Paderborn
Center for
Parallel
Computing

Julia for High-Performance Computing (HPC)

Carsten Bauer

November 7, 2023 @ ECAP
JuliaHEP Workshop

Plan for the Next Two Hours

First hour, three short **talks**:

- Carsten Bauer
- **Mose Giordano** (UCL)
- **Ludovic Räss** (ETHZ)

Second hour, **"HPC" tutorial**

- On Noctua 2 cluster (see image)
- https://github.com/carstenbauer/juliahep-hpctutorial

What is “HPC”?

“HPC” == I’m running code on a **supercomputer**?

- Efficiency?
- No **MPI** no HPC?

What about **GPU(s)**?

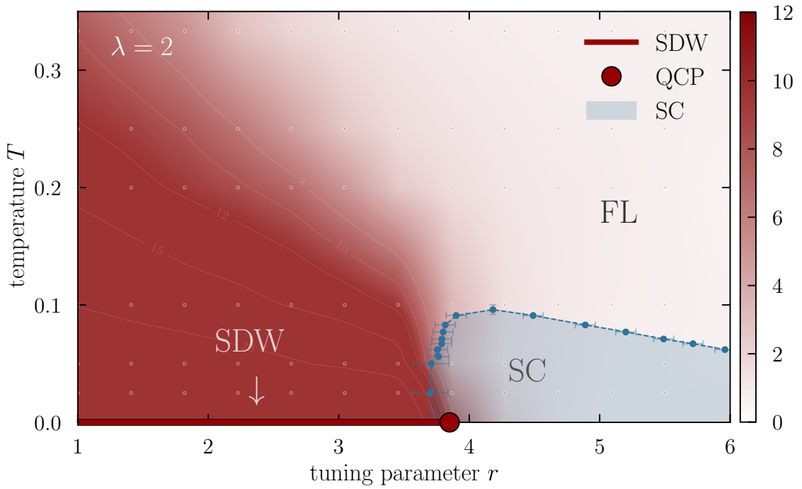
- NVIDIA A100 >> multiple CPU nodes

Trivial parallelisation (replicas)?

Where I Come From

Condensed matter physics / quantum field theory

- Large-scale Quantum Monte Carlo simulations
- O(15 Mio. CPU-core hours)
- O(100 TB)

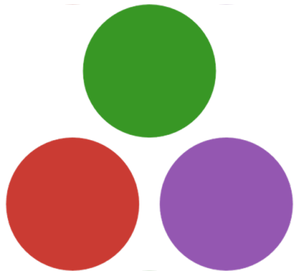


Domain Science

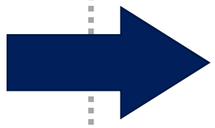
julia

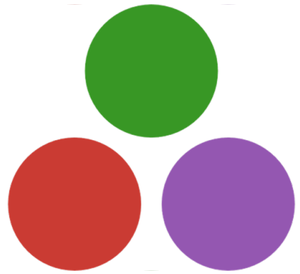
HPC

Inclusive HPC



Domain Science





HPC

LIKWID.jl + Pluto.jl

Counting Flops

```
x = rand(10_000);
```

```
function computation(x)
    x .+ x
end;
```

Counted Flops: 10000

How?

```
using LIKWID
```

```
metrics, events = @perfmon "FLOPS_DP" computation(x);
```

Compute from derived metrics

```
10000
```

```
begin
    flops_per_second = metrics["FLOPS_DP"][1]["DP [MFLOP/s]"] * 1e6
    runtime = metrics["FLOPS_DP"][1]["Runtime (RDTSC) [s]"]
    flops = round(Int, flops_per_second * runtime)
end
```

