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Developing a km-scale model system over the Alpine arc

HPC and other challenges

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⁷*University of Leeds*

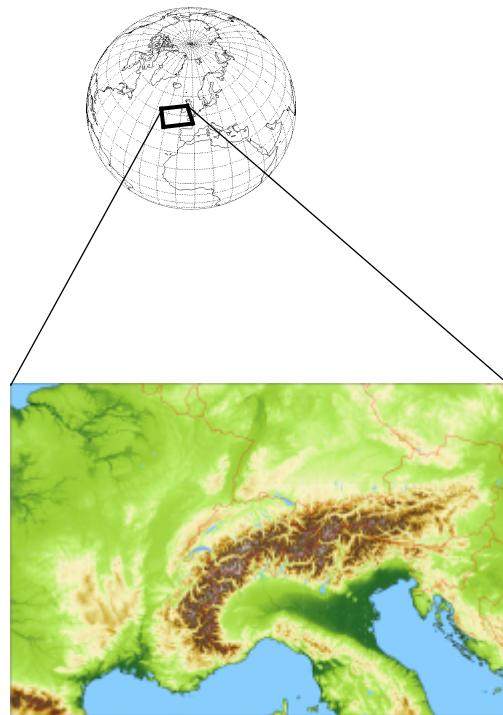
⁷*University of Innsbruck*

Greyzone Workshop, ECMWF, November 13-16, 2017

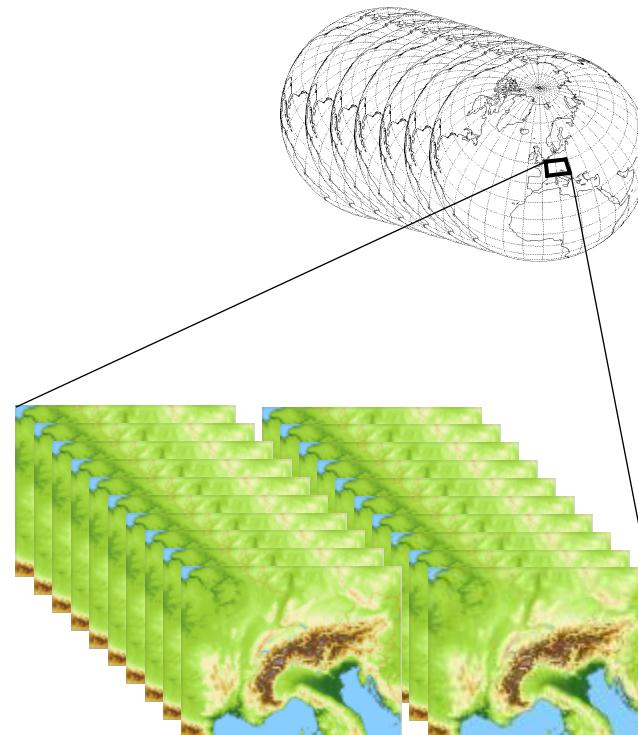


Operational system since 2016

IFS HRES



IFS ENS

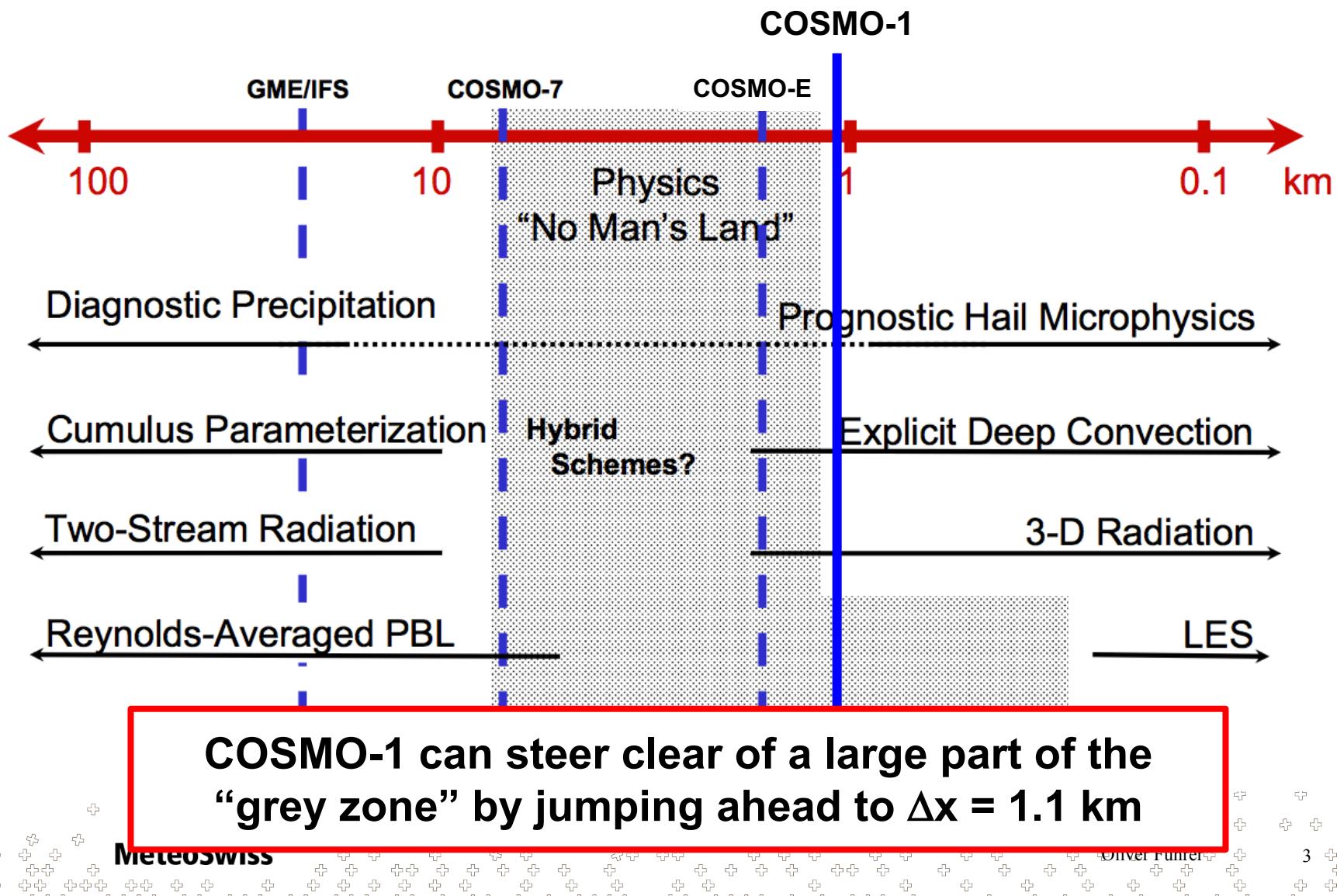


Ensemble data assimilation: LETKF (40 members)



Greyzone

(adapted from Klemp 2007)





The challenge of NWP in Switzerland



Flat-terrain cloudy BL



Cloudy BL over the Alps (Eggishorn)

