Separation of Concerns for Performance Portability and the wider context of the UK ExCALIBUR Programme

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WARWICK
THE UNIVERSITY OF WARWICK

- Traditional CPUs
  - Intel, AMD, ARM, IBM
  - multi-core (> 20 currently)
  - Deep memory hierarchy (cache levels and RAM)
  - longer vector units (e.g. AVX-512)
- GPUs
  - NVIDIA (A100), AMD (MI200) , Intel (Xe GPUs)
  - Many-core (> 1024 simpler SIMT cores)
  - CUDA cores, Tensor cores
  - Cache, Shared memory, HBM (3D stacked DRAM)
- Heterogeneous Processors
  - Different core architectures over the past few years
  - ARM *big.LITTLE*
  - NVIDIA *Grace.Hopper*
- XeonPhi (discontinued)
  - Many-core – based on simpler x86 cores
  - MCDRAM (3D stacked DRAM)
- FPGAs
  - Xilinx (AMD) and Intel
  - Various configurations
  - Low-level language / HLS tools for programming
  - Significant energy savings
- DSP Processors
  - Matrix 2000+ (MTP) DSP accelerator
  - [Yet to be announced Chinese Exascale system ?]
- TPUs (e.g. from Google), IPUs …

… Custom ASICs driven by AI ... in the cloud.

- Domain specific Hardware …
- Quantum [?]

But .. Even more diverse ways to programming them !

OpenMP, SIMD, CUDA, OpenCL, OpenMP4.0, OpenACC, SYCL/OneAPI, HIP/ROCm,
MPI, PGAS, Task-based (e.g Legion) ….

- Open standards (e.g OpenMP, SYCL)
  - So far have not been agile to catch up with changing architectures
- Proprietary models (e.g. CUDA, OpenACC, ROCm, OneAPI)
  - Restricted to narrow vendor specific hardware
- Need different code-paths/parallelization schemes to get the best performance
  - E.g. Coloring vs atomics vs SIMD vs MPI vs Cache-blocking tiling for unstructured mesh class of applications
- What about legacy codes ? There is a lot of FORTRAN code out there !

❑ What would an Exa-scale machine architecturally look like ?

- Perlmutter - Over 100 PFLOP/s - AMD EPYC CPUs (Milan) with NVIDIA A100 GPUs
- Aurora - 1 EFLOP Intel Xeon CPUs (Sapphire Rapids) with Intel Xe GPUs
- Frontier - 1.5 EFLOP/s AMD EPYC CPUs (Milan) with AMD Instinct GPUs
- El Capitan - 2 EFLOP/s AMD EPYC CPUs (Genoa) with AMD Instinct GPUs

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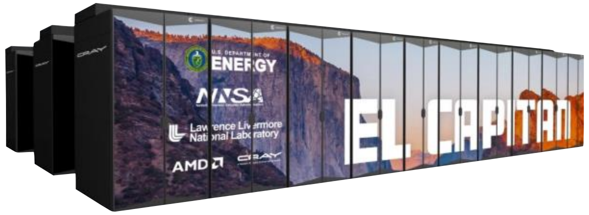
- LUMI - 0.5 EFLOP/s AMD EPYC CPUs with AMD Instinct GPUs
- LEONARDO - 0.3 EFLOP/s - Intel Xeon CPUs (Sapphire Rapids) with NVIDIA A100 GPUs
- MareNostrum5 - 2 distinct 100+ PFLOP/s systems possibly based on ARM/RISC-V

- ARCHER2- 28 PFLOP/s AMD EPYC CPUs (Rome)
- Many Tier-2 systems in the UK - Isambard-2 – ARM A64FX | Baskerville - NVIDIA A100 GPUs

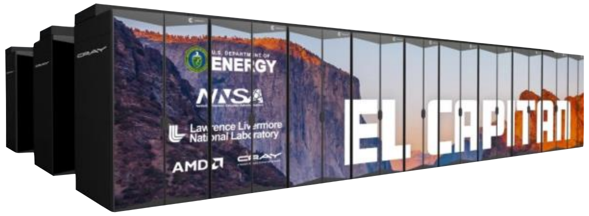


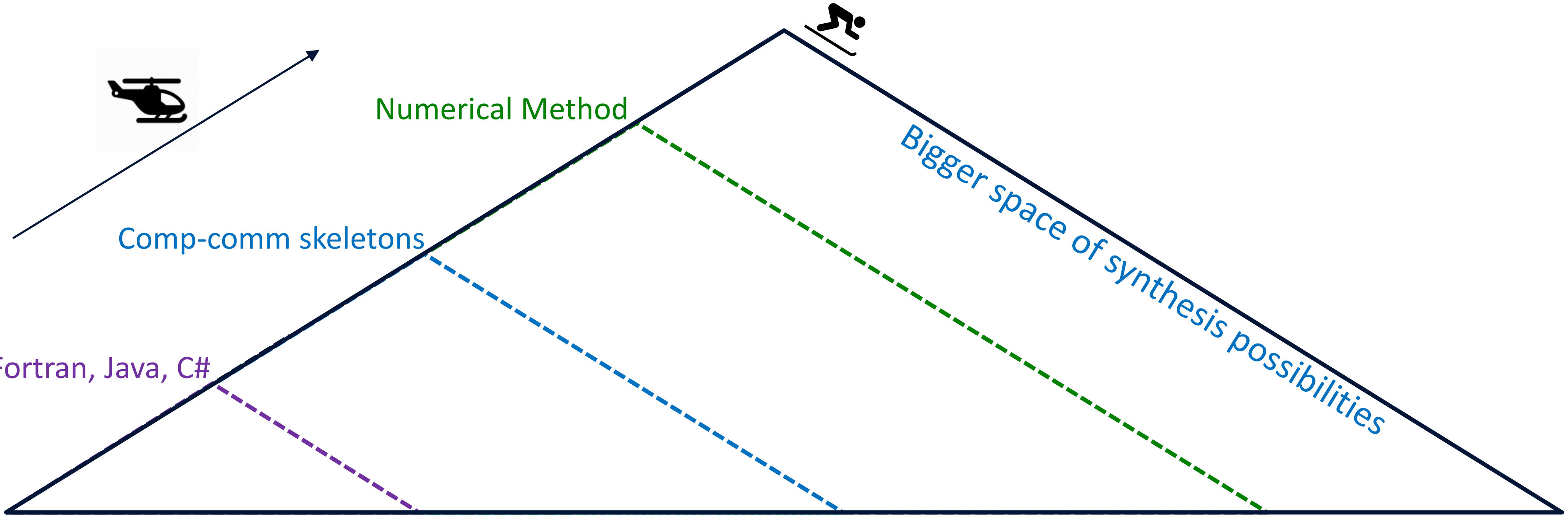
SOFTWARE CHALLENGE – A MOVING TARGET

- ❑ Each new platform requires new performance tuning effort
  - Deeper memory/cache hierarchies and/or shared-memory (including non-coherent)
  - Multiple (heterogeneous) memory spaces (device memory/host memory/near-chip memory)
  - Complex programming skills set needed to extract best performance on the newest architectures

- ❑ Not clear which architectural approach is likely to win in the long-term
  - Cannot be re-coding applications for each new type of architecture or parallel system
  - Nearly impossible for re-writing legacy codes

- ❑ Need to <u>future-proof</u> applications for their continued performance and portability
  - If not – significant loss of investment
  - Applications will not be able to make use of emerging architectures



