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Swiss Confederation

Federal Department of Home Affairs FDHA
Federal Office of Meteorology and Climatology MeteoSwiss

Operational numerical weather prediction on a GPU-accelerated cluster supercomputer

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C2SM
Center for Climate
Systems Modeling

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSCS
Swiss National Supercomputing Centre

OLD Meteoswiss operational system

Cray XE6 (Albis/Lema)

MeteoSwiss operational system

~4 years

OLD Meteoswiss operational system

ECMWF-Model

16 km gridspacing

2 x per day 10 day forecast

COSMO-7

Δx = 6.6 km, Δt = 60 s

393 x 338 x 60 cells

3 x per day 72 h forecast

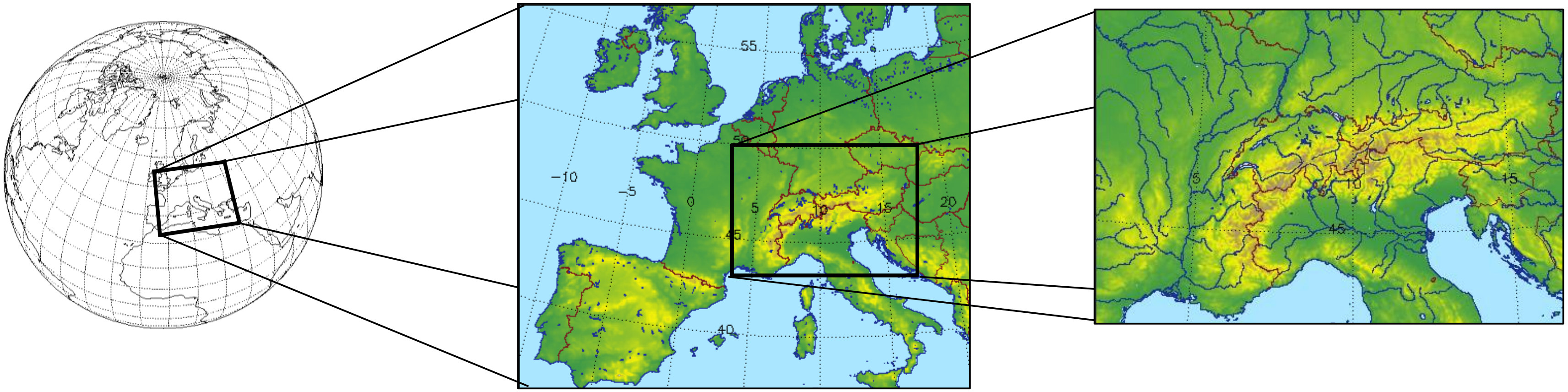
COSMO-2

Δx = 2.2 km, Δt = 20 s

520 x 350 x 60 cells

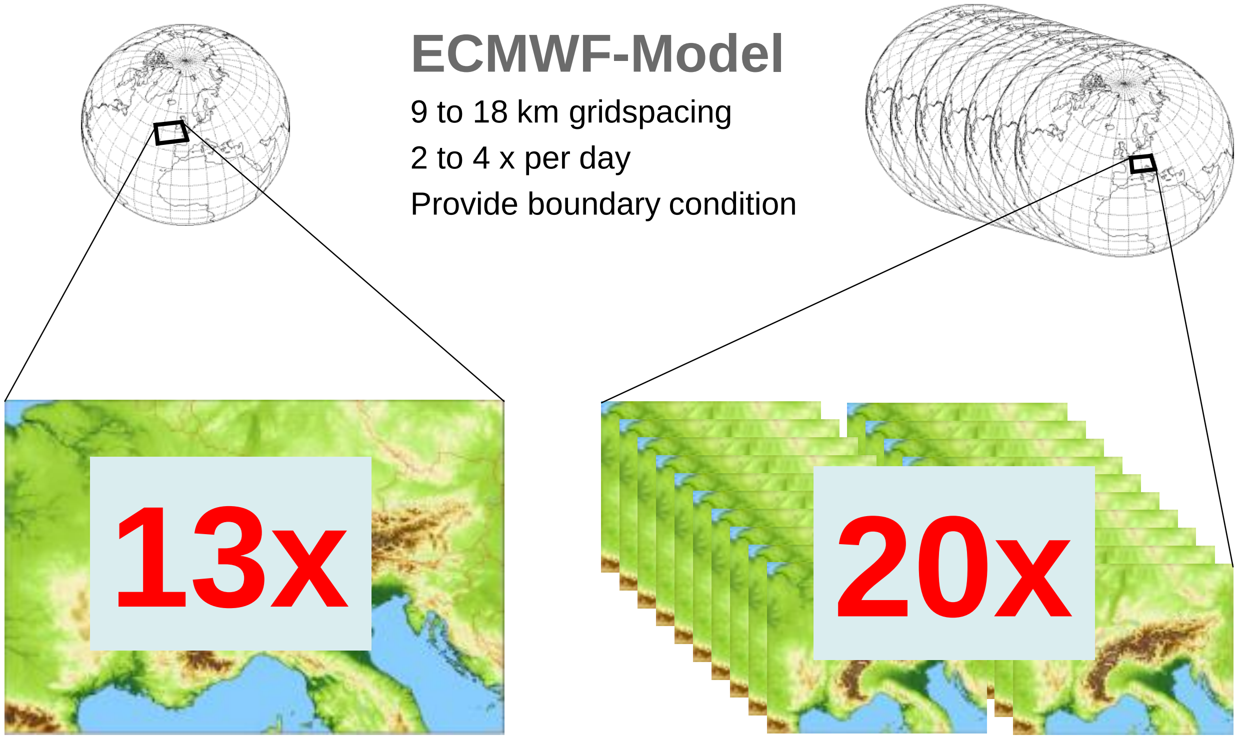
7 x per day 33 h forecast

1 x per day 45 h forecast



Requirements for New operational setup

- COSMO-1 (1 km high resolution) and COSMO-E (ensemble)
- Total computation cost for requirements = **40x**



ECMWF-Model

9 to 18 km gridspacing
2 to 4 x per day
Provide boundary condition

COSMO-1

1.1 km gridspacing
8 x per day
1 to 2 d forecast

(in production since
1/04/2016)

13x

20x

COSMO-E

2.2 km gridspacing
2 x per day
5 d forecast
21 members

(production planned
Mai/June 2016)

Ensemble **ation: LETKF**

7x

How to reach 40x in 5 years?

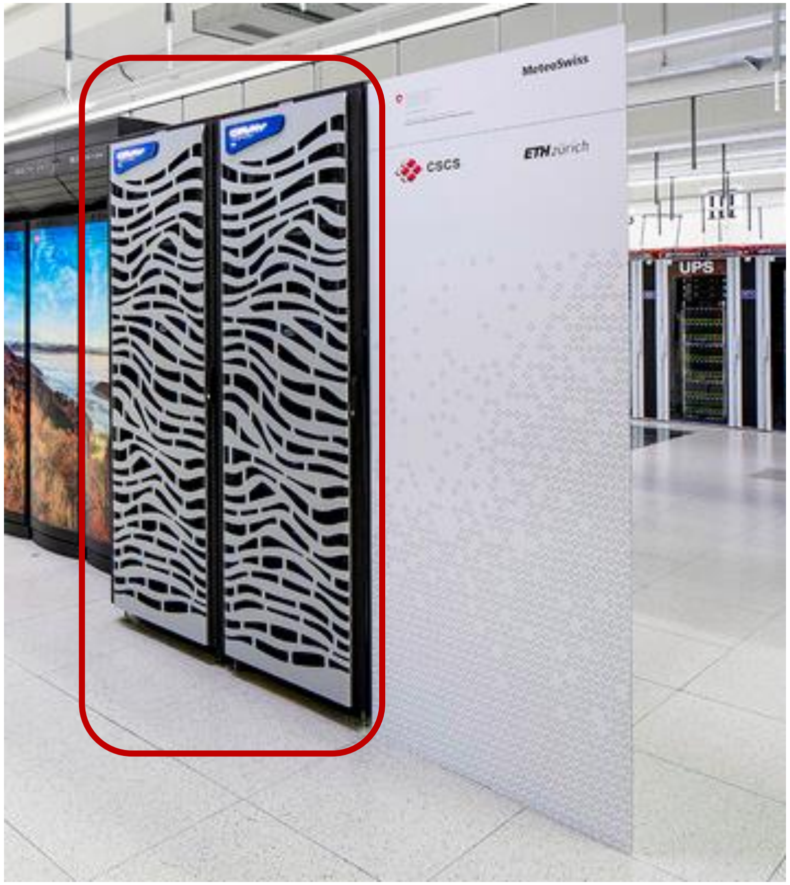
Key Ingredients

Processor performance (Moore’s Law)	~2.8x	
Increase in number of sockets	~1.3x	
Port to accelerators (GPUs)	~2.3x	~4x
Code improvement	~1.7x	
Increase utilization of system	~2.8x	