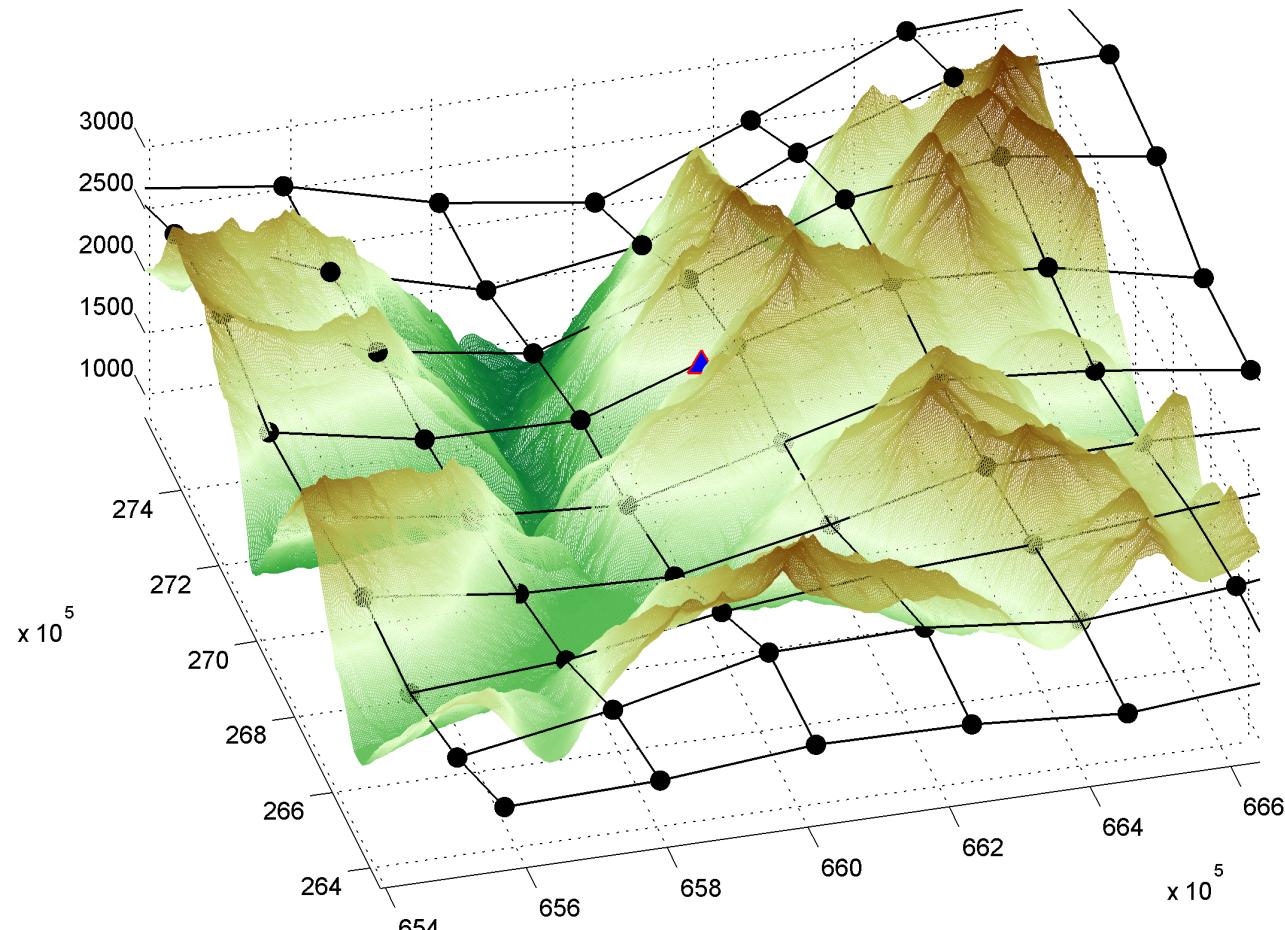
Two key issues for COSMO-1 and -E:

- ABLs over complex terrain
- Turbulence and shallow convection in greyzone



Complex topography

Model vs. real topography at $\Delta x = 2.2 \text{ km}$ (COSMO-E) at Guetsch (Andermatt)

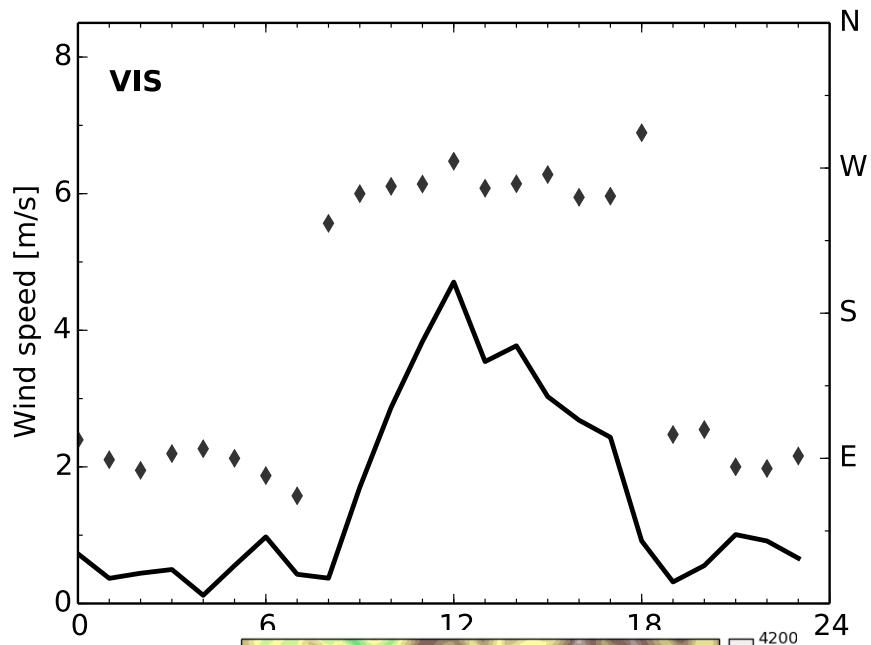




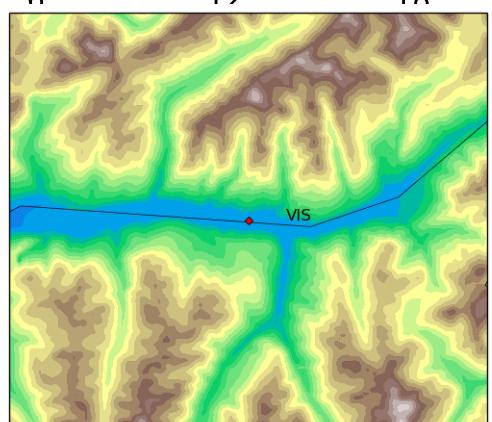
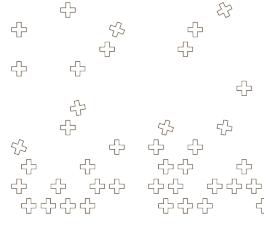
Mean diurnal cycle of valley winds

OBS

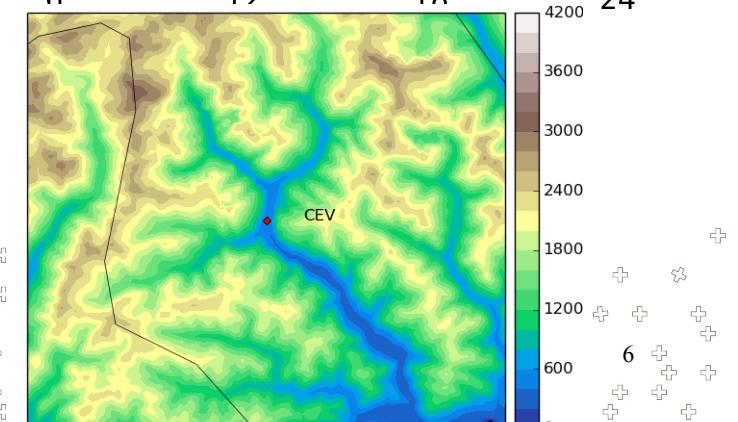
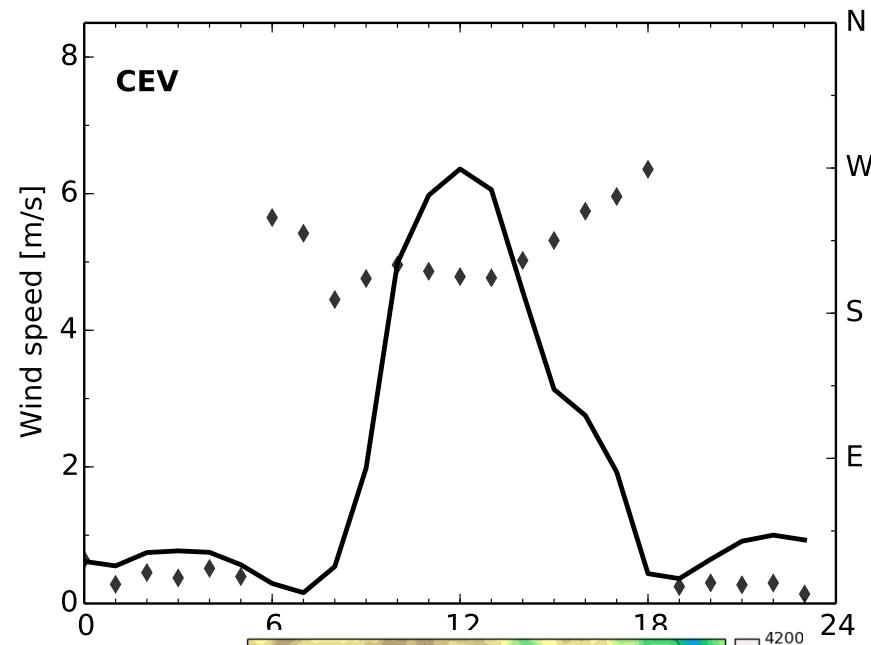
Visp (Rhone valley)



average — 27 July)



Cevio (Maggia valley)