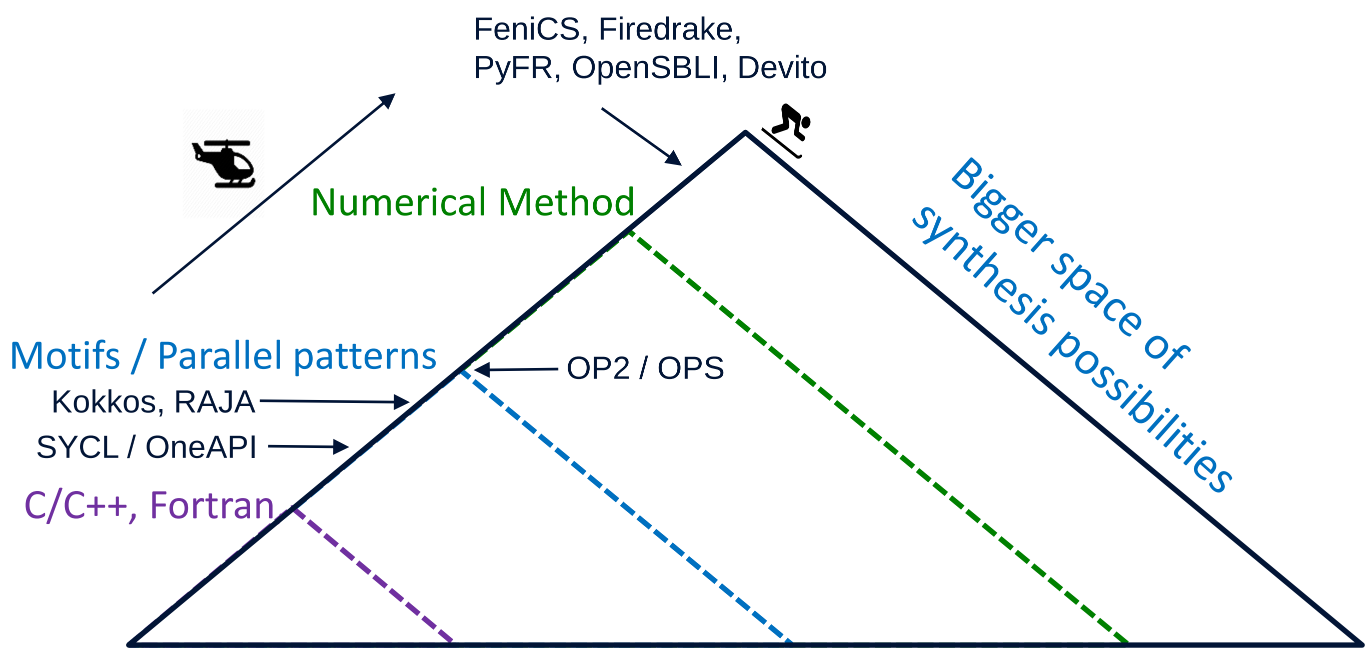


Adapted from: *Synthesis versus Analysis: What Do We Actually Gain from Domain-Specificity?* Keynote talk at the LCPC 2015. Paul H. J. Kelly (Imperial College London)

- Rise the abstraction to a specific domain of variability
- Concentrate on a narrower range (class) of computations
  - Computation-Communications skeletons - Structured-mesh, Unstructured-mesh, … 7 Dwarfs [Colella 2004] ?
  - (higher) Numerical Method - PDEs, FFTs, Monte Carlo …
  - (even higher) Specify application requirements, leaving implementation to select radically different solution approaches

DSLs / High-level Abstractions gaining traction

- FEniCS - PDE solver package - https://fenicsproject.org/
- Firedrake - automated system for the portable solution of PDEs using the finite element method https://www.firedrakeproject.org/
- PyFR - Python based framework for solving advection-diffusion type problems on streaming architectures using the Flux Reconstruction approach - http://www.pyfr.org/
- Devito - prototype DSL and code generation framework based on SymPy for the design of highly optimised finite difference kernels for use in inversion methods - http://www.opesci.org/devito-public
- GungHO project - Weather modelling codes (MetOffice)
- STELLA – DSL for stencil codes(Metro Swiss)
- Liszt – Stanford University : DSL for solving mesh-based PDEs - http://graphics.stanford.edu/hackliszt/
- Kokkos – C++ template library – SNL
- RAJA - C++ template libraries - LLNL



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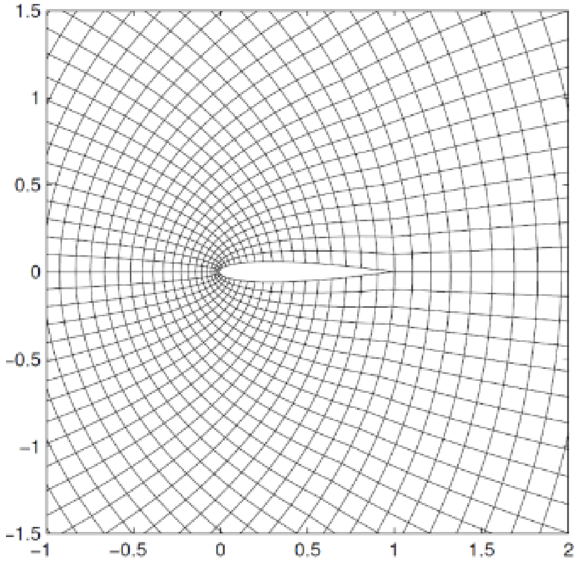
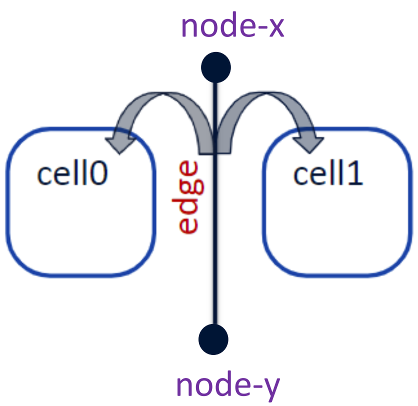
OP2 – Unstructured-mesh Applications Domain