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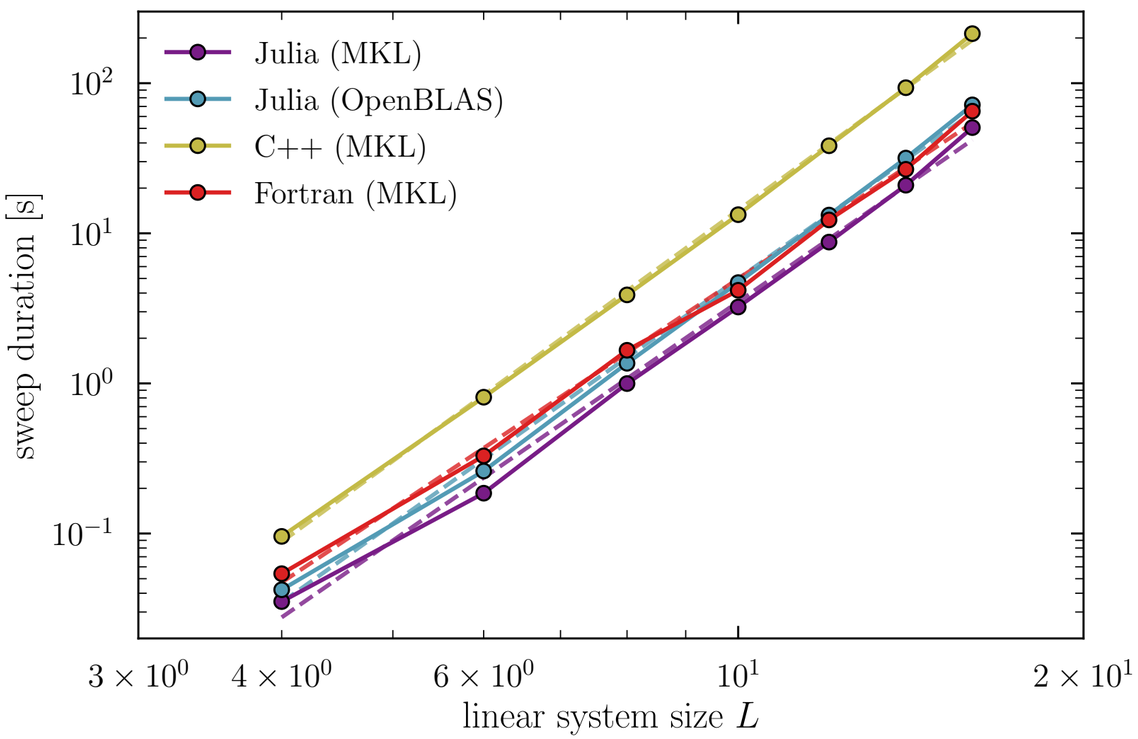
NHR FAU