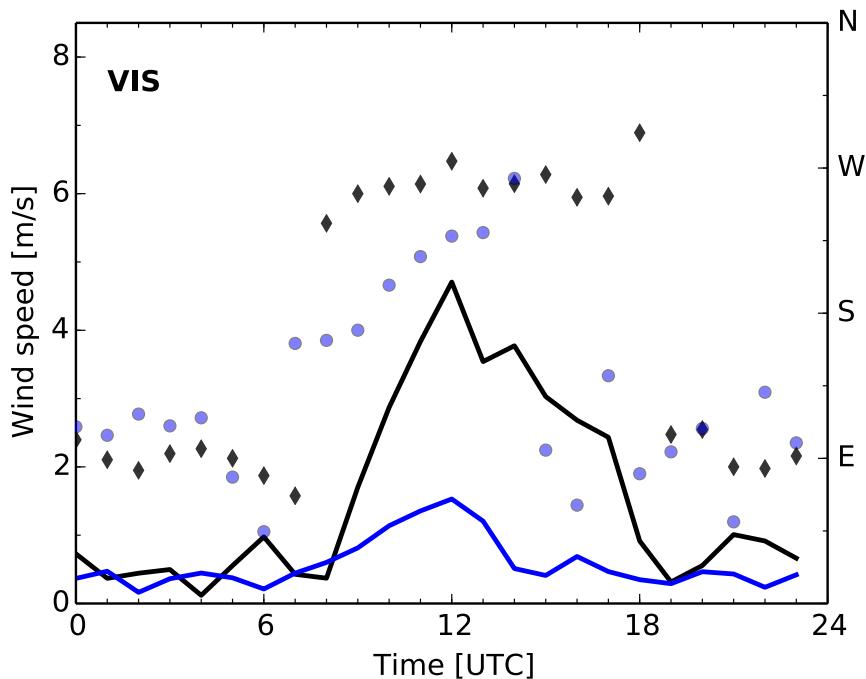
6



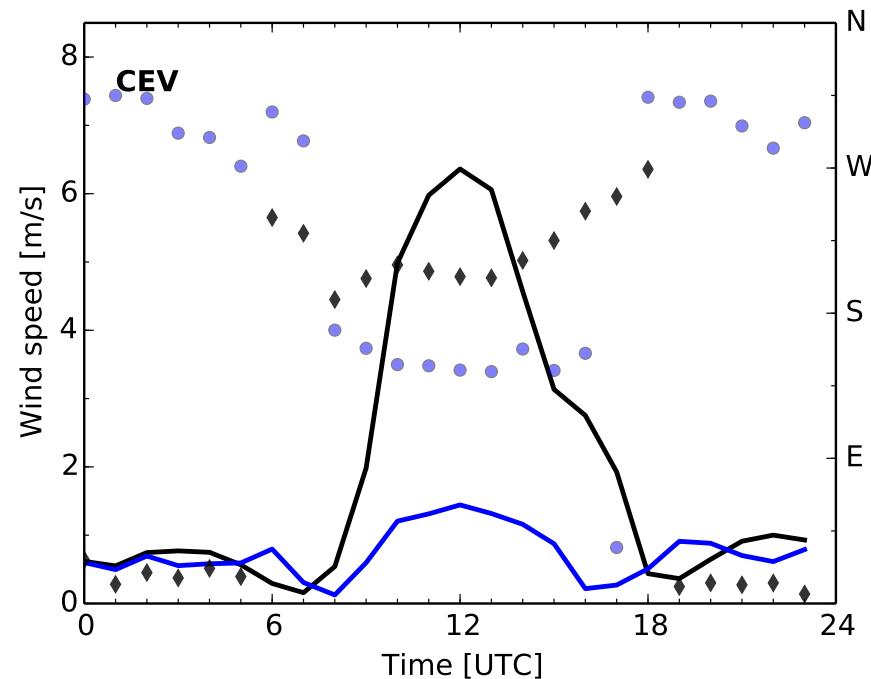
Mean diurnal cycle of valley winds

OBS 2 km

Visp (Rhone valley)



Cevio (Maggia valley)

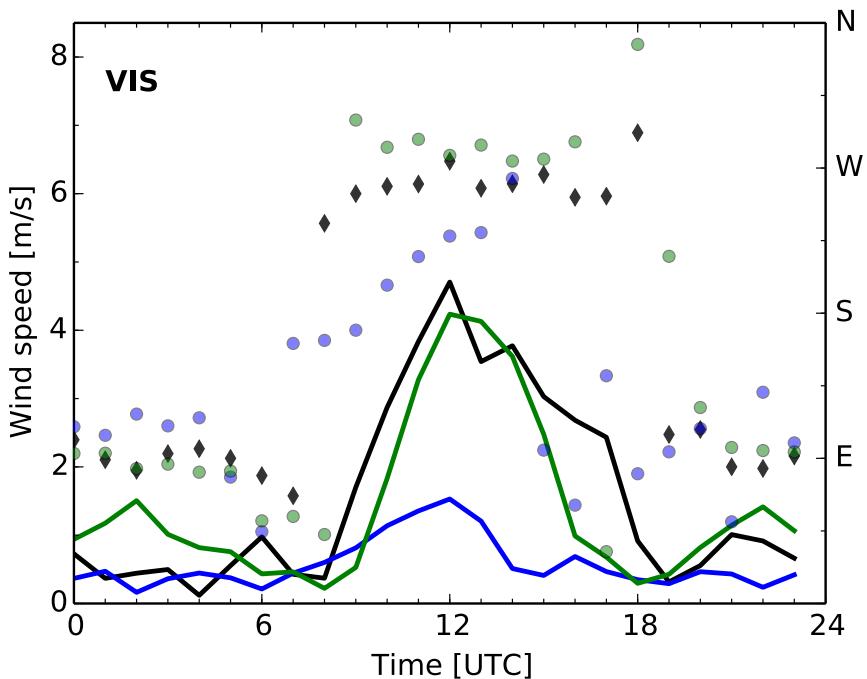




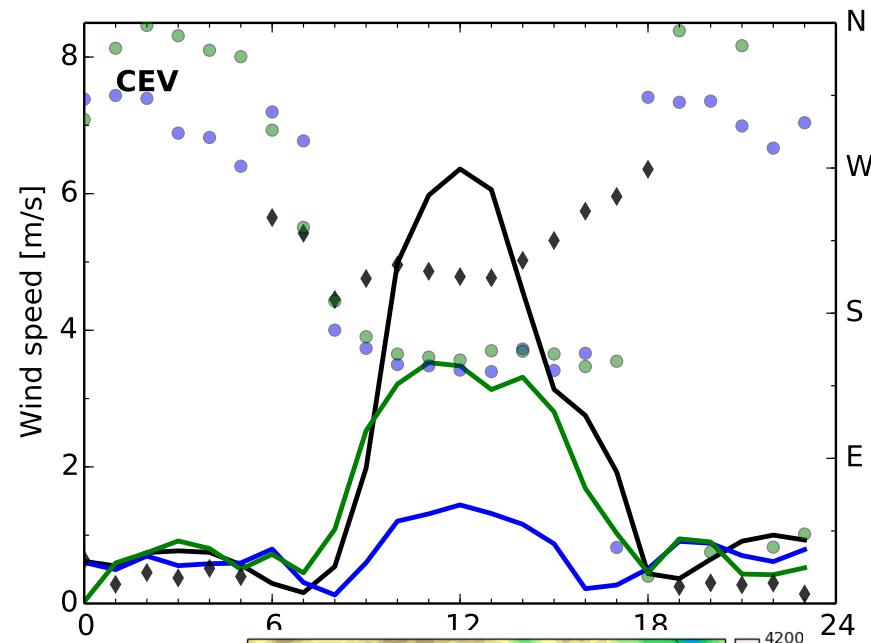
Mean diurnal cycle of valley winds

OBS 2 km 1 km

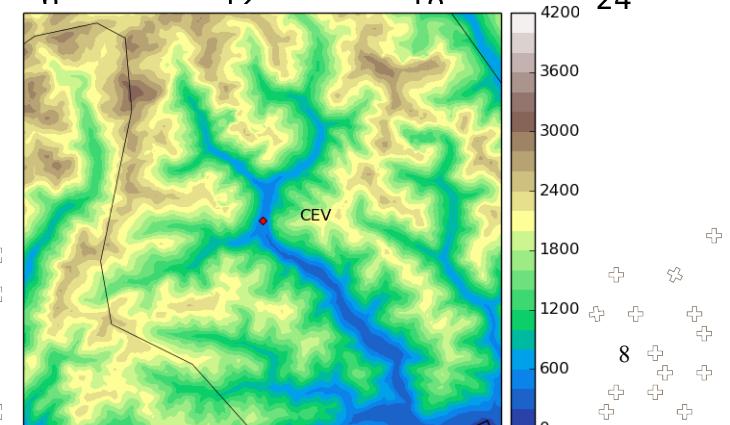
Visp (Rhone valley)



Cevio (Maggia valley)