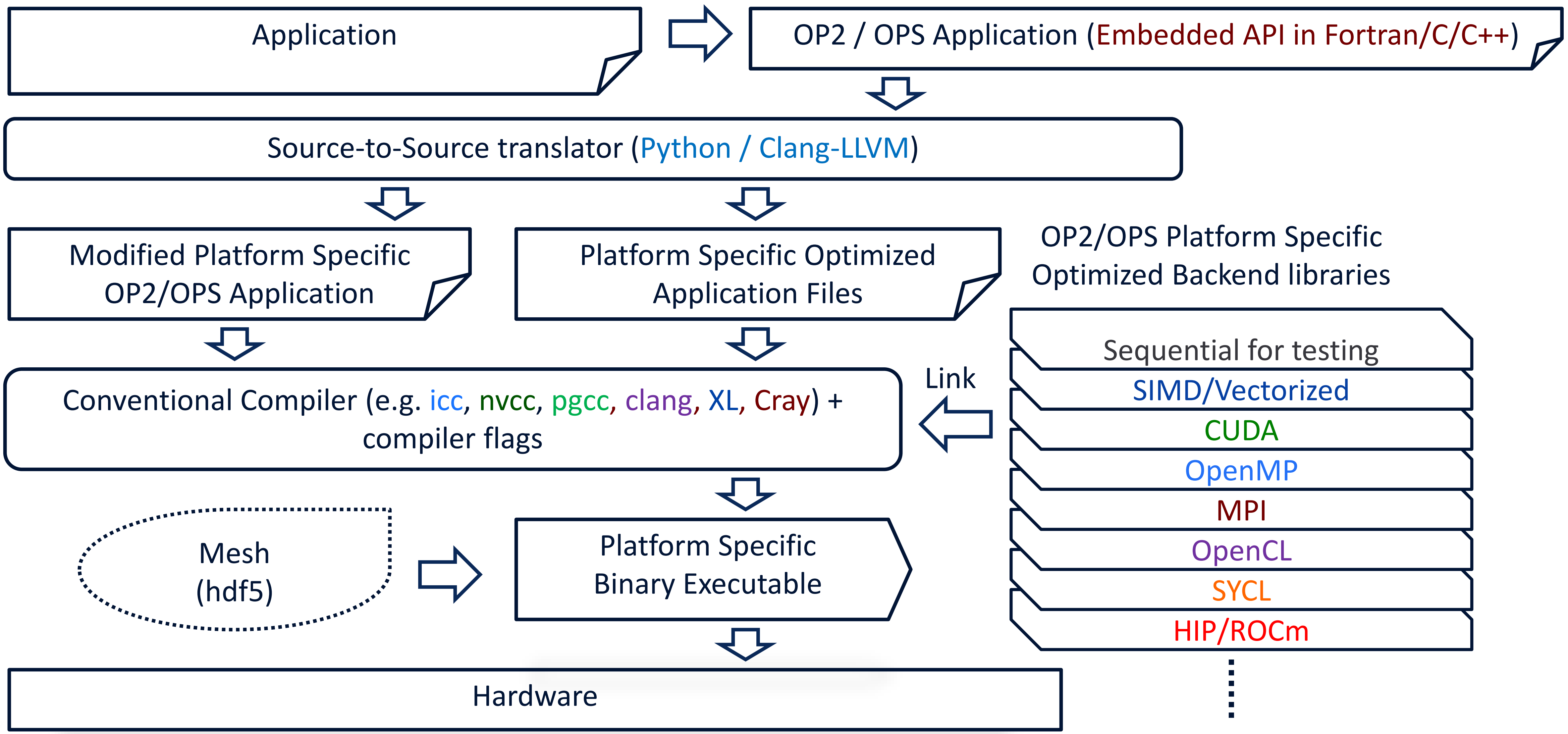
```
! Declaring the mesh with OP2
! sets
call op_decl_set(nnode,nodes,'nodes')
call op_decl_set(nedge,edges,'edges')
call op_decl_set(ncell,cells,'cells')
! maps
call op_decl_map(edges,nodes,2,edge ,pedge ,'pedge' )
call op_decl_map(edges,cells,2,ecell,pecell,'pecell')
! data
call op_decl_dat(nodes,2,'real(8)',x,p_x,'p_x')
call op_decl_dat(cells,4,'real(8)',q,p_q,'p_q')
call op_decl_dat(cells,1,'real(8)',adt,p_adt,'p_adt')
call op_decl_dat(cells,4,'real(8)',res,p_res,'p_res')
```






```
! Elemental kernel
subroutine res_calc(x1,x2,q1,q2,adt1,adt2,res1,res2)
  IMPLICIT NONE
  REAL(kind=8), DIMENSION(2), INTENT(IN) :: x1
  REAL(kind=8), DIMENSION(2), INTENT(IN) :: x2
  ...
  REAL(kind=8) :: dx,dy,mu,ri,p1,vol1,p2,vol2,f
  dx = x1(1) - x2(1)
  dy = x1(2) - x2(2)
  ...
  f = 0.5 * (vol1 * q1(1) + vol2 * q2(1)) + &
  &    mu * (q1(1) - q2(1))
  res1(1) = res1(1) + f
  res2(1) = res2(1) - f
  ...
! Calculate flux residual - parallel loop over edges
call op_par_loop_8 (res_calc, edges, &
& op_arg_dat(x,   1, edge,  2,"real(8)", OP_READ), &
& op_arg_dat(x,   2, edge,  2,"real(8)", OP_READ), &
& op_arg_dat(q,   1, ecell, 4,"real(8)", OP_READ), &
& op_arg_dat(q,   2, ecell, 4,"real(8)", OP_READ), &
& op_arg_dat(adt, 1, ecell, 1,"real(8)", OP_READ), &
& op_arg_dat(adt, 2, ecell, 1,"real(8)", OP_READ), &
& op_arg_dat(res, 1, ecell, 4,"real(8)", OP_INC ), &
& op_arg_dat(res, 2, ecell, 4,"real(8)", OP_INC ))
```