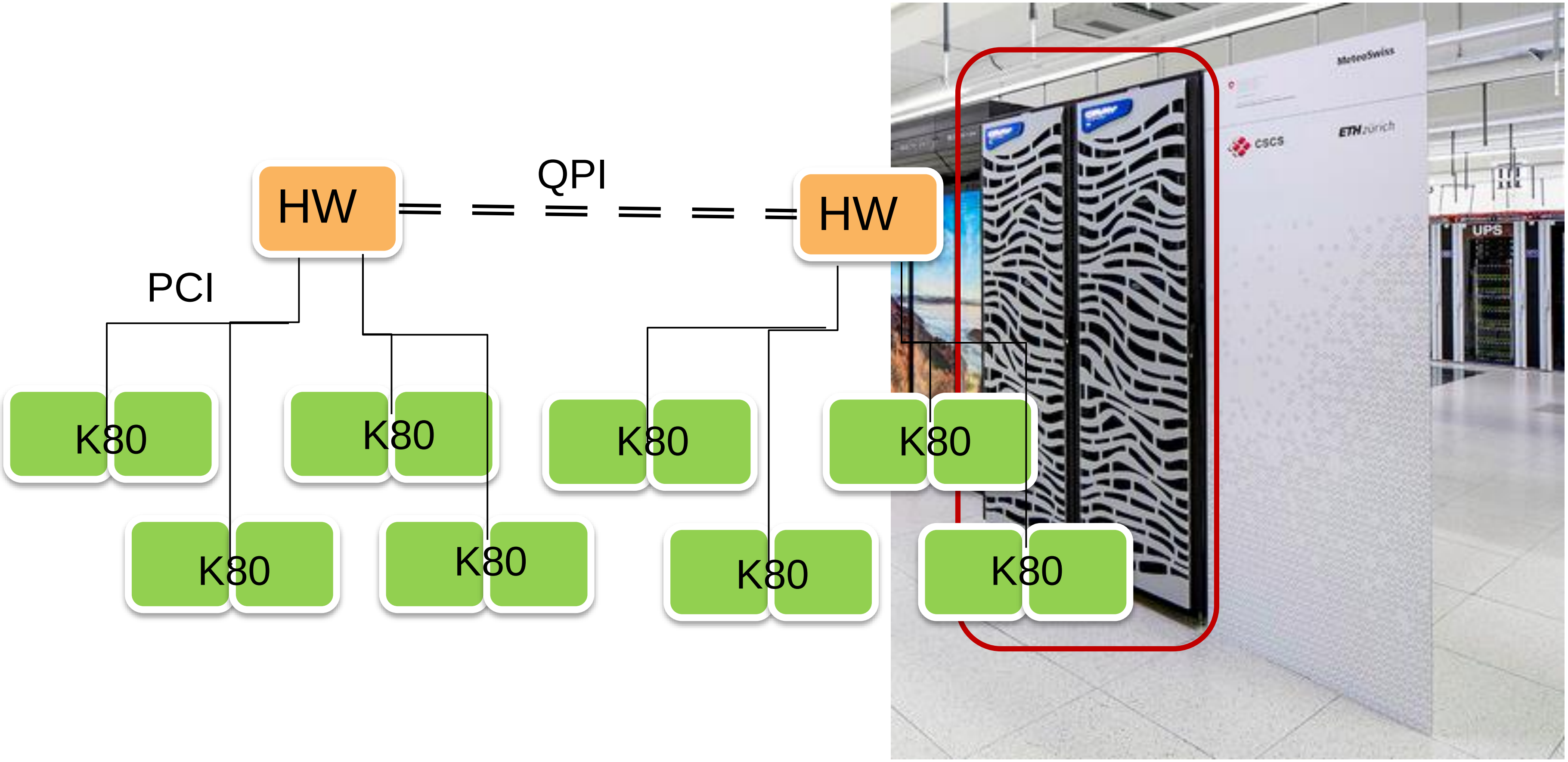
New MeteoSwiss hybrid HPC system

Piz Kesch (Cray CS Storm)

- 2 Cabinets (production & failover) installed at CSCS in July 2015
- 12 “Fat” compute nodes per cabinet
  - 2 Intel CPU Xeon E5 2690 (Haswell)
  - **8** Tesla K80 GPUs (each with 2 GK210 chip)

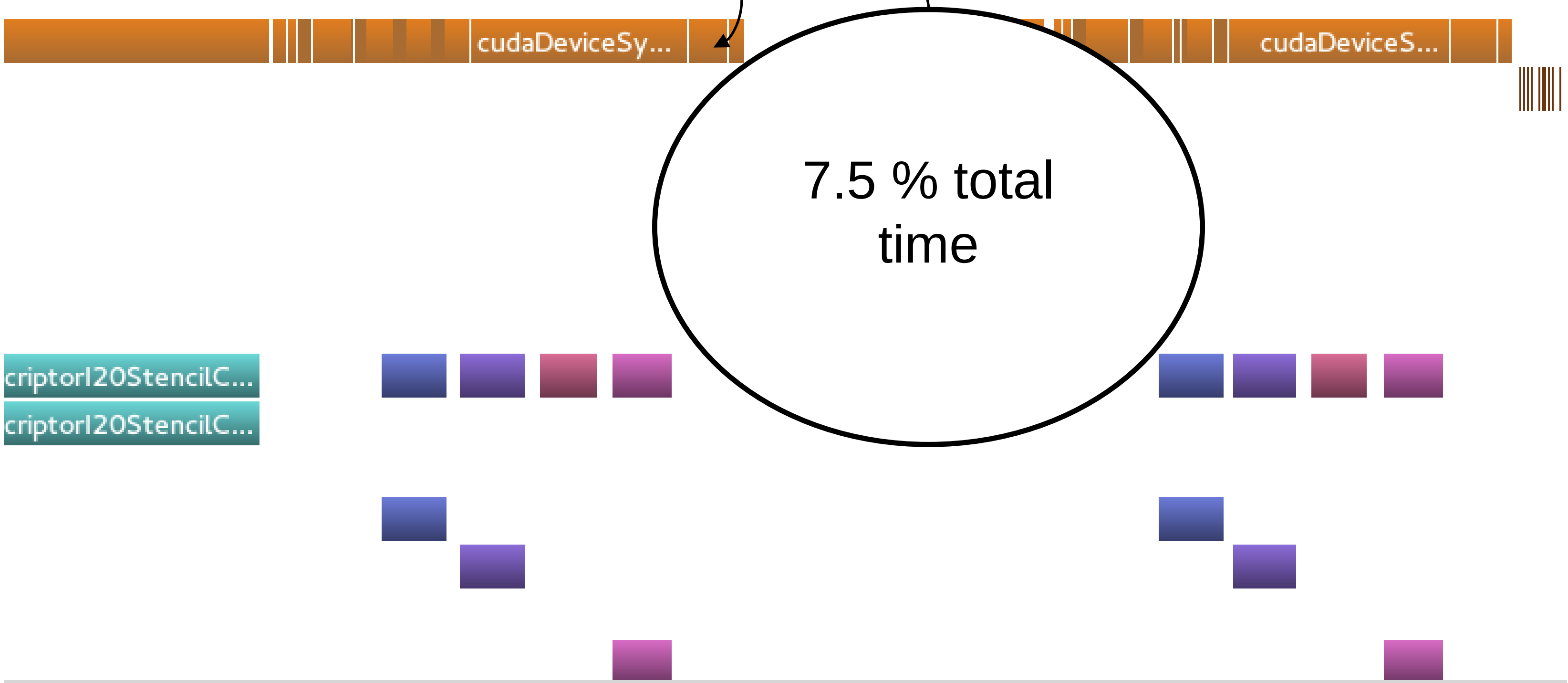


New MeteoSwiss hybrid HPC system



GPU communication with MPI

- Every Pack-MEvery pair GCL::Pack-MPI_Isend is generating large gaps in the streams due to delays in the host timeline (cudaDeviceSynchronize and cuda API calls)
- Collaboration with OSU, we will need mvapich2 GDS



cudaEventSynchronize

cudacudaEventElapsedTime
EventRecord

7.5 % total time

How to port a full weather model to GPUs?

Up or down?

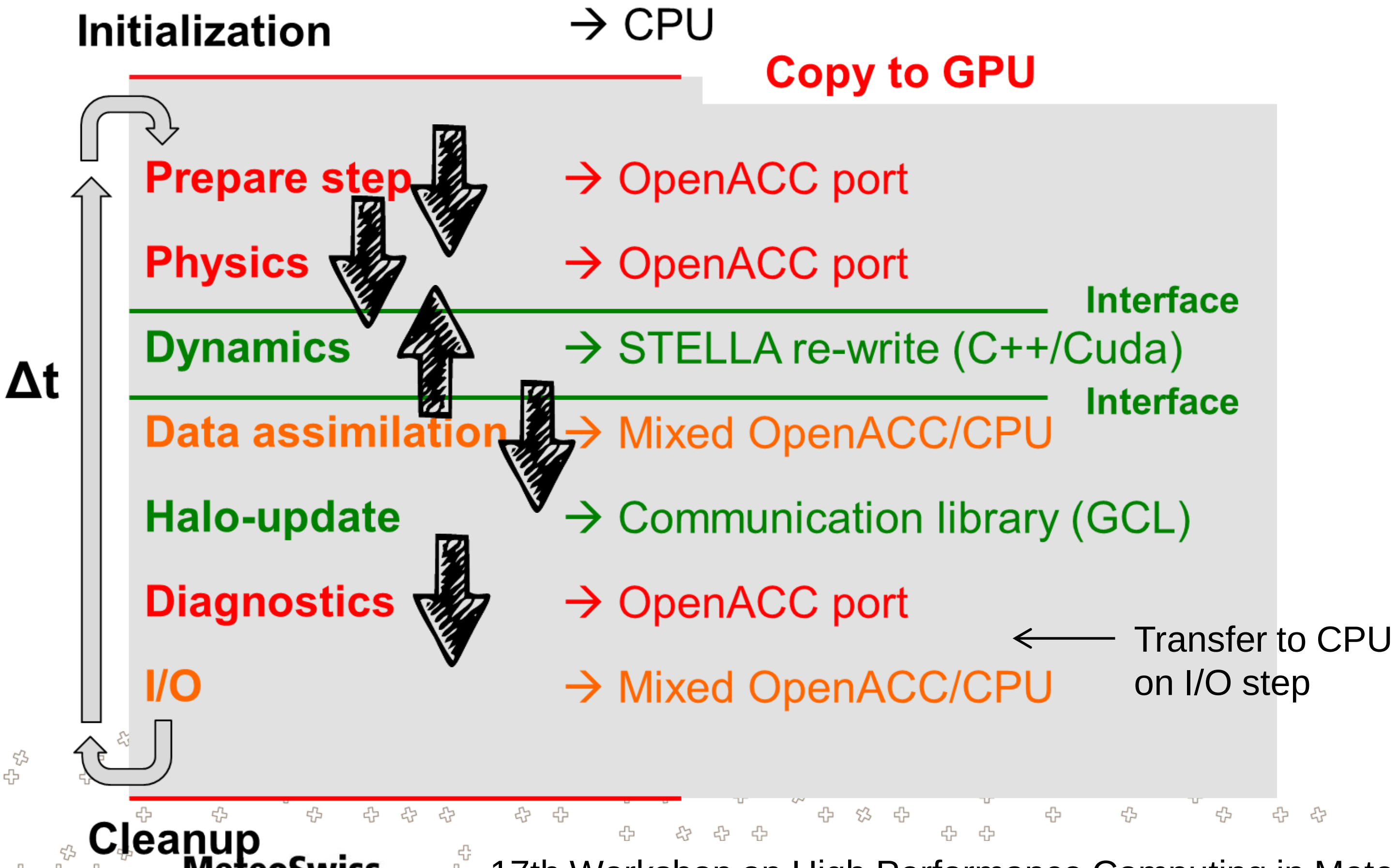
- **Increase level of abstraction**
  - Remove details of implementation
  - “Disruptive change”