NHR NATIONALES HOCHLEISTUNGS RECHNEN

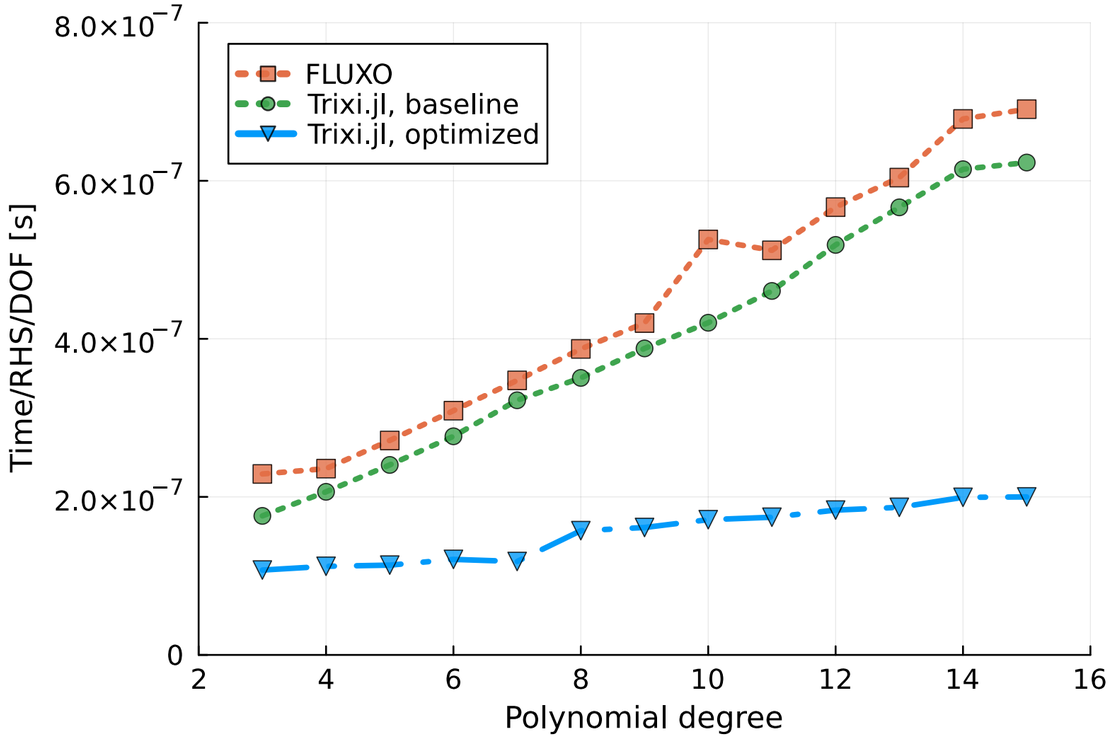
More: https://youtu.be/l2fTNfEDPC0

Julia Can Be Fast



QMC

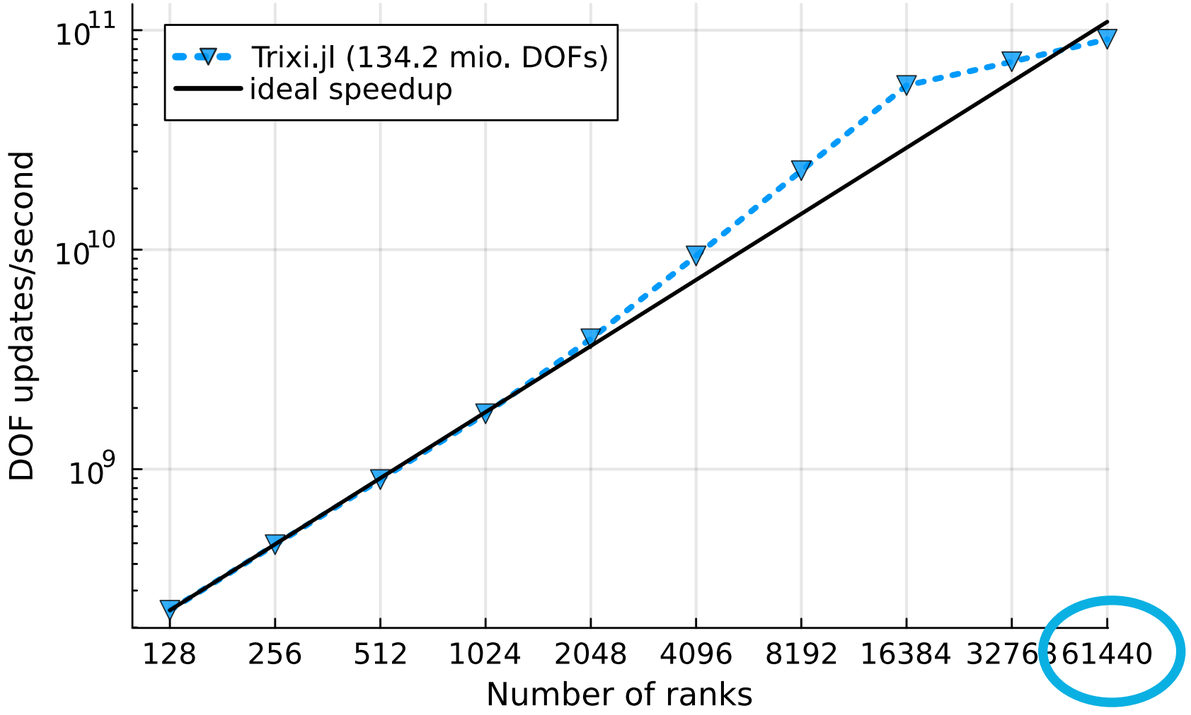
(MonteCarlo.jl)