OP2 – Application development workflow



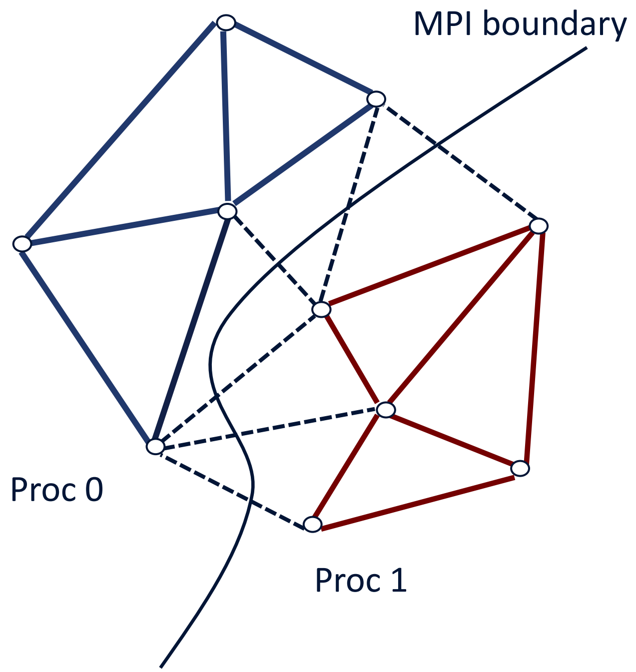
OP2 – Generated Code - CPU

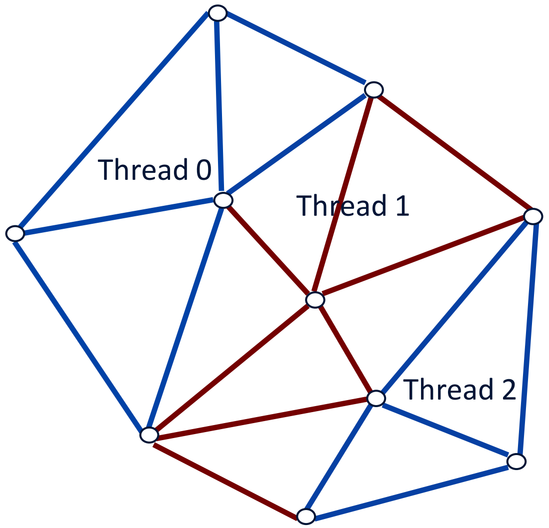
```fortran
! elemental kernel
SUBROUTINE res_calc(x1,x2,q1,q2,adt1,adt2,res1,res2)
...
END SUBROUTINE

! wrapper function - calls elemental kernel
SUBROUTINE op_wrap_res_calc( ... )
...
...
  DO i1 = bottom, top-1, 1
    IF (mod(i1,testfreq).eq.0) THEN
      call op_mpi_test_all(argc,args)
    END IF
    map1idx = opDat1Map(1 + i1 * opDat1MapDim + 0)+1
    map2idx = opDat1Map(1 + i1 * opDat1MapDim + 1)+1
    map3idx = opDat3Map(1 + i1 * opDat3MapDim + 0)+1
    map4idx = opDat3Map(1 + i1 * opDat3MapDim + 1)+1
    ! kernel call
    CALL res_calc(
         opDat1Local(1,map1idx), opDat1Local(1,map2idx),
         opDat3Local(1,map3idx), opDat3Local(1,map4idx),
         opDat5Local(1,map3idx), opDat5Local(1,map4idx),
         opDat7Local(1,map3idx), opDat7Local(1,map4idx))
    END DO
END SUBROUTINE
```

```fortran
! host function - setting up pointers and indirect accesses
SUBROUTINE res_calc_host( userSubroutine, set, opArg1, &
& opArg2, & opArg3, & opArg4, opArg5, opArg6, opArg7, opArg8)

  ! MPI halo exchanges
  n_upper = op_mpi_halo_exchanges(...)
  ...
  ...
  ! set up c to Fortran pointers
  CALL c_f_pointer(opArg1%data,opDat1Local, ...)
  CALL c_f_pointer(opArg1%map_data,opDat1Map, ...)
  ...
  ...
  ! compute over core iterations/elements
  CALL op_wrap_res_calc( opDat1Local, opDat3Local, &
                       & opDat5Local, opDat7Local, &
                       & opDat1Map, opDat1MapDim,  &
                       & opDat3Map, opDat3MapDim,  &
                       & 0, opSetCore%core_size, &
                       & numberOfOpDats,opArgArray,testfreq)

  ! wait for Halos to be received
  CALL op_mpi_wait_all(numberOfOpDats,opArgArray)

  ! compute over halo (redundant) iterations/elements
  CALL op_wrap_res_calc( opDat1Local, opDat3Local, &
  & opDat5Local, opDat7Local, &
  & opDat1Map, opDat1MapDim, opDat3Map, opDat3MapDim, &
  & opSetCore%core_size, n_upper,numberOfOpDats,&
  & opArgArray,2147483647)

  IF ((n_upper .EQ. 0) .OR. &
  &   (n_upper .EQ. opSetCore%core_size)) THEN
    CALL op_mpi_wait_all(numberOfOpDats,opArgArray)
  END IF

  ! mark halos dirty
  CALL op_mpi_set_dirtybit(numberOfOpDats,opArgArray)
  ....
  ....
END SUBROUTINE
END MODULE
```

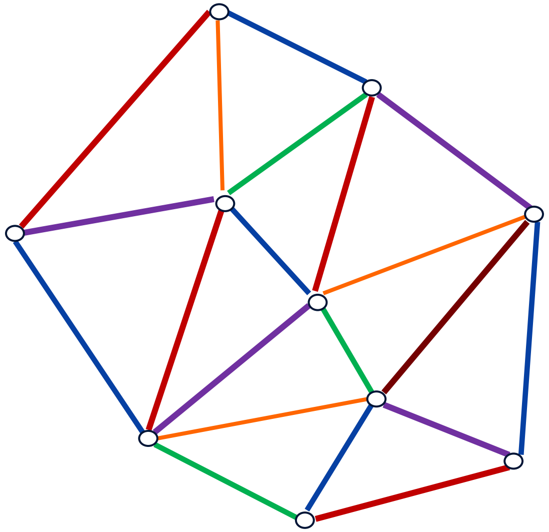
https://github.com/OP-DSL/OP2-APPS/blob/main/apps/fortran/airfoil/airfoil_hdf5/res_calc_seqkernel.F90

- ❑ Distributed memory parallelization
  - Mesh partitioning
  - Standard halo exchange methods
  - Redundant computation
- ❑ Single node – Inter-thread-block
  - Coloring
  - No two blocks of the same color update the same memory location
- ❑ Single node – Intra-thread block
  - Coloring
  - No two edges of the same colour update the same node
  - Use atomics





Threads 0 and 2 can run in parallel



OP2 – Generated Code – GPU with CUDA

```
SUBROUTINE res_calc_gpu(x1,x2,q1,q2,adt1,adt2,res1,res2)
  IMPLICIT NONE
  integer*4 istat
  REAL(kind=8)  :: x1(2)
  REAL(kind=8)  :: x2(2)
  REAL(kind=8), INTENT(IN) :: q1(4)
  REAL(kind=8), INTENT(IN) :: q2(4)
  REAL(kind=8), INTENT(IN) :: adt1
  REAL(kind=8), INTENT(IN) :: adt2
  REAL(kind=8) :: res1(4)
  REAL(kind=8) :: res2(4)
  REAL(kind=8) :: dx,dy,mu,ri,p1,vol1,p2,vol2,f
  dx = x1(1) - x2(1)
  dy = x1(2) - x2(2)
  ri = 1.0 / q1(1)
  p1 = 0.4 * (q1(4) - 0.5 * ri * (q1(2) * q1(2) + &
           & q1(3) * q1(3)))
  vol1 = ri * (q1(2) * dy - q1(3) * dx)
```

```
  ri = 1.0 / q2(1)
  p2 = 0.4 * (q2(4) - 0.5 * ri * (q2(2) * q2(2) + &
           & q2(3) * q2(3)))
  vol2 = ri * (q2(2) * dy - q2(3) * dx)
  mu = 0.5 * (adt1 + adt2) * 0.05
  f = 0.5 * (vol1 * q1(1) + vol2 * q2(1)) + &
         & mu * (q1(1) - q2(1))
  istat = atomicAdd(res1(1),+ f)
  istat = atomicAdd(res2(1),- f)
  f = 0.5 * (vol1 * q1(2) + p1 * dy + &
         & vol2 * q2(2) + p2 * dy) + mu * (q1(2) - q2(2))
  istat = atomicAdd(res1(2),+ f)
  istat = atomicAdd(res2(2),- f)
  f = 0.5 * (vol1 * q1(3) - p1 * dx + &
         & vol2 * q2(3) - p2 * dx) + mu * (q1(3) - q2(3))
  istat = atomicAdd(res1(3),+ f)
  istat = atomicAdd(res2(3),- f)
  f = 0.5 * (vol1 * (q1(4) + p1) + vol2 * (q2(4) + p2)) + &
         & mu * (q1(4) - q2(4))
  istat = atomicAdd(res1(4),+ f)
  istat = atomicAdd(res2(4),- f)
END SUBROUTINE
```

