F<:Function}
    Threads.@sync Threads.@threads for i in 1:N
        f(i, x...)
    end
end
#Multidimensional
function parallel_for((M, N)::Tuple{I,I}, f::F, x
    ...) where {I<:Integer,F<:Function}
    Threads.@sync Threads.@threads for j in 1:N
        for i in 1:M
            f(i, j, x...)
        end
    end
end
```

```
#JACC.Array and JACC.parallel_for on top of CUDA
function __init__()
    const JACC.Array = CUDA.CuArray{T,N} where {T,N}
end
#Unidimensional
function _parallel_for_cuda(f, x...)
    i = ( blockIdx().x - 1) * blockDim().x +
        threadIdx().x
    f(i, x...)
    return nothing
end
function JACC.parallel_for(N::I, f::F, x...) where
    {I<:Integer,F<:Function}
    maxPossibleThreads = attribute(device(),CUDA.
        DEVICE_ATTRIBUTE_MAX_BLOCK_DIM_X)
    cuda_threads = min(N, maxPossibleThreads)
    cuda_blocks = ceil(Int, N/cuda_threads)
    CUDA.@sync @cuda threads=cuda_threads blocks=
        cuda_blocks _parallel_for_cuda(N, f, x...)
end
#Multidimensional
function _parallel_for_cuda_MN(f,x...)
    i = ( blockIdx().x - 1) * blockDim().x +
        threadIdx().x
    j = ( blockIdx().y - 1) * blockDim().y +
        threadIdx().y
    f(i, j, x...)
    return nothing
end
function JACC.parallel_for((M, N)::Tuple{I,I}, f::
    F, x...) where {I<:Integer,F<:Function}
    numThreads = 16
    Mthreads = min(M, numThreads)
    Nthreads = min(N, numThreads)
    Mblocks = ceil(Int, M/Mthreads)
    Nblocks = ceil(Int, N/Nthreads)
    CUDA.@sync @cuda threads=(Mthreads, Nthreads)
        blocks=(Mblocks, Nblocks)
        _parallel_for_cuda_MN(f, x...)