- **Lower level of abstraction**
  - Add implementation details
  - „Incremental change“

Source: Oliver Fuhrer

The COSMO model on GPU

- Take advantage of the high computational capacity of GPUs
- Low compute intensity : avoid GPU-CPU data transfer
- Full GPU port strategy : all computations on the GPU



Initialization → CPU

Copy to GPU

Δt

Prepare step → OpenACC port

Physics → OpenACC port

Interface

Dynamics → STELLA re-write (C++/Cuda)

Interface

Data assimilation → Mixed OpenACC/CPU

Halo-update → Communication library (GCL)

Diagnostics → OpenACC port

I/O → Mixed OpenACC/CPU

← Transfer to CPU on I/O step

Cleanup

DOWN – Lower Level of abstraction

- Incremental adaptation to various programming models
- Traditionally OpenMP, OpenACC,
- Limited flexibility to custom platform dependent adaptations (#ifdef)

```
DO jb = i_startblk, i_endblk
    DO jc = i_startidx, i_endidx
        DO jk = slev, elev
            div_vec_c(jc,jk,jb) = vec_e(iid(ic,jb,1),jk,iblk(ic,jb,1)) * ptr_int%geofac_div(jc,1,jb) + &
                      vec_e(iid(ic,jb,2),jk,iblk(ic,jb,2)) * ptr_int%geofac_div(jc,2,jb) + &
                      vec_e(iid(ic,jb,3),jk,iblk(ic,jb,3)) * ptr_int%geofac_div(jc,3,jb)
        ENDDO
    ENDDO
ENDDO
```

DOWN – Lower Level of abstraction

- Incremental adaptation to various programming models
- Traditionally OpenMP, OpenACC,
- Limited flexibility to custom platform dependent adaptations (#ifdef)

```
!$ACC DATA COPYIN(vec_e) COPYOUT(div_vec_c)
!$ACC KERNELS LOOP, GANG(32), WORKER(8)
!OMP PARALLEL DO STATIC
                                             bl
                                             r_
                                             r_
     ENDDO
ENDDO
```

CPU

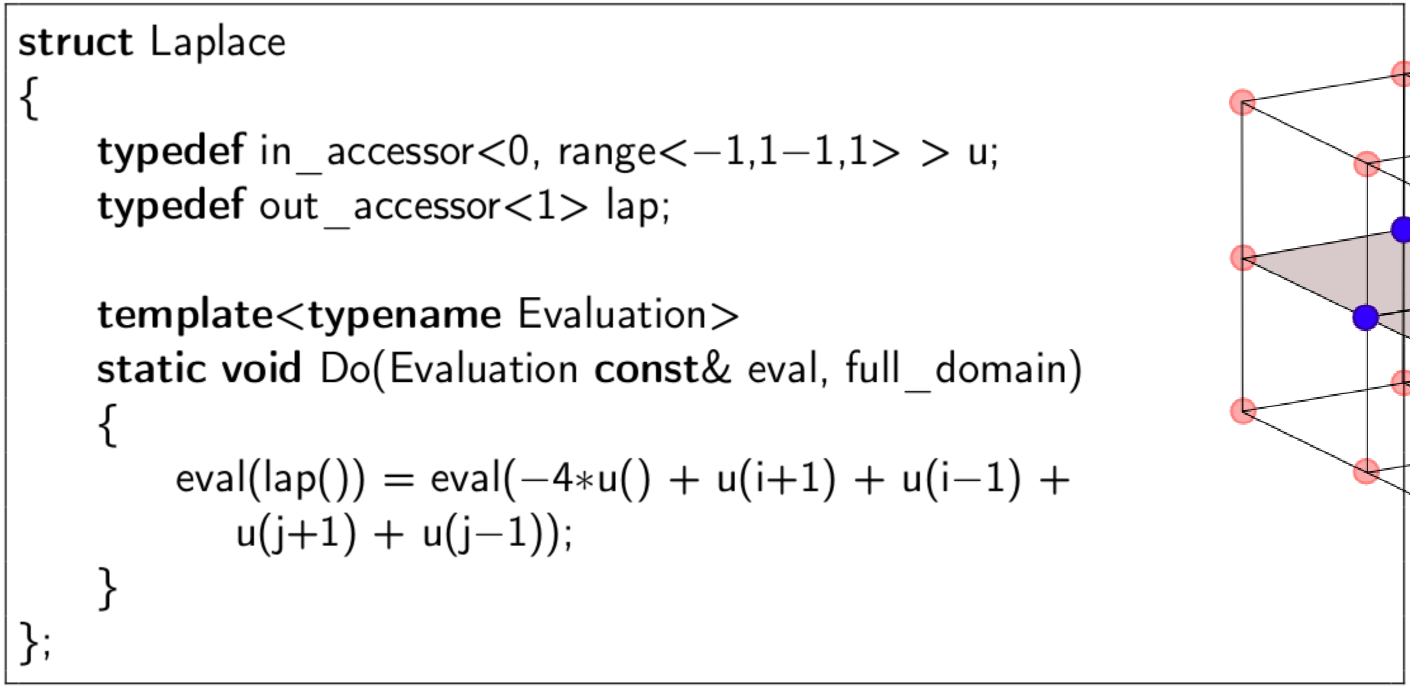
Algorithm: divergence
Language: Fortran
Grid: Structured
Data Layout: k, cell index, block index
Parallelism: block parallelism
Loop ordering: block index, cell index, k
Directives: OpenACC

GPU

Algorithm: divergence
Language: Fortran
Grid: Structured
Data Layout: cell index, k, block index
Parallelism: cell index
Loop ordering: block index, cell index, k
Directives: OpenACC

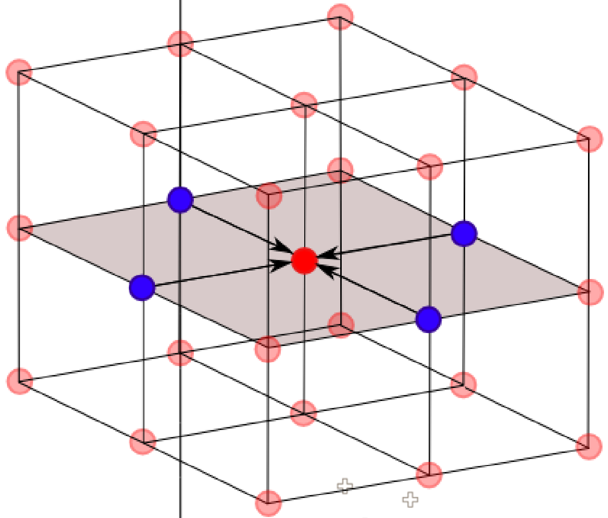
UP - STELLA / GridTools Library

- Domain-specific embedded language in C++
- Developed for stencil computations
- Separation of concern between model and hardware implementation
- Back-end optimized for different architectures (CPU,GPU)

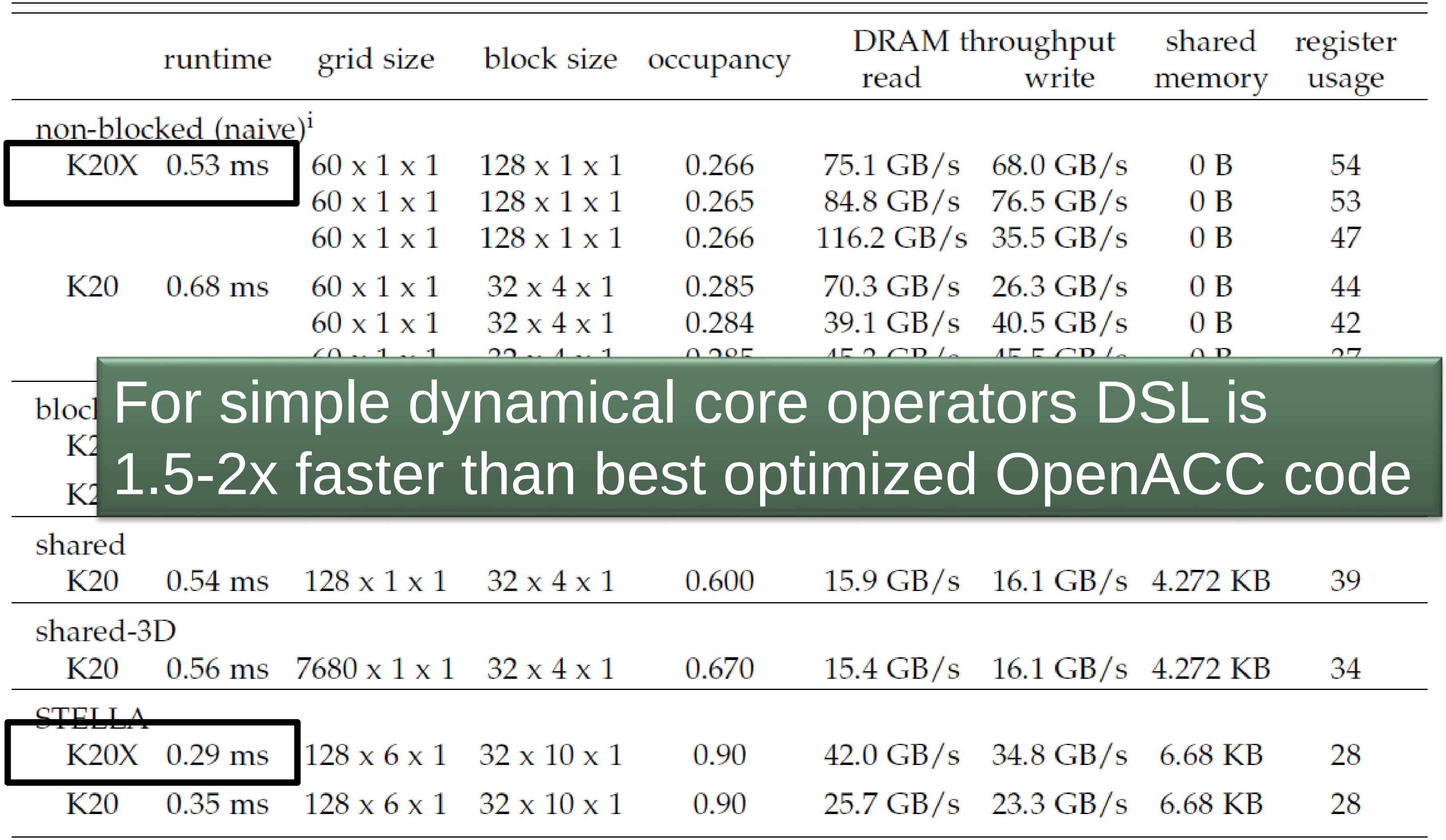


```
struct Laplace
{
    typedef in_accessor<0, range<-1,1-1,1> > u;
    typedef out_accessor<1> lap;

    template<typename Evaluation>
    static void Do(Evaluation const& eval, full_domain)
    {
        eval(lap()) = eval(-4*u() + u(i+1) + u(i-1) +
            u(j+1) + u(j-1));
    }
};
```