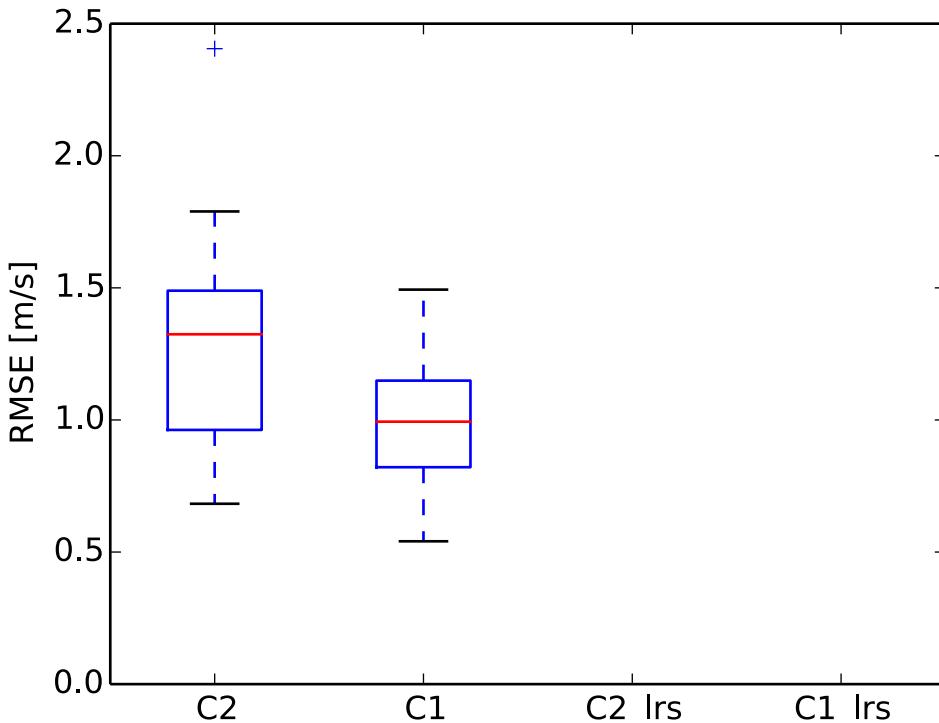
MeteoSwiss





Influence of surface data

“Diurnal wind” stations (21)



High-resolution surface data

- ASTER topography (30 m)
- GC2009 land cover (300 m)
- HWSD soil type (1 km)
- Raymond filter for topography (def: cutoff ~ 5 dx)

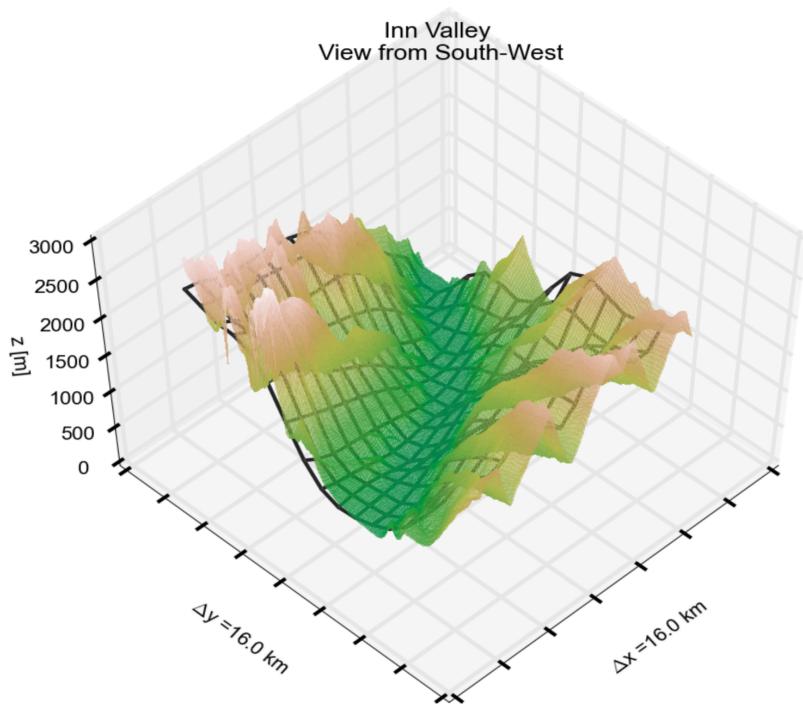
Low-resolution surface data (lrs)

- GLOBE topography (1 km)
- GLC2000 land cover (1 km)
- FAO DSMW (10 km)
- Raymond filter for topography (def: cutoff ~ 5 dx)

→ Coarse surface data: Only minor improvement for 1km!
→ Need high-resolution surface data for 1km simulation!



TKE budget in the Inn valley (i-Box)



Kohlsass station (545 masl)

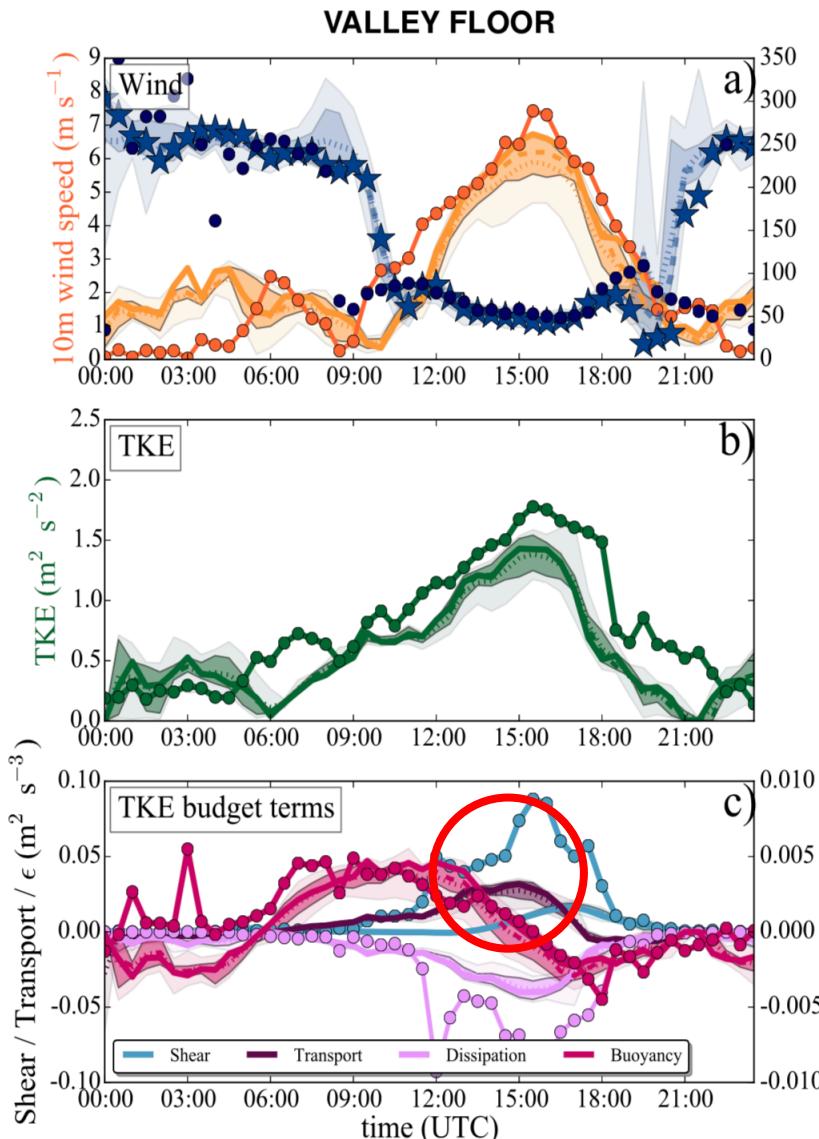


- Compare COSMO-1 against measurements (turbulent fluxes, TKE, TKE production terms)



1D Scheme

(1.5 order TKE closure)



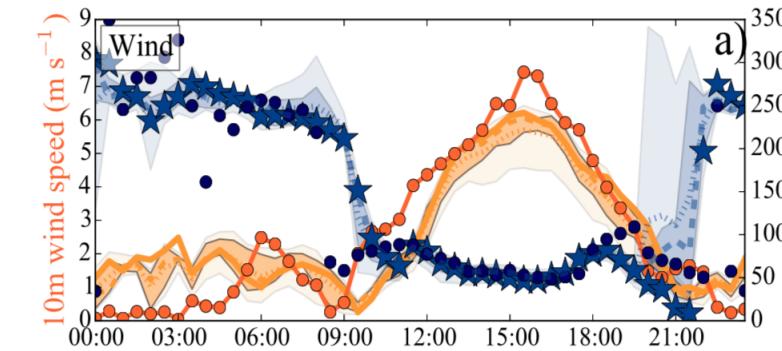
- **Morning**
 - Buoyant production dominates
 - TKE well simulated by model
- **Afternoon**
 - Vertical shear generation by valley wind
 - **Shear term drastically underestimated** (missing horizontal contributions)