CFD

(Trixi.jl)

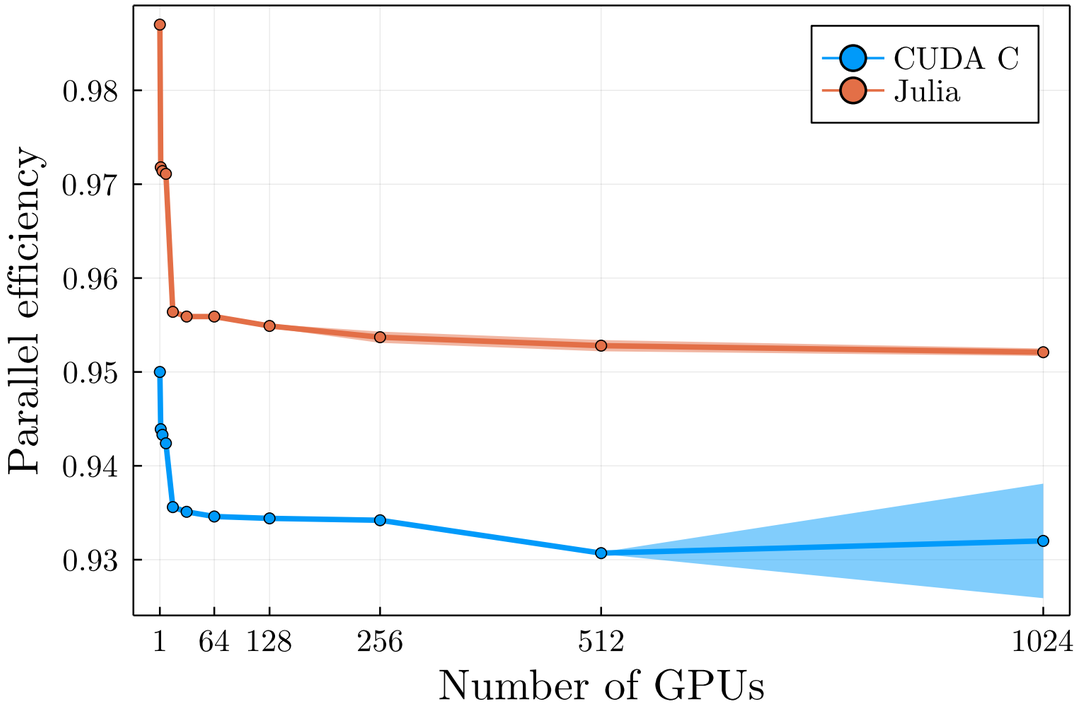
Julia Can Be Parallel



≈ 60k ranks

MPI-Parallel

(Trixi.jl)



