UNIVERSITY OF Southampton

Oak Ridge User Conference

Technical Challenges for Ab-inito Simulations of Low and High-Pressure Turbines

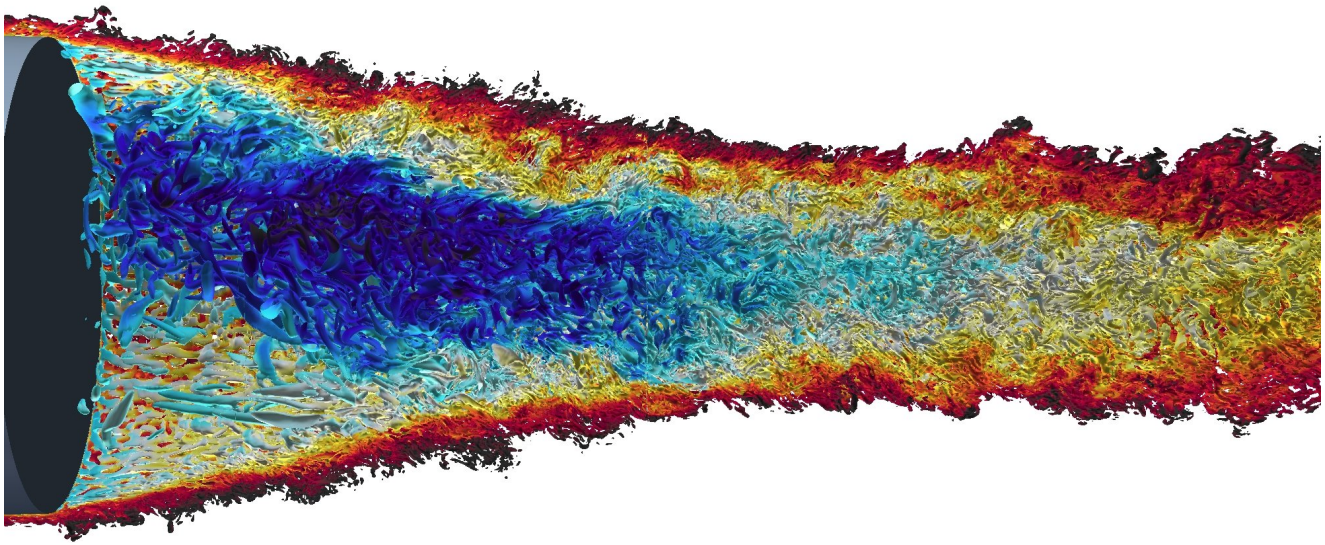
R. Pichler, R. D. Sandberg, V. Michelassi and G. Laskowski

Acknowledgements

- ORNL Directors Grant - access to a GPU system
- John Levesque and Tom Edwards from CRAY COE - initial porting
- Jeff Larkin - Nvidia

Outline

Research areas



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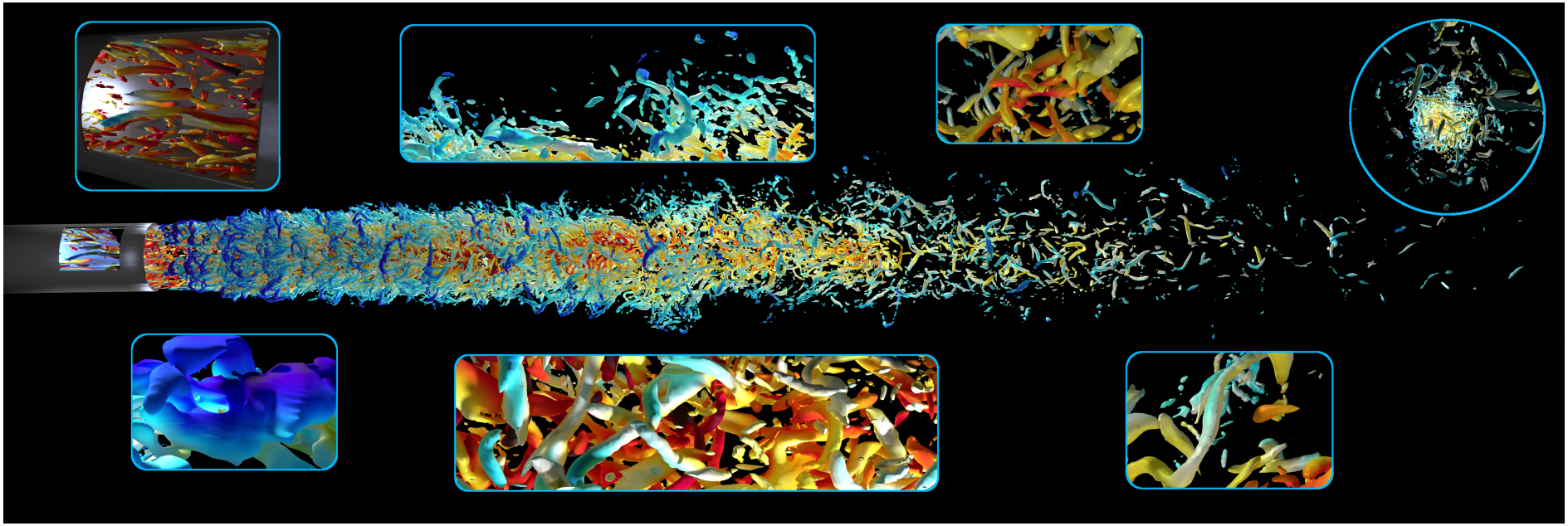

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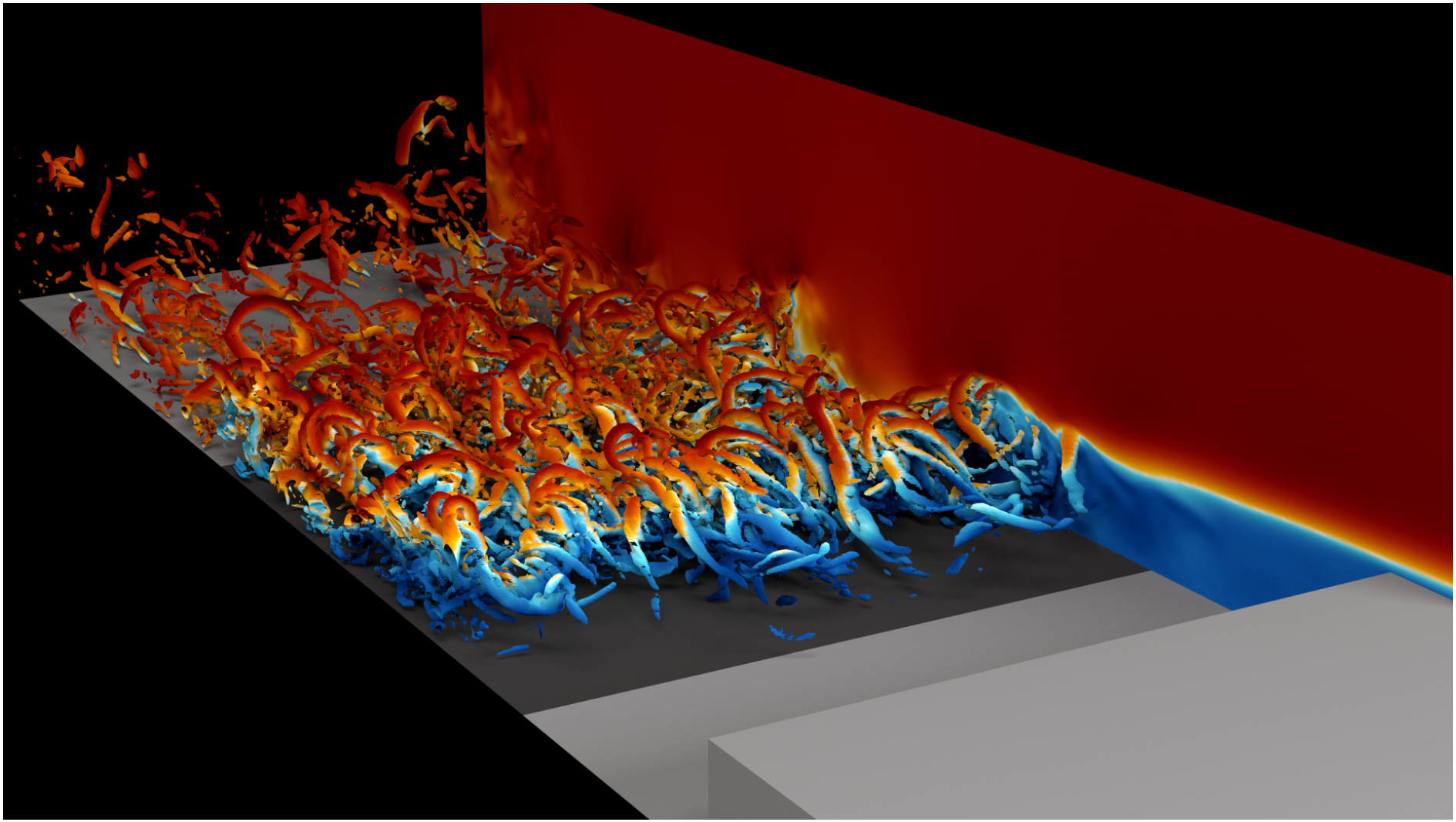