Hybrid Scheme

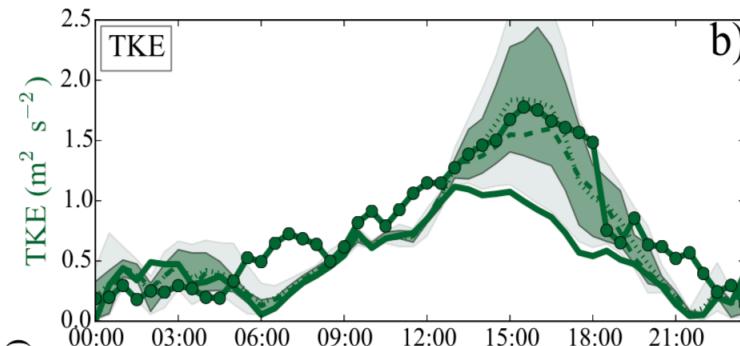
(+ TKE advection + horizontal shear contribution after Smagorinsky & Lilly)

VALLEY FLOOR

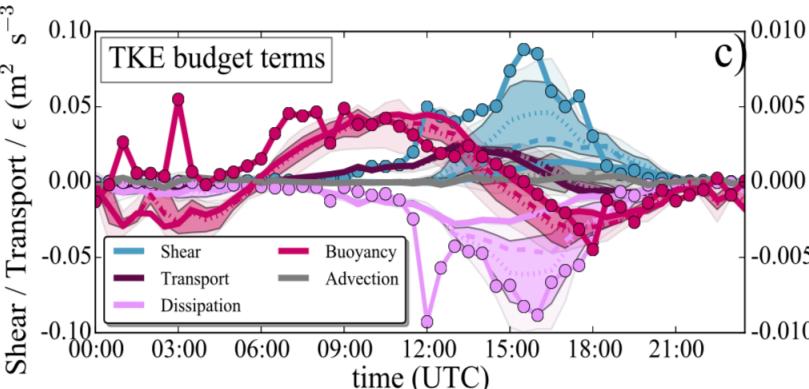


- Significant improvement in afternoon shear production

b)



c)



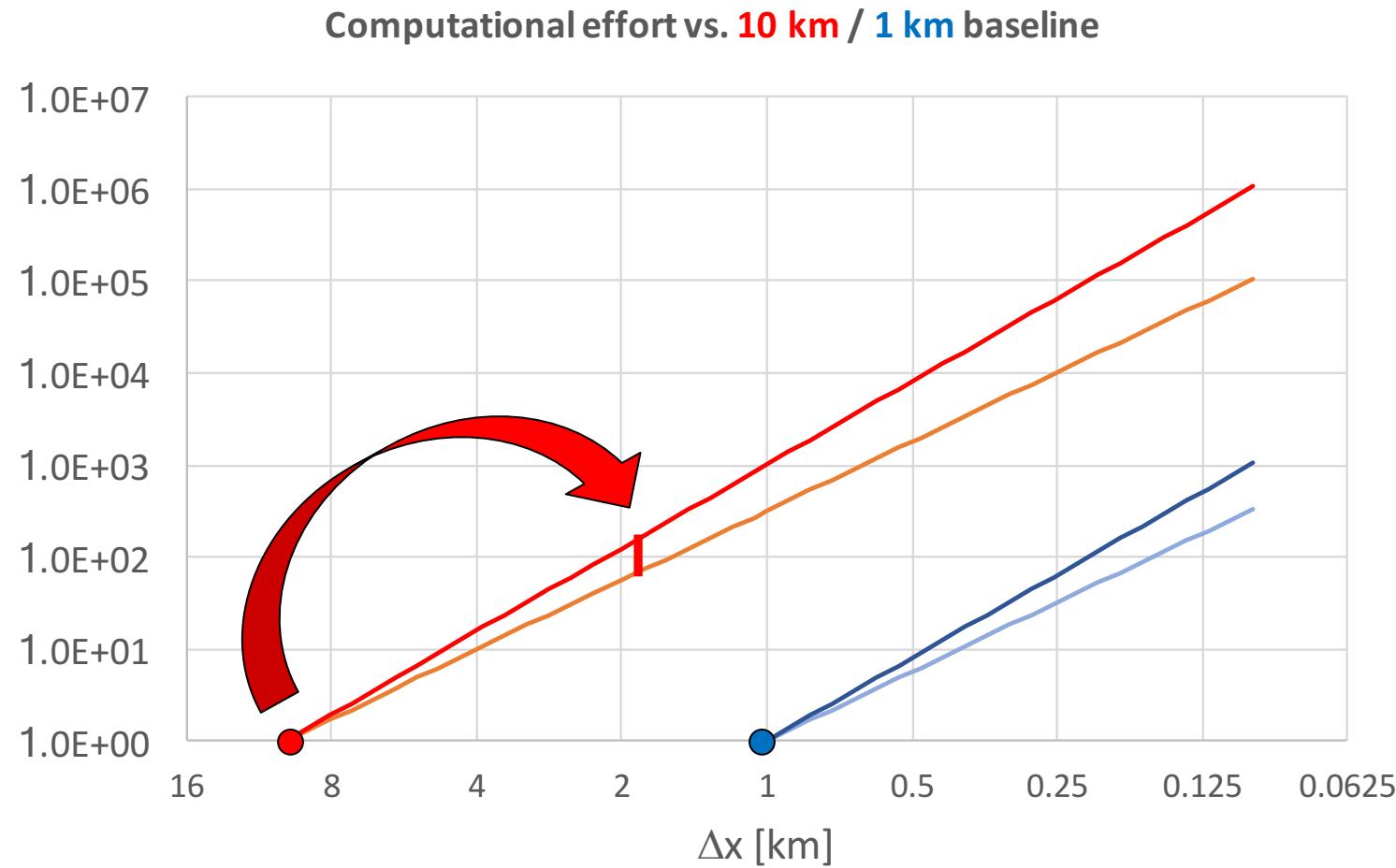
Oliver Fuhrer

Many shades to grey...





Jump across greyzone?

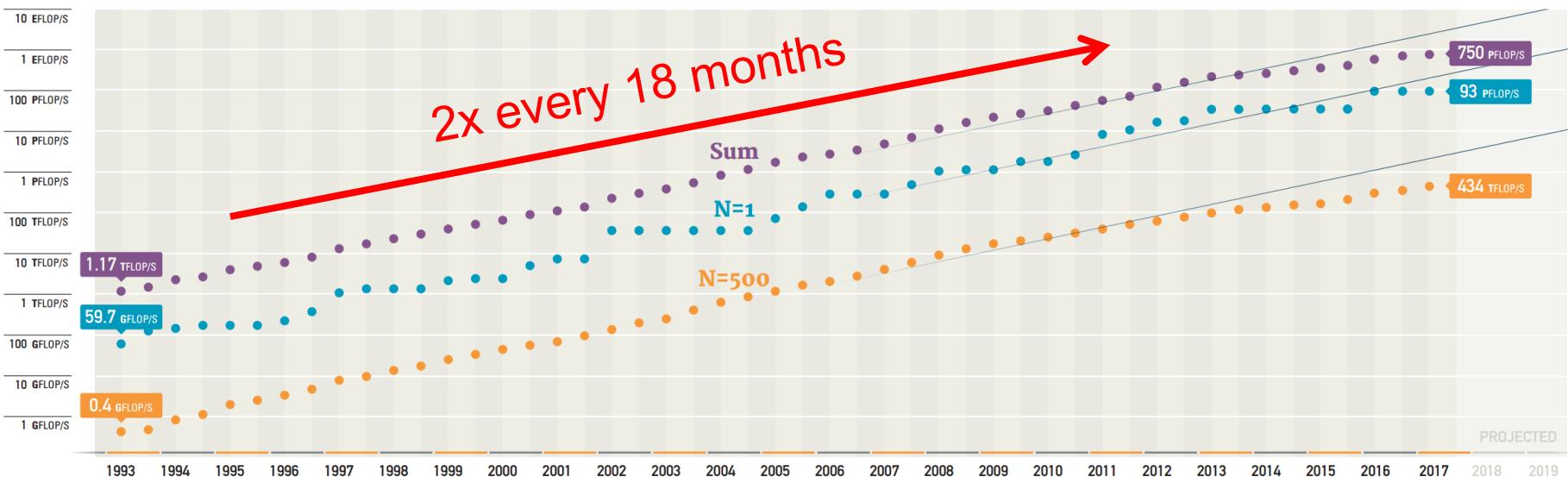




How to achieve a factor 100?

