PyFR and GiMMiK on Intel KNL

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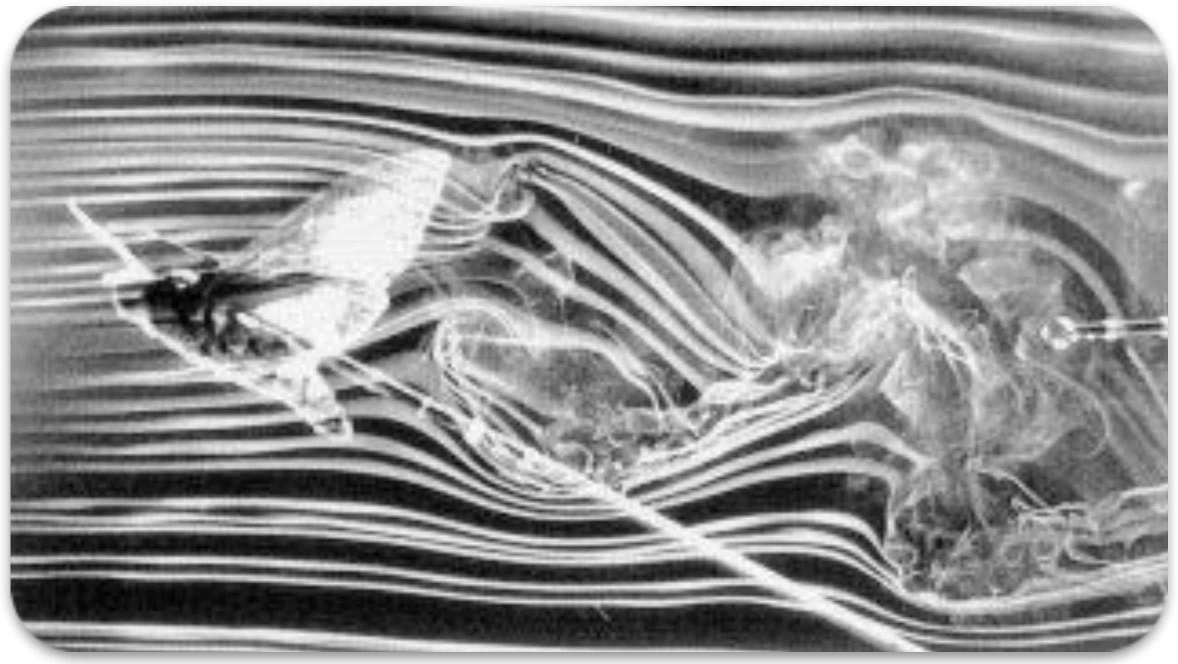
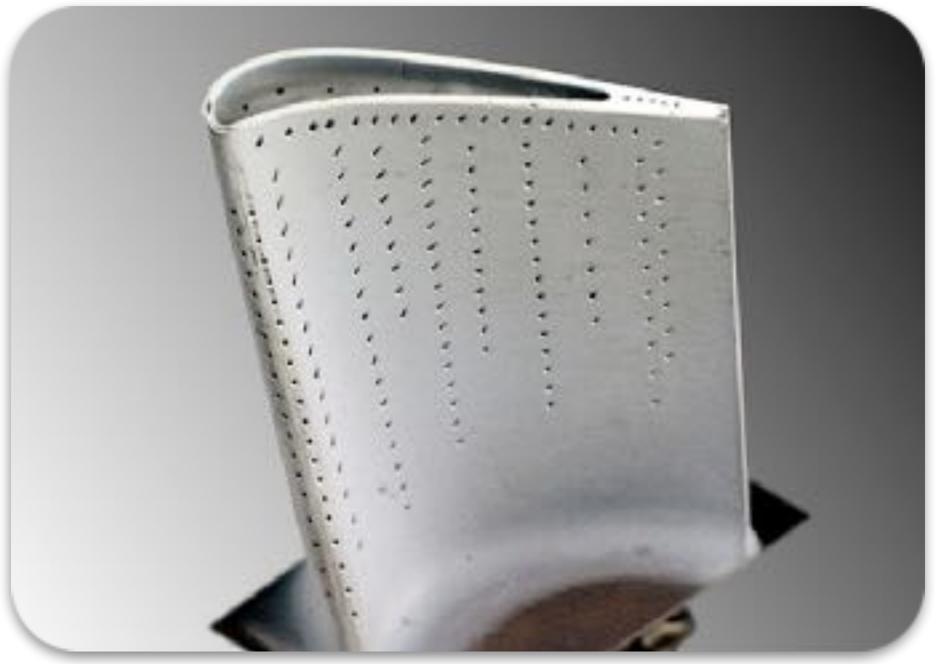
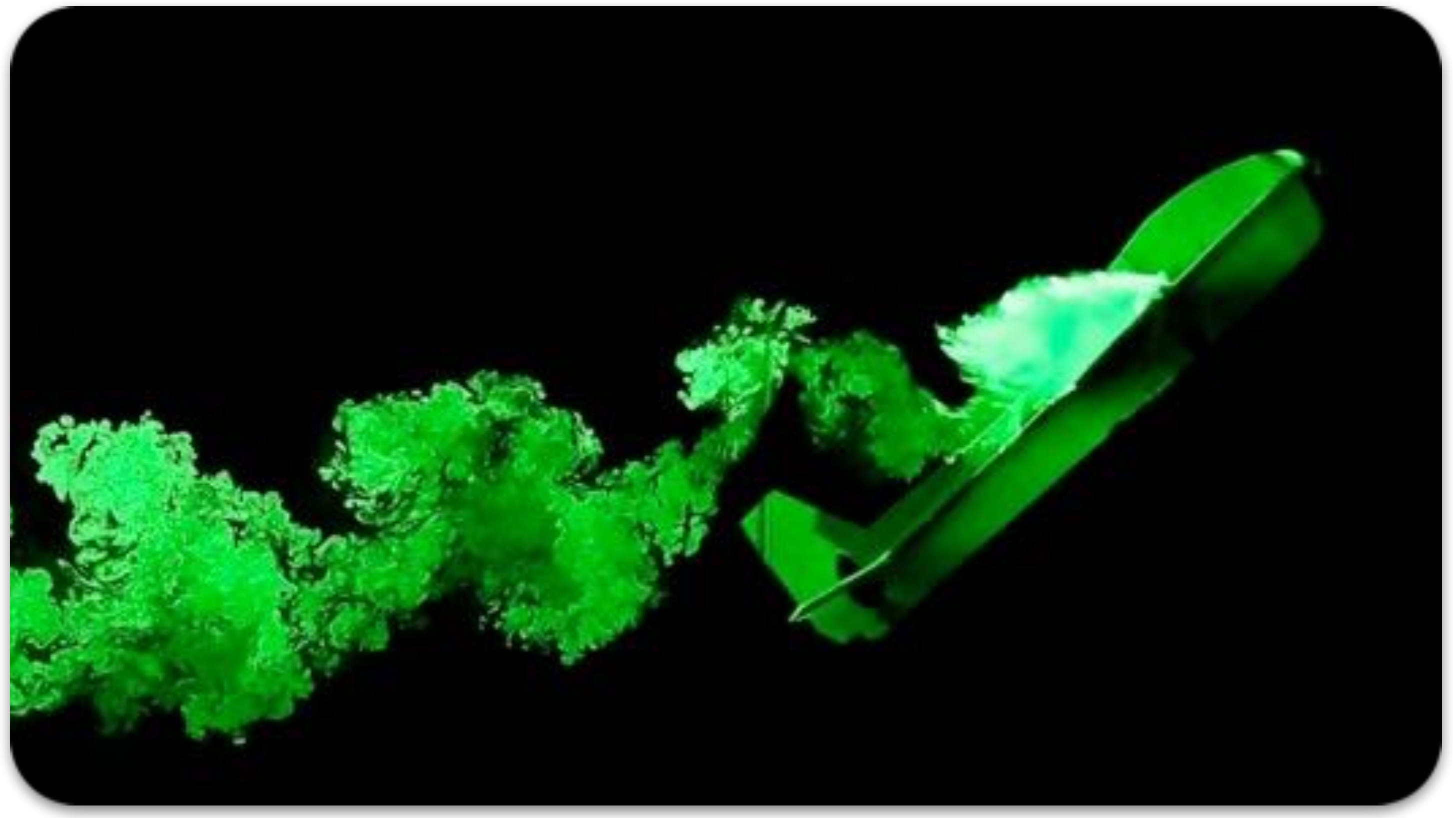
Motivation: Turbulent Flows