HiPSTAR

High Performance Solver for Turbulence and Aeroacoustic Research

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Solves unsteady 3d compressible Flow equations - continuum

- Conservation of mass
- Conservation of momentum (3x)
- Conservation of energy

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High Performance Solver for Turbulence and Aeroacoustic Research

Solves unsteady 3d compressible Flow equations - continuum

- Conservation of mass
- Conservation of momentum (3x)
- Conservation of energy
- Euler Frame of Reference
- neglect gravity

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(t_{ji}\right) \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho \vec{u}\right) + \rho\left(\vec{u}\cdot\nabla\right)\vec{u} = -\nabla p + \nabla\cdot\underline{t} \tag{2}$$

Numerical Approach

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(t_{ji}\right) \tag{3}$$

rewrite as

$$\frac{\partial}{\partial t}\left(\rho u_i\right) = \underbrace{-\frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(t_{ji}\right)}_{\textbf{RHS}} \tag{4}$$

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integrate numerically w.r.t time using explicit Runge-Kutta method

$$\rho u_i|_{n+1} = \rho u_i|_n + \Delta t \sum_{k=1}^{5} b_k \mathbf{RHS}|_n \tag{5}$$

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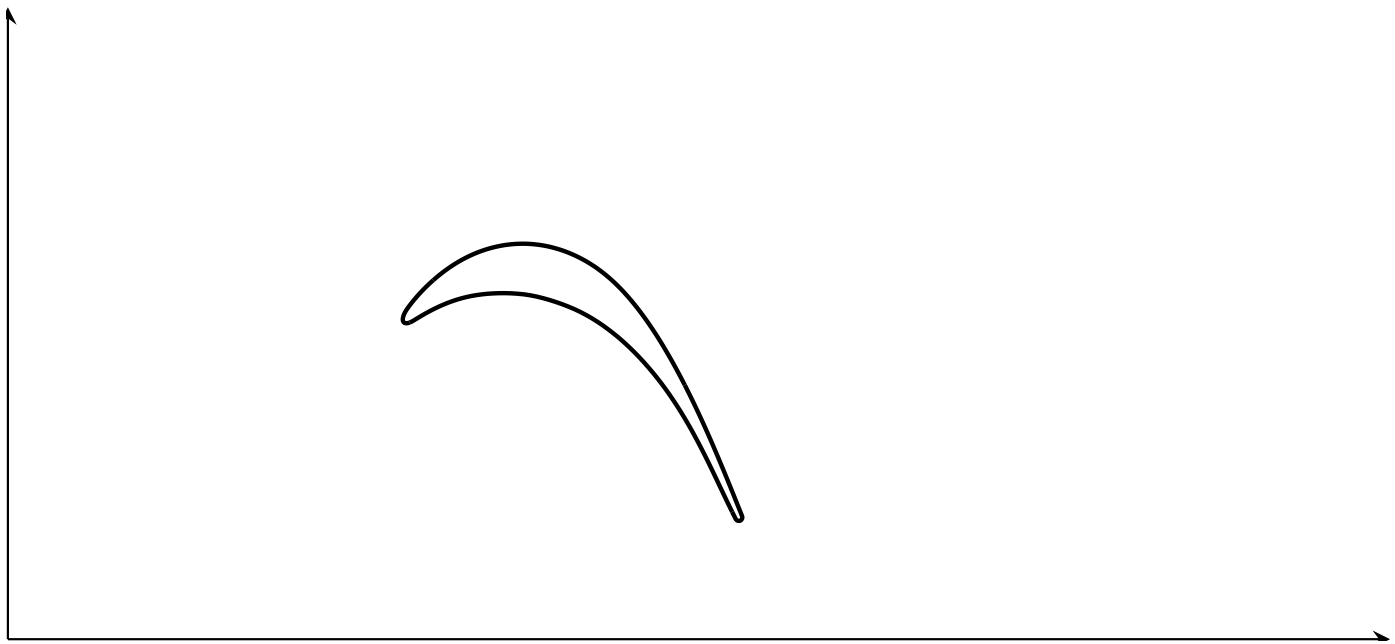
spatial derivative discretized by 4^{th} order finite differences and Fourier method

Parallelization

- discretize domain



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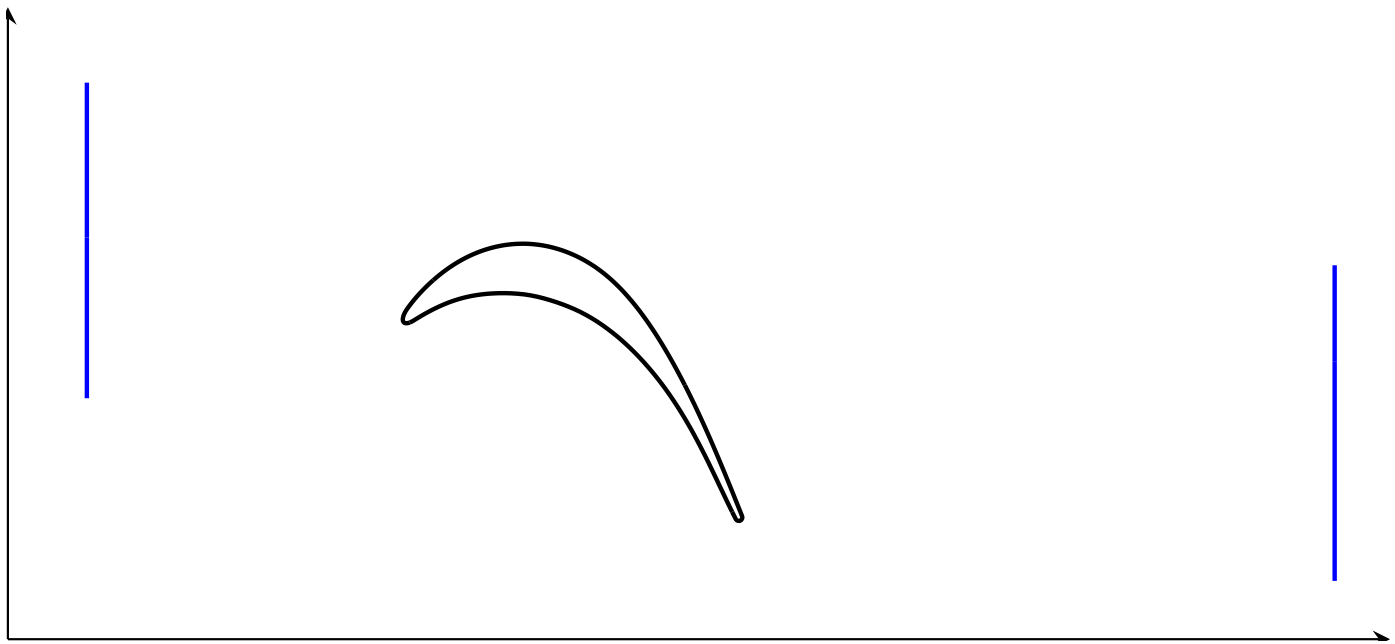