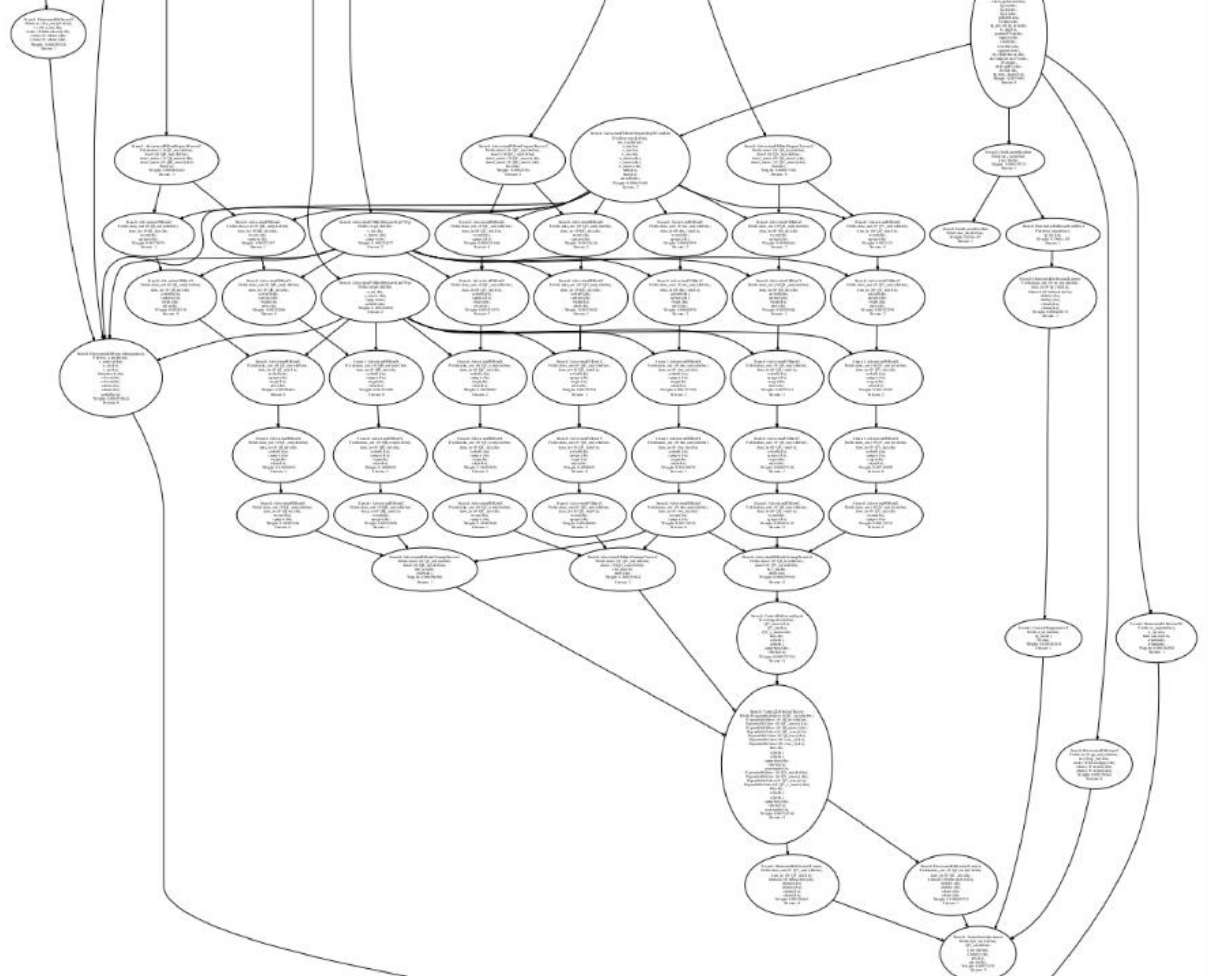


Performance Portability - Why UP (I)?



	runtime	grid size	block size	occupancy	DRAM throughput read	DRAM throughput write	shared memory	register usage
non-blocked (naive)[i]								
K20X	0.53 ms	60 x 1 x 1	128 x 1 x 1	0.266	75.1 GB/s	68.0 GB/s	0 B	54
		60 x 1 x 1	128 x 1 x 1	0.265	84.8 GB/s	76.5 GB/s	0 B	53
		60 x 1 x 1	128 x 1 x 1	0.266	116.2 GB/s	35.5 GB/s	0 B	47
K20	0.68 ms	60 x 1 x 1	32 x 4 x 1	0.285	70.3 GB/s	26.3 GB/s	0 B	44
		60 x 1 x 1	32 x 4 x 1	0.284	39.1 GB/s	40.5 GB/s	0 B	42
		60 x 1 x 1	32 x 4 x 1	0.285	45.3 GB/s	45.5 GB/s	0 B	37
bloc								
K2								
K2								
shared								
K20	0.54 ms	128 x 1 x 1	32 x 4 x 1	0.600	15.9 GB/s	16.1 GB/s	4.272 KB	39
shared-3D								
K20	0.56 ms	7680 x 1 x 1	32 x 4 x 1	0.670	15.4 GB/s	16.1 GB/s	4.272 KB	34
STELLA								
K20X	0.29 ms	128 x 6 x 1	32 x 10 x 1	0.90	42.0 GB/s	34.8 GB/s	6.68 KB	28
K20	0.35 ms	128 x 6 x 1	32 x 10 x 1	0.90	25.7 GB/s	23.3 GB/s	6.68 KB	28

For simple dynamical core operators DSL is 1.5-2x faster than best optimized OpenACC code



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Preparing for performance portability of future models

ESCAPE

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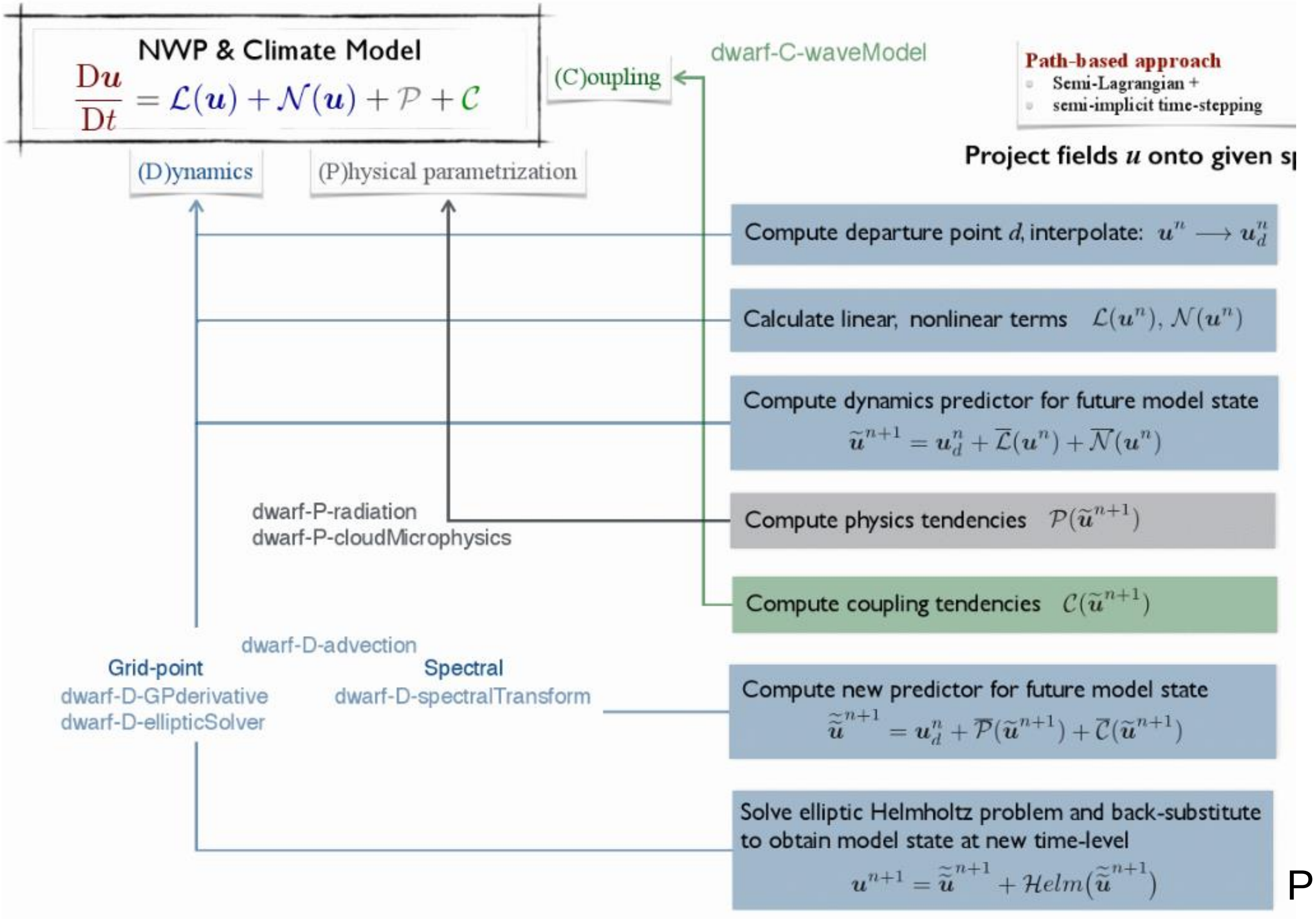
Energy efficient **SC**alable **A**lgorithms for weather **P**rediction at **E**xascale



NWP & Climate Model

$$\frac{D\boldsymbol{u}}{Dt} = \mathcal{L}(\boldsymbol{u}) + \mathcal{N}(\boldsymbol{u}) + \mathcal{P} + \mathcal{C}$$