- Interested in simulating unsteady, turbulent, flows.





The PyFR Framework

- Uses high-order **flux reconstruction** (FR) to solve the compressible **Navier–Stokes** equations on mixed **unstructured grids** with **explicit time stepping**.

The PyFR Framework

- **Performance portable** across a range of platforms.
- Finalist for the **2016 Gordon Bell Prize**.

The PyFR Framework

- Existing support for KNC based around **offloading via pyMIC**.

PyFR

- Python outer layer.

Python Outer Layer
(**Hardware Independent**)

- Setup
- Distributed memory parallelism
- Outer ‘for’ loop and calls to **hardware specific kernels**

PyFR

- Need to generate **hardware specific kernels**.

Python Outer Layer
(**Hardware Independent**)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to **hardware specific kernels**

PyFR

- In FR **two types** of kernel are required.

Python Outer Layer
(**Hardware Independent**)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to **hardware specific kernels**

Matrix Multiply Kernels

- Data interpolation/ extrapolation etc.

Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

PyFR

- Matrix multiplications are quite simple.

Python Outer Layer
(**Hardware Independent**)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to **hardware specific kernels**

Matrix Multiply Kernels

- Data interpolation/ extrapolation etc.

Call GEMM

Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

PyFR

- For the point-wise nonlinear kernels we use a DSL.

Python Outer Layer
(**Hardware Independent**)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to **hardware specific kernels**

Matrix Multiply Kernels

- Data interpolation/ extrapolation etc.

Call GEMM

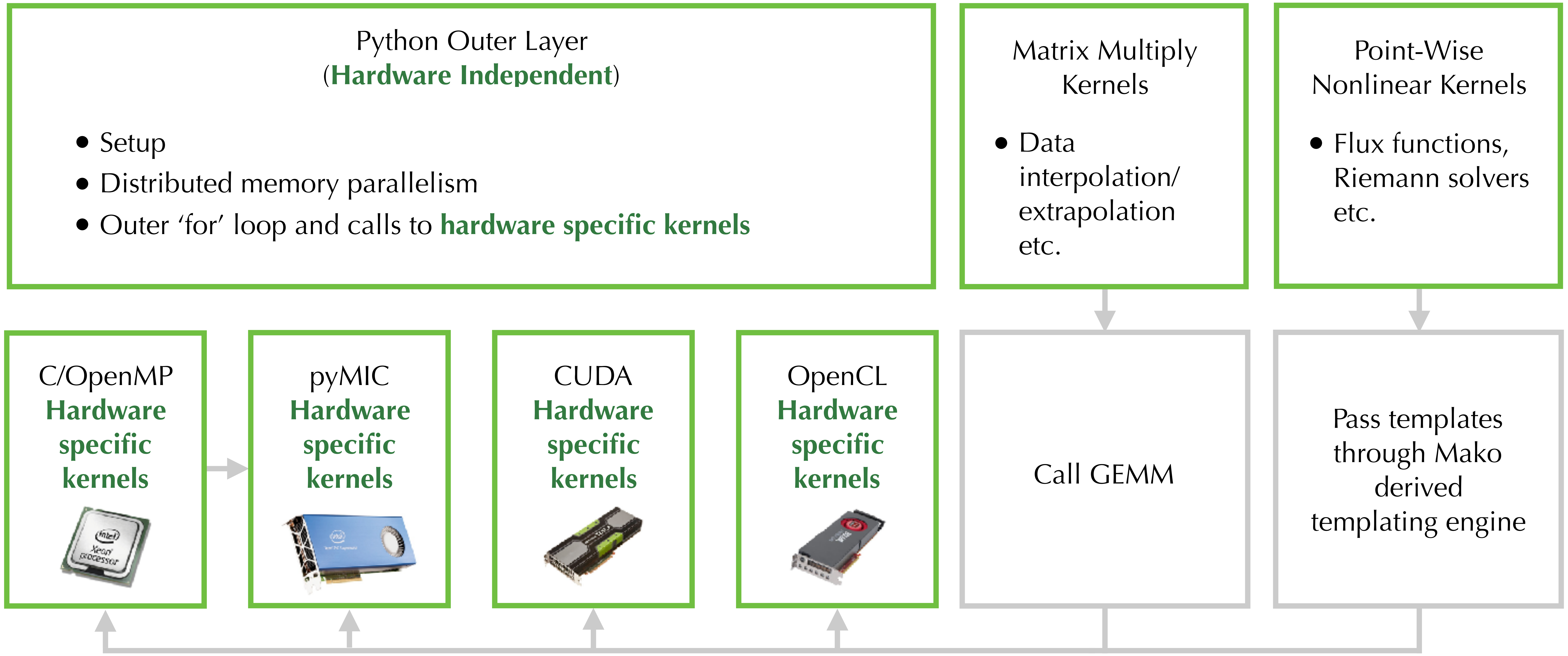
Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