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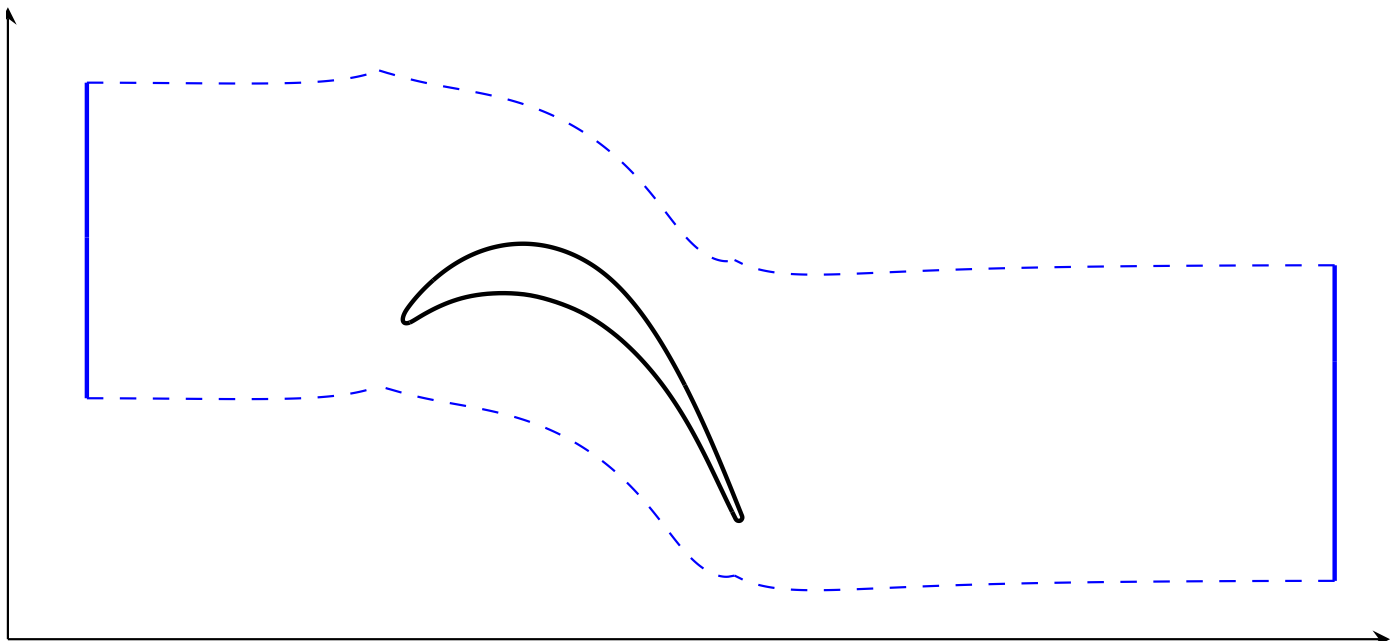
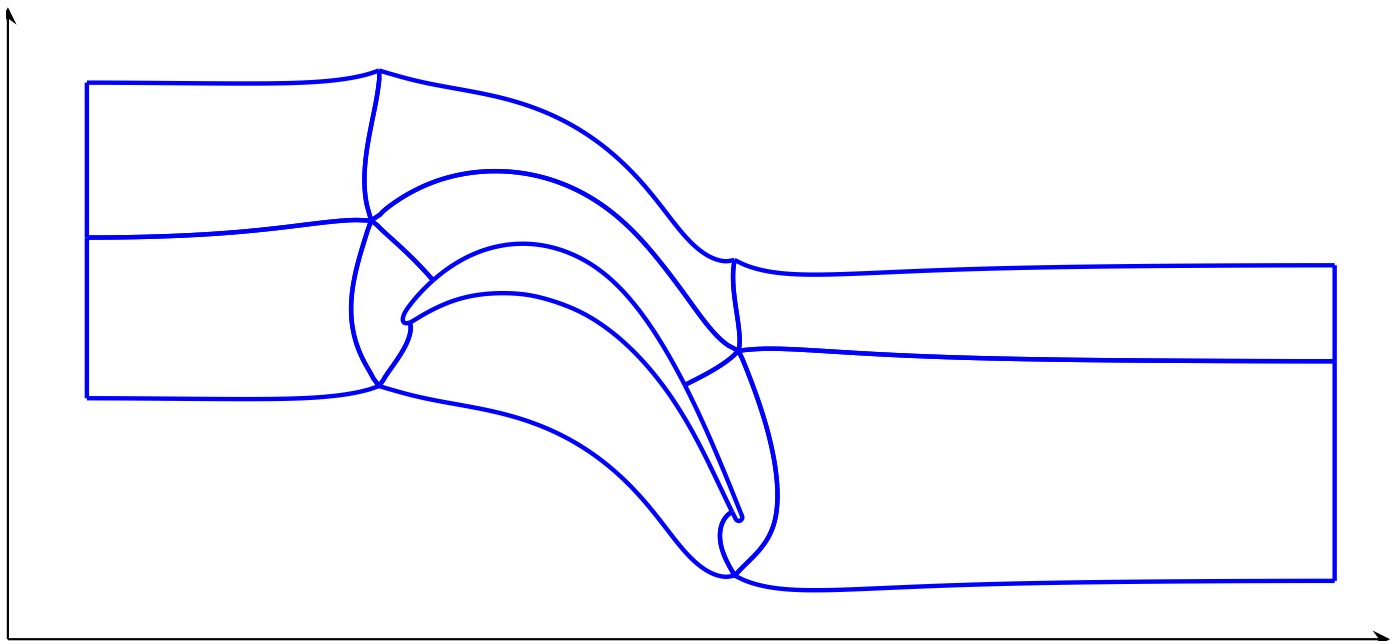


Parallelization

- discretize domain
- multi block grid for domain



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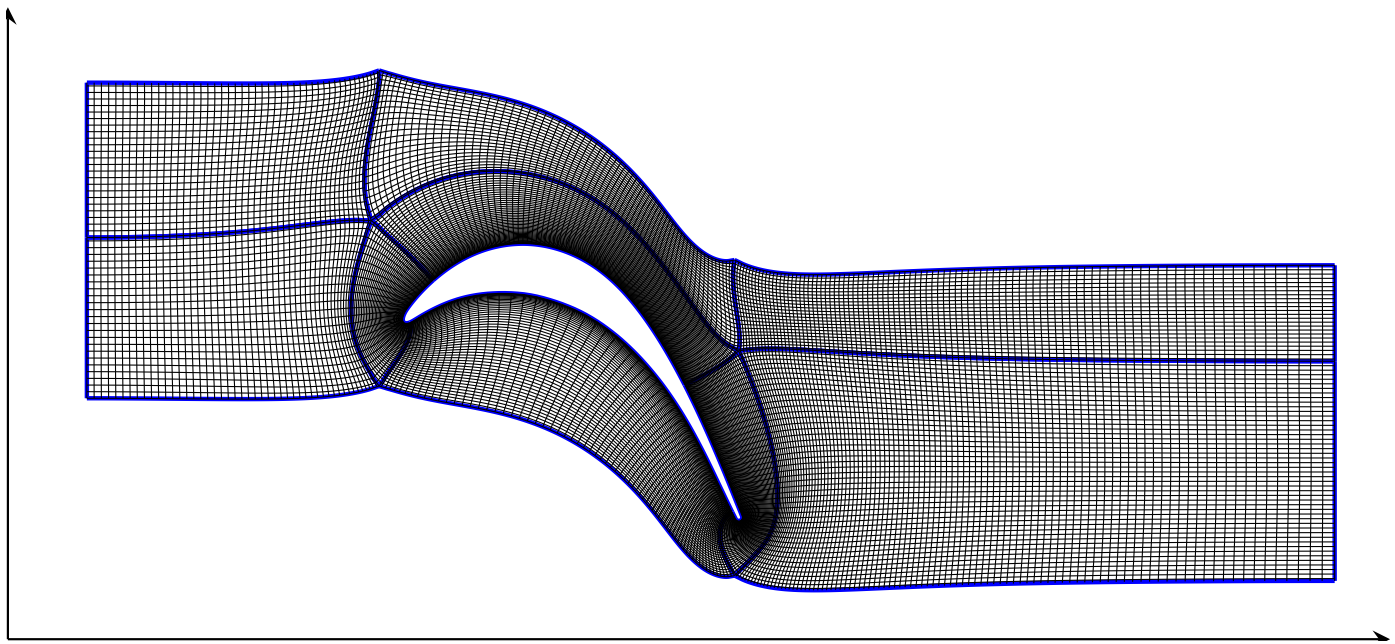