end
```

OK, but this is HPC, What about performance??



Julia as a unifying end-to-end workflow language on the Frontier exascale system. [SC Workshops 2023: 1989-1999](https://arxiv.org/abs/2309.10292)
<https://arxiv.org/abs/2309.10292>

Evaluating performance and portability of high-level programming models: Julia, Python/Numba, and Kokkos on exascale nodes. [IPDPS Workshops 2023: 373-382](https://arxiv.org/abs/2303.06195)
<https://arxiv.org/abs/2303.06195>

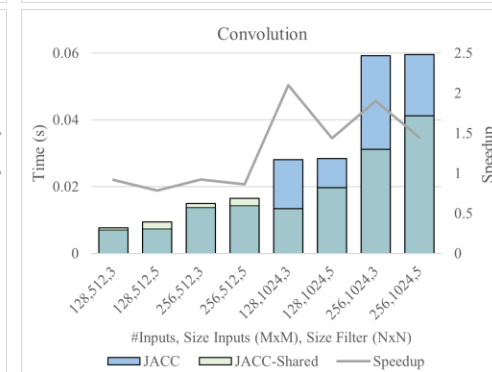
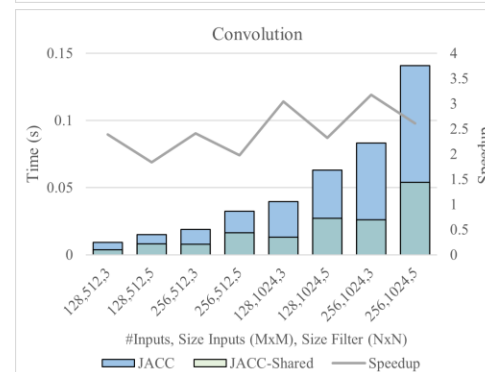
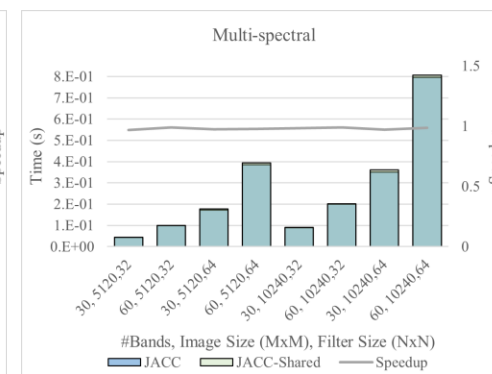
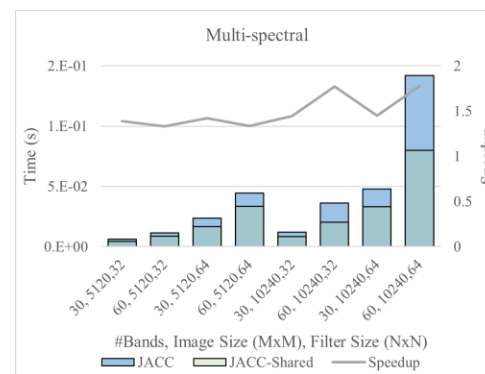
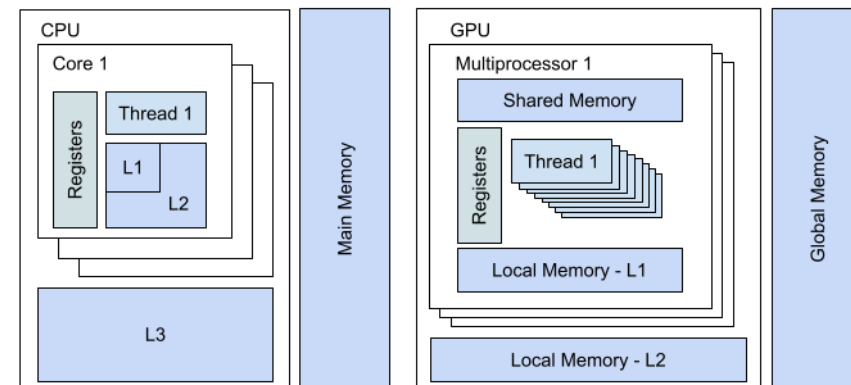
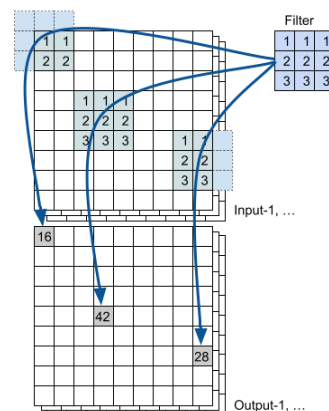
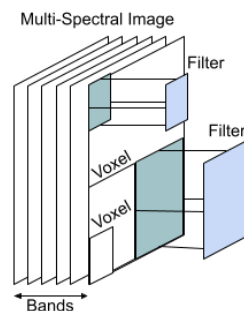
Ongoing efforts??

- JACC.Shared
 - Exploiting high-bandwidth programmable in-chip GPUs memory

```
function spectral(i, j, image, filter, num_bands)
  for b in 1:bands
    @inbounds image[b, i, j] *= filter[j]
  end
end
```

```
function spectral_shared(i, j, image, filter,
  num_bands)
  #Shared memory initialization
  filter_shared = JACC.shared(filter)
  for b in 1:bands
    @inbounds image[b, i, j] *= filter_shared[j]
  end
end
```

```
num_bands = 60
num_voxel = 10_240
size_voxel = 64*64
image = init_image(Float32,
  num_bands, num_voxel, size_voxel)
filter = init_filter(Float32, size_voxel)
jimage = JACC.Array(image)
jimage_shared = JACC.Array(image)
jfilter = JACC.Array(filter)
JACC.parallel_for((num_voxel, size_voxel),
  spectral[_shared], jimage, jfilter, num_bands)
```



Ongoing efforts??

