The exaFOAM project: bringing OpenFOAM to exaSCALE

Exploitation of Exascale Systems for Open-Source Computational Fluid Dynamics by Mainstream Industry

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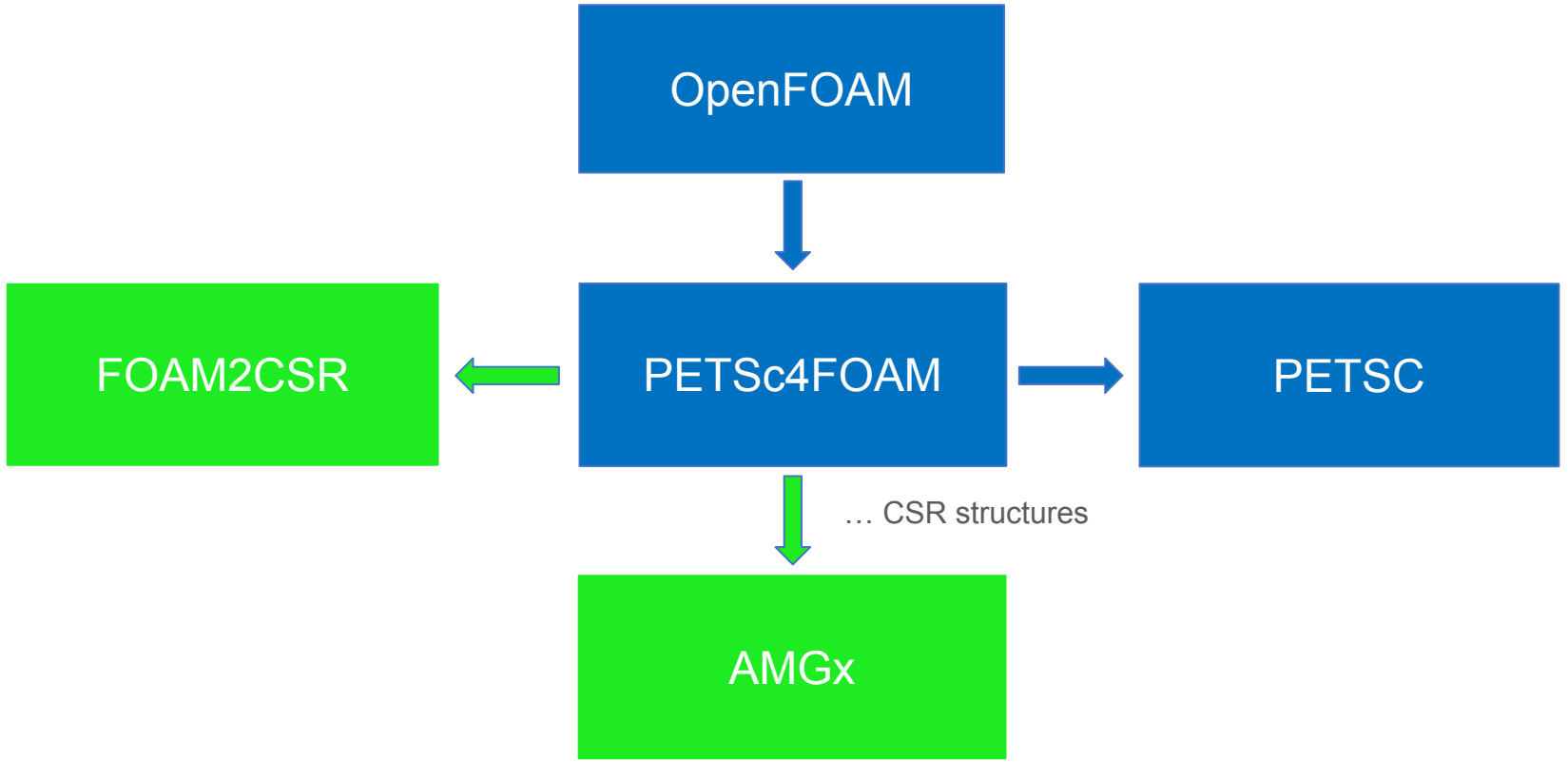
22th March 2024

esi-group.com

Porting to Accelerators: hybrid approach



[1] M. Martineau, S. Posey, F. Spiga, AMGX GPU solver developments for OpenFOAM, 2020

- **FOAM2CSR** has been implemented to convert the matrix from LDU-orderedCOO to CSR and to increase the amount of computational workload resident on the GPU [1]
- The **maximum speed-up** of this hybrid approach depends on how much time FOAM applications spend in the linear system solution. From experience this value is no more than **3X** on discrete GPUs (1 CPU-node vs 1 GPU-node)