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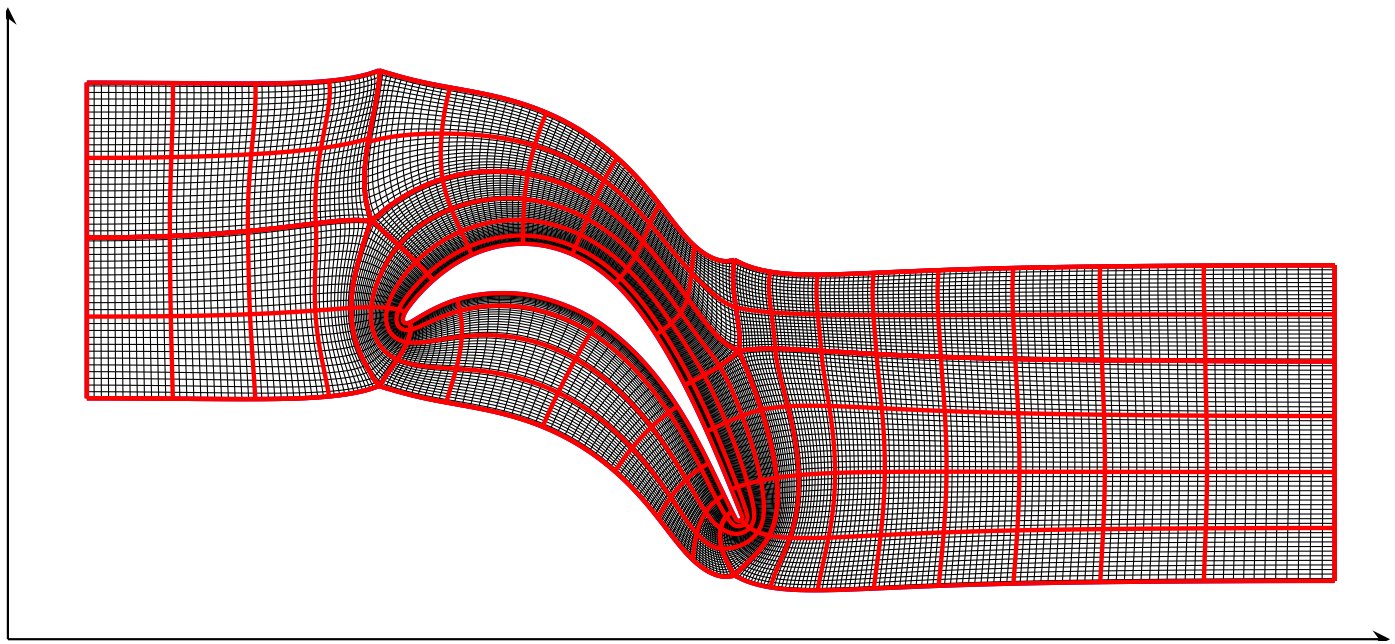
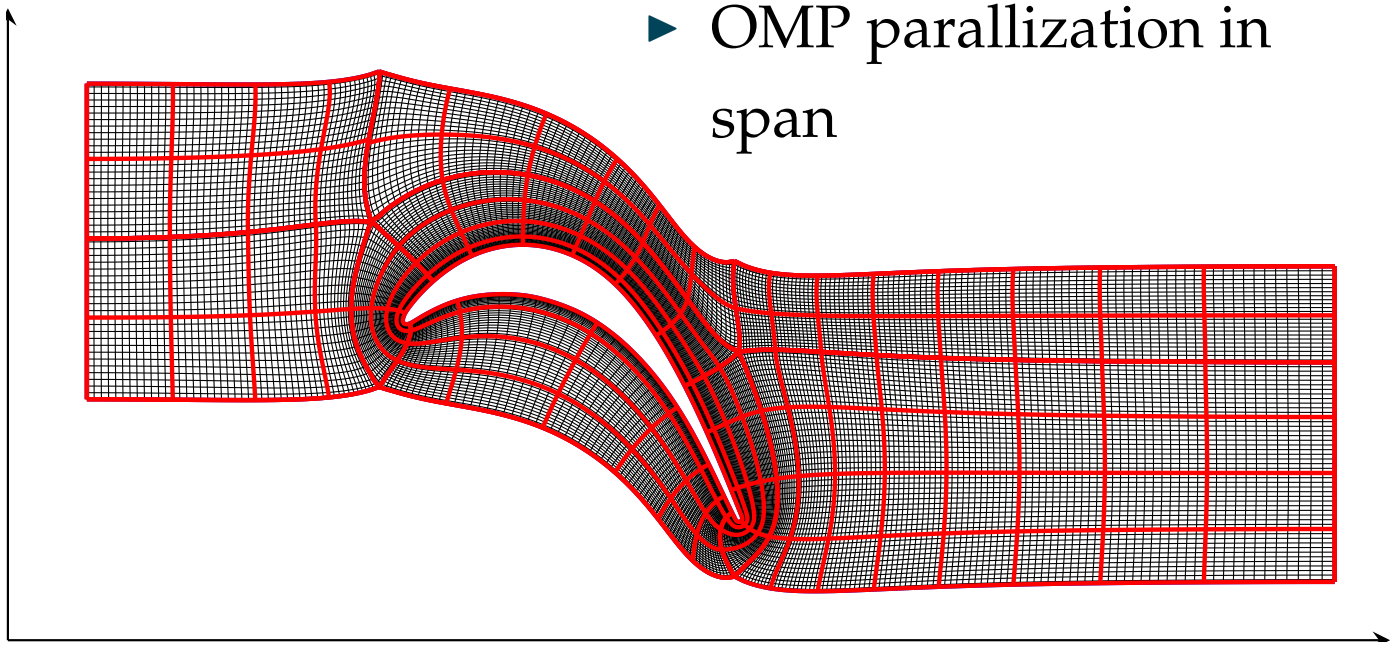
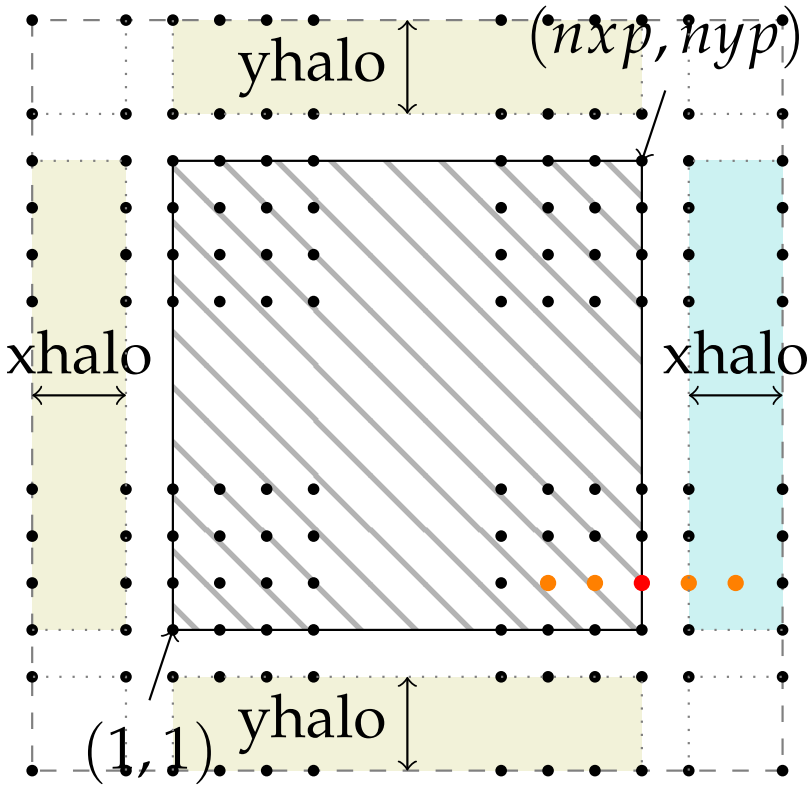


Parallelization

- discretize domain
- multi block grid for domain
- decompose grid using MPI
- OMP parallization in span