(C)oupling

dwarf-C-waveModel

(D)ynamics

(P)hysical parametrization

Path-based approach
- Semi-Lagrangian +
- semi-implicit time-stepping

Project fields $\boldsymbol{u}$ onto given s

Compute departure point d, interpolate: $\boldsymbol{u}^n \longrightarrow \boldsymbol{u}^n_d$

Calculate linear, nonlinear terms $\mathcal{L}(\boldsymbol{u}^n), \mathcal{N}(\boldsymbol{u}^n)$

Compute dynamics predictor for future model state

$$\tilde{\boldsymbol{u}}^{n+1} = \boldsymbol{u}^n_d + \overline{\mathcal{L}}(\boldsymbol{u}^n) + \overline{\mathcal{N}}(\boldsymbol{u}^n)$$

dwarf-P-radiation
dwarf-P-cloudMicrophysics

Compute physics tendencies $\mathcal{P}(\tilde{\boldsymbol{u}}^{n+1})$

Compute coupling tendencies $\mathcal{C}(\tilde{\boldsymbol{u}}^{n+1})$

dwarf-D-advection

Grid-point
dwarf-D-GPderivative
dwarf-D-ellipticSolver

Spectral
dwarf-D-spectralTransform

Compute new predictor for future model state

$$\tilde{\tilde{\boldsymbol{u}}}^{n+1} = \boldsymbol{u}^n_d + \overline{\mathcal{P}}(\tilde{\boldsymbol{u}}^{n+1}) + \overline{\mathcal{C}}(\tilde{\boldsymbol{u}}^{n+1})$$

Solve elliptic Helmholtz problem and back-substitute to obtain model state at new time-level

$$\boldsymbol{u}^{n+1} = \tilde{\tilde{\boldsymbol{u}}}^{n+1} + \mathcal{H}elm(\tilde{\tilde{\boldsymbol{u}}}^{n+1})$$

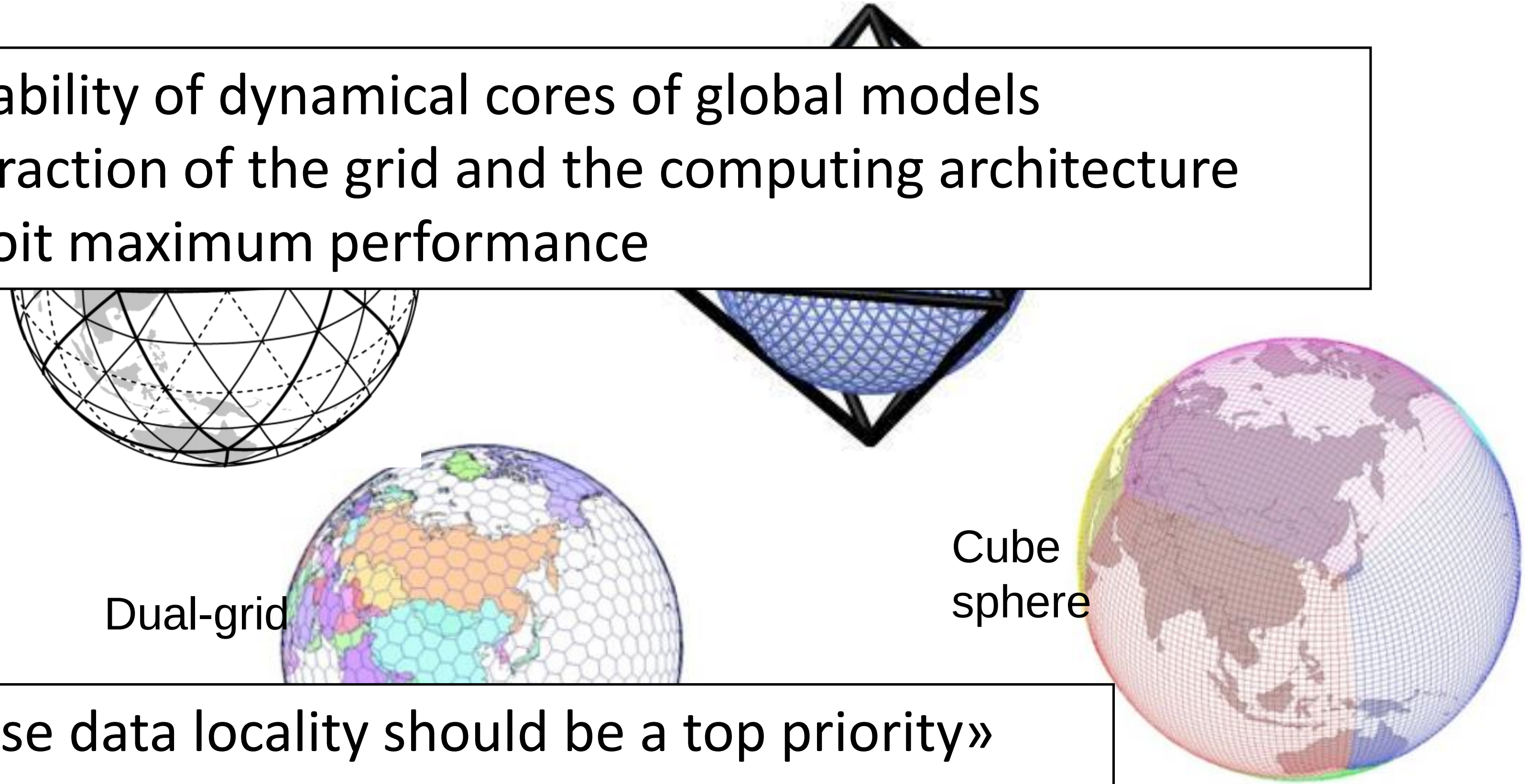
Peter Bauer

ECMWF · MeteoSwiss · DMI · RMI · NVIDIA · METEO FRANCE Toujours un temps d'avance · ICHEC · Deutscher Wetterdienst Wetter und Klima aus einer Hand · Optalysys · Bull atos technologies · PSNC · Loughborough University

UP - Preparing for future models

GridTools On Irregular Grids

- Portability of dynamical cores of global models
- Abstraction of the grid and the computing architecture
- Exploit maximum performance

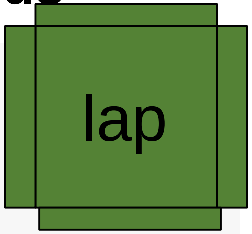

Dual-grid

Cube sphere

> «Increase data locality should be a top priority»
>
> Thomas Schulthess, HPC in Meteorology, 2016

Data Locality on unstructured meshes

Loop fusion and redundant computations on Lat-Lon grids



```
!OMP PARALLEL DO
DO iblock=1,nblocks
  DO k=1,nz
    DO j=jstart-1,jend+1
      DO i=istart-1,iend+1
        lap(i,j,k,iblock) =-4*u(i,j,k,iblock) + u(i+1,j,k,iblock) +
          u(i-1,j,k,iblock) + u(i,j+1,k,iblock) + u(i,j-1,k,iblock)
      ENDDO
    ENDDO
    DO j=jstart,jend
      DO i=istart,iend
        udiff(i,j,k,iblock) =-4*lap(i,j,k,iblock) + lap(i+1,j,k,iblock) +
          lap(i-1,j,k,iblock) + lap(i,j+1,k,iblock) + lap(i,j-1,k,iblock)
      ENDDO
    ENDDO
  ENDDO
ENDDO
```

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Data Locality on unstructured meshes

On irregular grids?

```
DO jb = i_startblk, i_endblk
   DO jc = i_startidx, i_endidx
      DO jk = slev, elev
          div(jc,jk,jb) = u(iid(ic,jb,1),jk,iblk(ic,jb,1)) * ptr_int%geofac_div(jc,1,jb) + &
                u(iid(ic,jb,2),jk,iblk(ic,jb,2)) * ptr_int%geofac_div(jc,2,jb) + &
                u(iid(ic,jb,3),jk,iblk(ic,jb,3)) * ptr_int%geofac_div(jc,3,jb)
      ENDDO
   ENDDO
ENDDO
Halo_exchange
DO jb = i_startbl
   DO jc = i_startidx, i_endidx
      DO jk = slev, elev
          div2 (jc,jk,jb) = div(iid(ic,jb,1),jk,iblk(ic,jb,1)) * ptr_int%geofac_div(jc,1,jb) + &
                div(iid(ic,jb,2),jk,iblk(ic,jb,2)) * ptr_int%geofac_div(jc,2,jb) + &
                div(iid(ic,jb,3),jk,iblk(ic,jb,3)) * ptr_int%geofac_div(jc,3,jb)
      ENDDO
   ENDDO
ENDDO
```

Are we abandoning Loop Fusion on unstructured meshes?