Pass templates through Mako derived templating engine

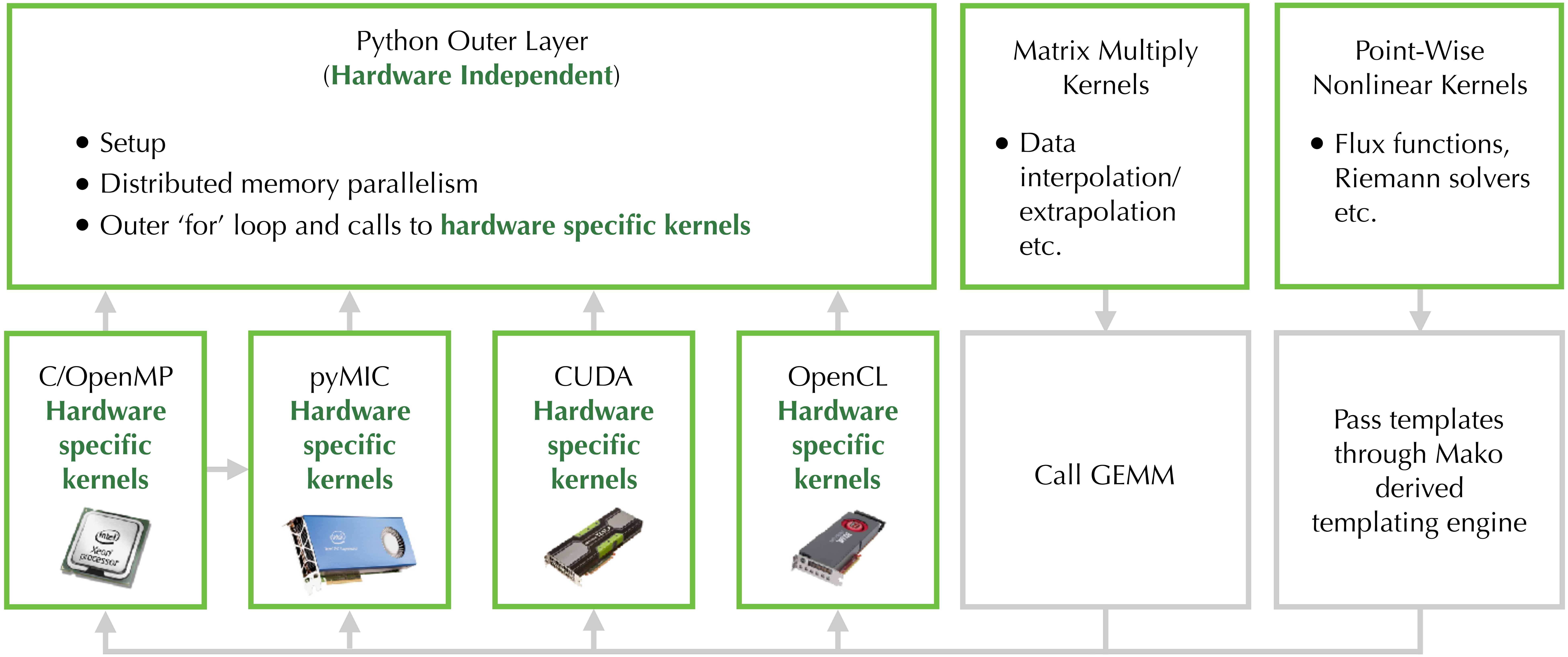
PyFR

- Kernels are generated and compiled at start-up.



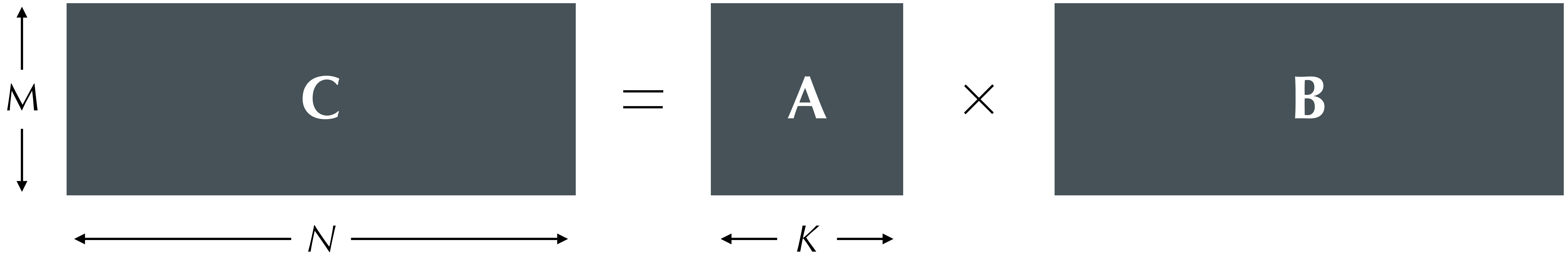
PyFR

- Which may then be called by the outer layer.



Matrix Multiplications in PyFR

- Multiplications are of the **block-by-panel** variety:



- where $N \sim 10^5$ with $N \gg (M, K)$ and **A is constant**.