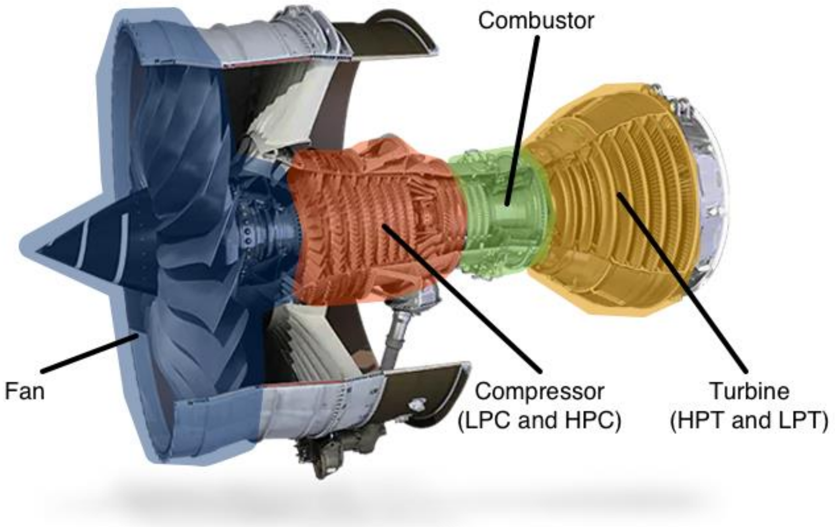
```
! CUDA kernel function
attributes (global) SUBROUTINE op_cuda_res_calc( &
& opDat1Deviceres_calc, opDat3Deviceres_calc,
& opDat5Deviceres_calc, opDat7Deviceres_calc,
& opDat1Map, opDat3Map, start, end, setSize)
...
...
  i1 = threadIdx%x - 1 + (blockIdx%x - 1) * blockDim%x
  IF (i1+start<end) THEN
    i3 = i1+start
    map1idx = opDat1Map(1 + i3 + setSize * 0)
    map2idx = opDat1Map(1 + i3 + setSize * 1)
    map3idx = opDat3Map(1 + i3 + setSize * 0)
    map4idx = opDat3Map(1 + i3 + setSize * 1)
    ! kernel call
    CALL res_calc_gpu( &
    & opDat1Deviceres_calc(1+map1idx*(2):map1idx*(2)+2), &
    & opDat1Deviceres_calc(1+map2idx*(2):map2idx*(2)+2), &
    & opDat3Deviceres_calc(1+map3idx*(4):map3idx*(4)+4), &
    & opDat3Deviceres_calc(1+map4idx*(4):map4idx*(4)+4), &
    & opDat5Deviceres_calc(1+map3idx), &
    & opDat5Deviceres_calc(1+map4idx), &
    & opDat7Deviceres_calc(1+map3idx*(4):map3idx*(4)+4), &
    & opDat7Deviceres_calc(1+map4idx*(4):map4idx*(4)+4))
  END IF
END SUBROUTINE
```

https://github.com/OP-DSL/OP2-APPS/blob/main/apps/fortran/airfoil/airfoil_hdf5/res_calc_kernel.CUF

EVOLVING PRODUCTION CODES – ROLLS-ROYCE HYDRA TO OP2-HYDRA

- Virtual certification of Gas Turbine Engines – EPSRC Prosperity Partnership (ASIMOV)
  - Main consortium with partners – EPCC, Warwick, Oxford, Cambridge, Bristol and Rolls-Royce plc.

- Grand Challenge 1 – Sliding Planes model of Rig250 (DLR test rig compressor)
  - 4.5 stage rotor-stator (10-row full annulus) | 4.58B mesh nodes.
  - Need to obtain 1 revolution of compressor in less than 24 hours
  - Current production estimates at 7 days

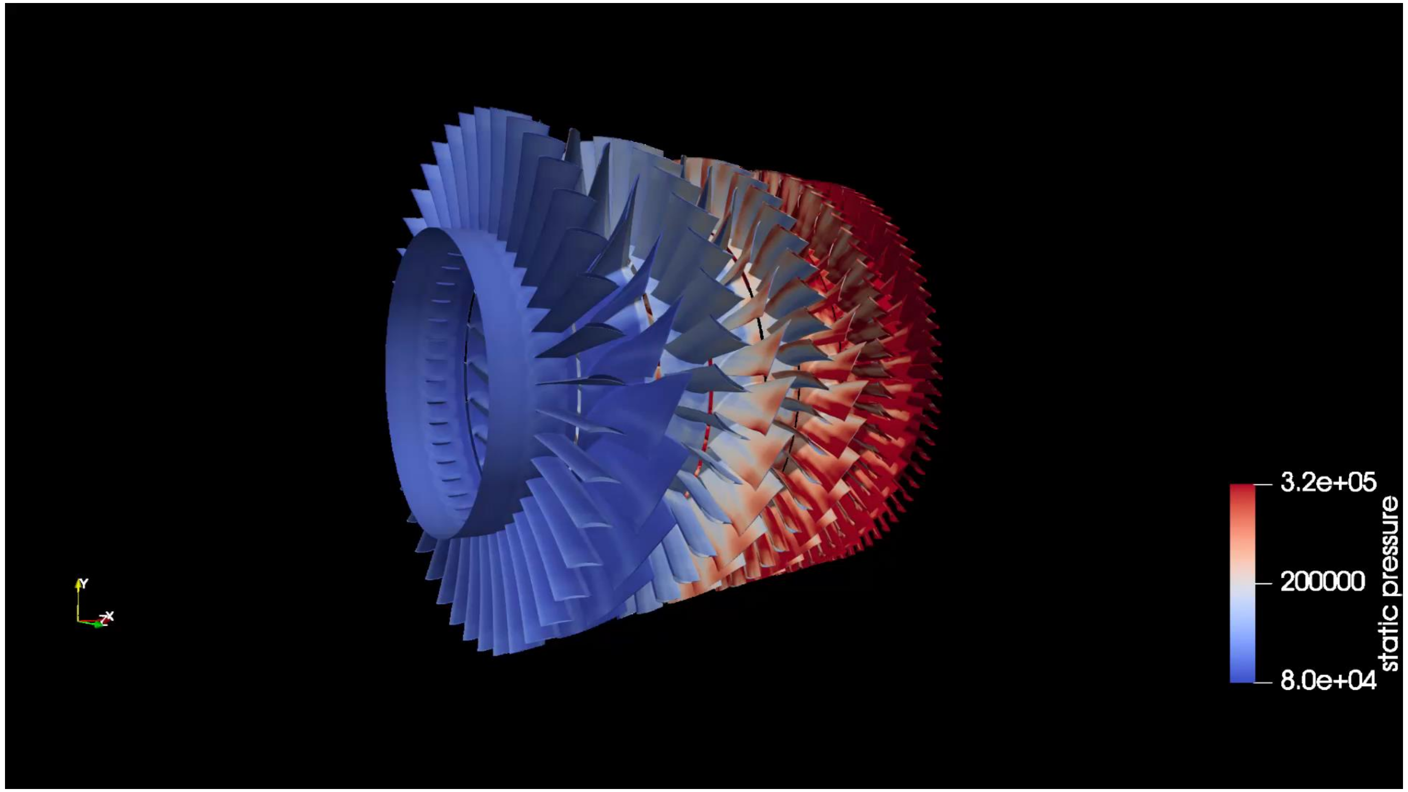


- Setup
  - Moving rotor-stator – sliding planes interfaces
  - Rotors and Stators modelled with Hydra CFD suite – URANS (360 degree models)
  - 10 rotor-stator interfaces
  - Code coupling for sliding planes – move from current monolithic (Hydra only) production code to coupling

- Challenges
  - Performance portability – run both CPUs and GPUs by multiple vendors
  - Preserve production code's scientific code and structure – cannot re-write, MUST "evolve" not overhaul !
  - Convince users to adopt ! (Ongoing for nearly 10 years now)

OP2-Hydra Performance *

System	ARCHER2 HPE Cray EX [6]	Cirrus SGI/HPE 8600 GPU Cluster [4]
Processor	AMD EPYC 7742 @ 2.25 GHz	Intel Xeon Gold 6248 (Cascade Lake) @ 2.5 GHz + NVIDIA Tesla V100-SXM2-16GN GPU
(procs×cores) /node	2×64	2×20 + 4×GPUs
Memory/node	256 GB	384 GB + 40GB/GPU
Interconnect	HPE Cray Slingshot 2×100 Gb/s bi-directional/node	Infiniband FDR, 54.5 Gb/s
OS	HPE Cray LE (based on SLES 15)	Linux CentOS 7
Compilers	GNU 10.2.0	nvfortran (nvhpc 21.2)
Compiler Flags	`-O2 -eF -fPIC`	
Power/node	660W	≈ 900W