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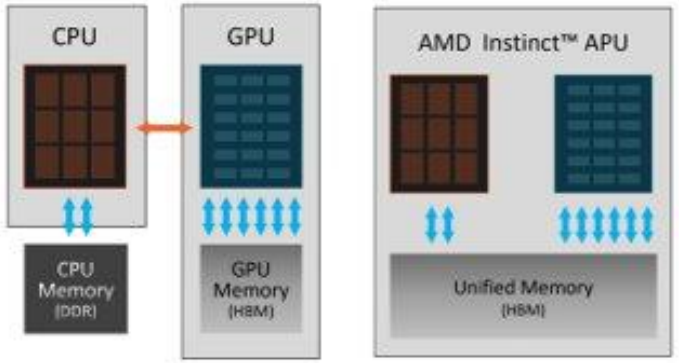
GPU porting approaches

We delivered a promising solution described in [1] based on **OpenMP target offloading** and **Unified Shared Memory** for APUs (e.g. AMD MI300A GPUs).

- Very few lines of code have been added (mainly #pragma directives)
- Usage of a Memory pool based on the Umpire library (OpenFOAM uses a lot of temporary arrays)
- No programming distinction between *host* and *device* memory spaces



[1] S. Tandon, L. Grinberg, D. Bercea, C. Bertolli, M. Olesen, S. Bnà and N. Malaya, Porting HPC applications to AMD Instinct TM MI300 APUs using unified memory and OpenMP, accepted, ISC High Performance 2024

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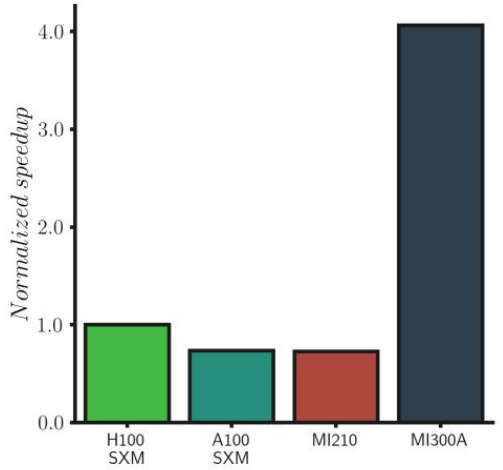
GPU porting approaches

Limitations to the openMP approach:

- Not all the compilers compile the code successfully (e.g. Nvidia compiler does not work)
- Not good performances on discrete GPUs (more than 65% of the time is spent in page migrations [1]). MI300A and GH are still not present in the current supercomputers. What about SMEs?
- This approach contains a lot of atomics operations. It relies on a good implementation of atomic on hardware (not the case with AMD MI200)

	CUDA		HIP		SYCL		Standard		OpenMP		OpenACC		Kokkos	
	C	F	C	F	C	F	C	F	C	F	C	F	C	F
NVIDIA	●	●	■	✖	▲	✖	●	●	◗	◗	●	●	▲	✖
AMD	■	✖	●	✖	■	✖	▲	✖	●	●	▲	▲	▲	✖
INTEL	■	✖	✖	✖	●	✖	◗	◗	●	●	✖	✖	▲	✖

● Full vendor support
◗ Partial vendor support
✖ Very limited or no support
▲ Comprehensive support, not from vendor
■ Indirect vendor support



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GPU porting approaches

ZeptoFoam, the successor of yoctoFOAM is a library built on top of OpenFOAM that refactors the core libraries (OpenFOAM, finiteVolume)

- Usage of a **Memory Pool** (currently only a naïve built-in implementation is available)
- Use of the **Visitor pattern** to separate, where possible, data structure from algorithms (e.g. same data structure (List of values) but several algorithms act on it (e.g. *std::memcpy* vs *cudaMemcpy* vs *hipMemCpy*)).
- Most of the kernels are confined into the **deviceFieldExecutor** class, the acronym name FOAM is still valid.
- **Explicit data managament** using the Memory Pool. This solution works fine both with the current discrete GPUs and APUs.
- All differential operators have been re-implemented in a new namespace (*devicefvm, devicefvc*)
- Rely on **third-party libraries** for linear algebra solvers and preconditioners (e.g. *AmgX* via *AmgX4Foam*). We implemented natively only *PCG* and *PBiCG* preconditioned by *Jacobi.*
- Regarding the *CUDA* implementation, we use *CUDA-aware MPI* wrapped by the *Pstream* library.