GPU-Parallel

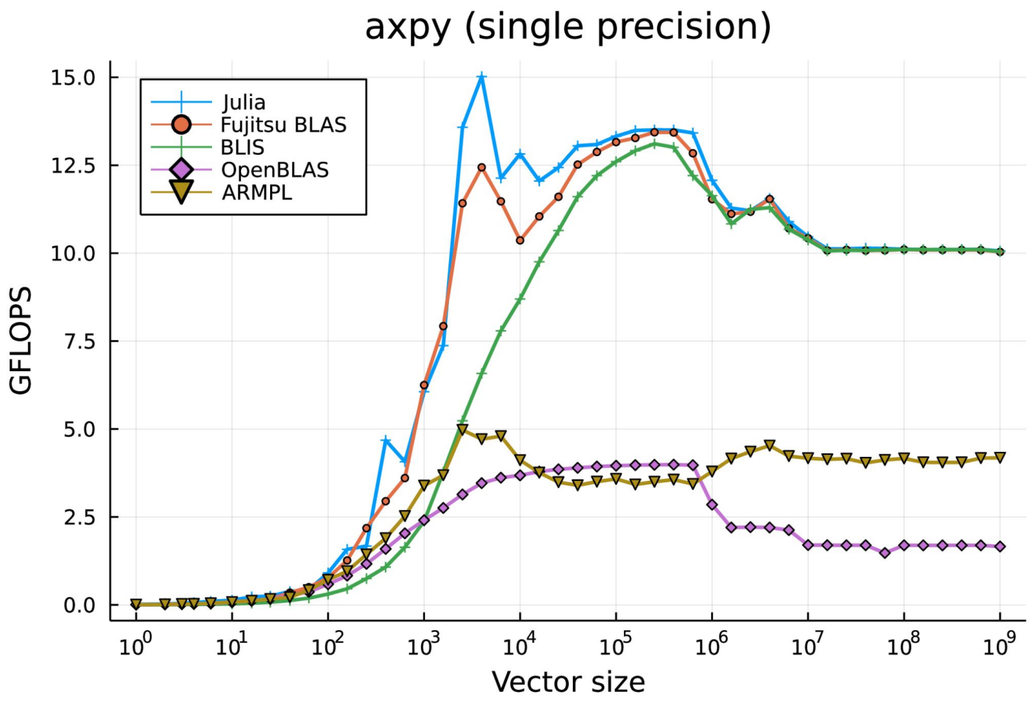
(ParallelStencil.jl)