Domain decomposition



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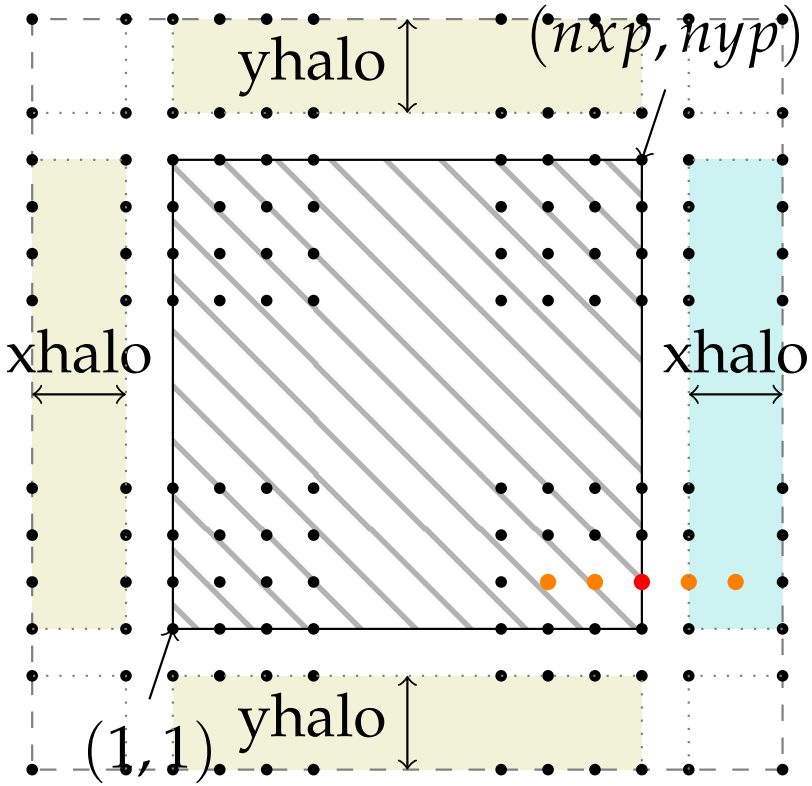

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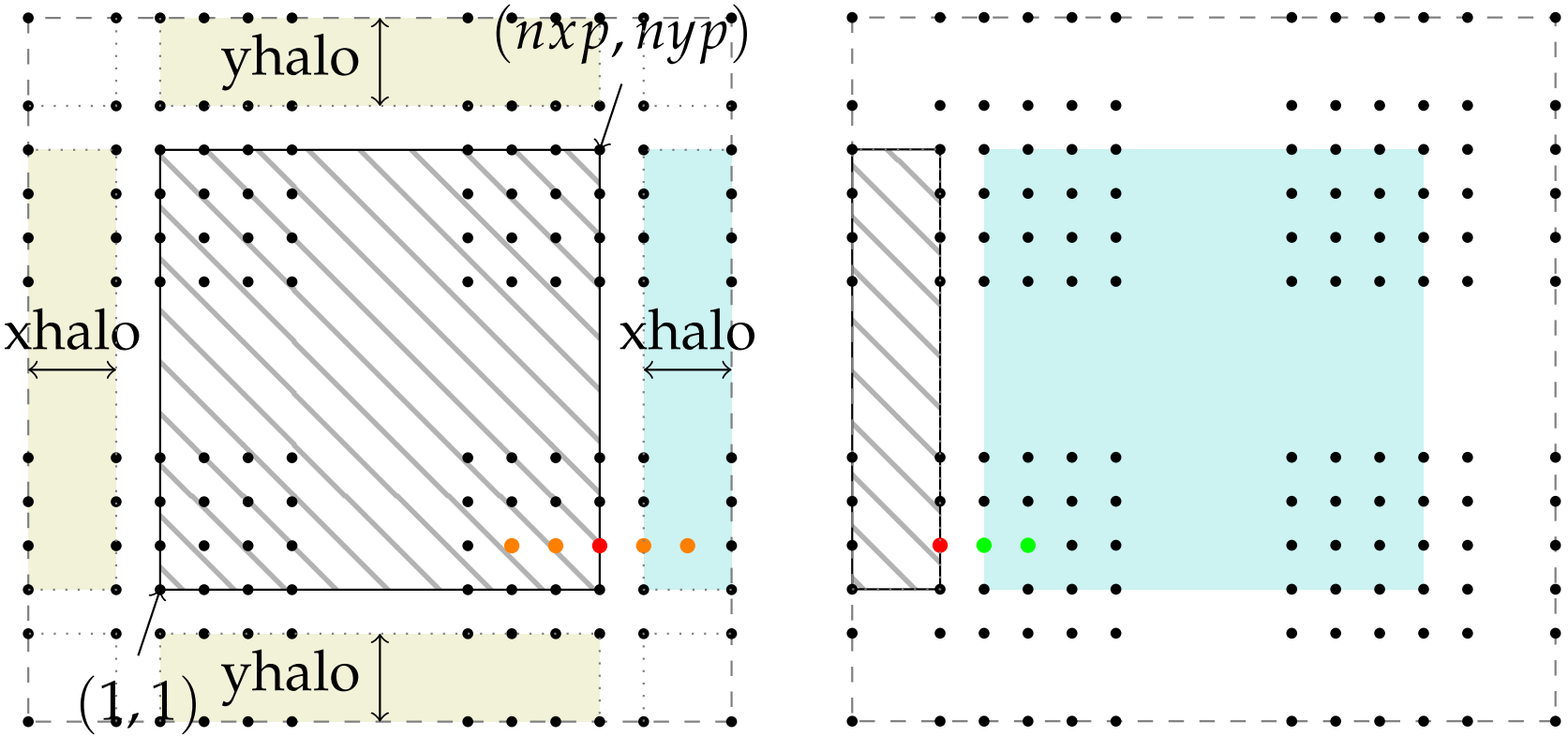
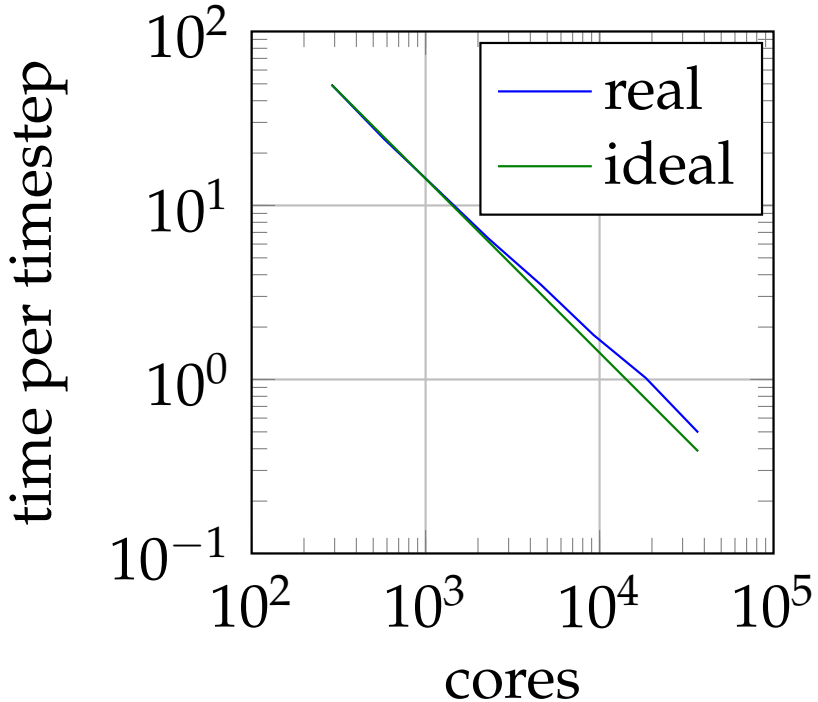
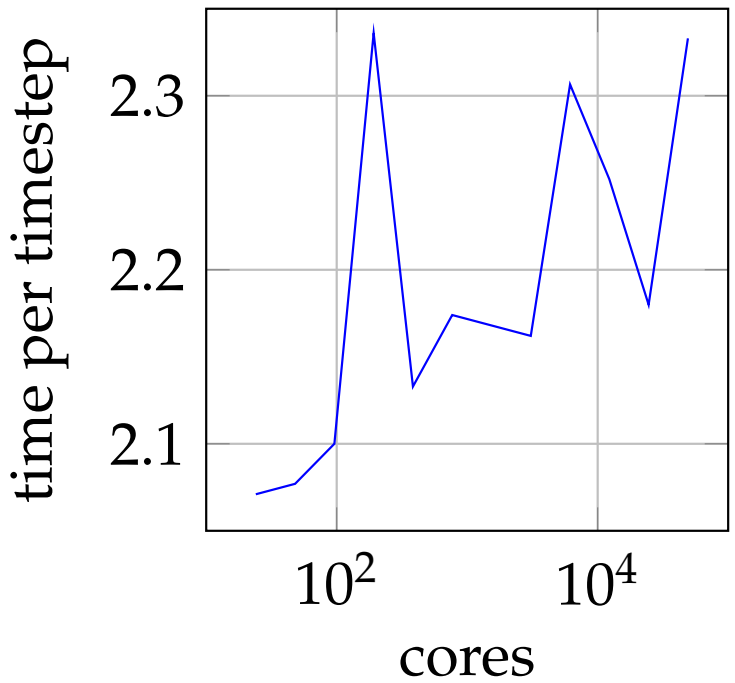