- Option 1: Money
- Option 2: Wait 10 years (Moore's law)

PERFORMANCE DEVELOPMENT

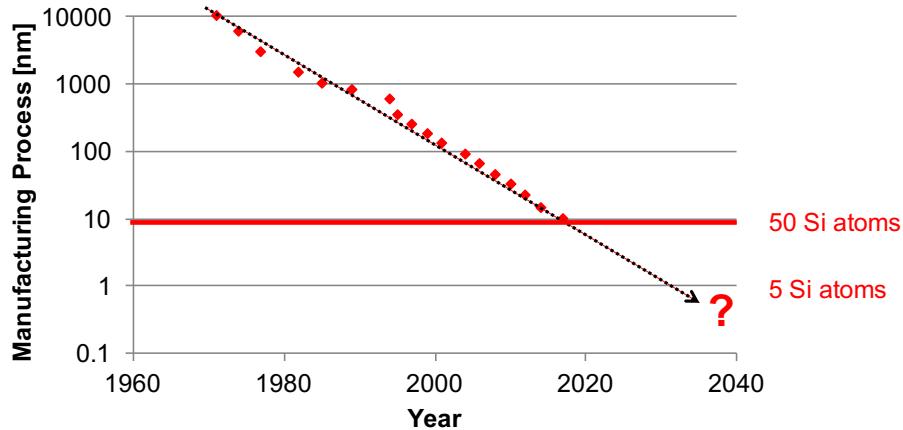


Source: top500.org

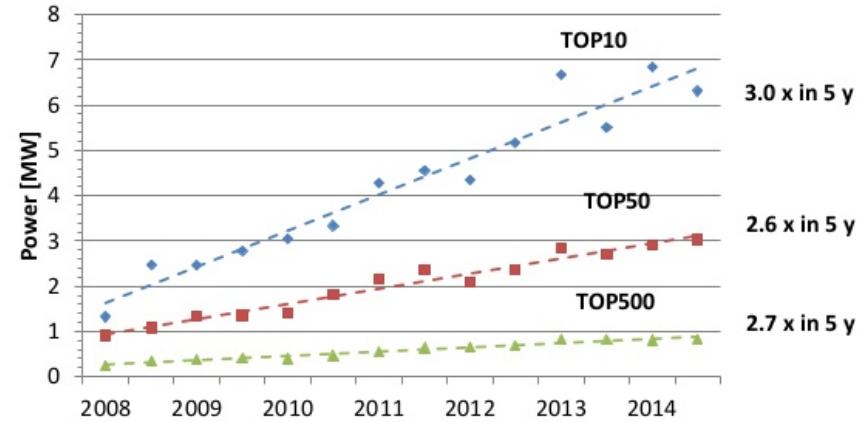


Moore's law is sick (or dead)

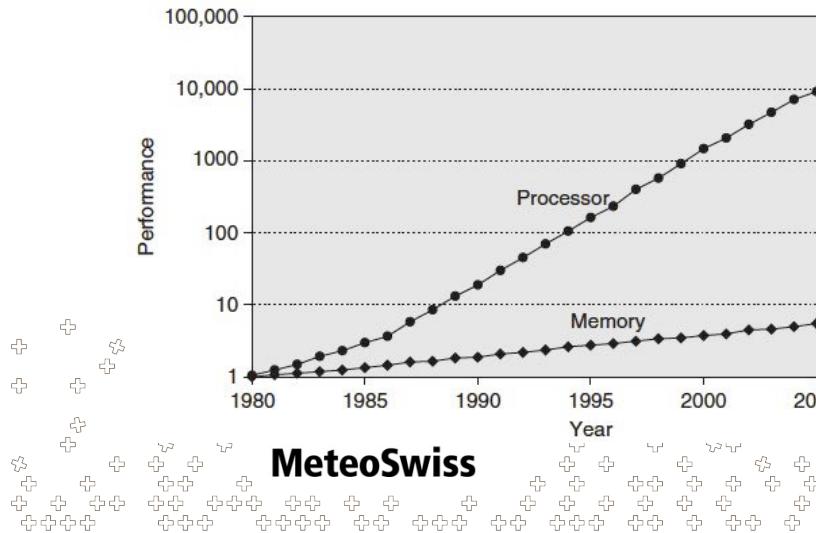
Decreasing feature size



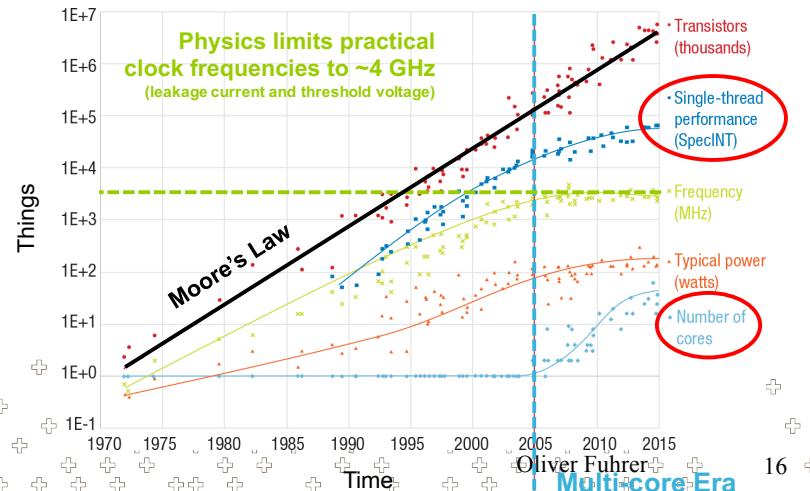
Increasing power consumption



Slower pace for bandwidth



Stagnating clock frequencies

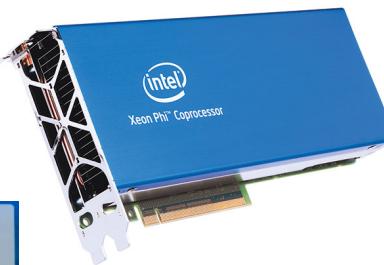
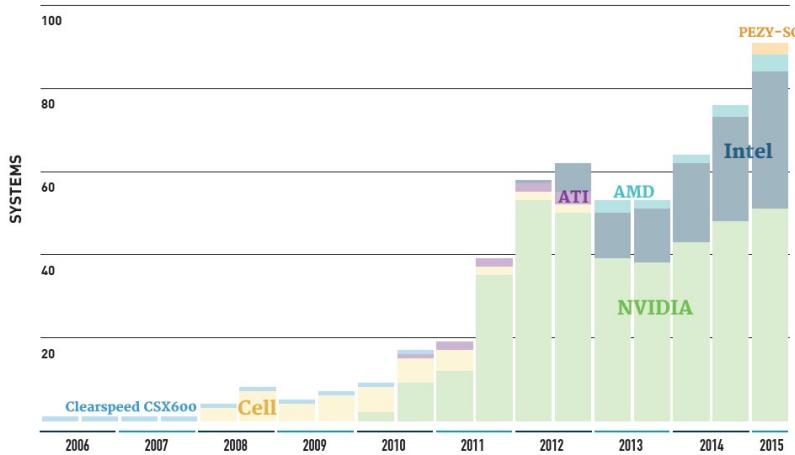




Specialization

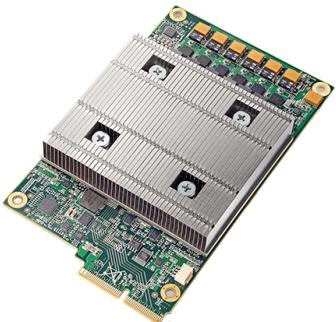
20% Systems on Top 500

ACCELERATORS/CO-PROCESSORS



Many-core
processors

GPUs



AI Accelerators
(e.g. Google Tensor Flow,
Intel Nervana)

Koenig et al. 2017, UCB
(accelerator for exact dot product)

MeteoSwiss

ARM

(e.g. Mont Blanc)



Oliver Fuhrer



Challenges

- **New design constraints**
 - Maximize parallelism
 - Minimize data movement and energy consumption
 - Minimize synchronizations
- **New programming models**
 - E.g. OpenMP 4.5, Coarray Fortran, CUDA, OpenACC
- **Rapid change**
 - Timescale of HPC system vs. Model





What to do?

300'000 lines of Fortran + MPI code



Libraries / System software



Up or down?



- **Increase level of abstraction**
 - Remove details of implementation
 - Can be “disruptive”
- **Lower level of abstraction**
 - Add implementation details
 - Often „incremental“



DOWN – Decrease level of abstraction



- **Approaches**

- Fortran + MPI + Directives (OpenMP, OpenACC)
- Optimize code for a specific hardware
- Custom implementations (#ifdef) or programming languages



Original Version

```
! solve tridiag(a,b,c) * x = d
!
! pre-computation
...
do j = jstart, jend
    !
    ! forward elimination
    do k = nk, 2, -1
        do i = istart, iend
            !CDIR ON ADB(d)
                d(i,j,k) = ( d(i,j,k) - d(i,j,k+1) * c(i,j,k) ) * b(i,j,k)
            end do
        end do
    !
    ! back substitution
    do k = 1, nk-1
        do i = istart, iend
            !CDIR ON ADB(x)
                x(i,j,k+1) = a(i,j,k+1) * x(i,j,k) + d(i,j,k+1)
            end do
        end do
    end do
```

- Algorithm: TDMA
- Language: Fortran
- Grid: Structured
- Data layout: (i,j,k)
- Parallelization: MPI in (i,j)
- Loop order: (jki)
- Blocking: (j)
- Vectorization: (i)
- Directives: NEC
- ...