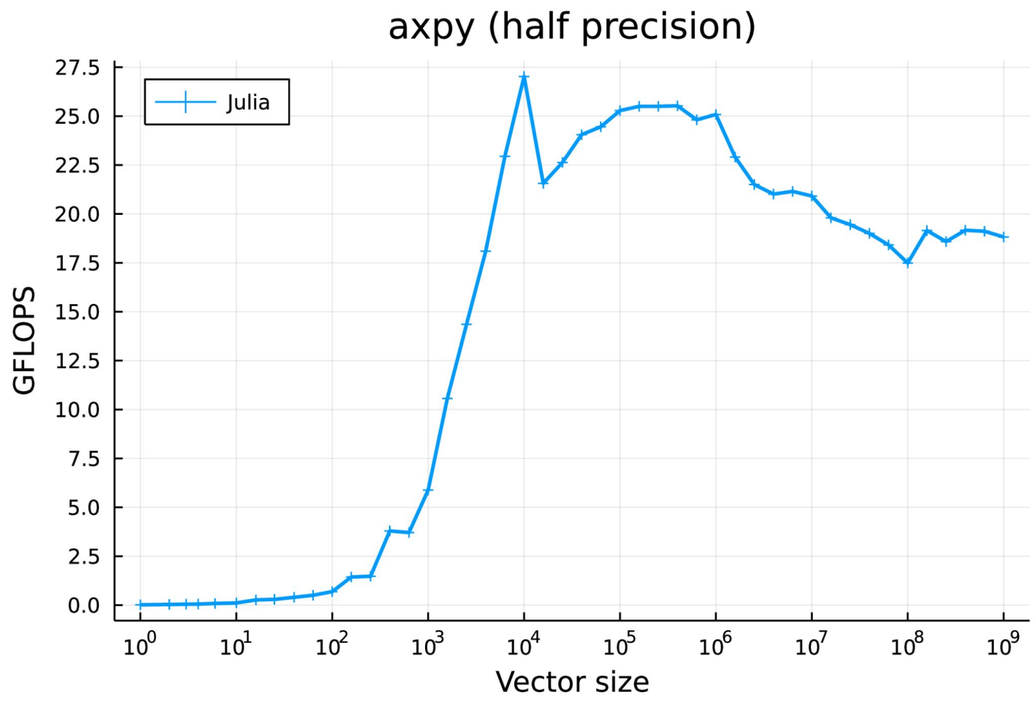
More on GPU → **Ludovic's talk**

Julia Can Be Generic

Fugaku performance benchmarks by Mose Giordano

- arxiv.org/abs/2207.12762





More on AXPY → **HPC tutorial**

Julia Code Is Portable

Laptop

```
➜  ~/myproject  tree
.
├── Manifest.toml
├── Project.toml
└── code.jl

0 directories, 3 files

➜  ~/myproject  cat Project.toml
[deps]
CUDA = "052768ef-5323-5732-b1bb-66c8b64840ba"
DifferentialEquations = "0c46a032-eb83-5123-abaf-570d42b7fbaa"
MKL = "33e6dc65-8f57-5167-99aa-e5a354878fb2"
MPI = "da04e1cc-30fd-572f-bb4f-1f8673147195"

➜  ~/myproject
```

HPC Cluster

```
➜  bauerc@n2login3 myproject  julia --project
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.7.2 (2022-02-06)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

(myproject) pkg> st
      Status `~/myproject/Project.toml`
➜ [052768ef] CUDA v3.11.0
➜ [0c46a032] DifferentialEquations v7.1.0
➜ [33e6dc65] MKL v0.5.0
➜ [da04e1cc] MPI v0.19.2
        Info packages marked with ➜ not downloaded, use `instantiat
e` to download

(myproject) pkg> instantiate
```

(As long as you stay within the Julia-verse. Using **system software** can be tricky.)

New Challenges (at Scale)

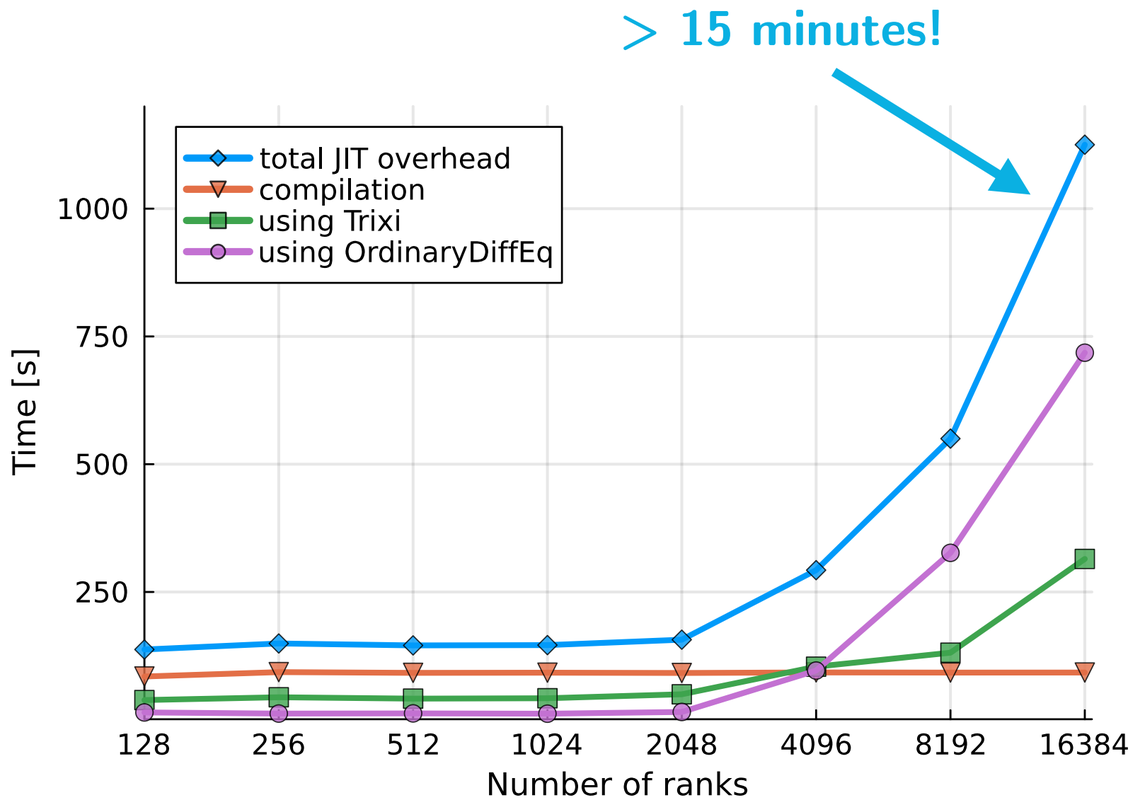
Julia depot can get under (a lot) of pressure!