- JACC.experimental
 - A separate JACC module to explore new ideas
 - Once the ideas are well implemented, these can be “promoted”
 - JACC.shared
- JACC.BLAS
 - BLAS library on top of JACC
 - Extend the capabilities of JACC to math libraries
 - Working on BLAS level-1 routines
 - Het Mankad
- JACC.multi
 - Support for multi-device
- JACC.auto
 - Support for auto-tuning
- DAGGER.jl
 - Having JACC as a backend or/and having DAGGER as a JACC backend (JACC.task)

Contents

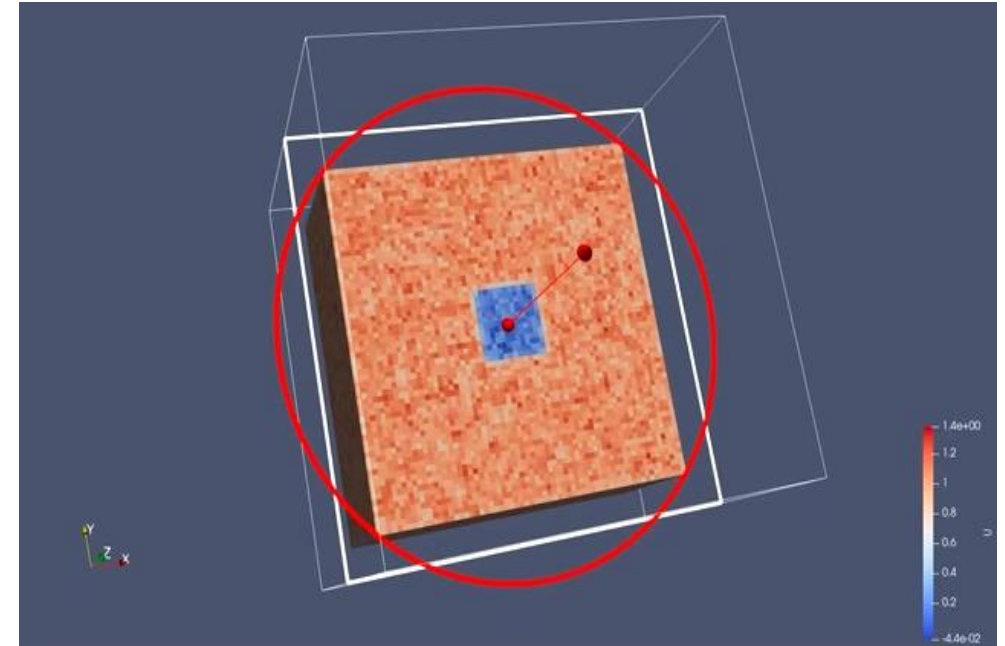
- Welcome
- Julia's value proposition for science: LLVM + Coordinated Ecosystem
- Update: Efforts in HPC
- **Resources: where to get started?**
- Acknowledgments

Contents

- Julia's value proposition for science: LLVM + Coordinated Ecosystem
- Efforts in HPC
- JACC: Julia for Accelerators
- **Resources: where to get started?**
- Acknowledgments

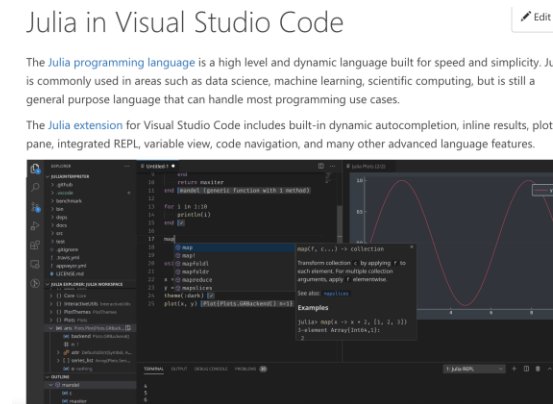
Tutorial Material

- <https://github.com/JuliaORNL/GrayScott.jl>
- Simple 3D 2-variable diffusion-reaction solver
 - Branch “GrayScott-JACC”
 - CPU Threads, CUDA.jl and AMDGPU.jl backends using JACC and [weakdependencies]
 - Parallel I/O ADIOS2, can be visualized with ParaView
 - MPI.jl for communication
 - Configuration and job scripts for Odo/Frontier under ./scripts/



Where to get started?