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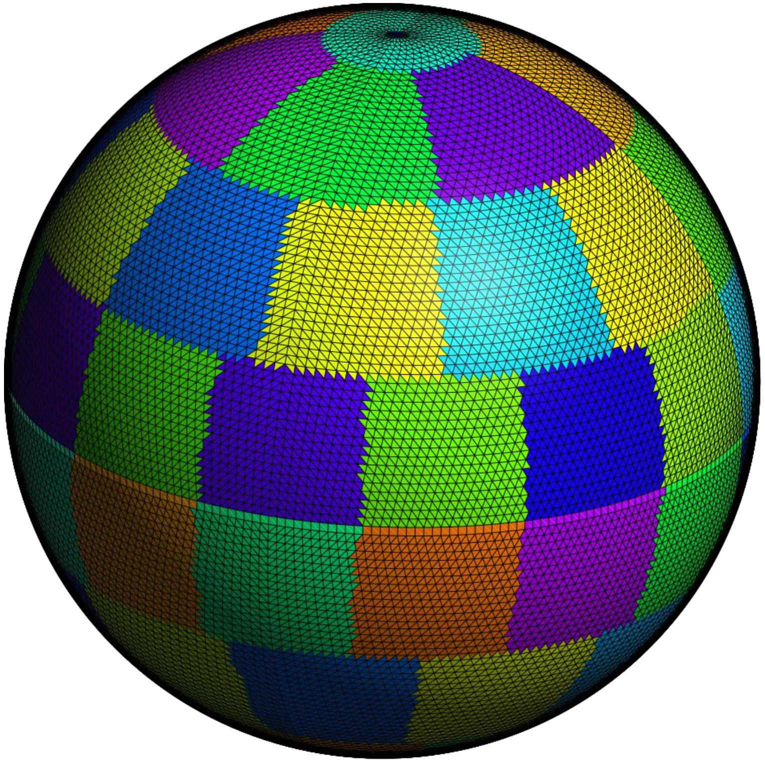
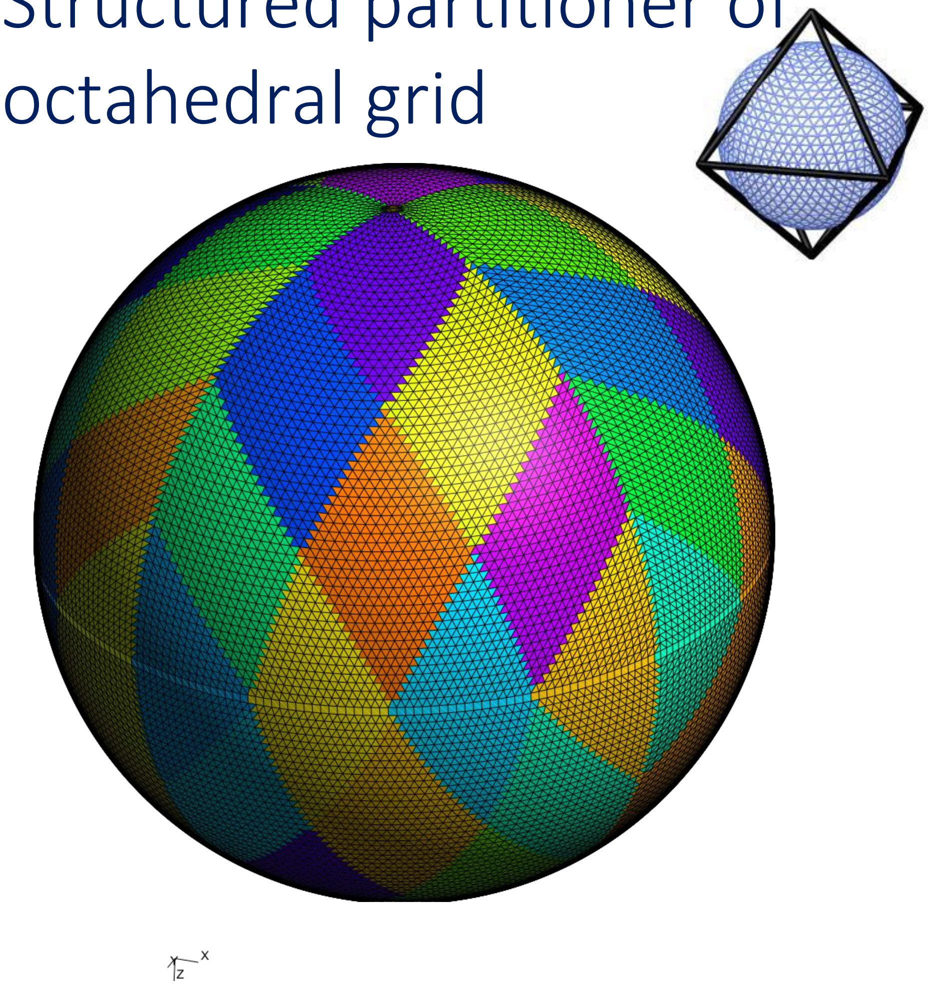
Equal partitioner of octahedral grid



Structured partitioner of octahedral grid



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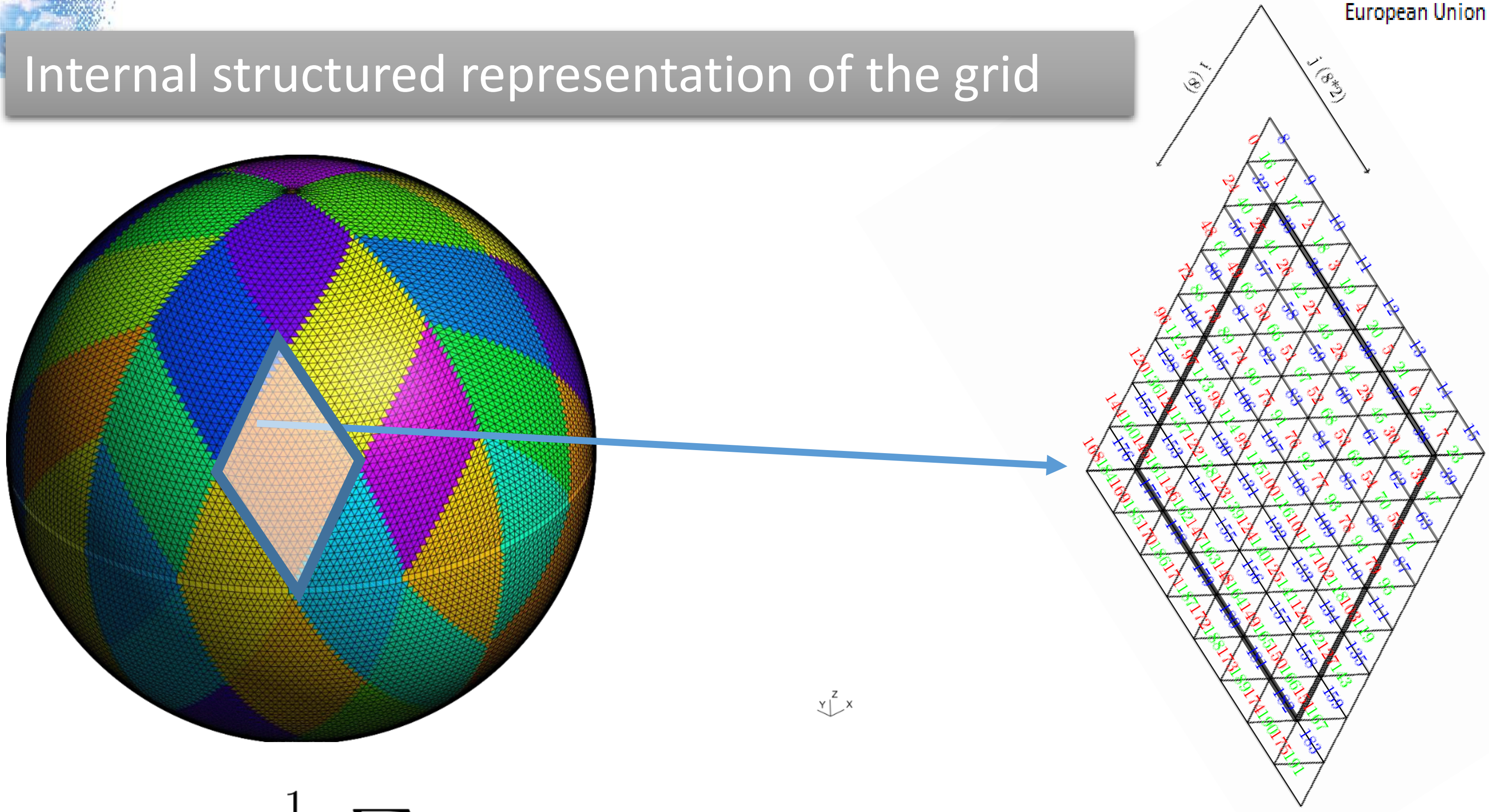
Internal structured representation of the grid



$$\mathrm{div}(\mathbf{v})_i := \frac{1}{A_i} \sum_{l \in \mathcal{E}(i)} v_{n_l} (\mathbf{N}_l \cdot \mathbf{n}_{i,l}) l$$

Unstructured DSL syntax

```
on_edges(sum_reduction, v(), l()) / A();
```

ECMWF
MeteoSwiss
DMI
RMI
NVIDIA
METEO FRANCE Toujours un temps d'avance
ICHEC Irish Centre for High-End Computing
Deutscher Wetterdienst Wetter und Klima aus einer Hand DWD
Optalysys
Bull atos technologies
PSNC
Loughborough University

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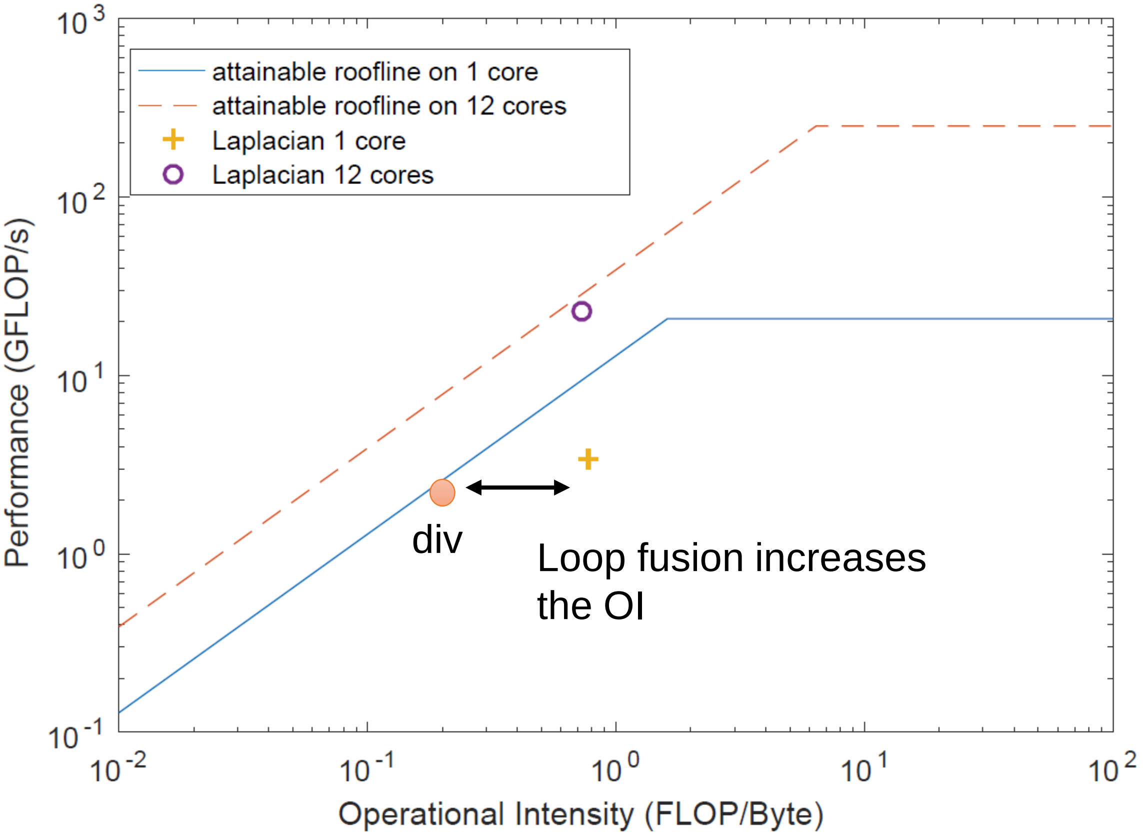
$$(\nabla_d^2 \mathbf{v})_l \cdot \mathbf{N}_l := \mathrm{grad}_n \Big[\mathrm{div}(\mathbf{v})\Big]_l - \mathrm{grad}_\tau \Big[\mathrm{curl}(\mathbf{v})\Big]_l$$