OP2-Hydra Performance *

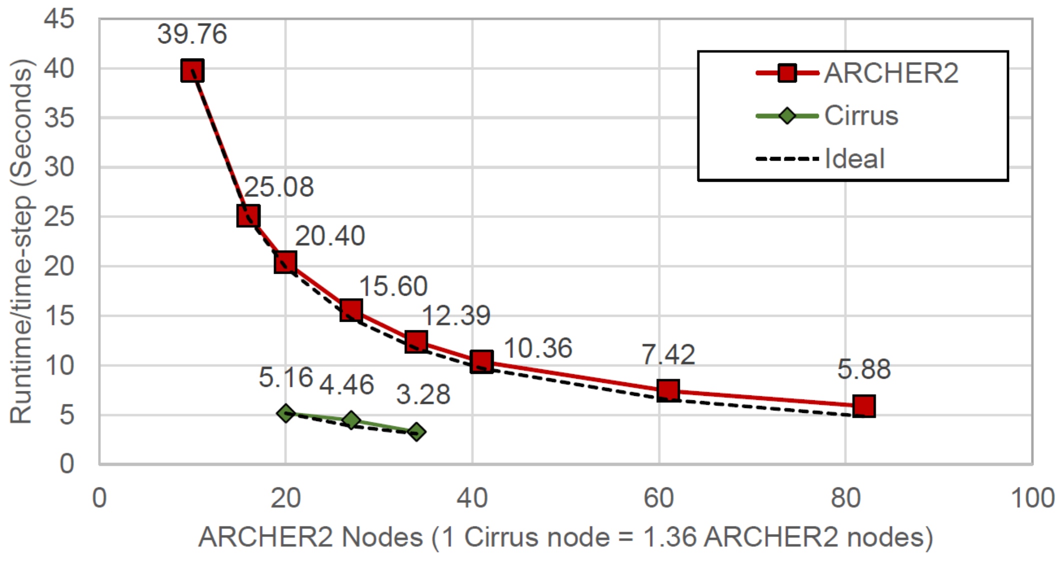
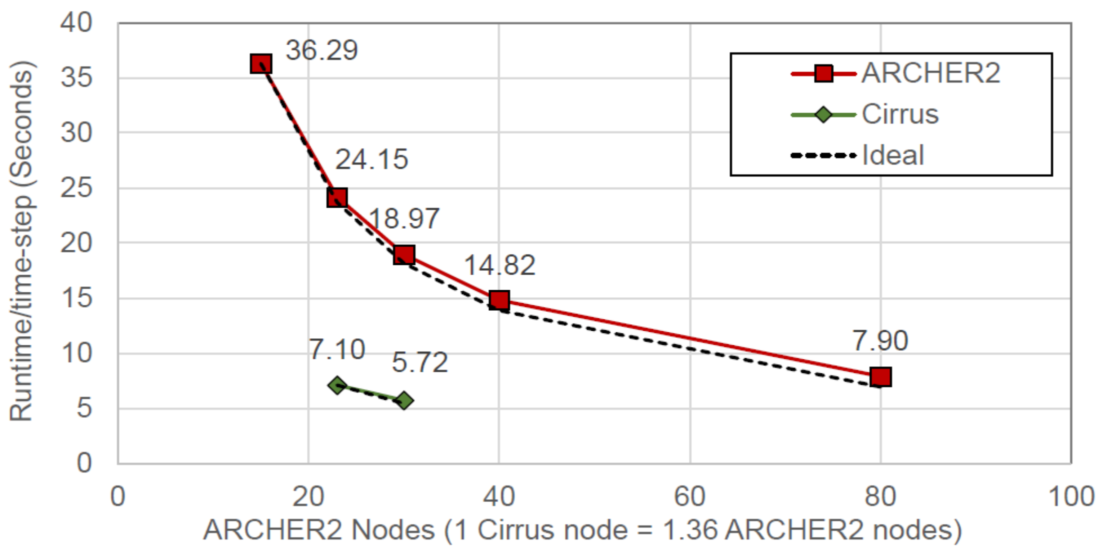


Figure 7: Rig250 $1 - 10_{430M}$ Mesh Runtime



Rig250 $1 - 2_{653M}$ Mesh Runtime

- ARCHER2 @ 34 nodes
  - 94% parallel efficiency
  - 10% coupling overhead
- Cirrus @ 25 nodes
  - 94% parallel efficiency
  - 20% coupling overhead
- ARCHER2 @ 82 nodes
  - 82% parallel efficiency
  - 20% coupling overhead

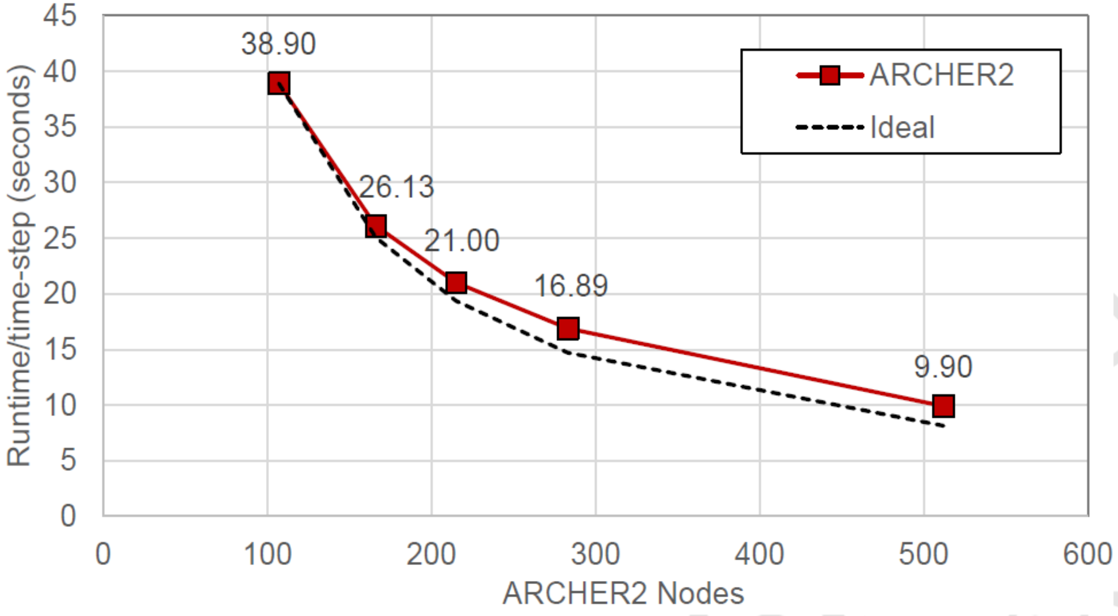
3.7- 4x speedup

- ARCHER2 @ 80 nodes
  - 88% parallel efficiency
  - 8% coupling overhead
- Cirrus @ 22 nodes
  - 94% parallel efficiency
  - 12% coupling overhead
- Cirrus @ 22 nodes
  - 94% parallel efficiency
  - 12% coupling overhead

3.3 - 3.4x speedup

* Results under review

OP2-Hydra Performance *



Rig250 $1-10_{4.58B}$ Mesh Runtime

- ARCHER2 @ 512 nodes:
  - 82% parallel efficiency (vs 107 node run)
  - 15% coupling overhead

Achieved (A) and *Projected (P)* times to solution (hours) : Rig250, 1 revolution