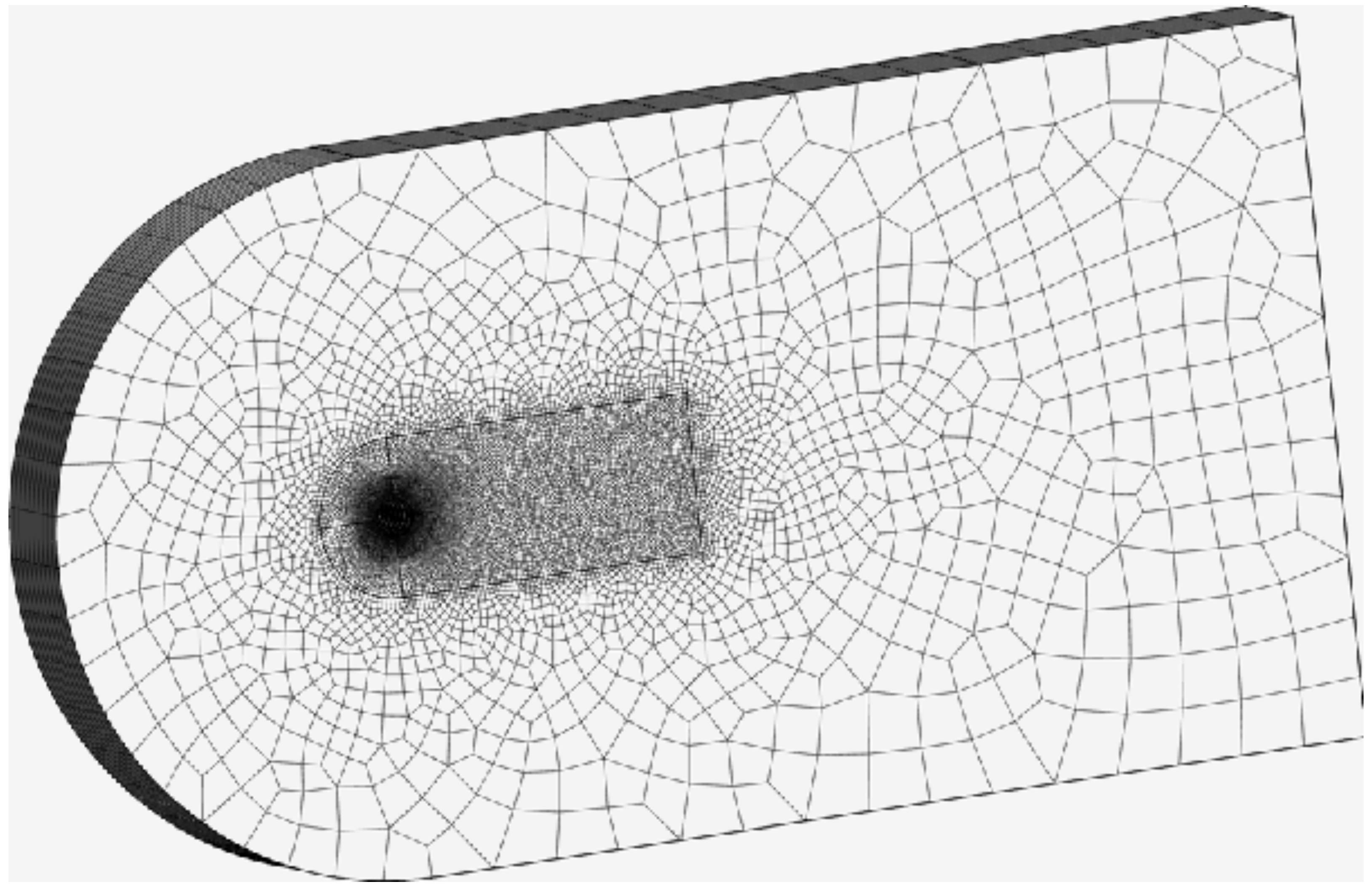
GEMM in PyFR

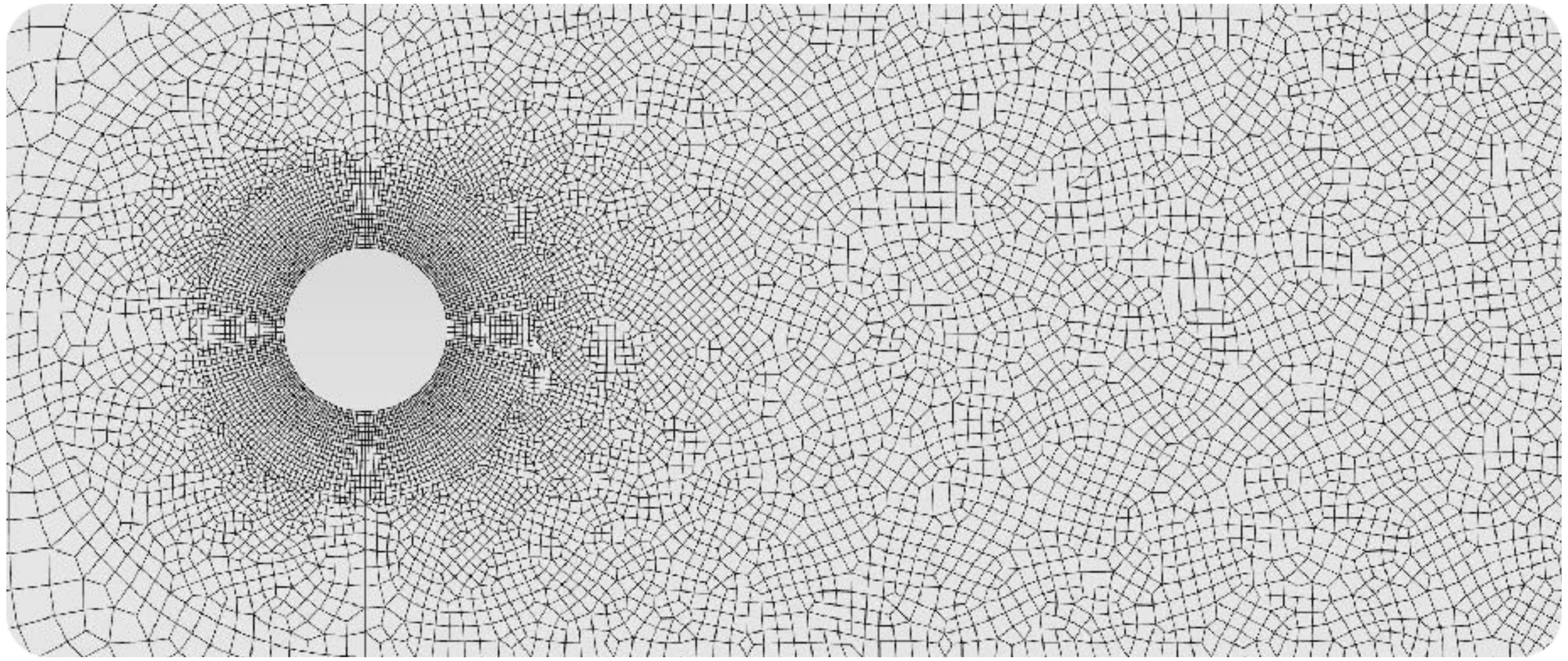
- On x86 S/DGEMM has **three kernels providers**.

	Dense A (Small)	Dense A (Large)	Sparse A (Small)	Sparse A (Large)
MKL	∅	★	∅	∅
GiMMiK	★	∅	★	★
Libxsmm (new)	★★	▲	★★	▲