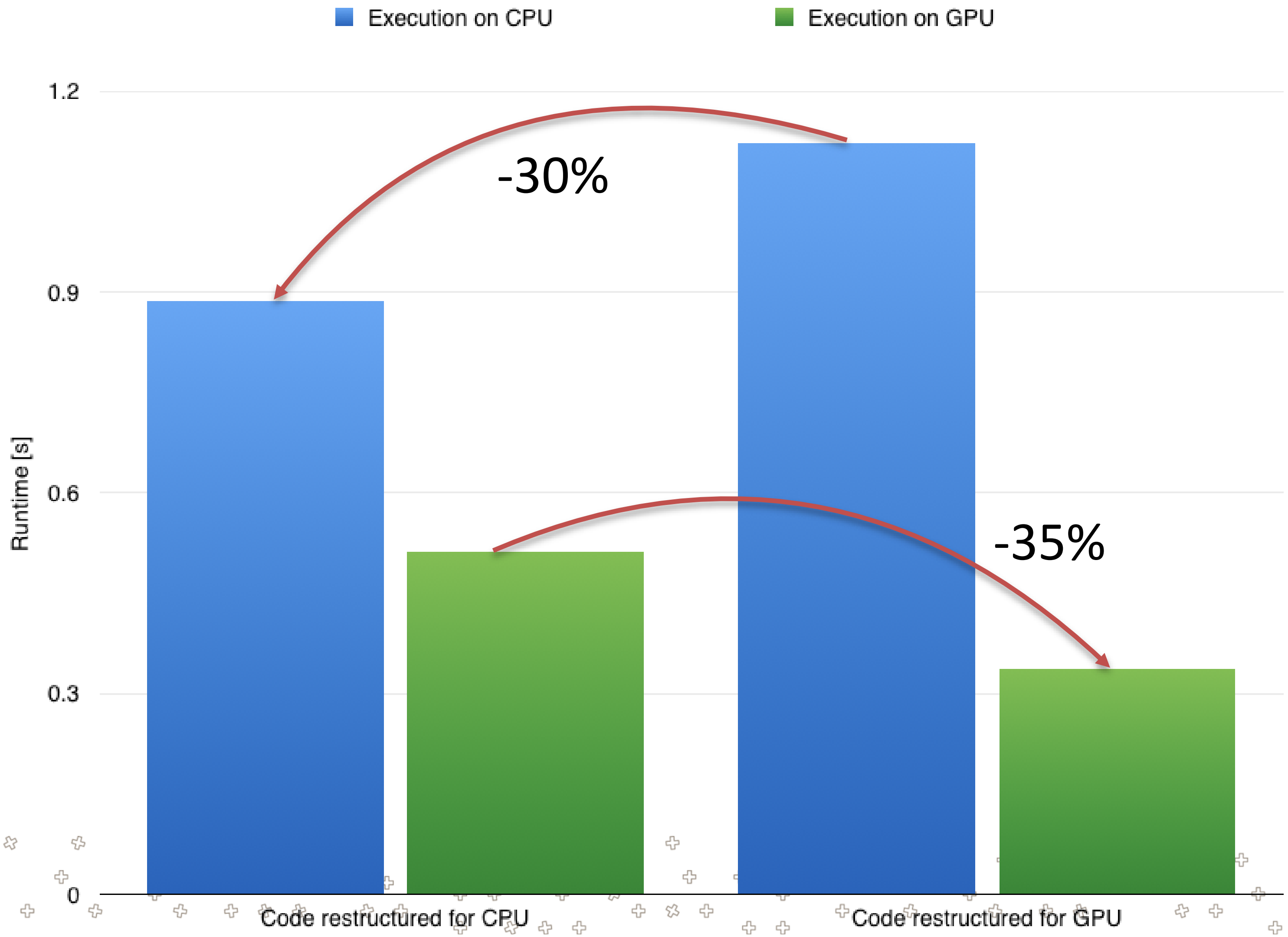


Loop fusion increases the OI

Domain size	1 core			12 cores			GPU	
	Fortran	GridTools	speedup	Fortran	GridTools	speedup	Gridtools	speedup
256*256*50	0.784	0.3829	**2.05x**	0.1279	0.0569	**2.25x**	0.0473	**2.7x**

DOWN - Preparing for future models

Performance portability: COSMO Radiation



CLAW: Low-level transformations

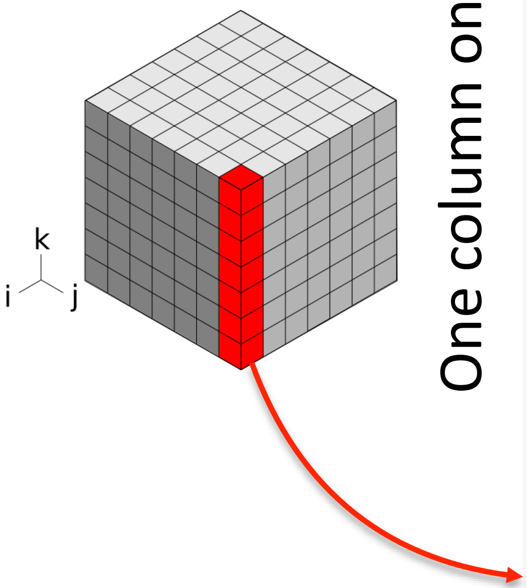
```
!$acc parallel loop
!$claw loop-interchange
DO k=1,nz
  !$claw loop-extract fusion
  CALL fct()
  !$claw loop-fusion group(j)
  !$acc loop
  DO j=1,nproma
    ! 1st loop body
  END DO
  !$claw loop-fusion group(j)
  !$acc loop
  DO j=1,nproma
    ! 2nd loop body
  END DO
  !$claw loop-fusion group(j)
  !$acc loop
  DO j=1,nproma
    ! 3rd loop body
  END DO
END DO
!$acc end parallel
```

```
!$acc parallel loop
DO j=1,nproma
  !$acc loop
  DO k=1,nz
    CALL fct()
    ! 1st loop body
    ! 2nd loop body
    ! 3rd loop body
  END DO
END DO
!$acc end parallel
```

CLAW Compiler low-level transformations:

- Loop fusion
- Loop reordering
- Loop extraction
- Loop hoisting
- Caching
- On the fly computation
- Array notation to do statement
- Code removal
- Conditional directive enabling

CLAW One column abstraction

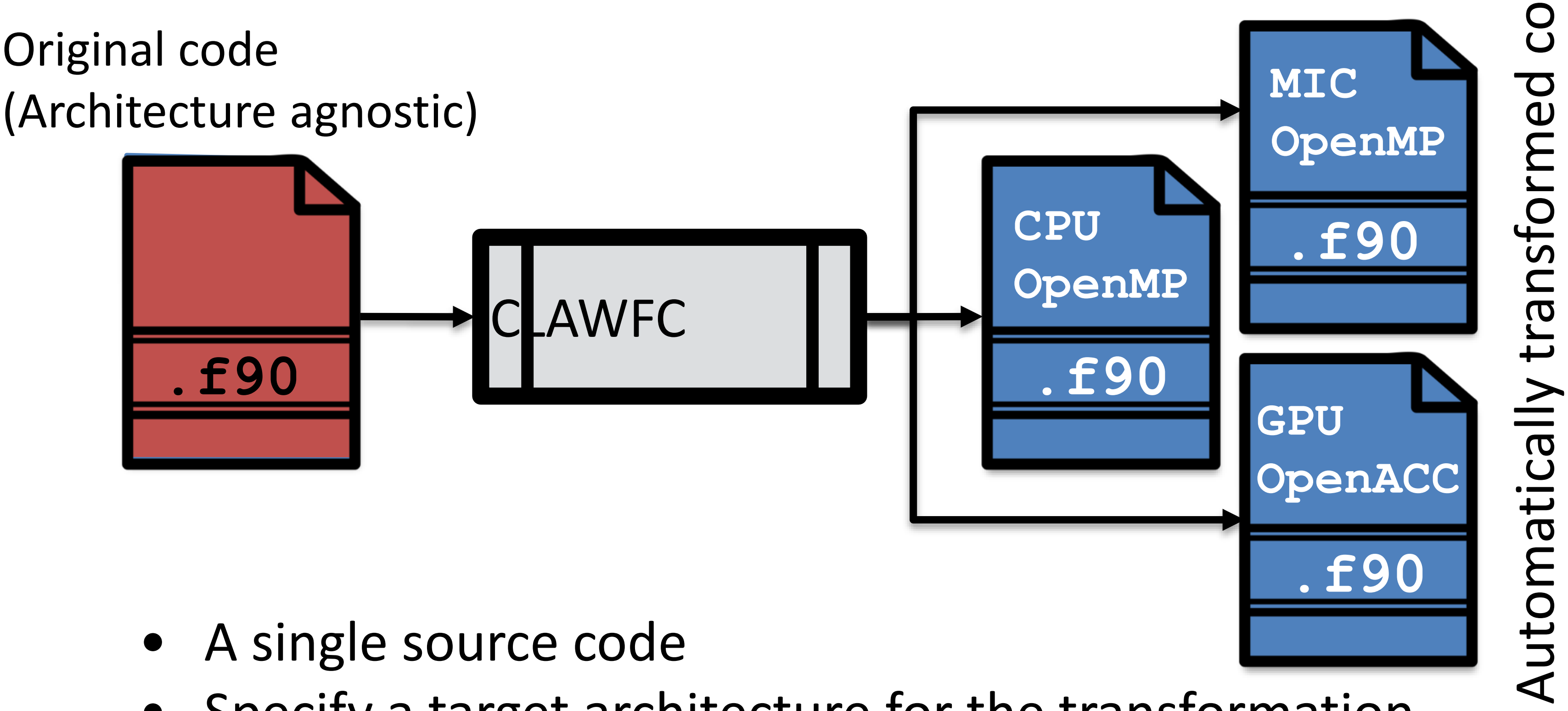


One column only

```
SUBROUTINE lw_solver(…)
     !$claw define dimension icol(1:ncol) &
     !$claw parallelize
     DO igpt = 1, ngpt
       DO ilev = 1, nlay
              tau_loc(ilev) = max(tau(ilev,igpt) …
         END DO
         DO ilev = 1, nlay
              trans(ilev) = exp(-tau_loc(ilev))
         END DO
         DO ilev = nlay, 1, -1
              radn_dn(ilev,igpt) = trans(ilev) *
              radn_dn(ilev+1,igpt) + …
         END DO
         DO ilev = 2, nlay + 1
              radn_up(ilev,igpt) = trans(ilev-1) * radn_up(ilev-
              1,igpt) + …
         END DO
     END DO
     radn_up(:,:) = 2._wp * pi * quad_wt * radn_up(:,:)
     radn_dn(:,:) = 2._wp * pi * quad_wt * radn_dn(:,:)
END SUBROUTINE lw_solver
```