Rig250 Problem	ARCHER2 Runime	ARCHER2 #nodes	Cirrus Runtime	Cirrus #nodes
$1-10_{430M}$ - Monolithic	*93.0 (P)*	*8*		
$1-10_{430M}$ - Coupled	*85.0 (P)*	*8*	*2.9 (P)*	*15*
$1-10_{430M}$ - Coupled	*3.3 (P)*	*80*	*1.8 (P)*	*25*
$1-2_{653M}$ - Monolithic	*110.0 (P)*	*8*		
$1-2_{653M}$ - Coupled	*40.0 (P)*	*8*	*3.9 (P)*	*17*
$1-2_{653M}$ - Coupled	*8.2 (P)*	*40*	*3.2 (P)*	*22*
$1-10_{4.58B}$ - Coupled	*14.5 (A)*	*166*	*4.7 (P)*	*122*
$1-10_{4.58B}$ - Coupled	*9.4 (A)*	*256*		
$1-10_{4.58B}$ - Coupled	*5.5 (A)*	*512*		

- 122 Cirrus nodes is power equivalent to 166 ARCHER2 nodes
- ARCHER2 needs just over 3x more number of *power equivalent* nodes (512) to match Cirrus's runtime (4.7 hours)

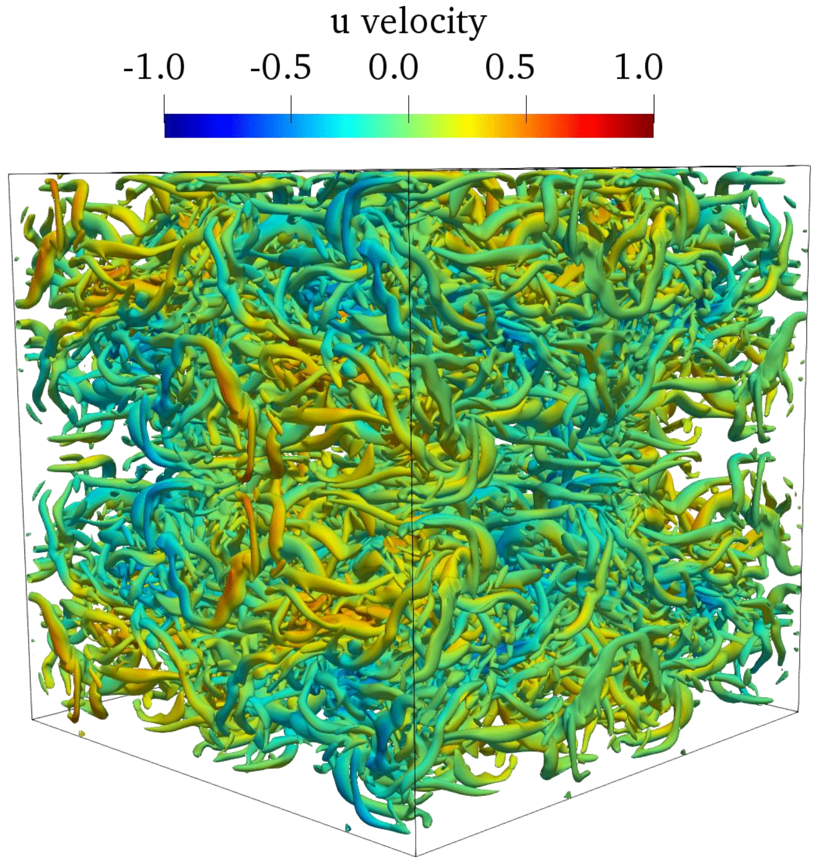
* Results under review

Production Apps – OpenSBLI (Uni. of Southampton)

- Compressible Navier-Stockes solver
  - With shock capturing WENO/TENO
  - 4th order Finite Difference
  - Single/double precision
- OpenSBLI is a Python framework
  - Write equations in SymPy expressions
  - OPS code generated

OpenSBLI

https://opensbli.github.io/



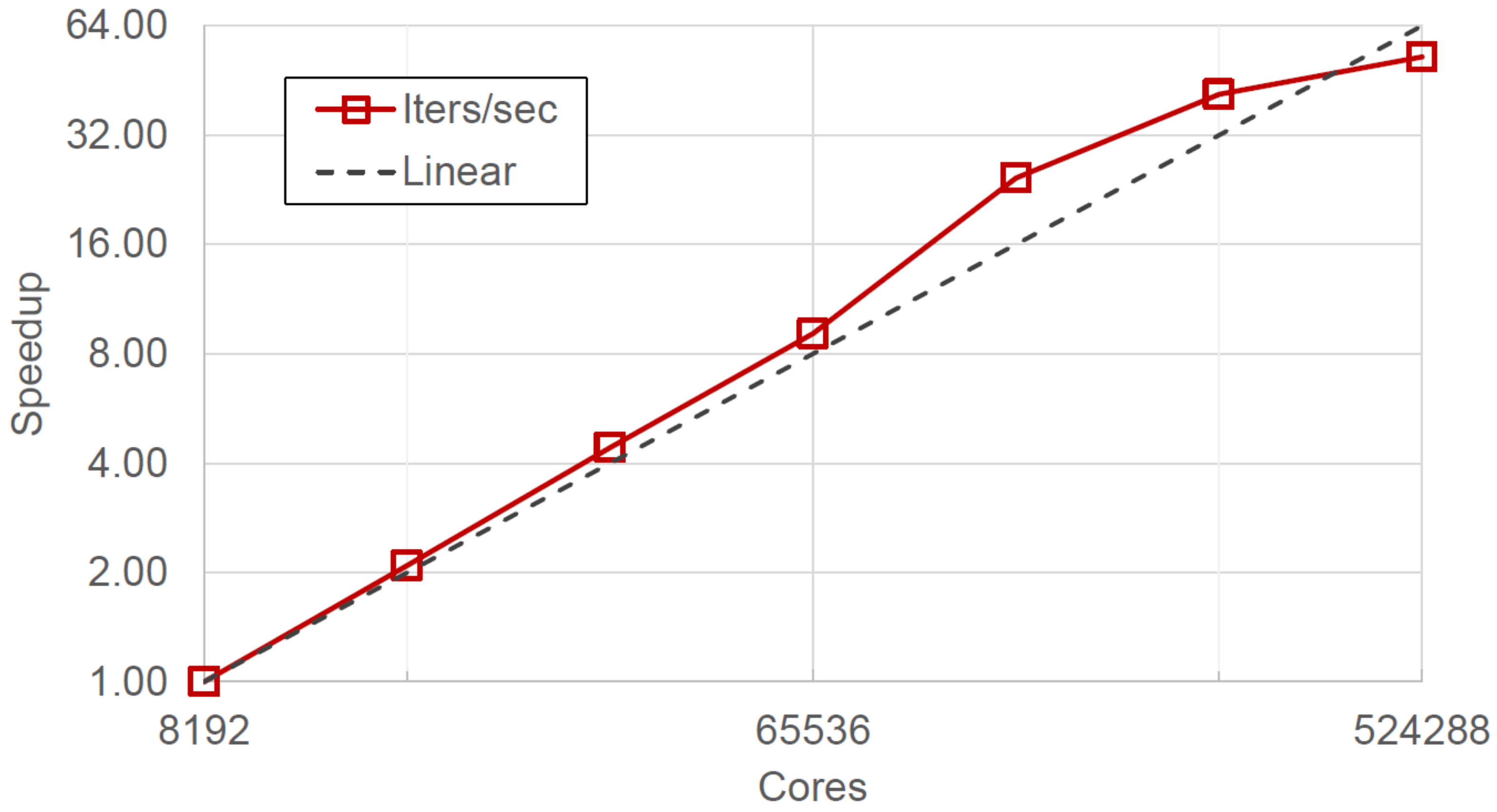

```
ndim = 3
sc1 = "**{\'scheme\':\'Teno\'}"
# Define the compresible Navier-Stokes equations in Einstein notation.
mass = "Eq(Der(rho,t), - Conservative(rhou_j,x_j,%s))" % sc1
momentum = "Eq(Der(rhou_i,t) , -Conservative(rhou_i*u_j + KD(_i,_j)*p,x_j , %s) + Der(tau_i_j,x_j) )" % sc1
energy = "Eq(Der(rhoE,t), - Conservative((p+rhoE)*u_j,x_j, %s) - Der(q_j,x_j) + Der(u_i*tau_i_j ,x_j) )" % sc1
stress_tensor = "Eq(tau_i_j, (mu/Re)*(Der(u_i,x_j)+ Der(u_j,x_i) - (2/3)* KD(_i,_j)* Der(u_k,x_k)))"
heat_flux = "Eq(q_j, (-mu/((gama-1)*Minf*Minf*Pr*Re))*Der(T,x_j))"
# Numerical scheme selection
Avg = RoeAverage([0, 1])
LLF = LLFTeno(teno_order, averaging=Avg)
cent = Central(4)
rk = RungeKuttaLS(3, formulation='SSP')
# Specifying boundary conditions
boundaries[direction][side] = IsothermalWallBC(direction, 0, wall_eqns)
# Generate a C code
alg = TraditionalAlgorithmRK(block)
OPSC(alg)
```