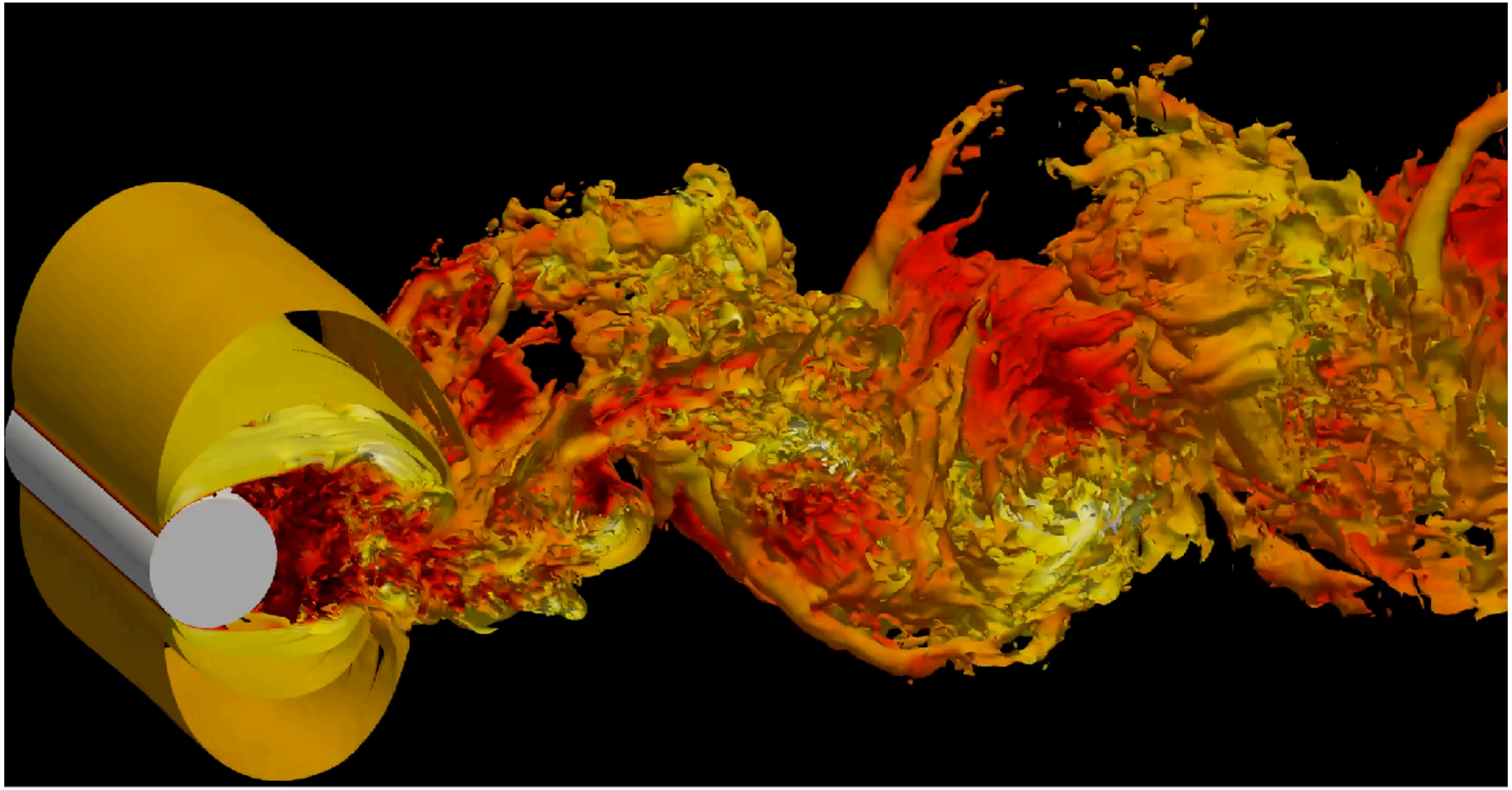
Initial Results

- Flow over a cylinder at **Re = 3,900** and **Ma = 0.2**.
- Quadratically curved hexahedral mesh with **N_E = 118,820**.



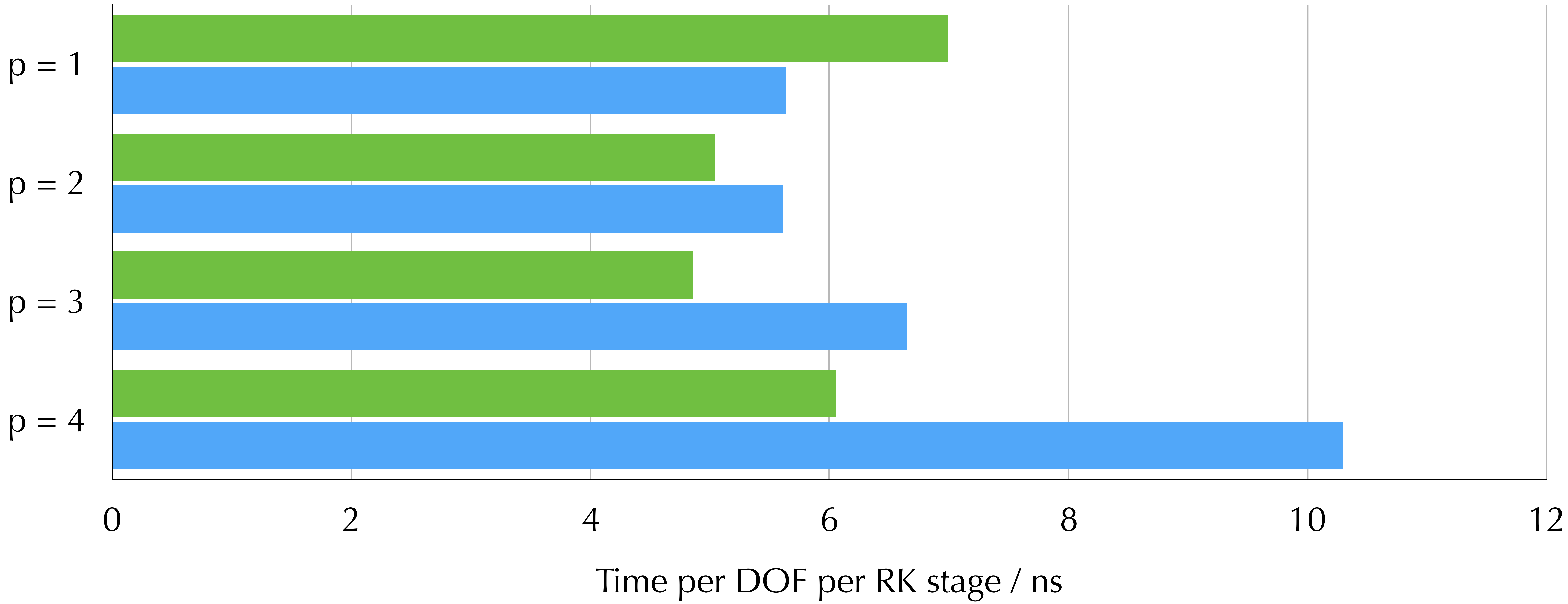


Initial Results



Initial Results

- PyFR 1.4.0: **K40c (cuBLAS)** vs **KNL 7250F (MKL)**.



Initial Results

- Profiling indicates **point-wise kernels** are the bottleneck.
  - **Surprising!**
- Must therefore **rethink our data layout** and **push for further vectorisation**.

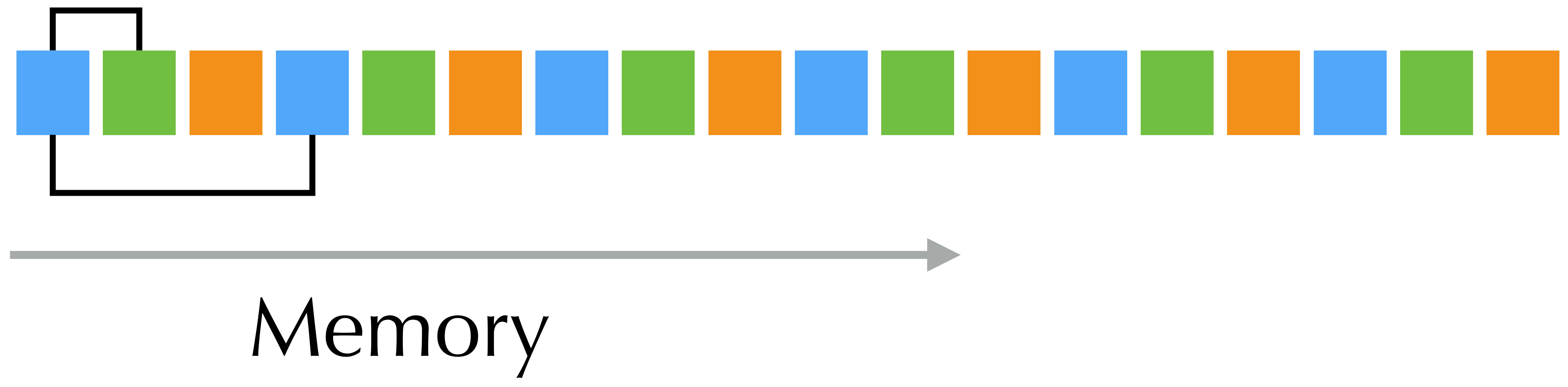
Data Layout 101

- Three main layouts:
  - AoS
  - SoA (used by PyFR 1.4.0)
  - AoSoA(k)