CPU scaling - Plane jet

- Archer - UK national facility XC30
- strong scaling: speed up of 102 vs. 128
- weak scaling: 24 to 49152 cores





Code structure - CPU profile

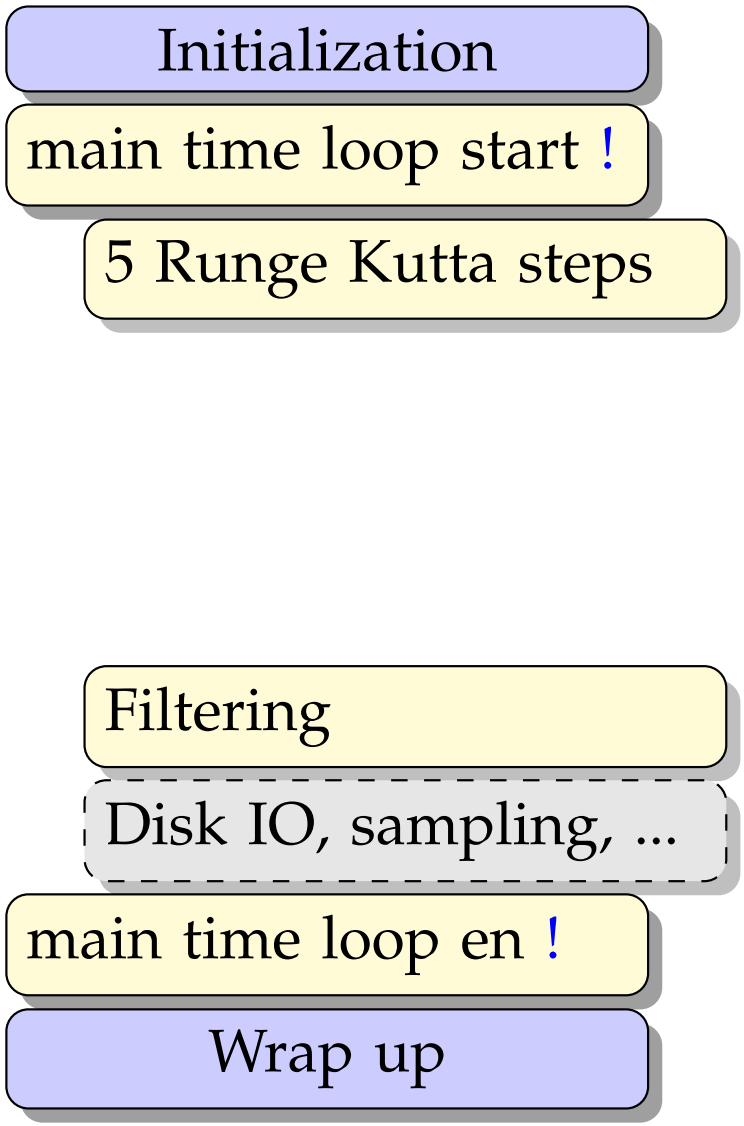
Initialization

main time loop start !

main time loop en !

Wrap up

Code structure - CPU profile



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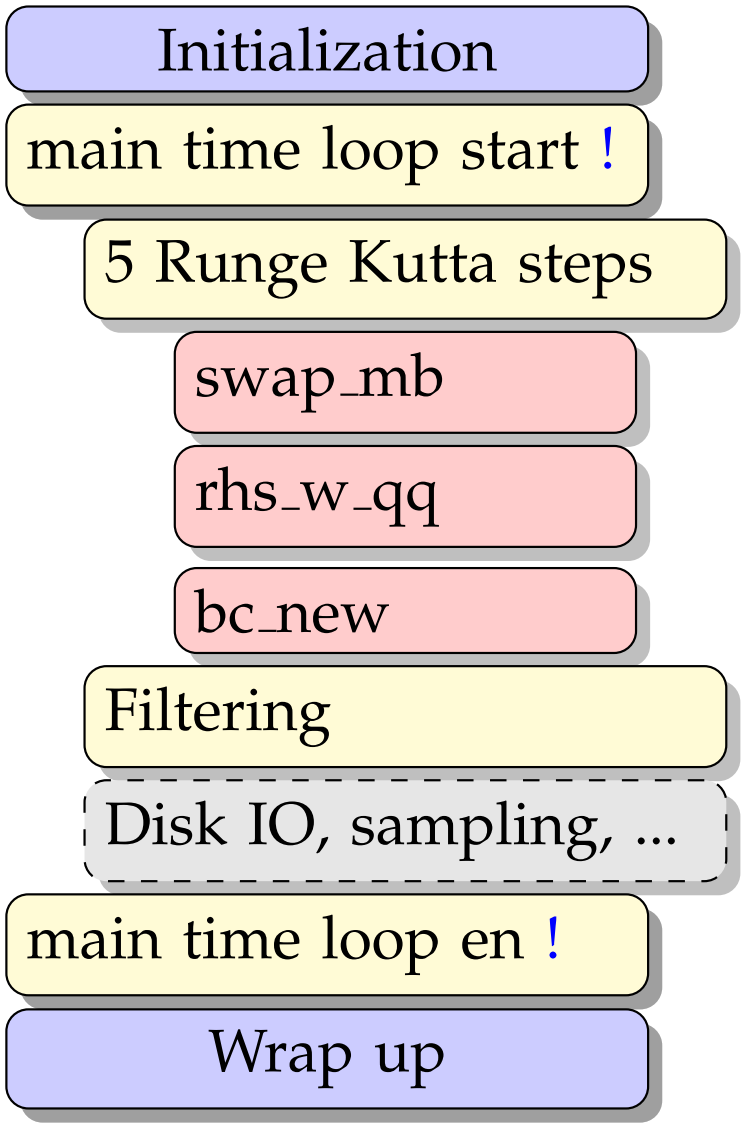

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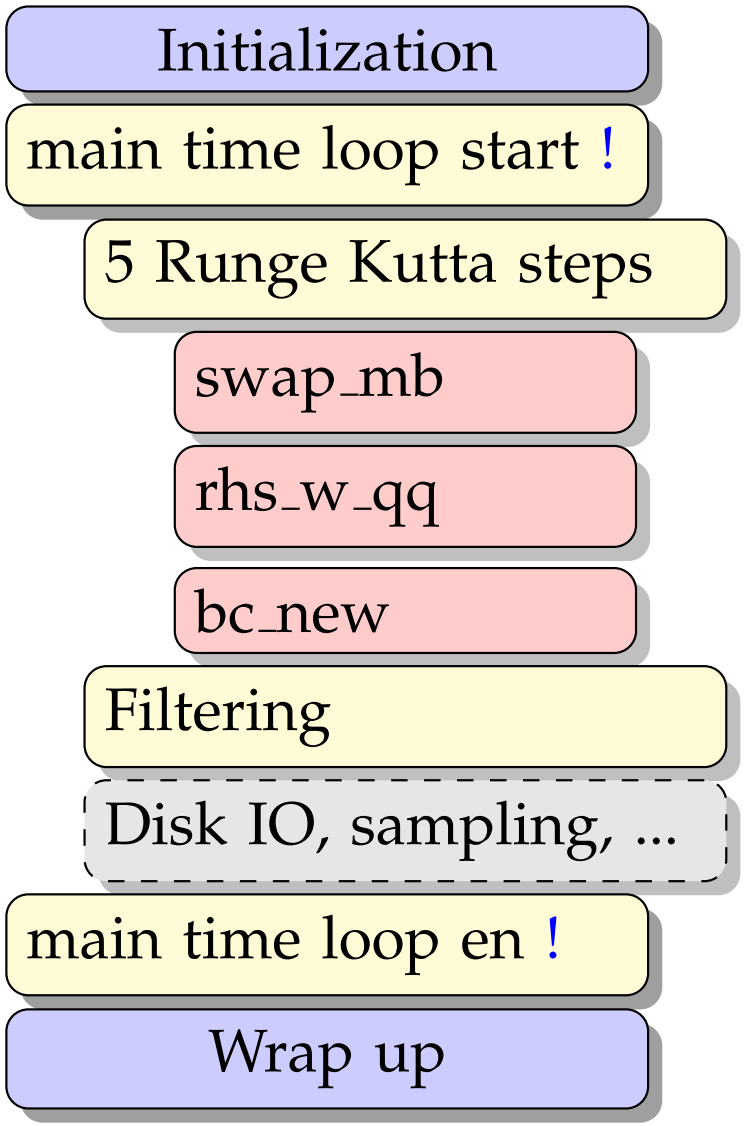