- Location matters (NFS vs GPFS vs RAM)

Memory footprint, O(1 GB) per proc.

- Increasing since Julia 1.6 😢

Multithreading + GC



Many more challenges: "interactivity at scale", tooling, ...

Julia HPC Projects

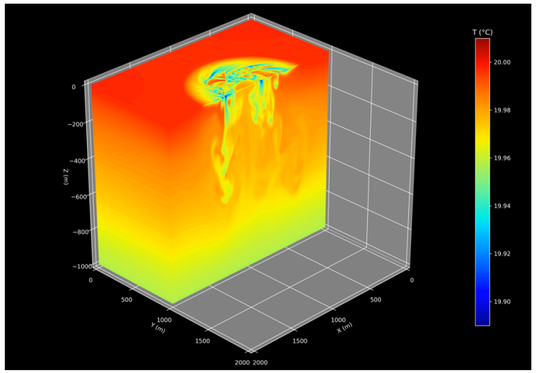
CliMA @ Caltech
- Climate Modeling Alliance

CESMIX @ MIT
- Exascale simulation of materials in extreme environments

Trixi @ RWTH Aachen / HLRS
- Computational fluid dynamics

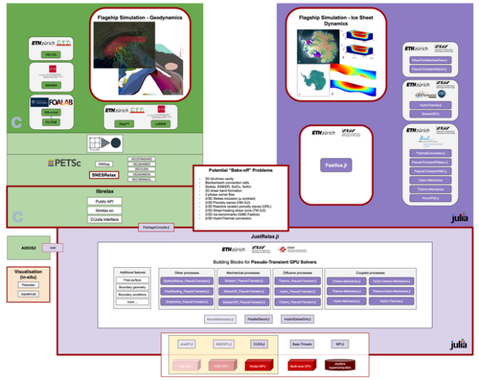
GPU4GEO @ ETH / CSCS
- Computational earth science
- → **Ludovic's talk**

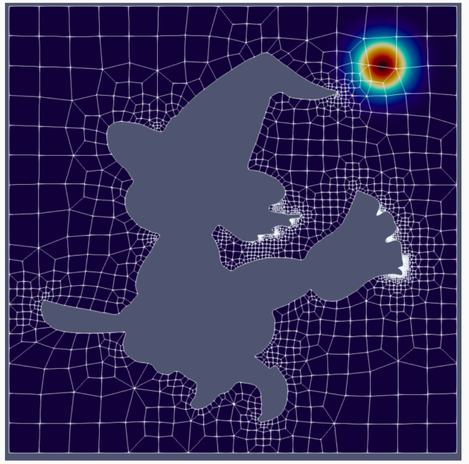
...