Jacobs, C. T., Jammy, S. P., Sandham N. D. (2017). OpenSBLI: A framework for the automated derivation and parallel execution of finite difference solvers on a range of computer architectures. *Journal of Computational Science*, 18:12-23, DOI: 10.1016/j.jocs.2016.11.001

OPENSBLI ON ARHCER2

- Taylor – Green Vortex Problem – ARCHER2 benchmark
  - Strong Scaling - 1024^3 Mesh
  - Double precision
  - Speedup calculated from 1000 iterations – includes start up time.

From recent benchmarking runs done by Andrew Turner and the ExCALIBUR Benchmarking team (Oct 2021)



ExCALIBUR and Current Projects

❑ CCP – Turbulence

- Direct solver libraries – Tri-, penta-, 7-, 9-, 11 diagonal, multi-dimensional solvers
- Integrate directsolver libraries to be called within OPS
- OpenSBLI type high-level (Python) framework for XCompact3D – High Order FD framework

UK TURBULENCE CONSORTIUM

UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

❑ ExCALIBUR Phase 1B – Turbulence at the Exascale (one of 3 funded, £2.6M)

- Imperial, Warwick, Newcastle, Southampton, Cambridge, STFC collaboration | UKTC and UKCTRF Communities
- Xcompact3D and Wind Energy, OpenSBLI and Green Aviation, uDALES and Air Quality, SENGA+ and Net-Zero Combustion
- Extending OPS capability – robust code-gen tools and parallel transformations | support future-proof code development
- UQ, I/O, Coupling and Visualization
- Machine Learning Algorithms for Turbulent Flow

ExCALIBUR

❑ UK AEA Mini-Apps Project

- Collaboration with University of York
- Developing Prototype miniApps for UKAEA workload
- Investigate / advise on performance portability techniques and current state-of-the-art.

UK Atomic Energy Authority

Wider ExCALIBUR Projects of Interest – Separation of Concerns

- xDSL Project - Efficient Cross-Domain DSL Development for Exascale [https://xdsl.dev/index] : Tobias Grosser, Paul Kelly, Gerard Gorman et al.
  - A common ecosystem for DSL development
  - Funded as the ExCALIBUR Crosscutting research for exascale software and algorithms (2021)
  - Aims to offer software ecosystem for DSL building based on MLIR and LLVM

- Integrated Simulation at the Exascale: Coupling, Synthesis and Performance : Garth Wells and David Emerson et al.
  - Devlop mathematical and software tools to enable coupled simulations
  - Funded as the ExCALIBUR Crosscutting research for exascale software and algorithms (2021)
  - Coupled simulation of fusion modelling,
  - Strong coupling of electromagnetic, thermal, mechanical and fluid processes – electric propulsion

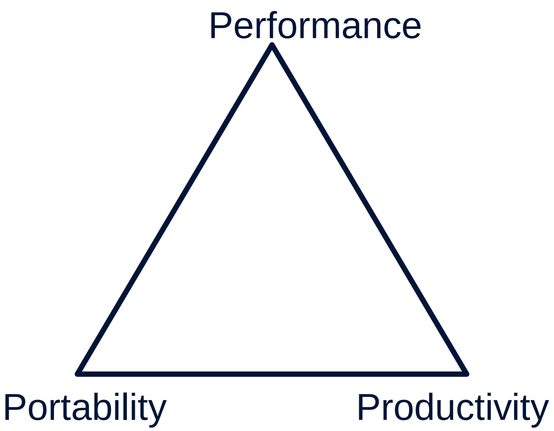
Wider ExCALIBUR Projects of Interest – Separation of Concerns

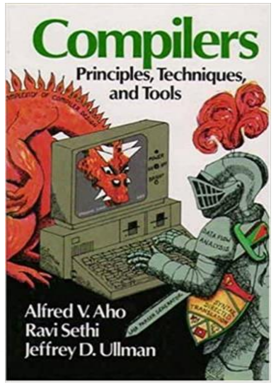
- SysGenX: Composable software generation for system-level simulation at exascale : Garth Wells, David Ham et al.
  - Funded as one of the 3 ExCALIBUR Phase 1b projects (£2.5M)
  - Developments for Firedrake, FEniCS and Bempp
  - Automatic code generation for very high-level problem description
  - Partners include Culham Centre for Fusion Energy Nvidia and Codeplay Software.

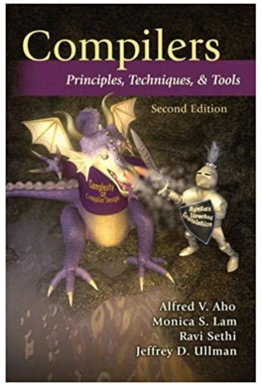
- Particles At eXascale on High Performance Computers (PAX-HPC) : group led by UCL
  - Developing exascale software for "efficiently calculating the interacting particles on vast numbers of computer cores"
  - The final one of the 3 ExCALIBUR Phase 1b projects (£3M)
  - Again, a core aim seems to be moving established software for exascale systems and extream scaling

- ExCALIBUR NEPTUNE Project – see Setven Wright's Talk on this later today.

- Utilizing domain knowledge will expose things that the compiler does not know
  - Iterating over the same mesh many times without change
  - Mesh is partitioned and colourable
- Compilers are conservative
  - Force it to do what you know is right for your code !
- Let go of the conventional wisdom that higher abstraction will not deliver higher performance
  - Higher abstraction leads to a bigger space of code synthesis possibilities
  - We can automatically generate significantly better code than what (most) people can (reasonably) write
  - Do not destroy performance portability by (hand-) tuning at a very low level to a specific platform







"Fundamentals and abstractions have more staying power than the technology of the moment"
Alfred Aho and Jeffrey Ullman (Turing Award Recipients 2020)

Downloads and More Information

- GitHub Repositories
  - OP2 – https://github.com/OP-DSL/OP2-Common
  - OPS – https://github.com/OP-DSL/OPS

  - OP-DSL Webpage - https://op-dsl.github.io/

- Contact

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