GPU porting approaches

- Same **DSL**
- Implemented as a **library** built on-top of OpenFOAM, no modifications are required to the source code of OpenFOAM
- Same inputs as OpenFOAM, it relies on the same runTime Selection Table
- **Duplicate code**
- Better integration with OpenFOAM will reduce duplicate code but will probably requires modifications to the source code of OpenFOAM

```
deviceFvMatrix<vector> UEqn
(
      devicefvm::ddt(devU)
    + devicefvm::div(devphi, devU)
    - devicefvm::laplacian(devnu, devU)
);
solve(UEqn == -devicefvc::grad(devp));

// --- PISO loop
while (piso.correct())
{
    deviceVolumeField<scalar> rAU(UEqn.A().ref().reciprocal());
    deviceVolumeField<vector> HbyA(constrainHbyA(rAU*UEqn.H(), devU, devp));
    deviceSurfaceField<scalar> phiHbyA
    (
        "phiHbyA",
        devicefvc::flux(HbyA)
      // + fvc::interpolate(rAU)*fvc::ddtCorr(U, phi)
    );

    adjustPhi(phiHbyA, devU, devp);

    // Update the pressure BCs to ensure flux consistency
    constrainPressure(devp, devU, phiHbyA, rAU);

    // Non-orthogonal pressure corrector loop
    while (piso.correctNonOrthogonal())
    {
        // Pressure corrector
        deviceFvMatrix<scalar> pEqn
        (
            devicefvm::laplacian(rAU, devp) == devicefvc::div(phiHbyA)
        );

        pEqn.setReference(pRefCell, pRefValue);

        pEqn.solve(p.select(piso.finalInnerIter()));

        if (piso.finalNonOrthogonalIter())
        {
            devphi = phiHbyA - pEqn.flux();
        }
    }

    // #include "continuityErrs.H"

    devU = HbyA - rAU*devicefvc::grad(devp);
    devU.correctBoundaryConditions();
```

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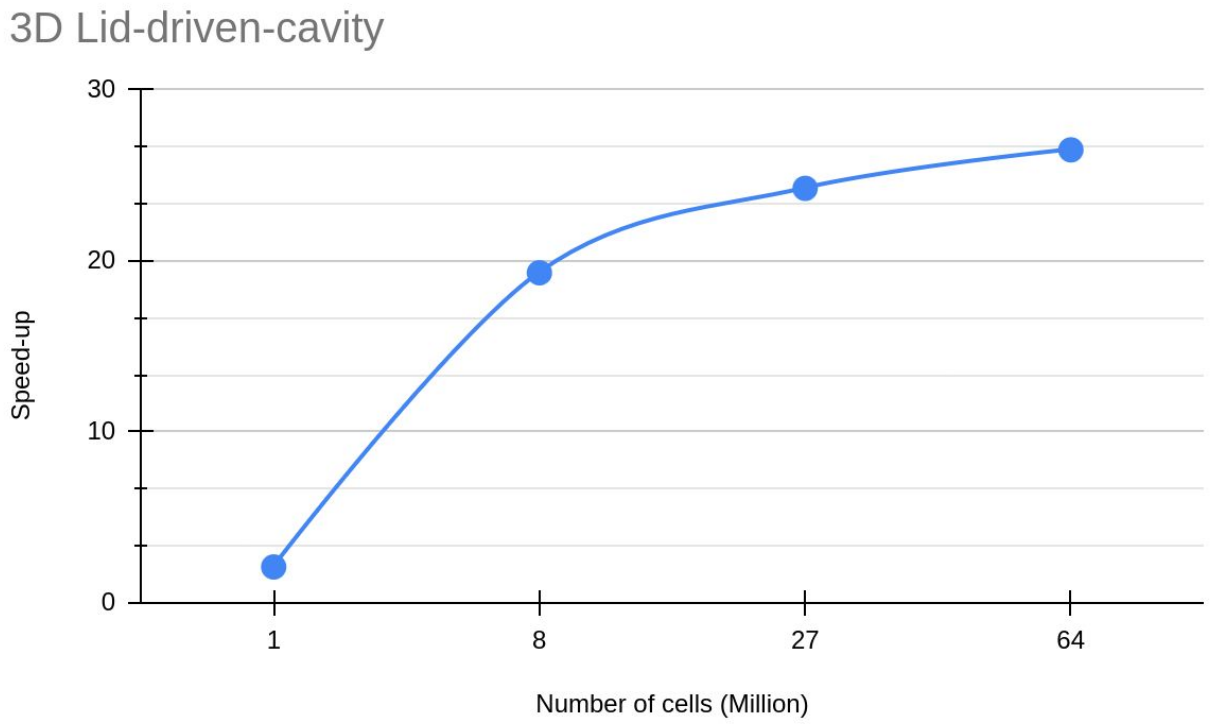
zeptoFOAM results

3D-Lid-driven-Cavity: **saturation** tests on Leonardo (1 node with 4 GPUs A100 "Da Vinci")
PCG+Jacobi for p (fixed Iters: 250 (S), 650 (M), 1600 (L), 3000(XL)), BiCG+Jacobi for U



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zeptoFOAM results

3D-Lid-driven-Cavity: **saturation+strong scaling** tests on Leonardo (CPU Intel Ice Lake (32 core) vs GPU A100 "Da Vinci")
PCG+Jacobi for p (fixed Iters: 250 (S), 650 (M), 1600 (L), 3000 (XL)), BiCG+Jacobi for U