- Pick a gentle tutorial: <https://techytok.com/from-zero-to-julia/>
- <https://github.com/ornl-training/julia-basics> (training by WF Godoy & Philip Fackler) OLCF Tutorial: <https://juliaornl.github.io/TutorialJuliaHPC/applications/GrayScott/01-Solver.html>
- Use VS Code as the official IDE + debugger
- JuliaCon talks are available on YouTube
- <https://discourse.julialang.org/> Stackoverflow might be outdated, <https://julialang.slack.com/>
- Julia docs and standard library: <https://docs.julialang.org/en/v1/>
- Learn: Project.toml, Testing.jl @testset @test, Pluto.jl , CUDA.jl/AMDGPU.jl , JACC.jl, KernelAbstractions.jl, LinearAlgebra.jl , Makie.jl , Plots.jl and Flux.jl (AI/ML), how to build a sysimage with PackageCompiler.jl
- **Pick problems you care about! Let us know if you're interested in a hackathon.**
- Patience and community reliance: learning a language is a big investment.



GitHub Copilot (GPT-3/Codex), Large Language Models + Julia

Julia is a more targeted language (like Fortran)

Julia + LLMs are a powerful combination for
productivity

GitHub Copilot on VS Code \$100/year/account

Compared several languages + parallel
programming models

C++, Fortran, Python, Julia. Fortran and Julia
scored high!

RESEARCH-ARTICLE

Evaluation of OpenAI Codex for HPC Parallel Programming Models Kernel Generation

Authors: William Godoy, Pedro Valero-Lara, Keita Teranishi, Prasanna Balaprakash, Jeffrey Vetter [Authors Info & Claims](#)

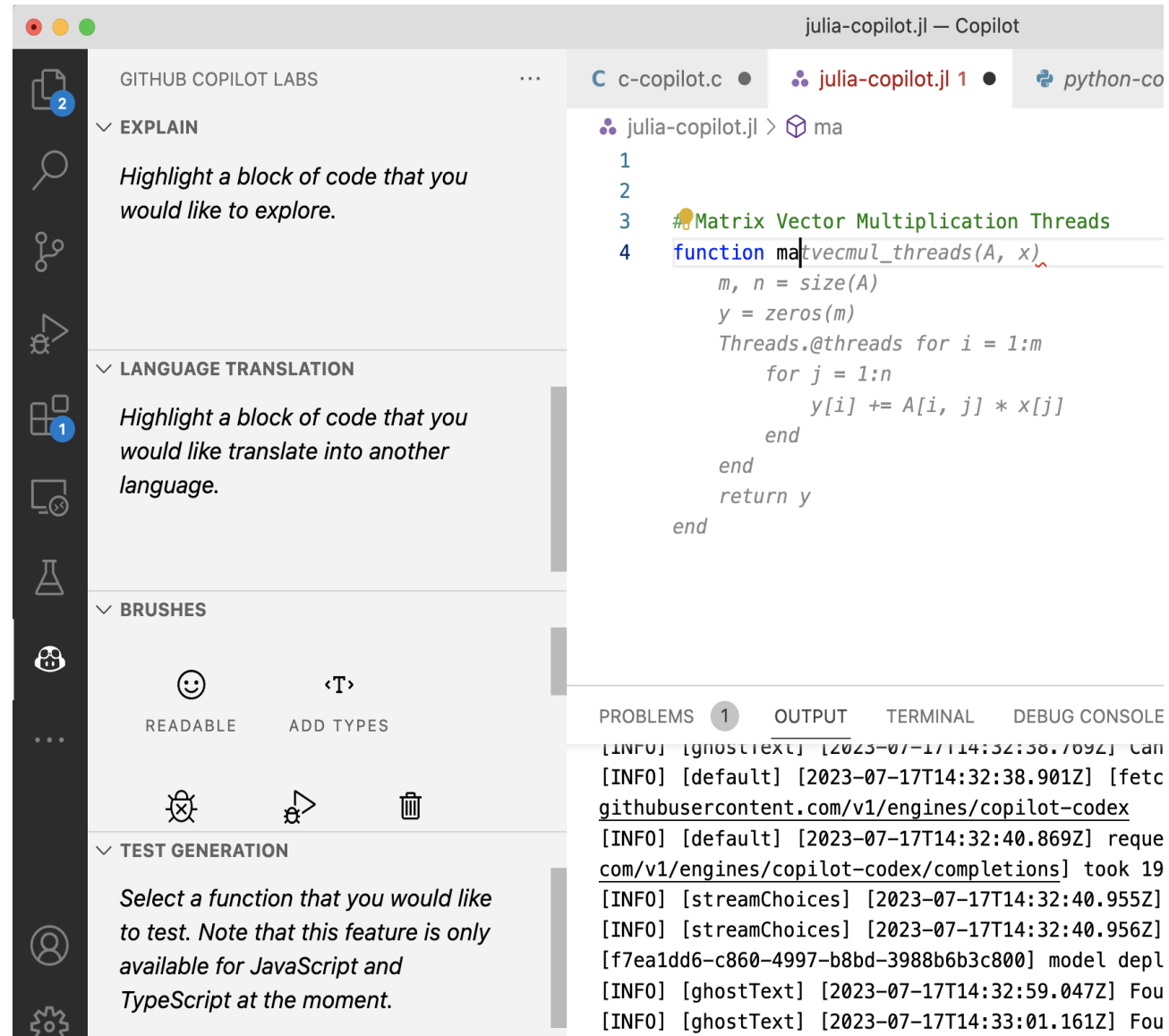
ICPPW '23: Proceedings of the 52nd International Conference on Parallel Processing Workshops • August 2023 • Pages 136–144
• <https://doi.org/10.1145/3605731.3605886>

Comparing Llama-2 and GPT-3 LLMs for HPC kernels generation

Pedro Valero-Lara¹, *0000-0002-1479-4310],
Alexis Huante²0009-0008-2818-0265],
Mustafa Al Lai²0009-0000-0326-6363],
William F. Godoy¹0000-0002-2590-5178],
Keita Teranishi¹0000-0001-6647-2690],
Prasanna Balaprakash¹0000-0002-0292-5715],
Jeffrey S. Vetter¹0000-0002-2449-6720]

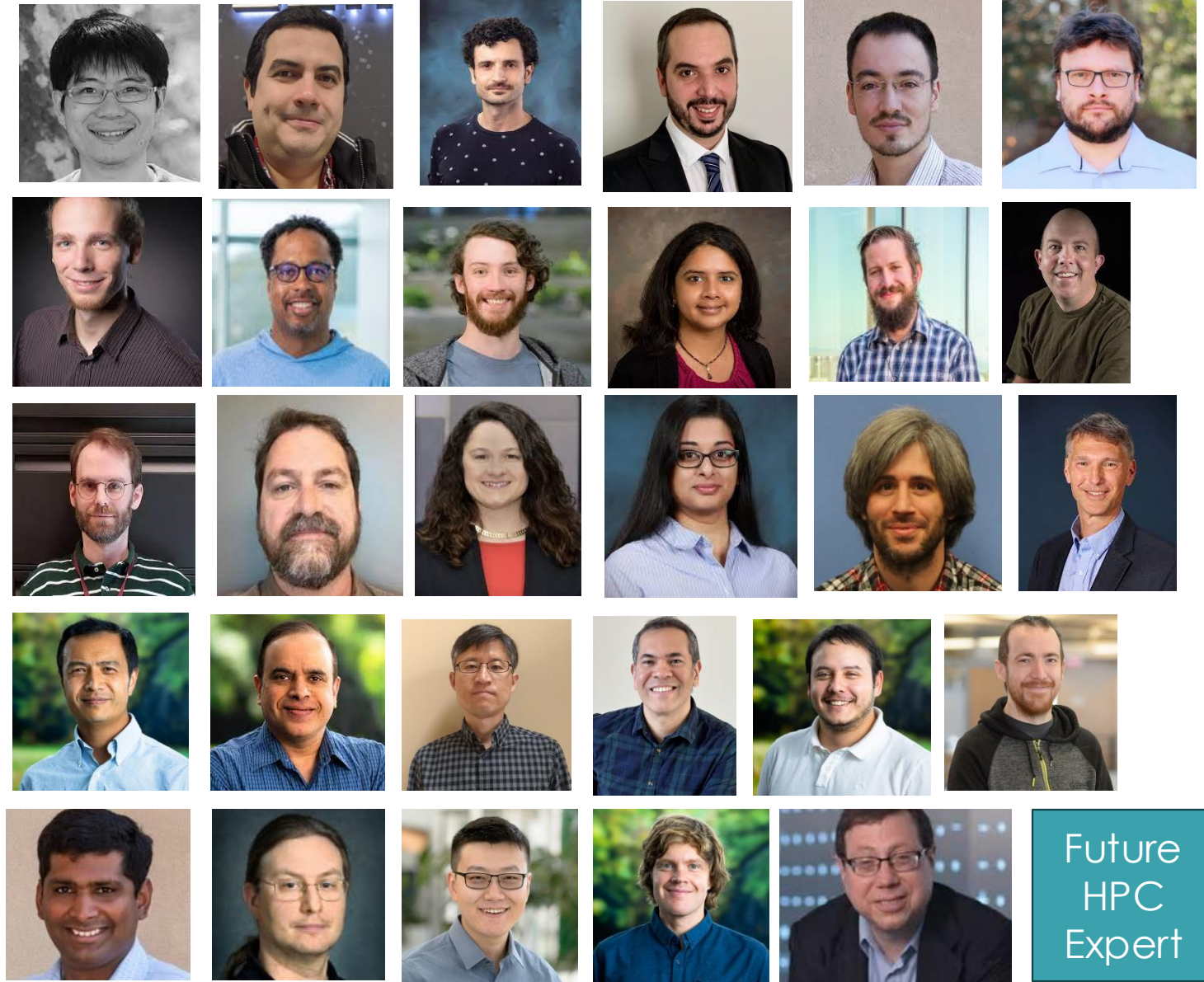
¹ Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
² Texas A&M International University, Laredo, Texas 78041, USA

*Corresponding author: valerolarap@ornl.gov



S4PST: Stewardship of Programming Systems and Tools (2024-2029)

- PI: Keita Teranishi (ORNL), Co-PIs: Pedro Valero-Lara, William F Godoy
- 8 National Laboratories:
 - Oak Ridge National Laboratory
 - Argonne National Laboratory
 - Lawrence Livermore National Laboratory
 - Lawrence Berkeley National Laboratory
 - Sandia National Laboratories
 - Brookhaven National Laboratory
 - Los Alamos National Laboratory
 - SLAC National Accelerator Laboratory
- University Partners:
 - University of Delaware
 - Massachusetts Institute of Technology
- Collaborations:
 - Louisiana State University
 - Pacific Northwest National Laboratory
 - Carnegie Mellon University
 - University of Tennessee, Knoxville
 - Stanford University
 - Other 6 NSSGT projects



Acknowledgements

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

Co-authors:

- William F Godoy (ORNL-CSMD)
- Pedro Valero-Lara (ORNL-CSMD)
- Het Mankad (ORNL-CSMD)

Organizers: OSDX 2024

Sponsors:

The [ASCR Bluestone Project](#)
[CASS PESO and S4PST projects](#)
OLCF/NERSC



Thanks to the
audience!