Optimized GPU Version

```
! solve tridiag(a,b,c) * x = d
!
!$ACC DATA COPYIN(a,b,c,d) COPYOUT(x)
!
!$ACC KERNELS LOOP, GANG(32), WORKER(8)
do i = istart, iend
do j = jstart, jend
    ! pre-computation
    ...
    ! forward elimination
    do k = nk, 2, -1
        d(i,j,k) = ( d(i,j,k) - d(i,j,k+1) * c(i,j),
    end do
    ! back substitution
    do k = 1, nk-1
        x(i,j,k+1) = a(i,j,k+1) * x(i,j,k) + d(i,j,k+1)
    end do
end do
end do
!$OMP END KERNELS LOOPS
!
!$ACC END DATA
```

- Algorithm: TDMA
- Language: Fortran
- Grid: Structured
- Data layout: (i,j,k)
- Parallelization: Nodes (i,j) and Blocks (i,j)
- Loop order: (ijijk)
- No Blocking
- Vectorization: SIMD Threads (i,j)
- Directives: OpenACC
- ...



DOWN – Discussion



- Easy to learn
- Incremental



- Harder to understand / adapt
- Increased maintenance effort
- Performance compromise

- **Is it possible to reach a good compromise?**

- Near optimal performance
- Multiple hardware architectures
- Maintainable code



UP – Increase level of abstraction



- **Approaches**
 - Compilers
 - Libraries / Frameworks
 - Code generators and source-to-source translators
 - Domain-specific languages (DSL)



Domain-specific language (DSL)

```

function avg {
    offset off
    storage in

    avg = 0.5 * ( in(off) + in() )
}

function coriolis_force {
    storage fc, in

    coriolis_force = fc() * in()
}

operator coriolis {
    storage u_tend, u, v_tend, v, fc

    vertical_region ( k_start , k_end ) {
        u_tend += avg(j-1, coriolis_force(fc, avg(i+1, v)))
        v_tend -= avg(i-1, coriolis_force(fc, avg(j+1, u)))
    }
}
}

```

Example: gtclang

- Coriolis force

$$\frac{\partial u}{\partial t} = \dots + fv$$

$$\frac{\partial v}{\partial t} = \dots - fu$$

- No loops
- No data structures
- No halo-updates



UP – Discussion

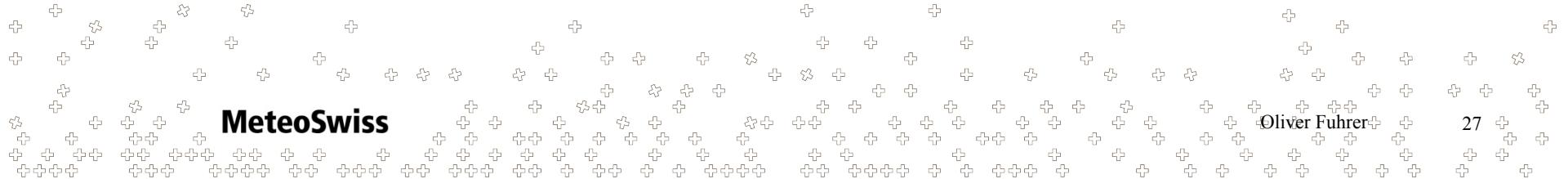


- User code easy to understand / modify
- Performance portability
- High performance
- Safety / correctness can be imposed



- No turn key solutions available
- Disruptive change
- Maintenance of DSL / compiler

- **Can be achieve a community solution?**

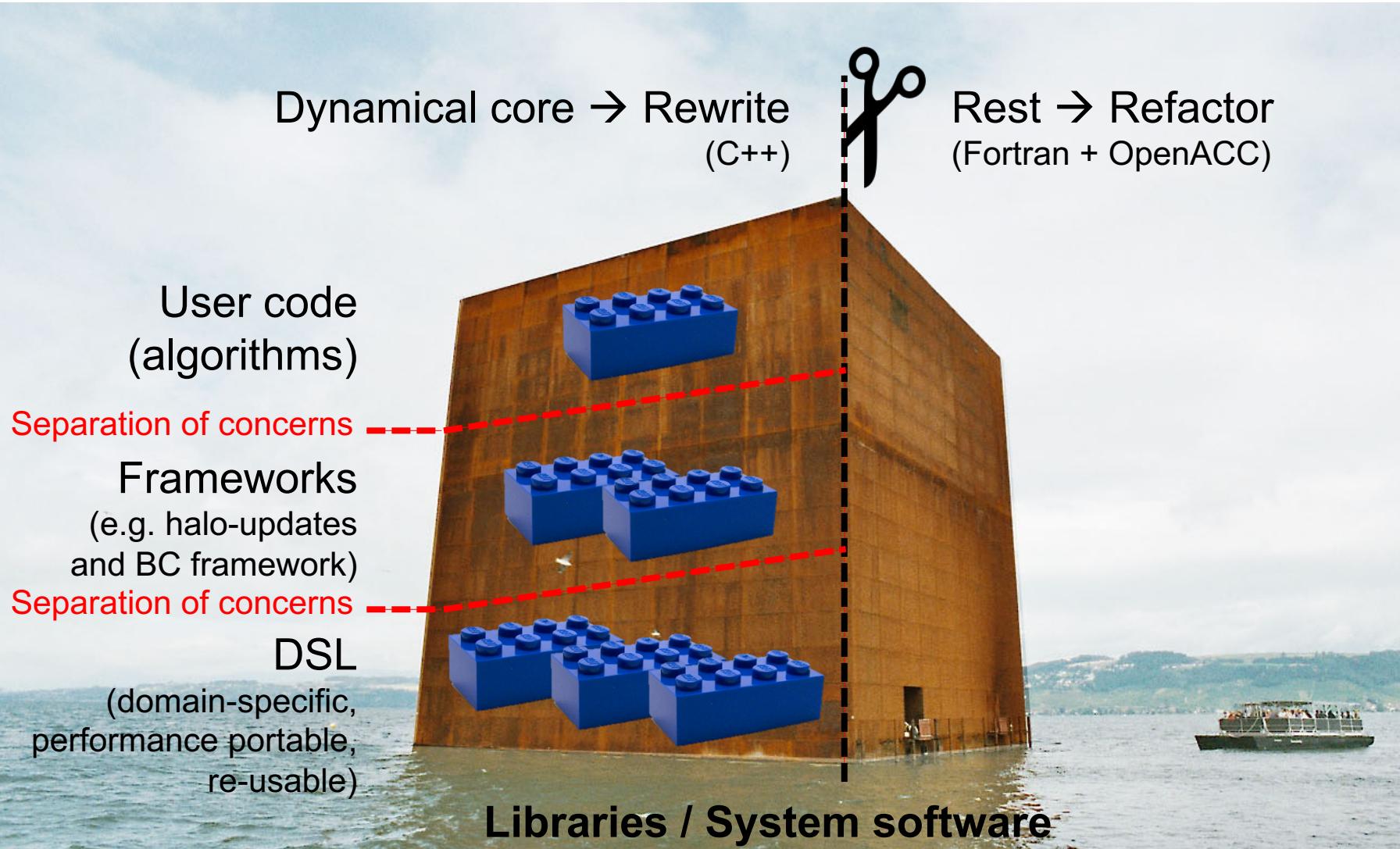




Both approaches for COSMO

Führer et al., 2014, doi:[10.14529/jsfi1401](https://doi.org/10.14529/jsfi1401)

Lapillonne and Führer, 2014, doi: [10.1142/S0129626414500030](https://doi.org/10.1142/S0129626414500030)





Operational system in 2016



Piz Kesch (Cray CS Storm)

- GPU-accelerated hybrid system
- “Fat” compute nodes with
 - 2 x Intel Haswell E5-2690v3
 - 8 x NVIDIA Tesla K80
- 12 nodes per rack
- Including service nodes, post-processing nodes, file system, ...
- 2 redundant racks

Increase in computational problem size of 40x in 4-5 years with constant budget and running costs.