- Piz Daint - Xeon E5-2670 8C 2.600GHz
- CrayPAT - trace MPI and user functions in main loop

Code structure - CPU profile

- Initialization
- main time loop start !
  - 5 Runge Kutta steps
    - swap_mb
    - rhs_w_qq
    - bc_new
  - Filtering
  - Disk IO, sampling, ...
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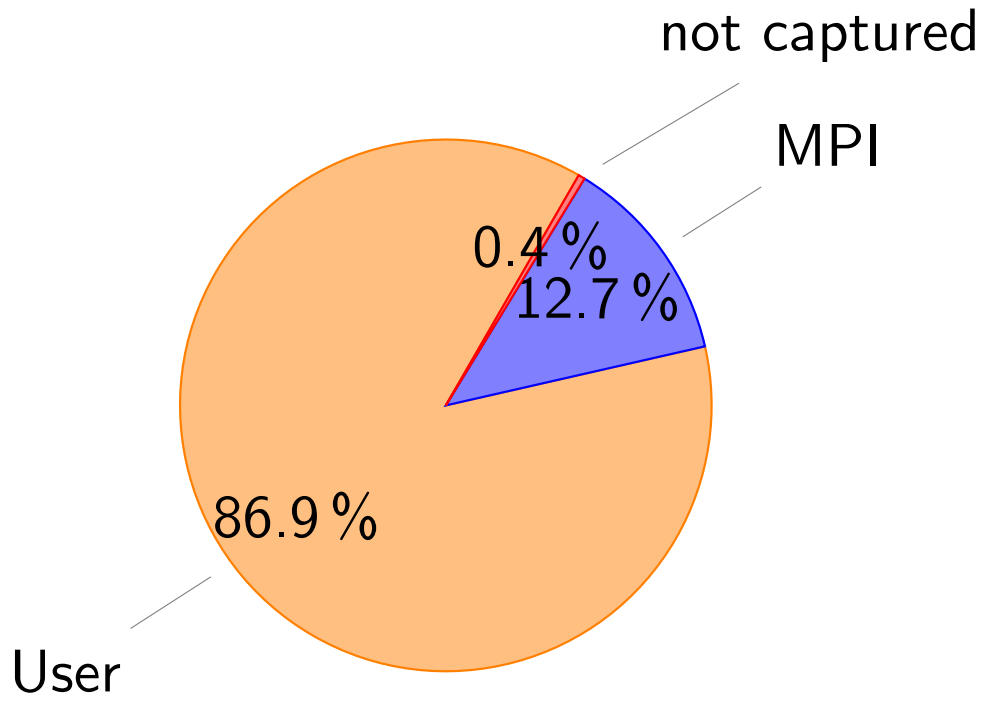

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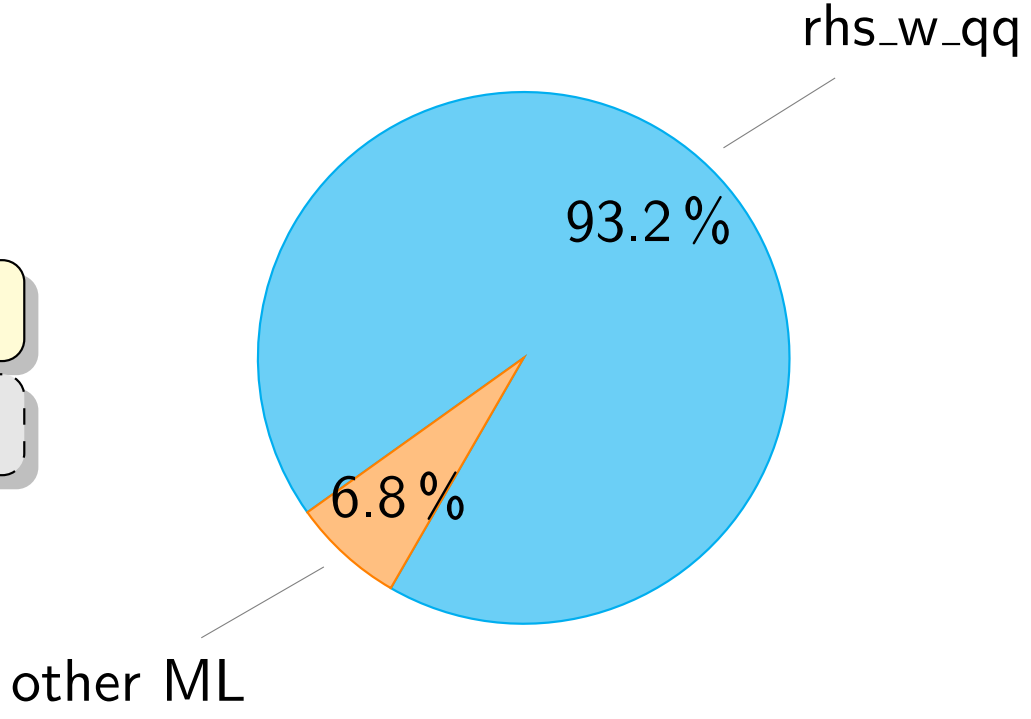

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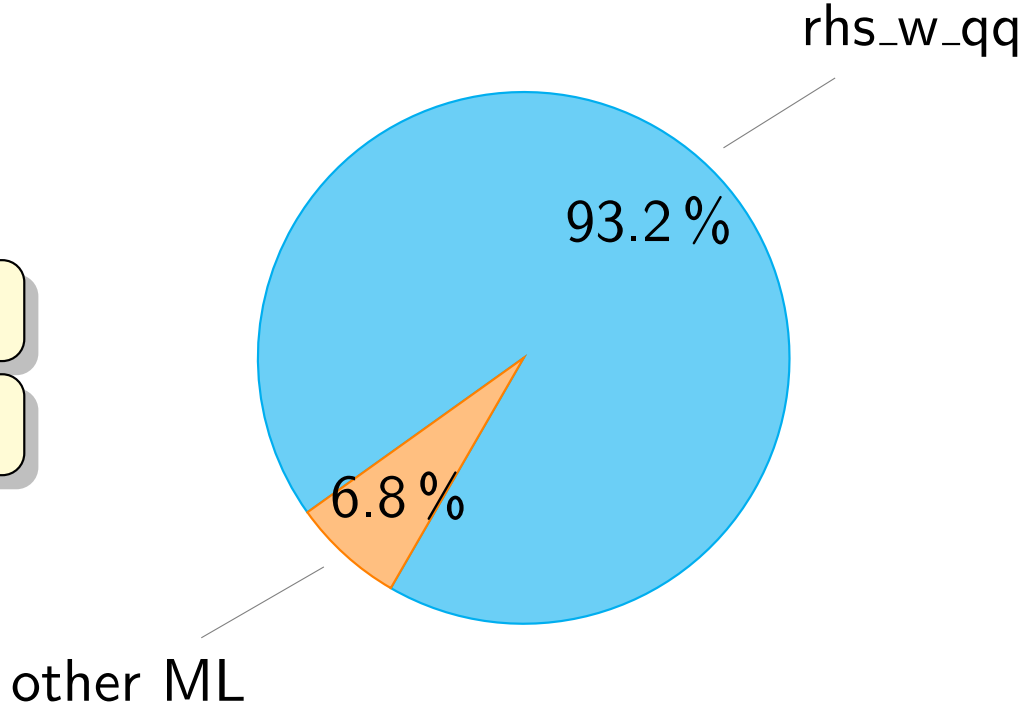