AoS

```
struct
{
    float rho;
    float rhou;
    float E;
} data[NELES];
```

AoS

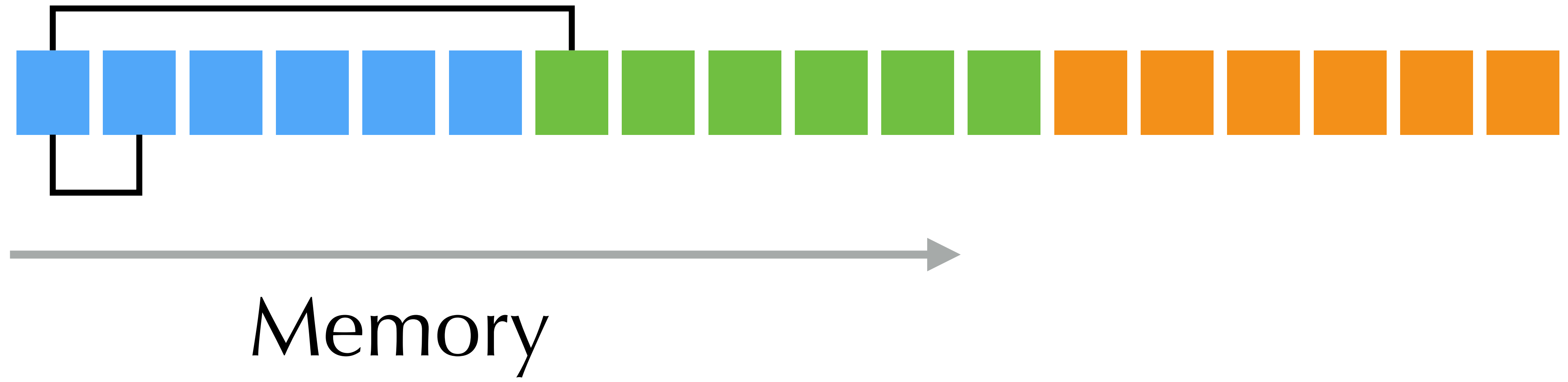


- Cache and TLB friendly.
- Difficult to vectorise.

SoA

```
struct
{
    float rho[NELES];
    float rhou[NELES];
    float E[NELES];
} data;
```

SoA

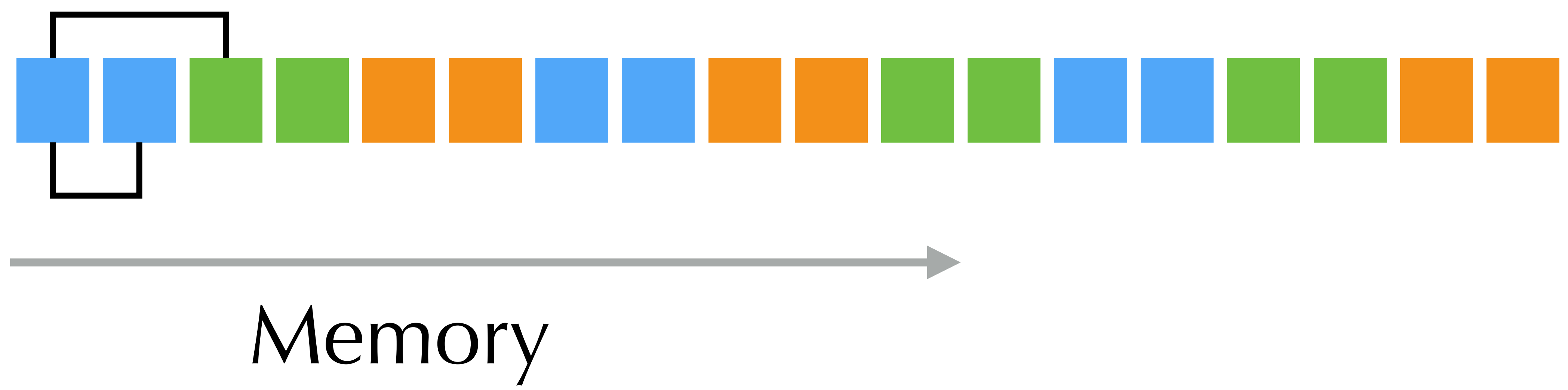


- Trivial to vectorise.
- Can put pressure on TLB and/or hardware pre-fetchers.

AoSoA(k = 2)

```
struct
{
    float rho[k];
    float rhou[k];
    float E[k];
} data[NELES / k];
```

AoSoA(k = 2)



- Can be vectorised efficiently for suitable k.
- Cache and TLB friendly.

AoSoA($k = 2$)

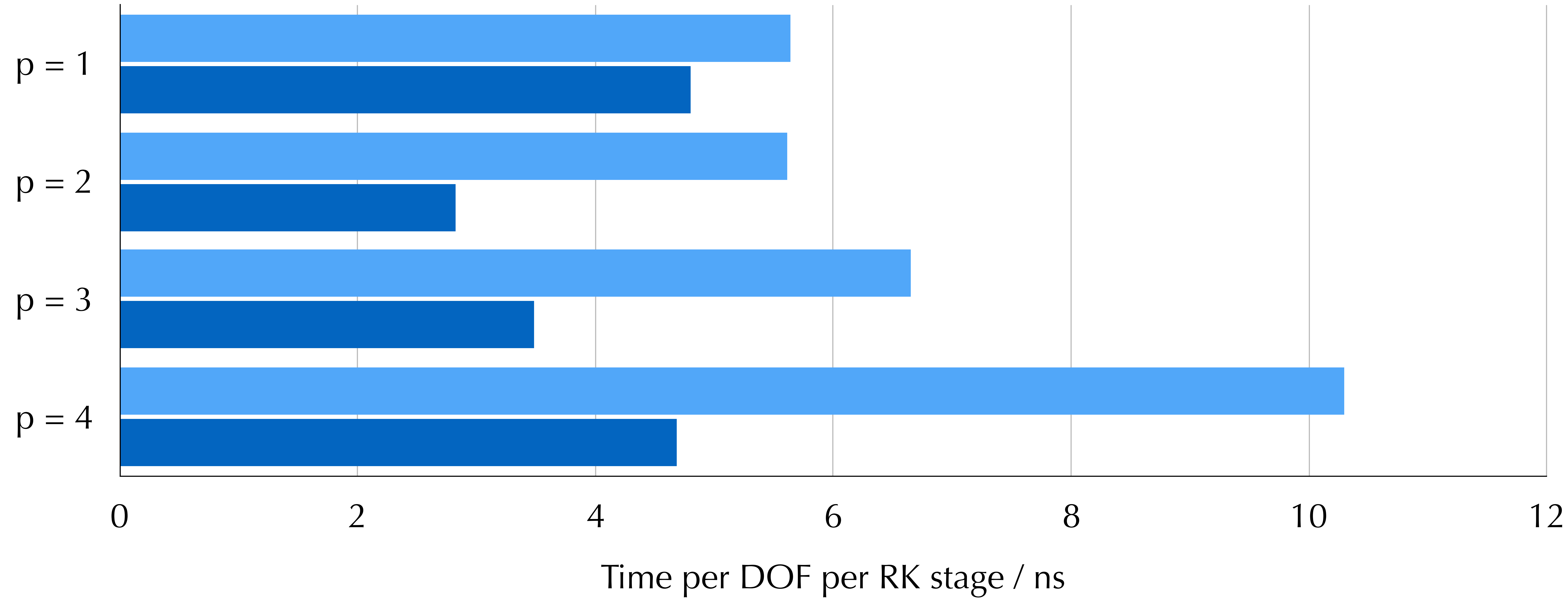
- The Goldilocks solution
  - …albeit at the cost of **messy indexing**
  - …also requires **coaxing for compilers to vectorise**.