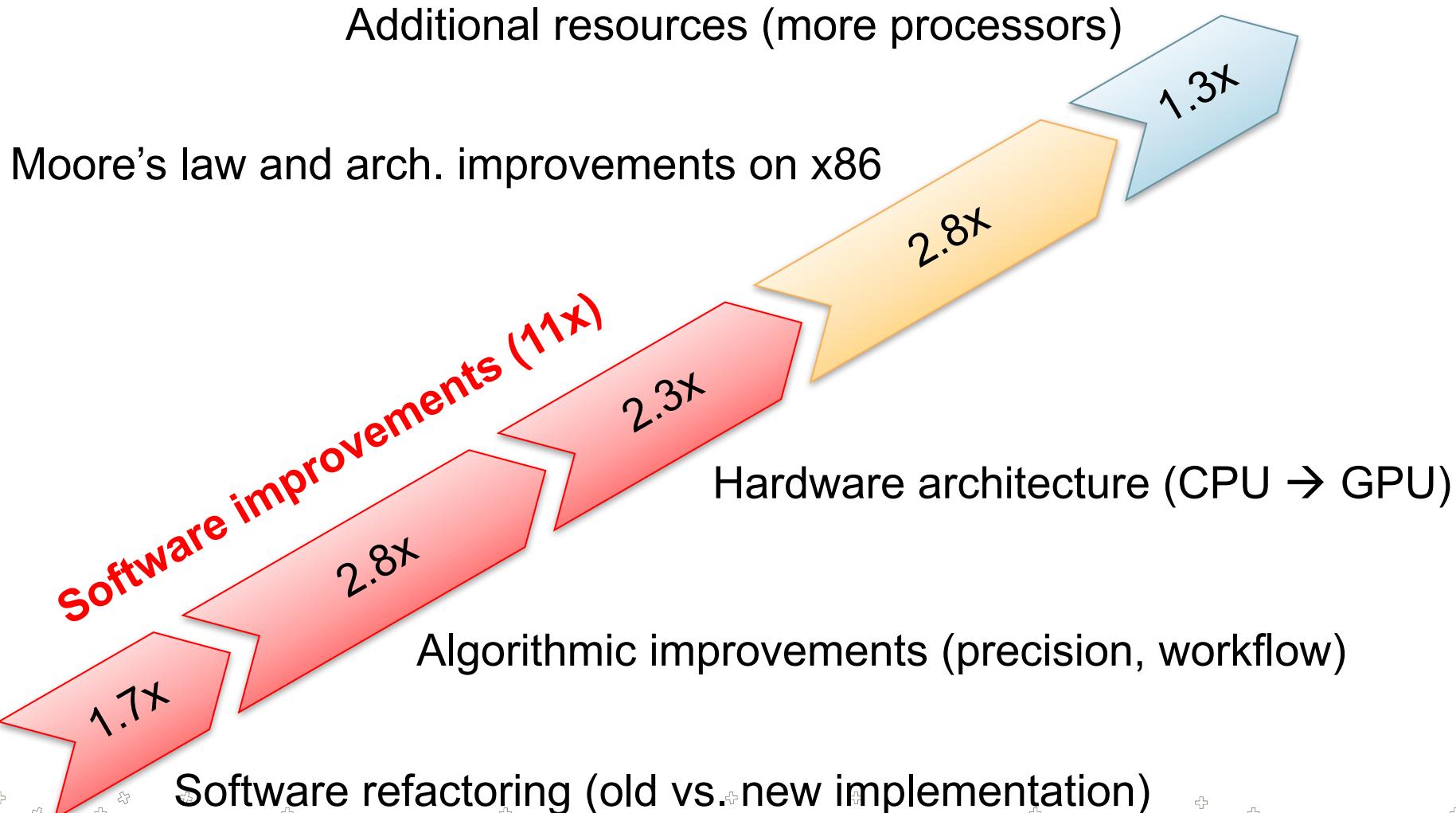
Learnings (so far)

- **Co-design approach:** Team of computer scientists, computational scientists, domain scientists, system architects and vendors
- Trading off options and **taking compromises** is important
 - e.g. cannot re-write everything in one go
 - e.g. data-assimilation is not a good match for GPUs
- Consider **full workflow**
(including I/O, pre-/post-processing, ...)
- Aim for **sustainable solutions**
 - Consider development and maintenance effort





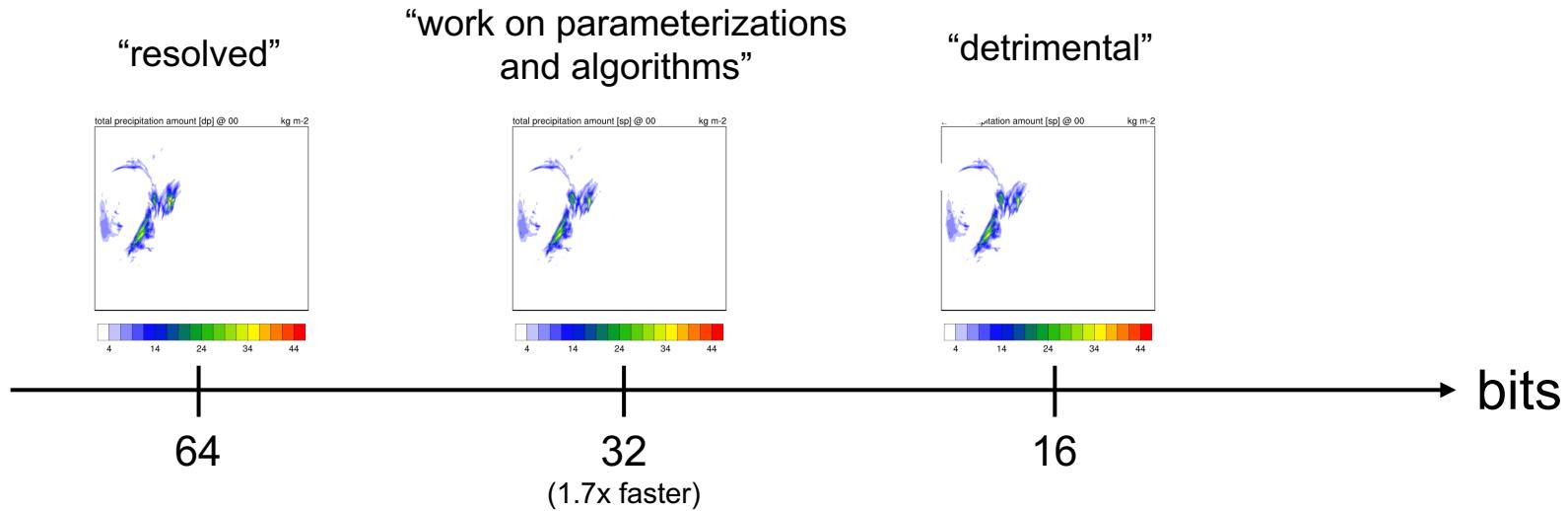
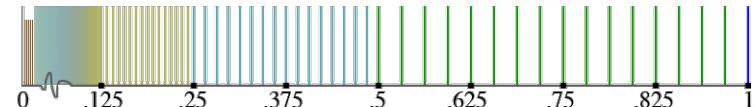
How was factor 40x achieved?





Greyzone of precision

- Discretization of number space
- Higher precision → more data movement / energy

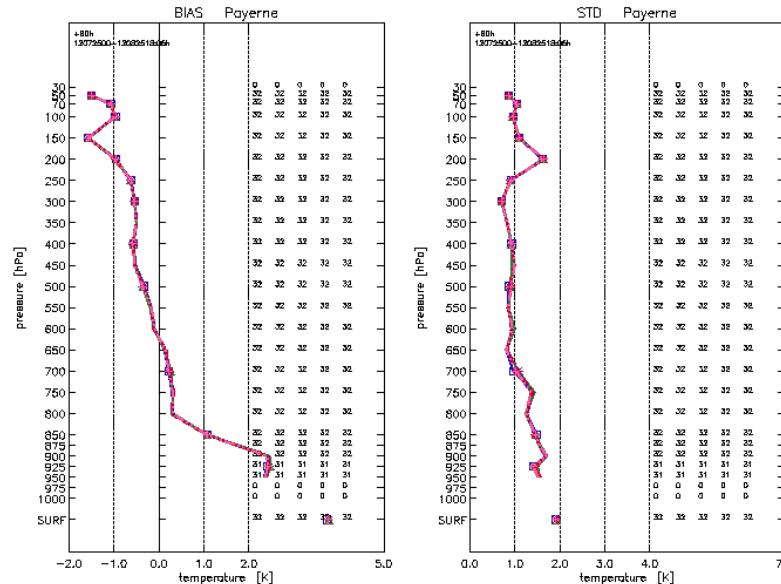


- Tradeoff: algorithm, precision, resolution, ensemble size



COSMO in single precision

- Results not distinguishable between single / double precision (e.g. upper air verification)



- Ensemble runs are in single precision (60% more members)
- Issues with data assimilation code



Summary

- Key issues for O(1-2 km) modeling over complex terrain
 - ABLs over complex terrain
 - Turbulence and shallow convection in greyzone
- Exponentially increasing compute power is no longer a given
 - Specialization of hardware
 - New programming models
- Urgent need to also address HPC issues in order not to get stuck in greyzone!





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