Dependency on the vertical dimension only

CLAW One column abstraction



- A single source code
- Specify a target architecture for the transformation
- Specify a compiler directives language to be added

```
clawfc --directive=openacc --target=gpu -o mo_lw_solver.acc.f90 mo_lw_solver.f90
```

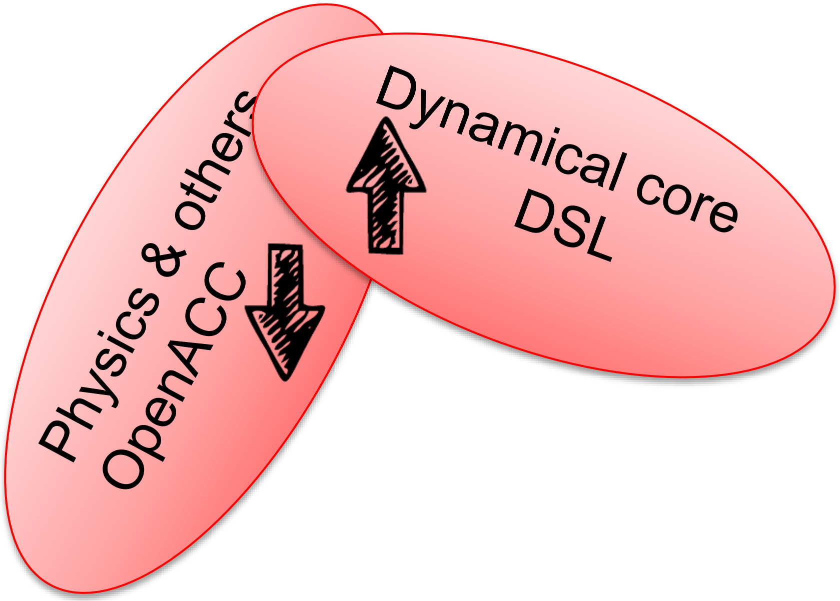
```
clawfc --directive=openmp --target=cpu -o mo_lw_solver.omp.f90 mo_lw_solver.f90
```

```
clawfc --directive=openmp --target=mic -o mo_lw_solver.mic.f90 mo_lw_solver.f90
```

pictures: Por Suppasit from Noun Project

Conclusions

- New setup COSMO-1 and COSMO-E running on hybrid GPU system
- About 4x was gained by moving to GPUs as compare to traditional CPUs



Performance comparison with CPU only system

Piz Dora (Cray XC40)

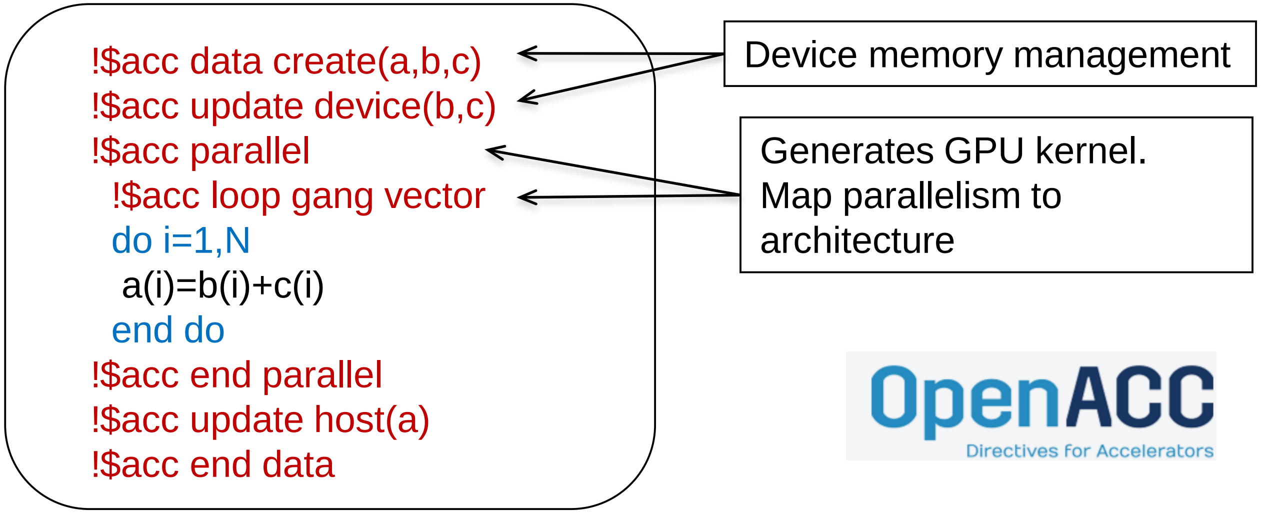
- “Traditional” CPU based system
- Compute nodes with 2 Intel Xeon E5-2690 v3 socket (Haswell)
- Pure compute rack
- Rack has 192 compute nodes
- Very high density (supercomputing line)

- Performance comparison for the COSMO-E ensemble members

Results

	Piz Dora	**Piz Kesch**	Factor
Energy per member	10 kWh	2.1 kWh	**4.8 x**
Time with 8 sockets per member	3.9 h	1.0 h	**3.9 x**
Cabinets required to run ensemble at required time-to-solution	1.4	0.38	**3.8 x**

Porting with OpenACC directives



```
!$acc data create(a,b,c)
!$acc update device(b,c)
!$acc parallel
  !$acc loop gang vector
  do i=1,N
   a(i)=b(i)+c(i)
  end do
!$acc end parallel
!$acc update host(a)
!$acc end data
```

Device memory management

Generates GPU kernel.
Map parallelism to
architecture

- Directive-based programming model for C++ and Fortran
- Provides abstraction to define parallel region, data locality (GPU, CPU) and mapping to specific hardware parallelism (gang, worker, vector)
- Enable to port large codes to GPU with acceptable efforts
- Used for porting the physics, assimilation, I/O.

Performance portability with OpenACC

- In some cases CPU and GPU have different optimization requirement

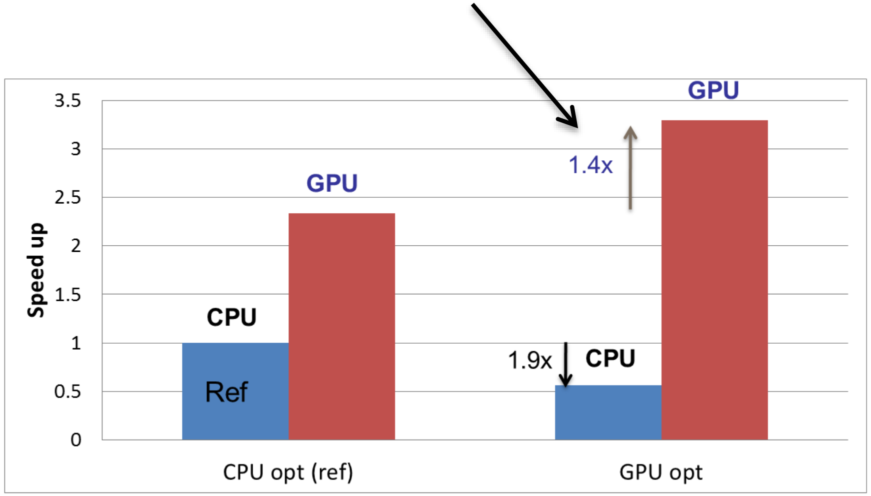
CPU : compute bound

- Auto-vectorization : small loop
- Pre-computation

GPU : memory bound limited

- Benefit from large kernels : reduce kernel launch overhead, better computation/memory access overlap
- Loop re-ordering and scalar replacement
- On the fly computation

Optimize code for GPU runs 1.9x slower on CPU



Radiation parametrization, domain 128x128x60, 1 Sandy Bridge CPU vs 1 K20x CPU

- Current solution : different code paths for time critical components with pre-processor macros

CLAW approach

- Goal : Provide language abstraction for performance portability in climate and weather model
- Directives with code transformation

```
SUBROUTINE inv_th(pclc,pca1, …)
  INTEGER:: ki1sd

  !$acc parallel
  !$acc loop collapse(3)
  !$claw loop-interchange (k,i,j)
  DO i=istart,iend
    DO j=jstart,jend
      DO k=kstart,kend
        ! Computation is done here
      END DO
    END DO
  END DO
  !$acc end parallel

END SUBROUTINE inv_th
```

CLAW

- Code manipulation with AST
- Based on the OMNI compiler
- Transformed code can be compile with standard compiler

CLAW language definition are available on github :

https://github.com/C2SM-RCM/claw-language-definition

References

Lapillonne, X. and Fuhrer, O. (2014). Using compiler directives to port large scientific applications to GPUs: An example from atmospheric science. *Parallel Processing Letters*, *24*(01), 1450003.

Fuhrer, O. and *al.* (2014). Towards a performance portable, architecture agnostic implementation strategy for weather and climate models. *Supercomputing frontiers and innovations*, *1*(1), 45-62.

Gysi, T. and *al.* (2015). STELLA: a domain-specific tool for structured grid methods in weather and climate models. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (p. 41). ACM.

Thank you

Increase of x40 in computational cost of operational setup

Key ingredients

Processor performance (Moore’s law)	~2.8 x
Code refactoring and port to GPUs	~3.9 x
Increase utilization of system	~2.8 x
Increase in number of sockets	~1.3 x

- Target system architecture to application

Image: Cray