Case	32CPUs (1 CPU node)	1 GPU	2 GPUs	4 GPUs (1 GPU node)	1 CPU node/ 1 GPU node
S (1M)	3.43 [s]	1.92 [s]	1.62 [s]	1.63 [s]	2.1x
M (8M)	166.97 [s]	27.63 [s]	15.73 [s]	8.65 [s]	19.3x
L (27M)	1416.31 [s]	204.73 [s]	109.75 [s]	58.42 [s]	24.2x
XL (64M)	6250.03 [s]	N.A.	N.A.	236.10 [s]	26.5x

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zeptoFOAM results

3D-Lid-driven-Cavity: **solver comparison** on Leonardo (1 GPU A100 "Da Vinci")
PCG+Jacobi vs PCG+AMG+BlockJacobi with AmgX for p (fixed iters: 250 (S), 650 (M)), BiCG+Jacobi for U

Case	PCG+Jacobi (1 GPU)	PCG+AMG (1 GPU)	Speed-up
S (1M)	4.62 [s]	3.28 [s]	1.4x
M (8M)	66.8 [s]	23.73 [s]	2.8x

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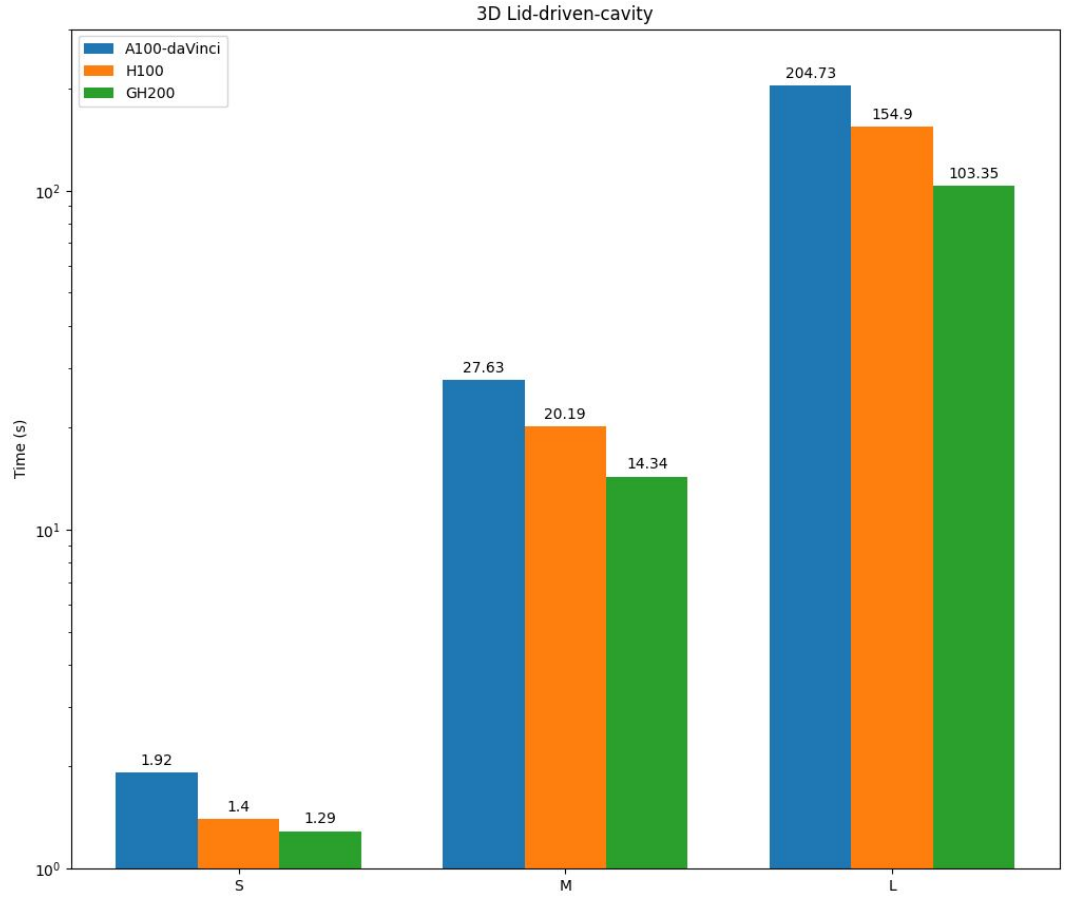
zeptoFOAM results

3D-Lid-driven-Cavity: **hardware comparison** between A100 "Da Vinci", H100 and GH200
PCG+Jacobi for p (fixed iters: 250 (S), 650 (M), 1600 (L)), BiCG+Jacobi for U



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Any Questions?

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