Oceananigans.jl

EXASCALE COMPUTING PROJECT





Credit: Andrew R. Winters

Julia HPC Community

Julia Slack

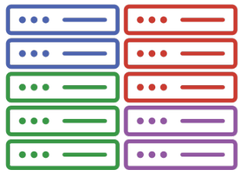
- #hpc
- #distributed
- #performance-helpdesk

Monthly Julia HPC call

- https://julialang.org/community/#events

At conferences

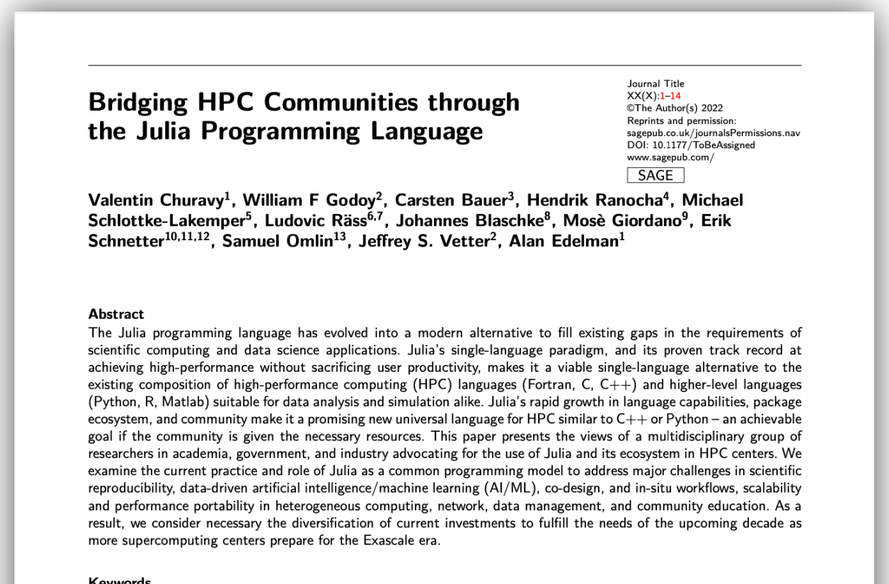
- JuliaCon23, **SC23**, PASC23, SIAM CSE 23, ...

JULIA FOR HPC

JuliaCon 2023 Minisymposium

arxiv.org/abs/2211.02740



Bridging HPC Communities through the Julia Programming Language

Journal Title
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DOI: 10.1177/ToBeAssigned
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Valentin Churavy[1], William F Godoy[2], Carsten Bauer[3], Hendrik Ranocha[4], Michael Schlottke-Lakemper[5], Ludovic Räss[6,7], Johannes Blaschke[8], Mosè Giordano[9], Erik Schnetter[10,11,12], Samuel Omlin[13], Jeffrey S. Vetter[2], Alan Edelman[1]

Abstract

The Julia programming language has evolved into a modern alternative to fill existing gaps in the requirements of scientific computing and data science applications. Julia's single-language paradigm, and its proven track record at achieving high-performance without sacrificing user productivity, makes it a viable single-language alternative to the existing composition of high-performance computing (HPC) languages (Fortran, C, C++) and higher-level languages (Python, R, Matlab) suitable for data analysis and simulation alike. Julia's rapid growth in language capabilities, package ecosystem, and community make it a promising new universal language for HPC similar to C++ or Python – an achievable goal if the community is given the necessary resources. This paper presents the views of a multidisciplinary group of researchers in academia, government, and industry advocating for the use of Julia and its ecosystem in HPC centers. We examine the current practice and role of Julia as a common programming model to address major challenges in scientific reproducibility, data-driven artificial intelligence/machine learning (AI/ML), co-design, and in-situ workflows, scalability and performance portability in heterogeneous computing, network, data management, and community education. As a result, we consider necessary the diversification of current investments to fulfill the needs of the upcoming decade as more supercomputing centers prepare for the Exascale era.

Summary

- **Julia can be a great option for HPC!**
  - serial and parallel performance on-par with Fortran/C/C++
  - portability and high-productivity
  - new opportunities, e.g. interactive HPC

- **New challenges**
  - workflow / interactivity at scale, Julia depot, system binaries, …

- **“Early adoption” cost**
  - Julia for HPC is a niche
  - lack of support, tooling, …

The Julia for HPC community is small but vibrant. Join us!