AoSoA($k = 2$)

- Here PyFR's DSL **pays dividends**.
- Iteration and indexing are **hidden from kernels**.
- Can therefore **change data structures with ease**.

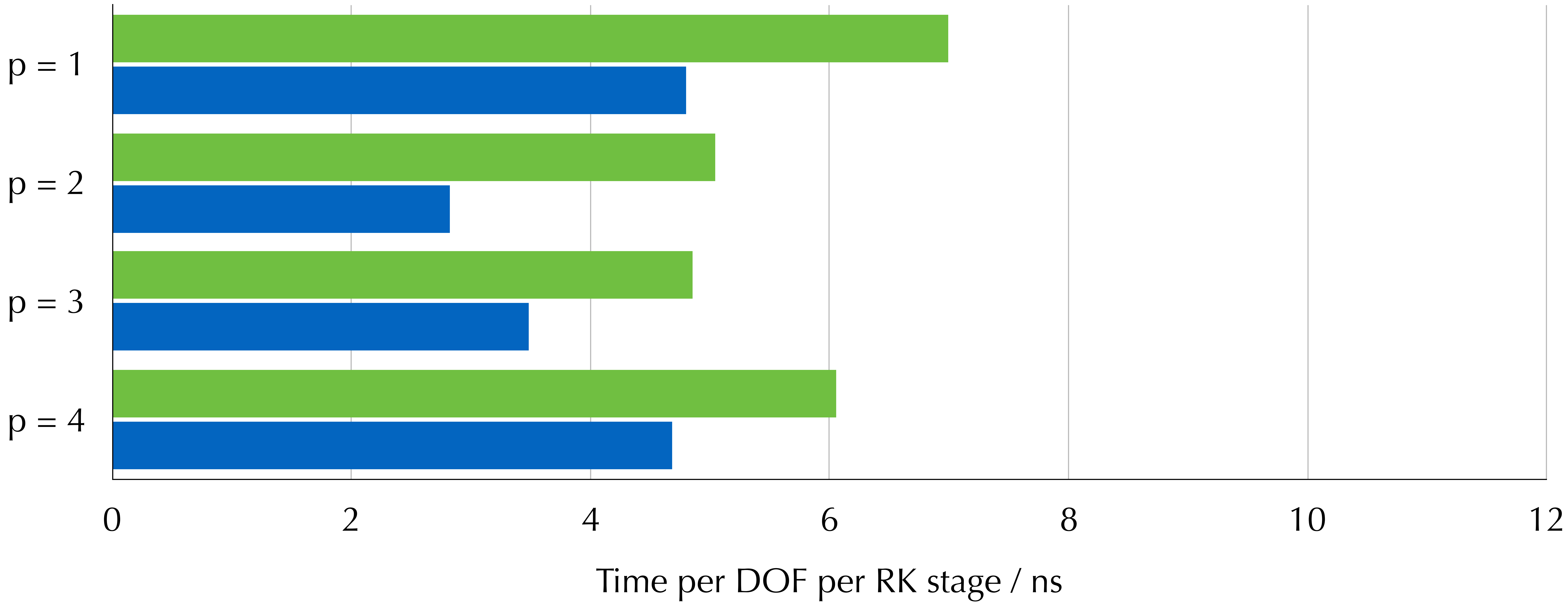
AoSoA(k) Results

- PyFR 1.4.0 **KNL (MKL)** vs PyFR 1.5.0 **KNL (MKL)**.



AoSoA(k) Results

- Comparing with PyFR 1.4.0 **K40c (cuBLAS)**

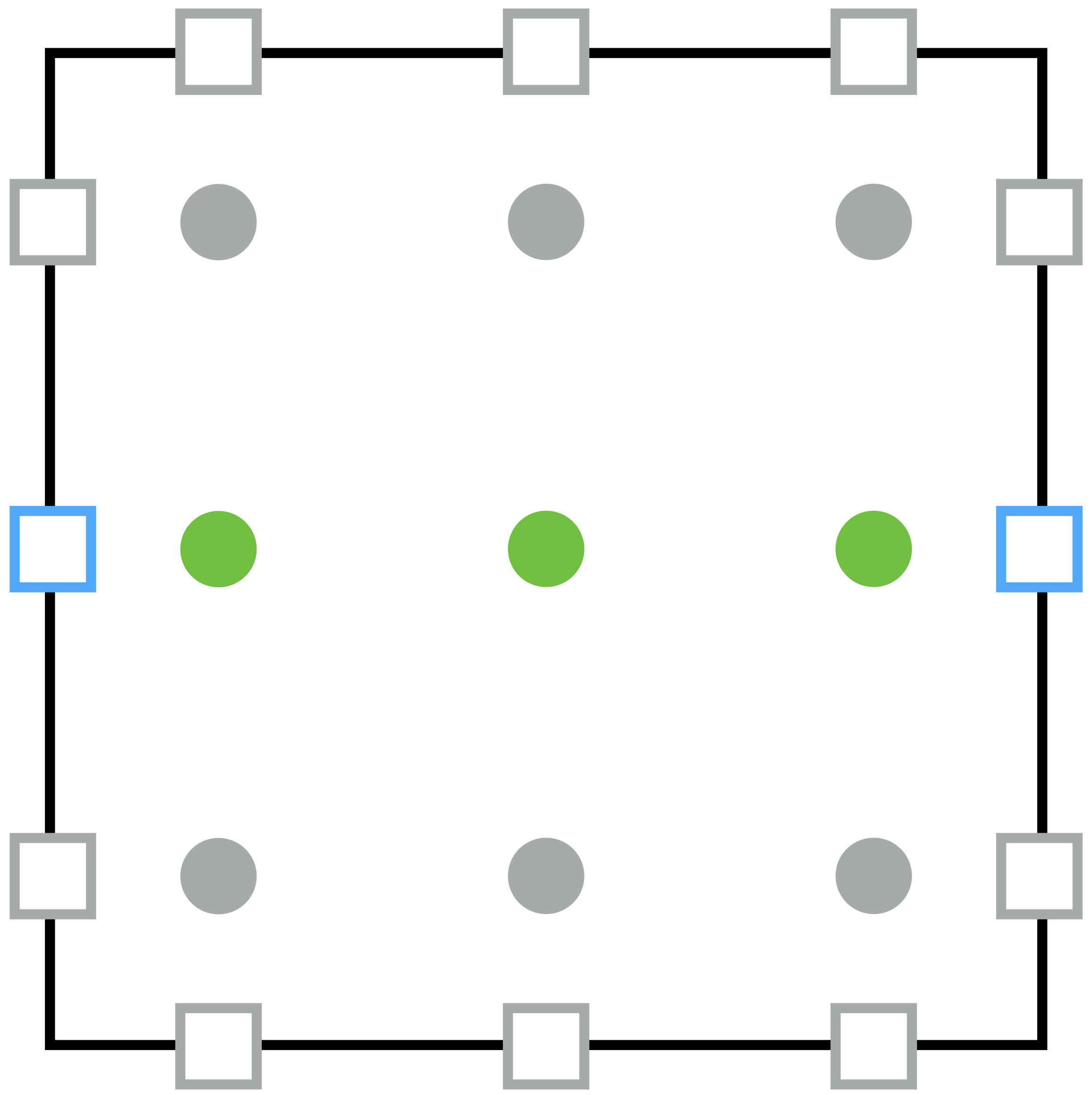


AoSoA(k) Results

- Large **performance boost**.
    - KNL now outperforms a K40c in the **dense regime**.
    - Other backends improve, too, but only slightly.

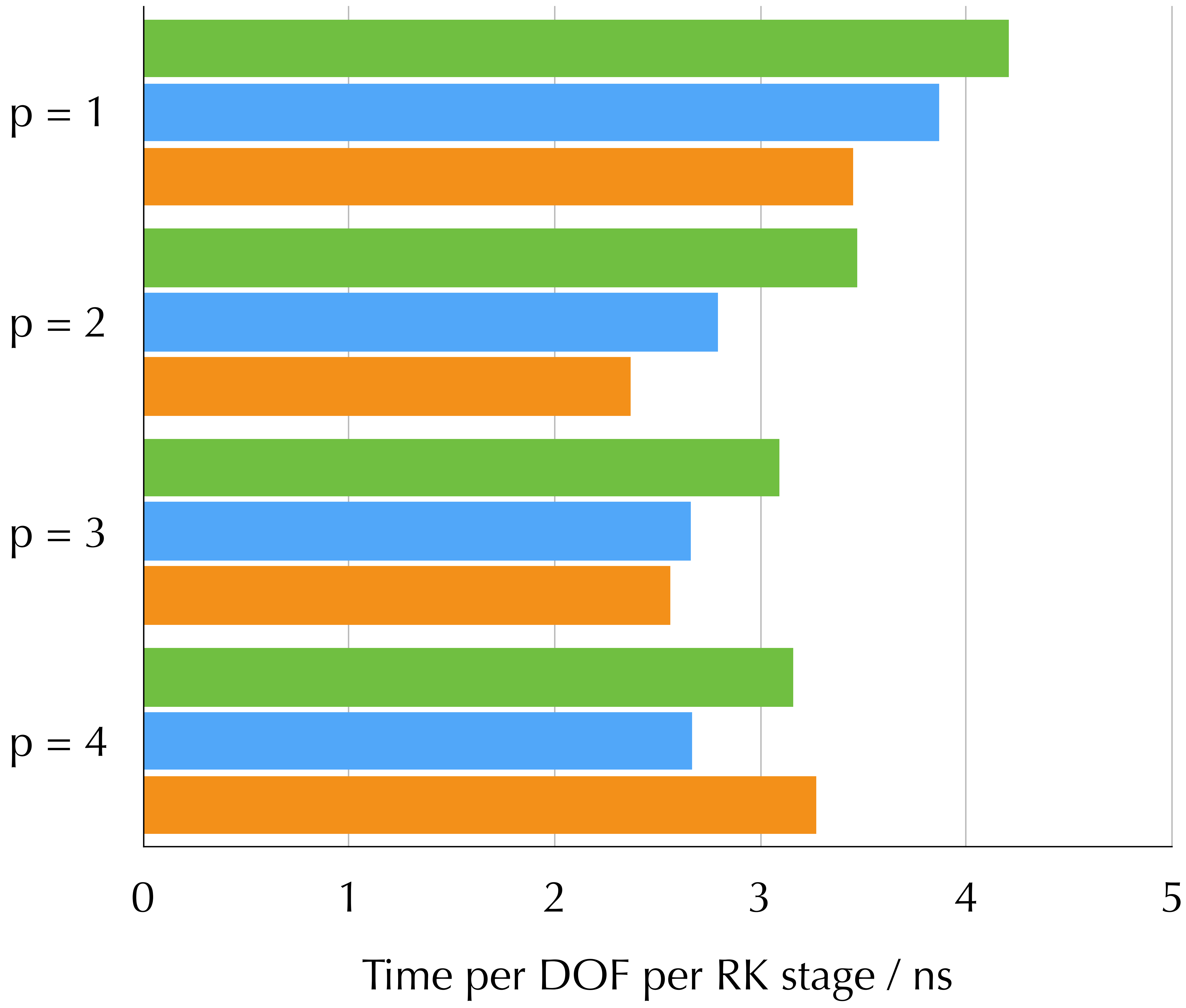
Sparsity Exploitation

- Hexahedral operator matrices are **sparse**.
- Can therefore use **GiMMiK/libxsmm**.



Sparsity Exploitation

- All with PyFR 1.5.0
  - **K40c (GiMMiK)**
  - **KNL (GiMMiK)**
  - **KNL (libxsmm)**



Summary

- Performance is **promising**.
- Lots of room for improvement in **GiMMiK and libxsmm**.

Acknowledgements

- **Air Force Office of Scientific Research** for support under grant FA9550-14-1-0186.

Backup Slides

Start Up Time

- Normally start up time is a non-issue for PyFR.
- A **few minutes** for a simulation which will run for **hours to days**.

Start Up Time

- Time is split roughly equally between

  (i) running **serial Python code**;

  (ii) using **ICC** to compile run-time generated kernels.

Start Up Time

- Difficult to improve
  - ...Python is **virtually impossible to JIT**
  - ...and due to the **GIL** does not benefit from multi-threading.

Start Up Time

- But did add a **kernel cache**.
- Huge reduction in time for **$p = 4$** cylinder case with GiMMiK.