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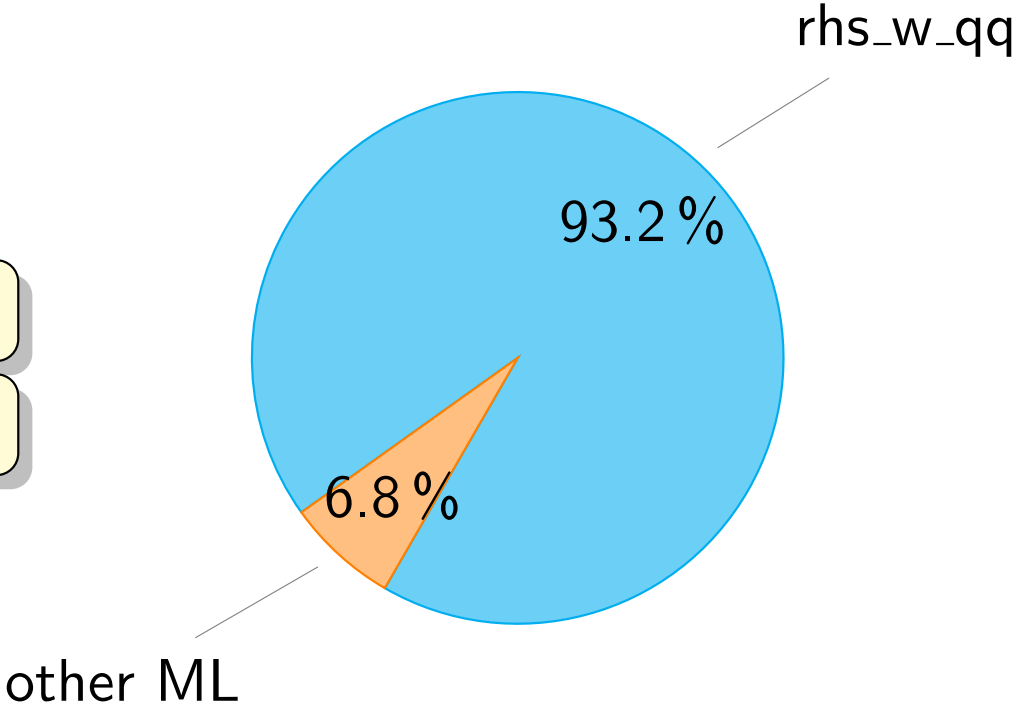

1. step: port rhs_w_qq ⇒ data transfer

Step 1 - Computationally heavy Part

- “Only” 30% of the code have to be ported
- done by John Levesque and Tom Edwards (Cray)

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- "Only" 30% of the code have to be ported
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- add ACC statements to loops
- define data regions $\Rightarrow$ CPU-GPU data transfer

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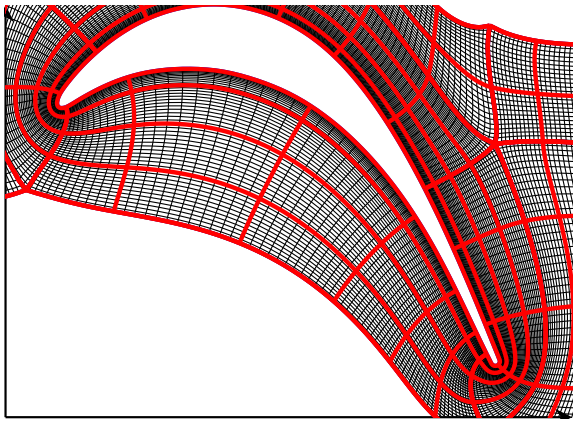
$$\mathbf{RHS} = -\frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(t_{ji}\right)$$



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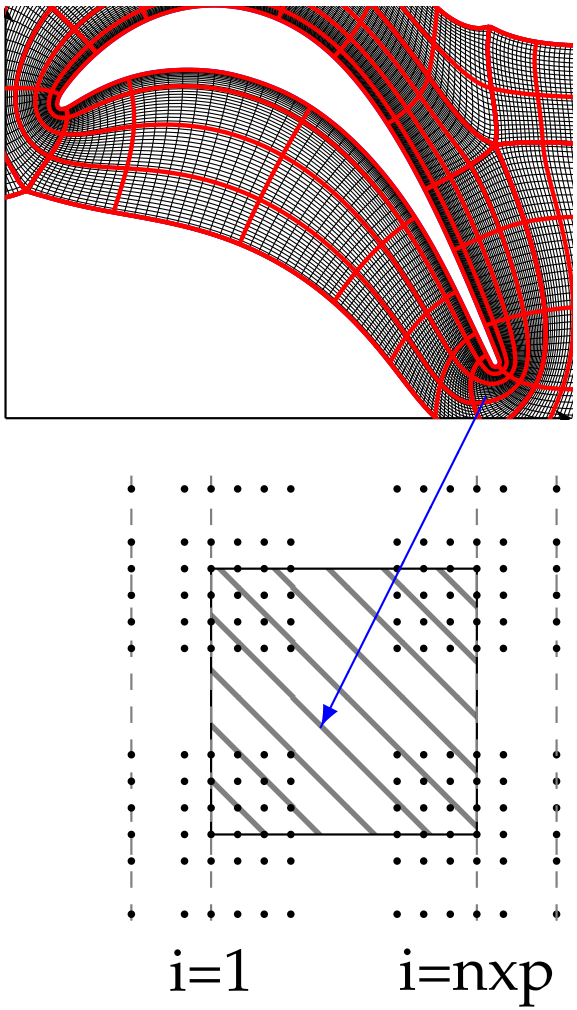

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$$\mathbf{RHS} = -\frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(t_{ji}\right)$$

```
do k=nzp_start,nzp_end

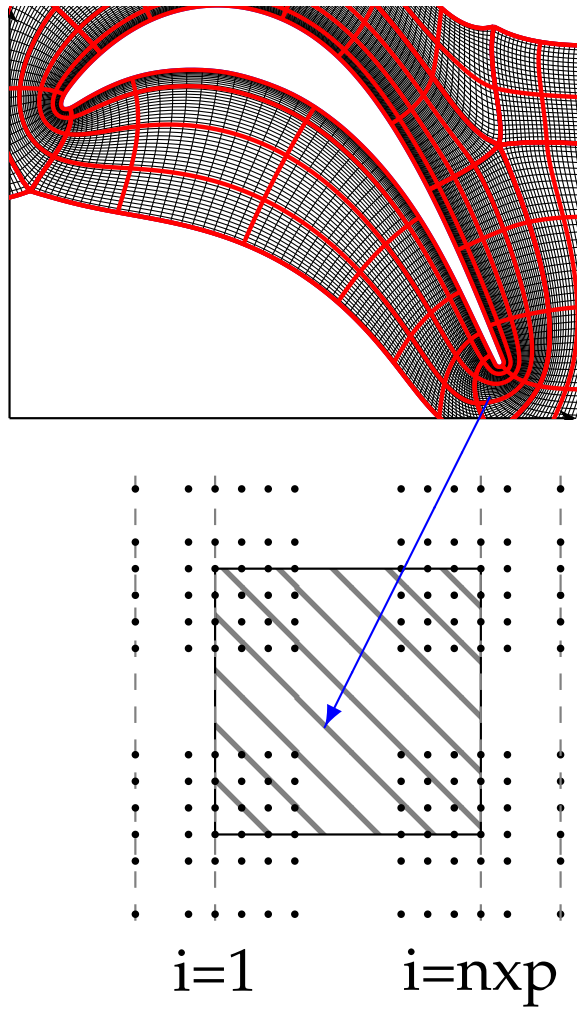
  do j=jbegwp,jendwp

    do i=ibegwp,iendwp
      ddw4(i,j,1) = qph(i,j,k,2)*r_et(i,j)
    end do
  end do


  call ddxi(ddw4(1-xhalo,1-yhalo,1)
&           ,ddw1(1-xhalo,1-yhalo,1) ,1)


  do j=1,nyp

    do i=1,nxp
      q(i,j,k,2)= q(i,j,k,2)+ddw1(i,j,1)
    end do
  end do
end do
```



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      ddw4(i,j,k) = qph(i,j,k,2)*r_et(i,j)
    end do
  end do
end do

  call ddxi_all(ddw4(1-xhalo,1-yhalo,1)
&             ,ddw1(1-xhalo,1-yhalo,1) ,nzp)

do k=nzp_start,nzp_end

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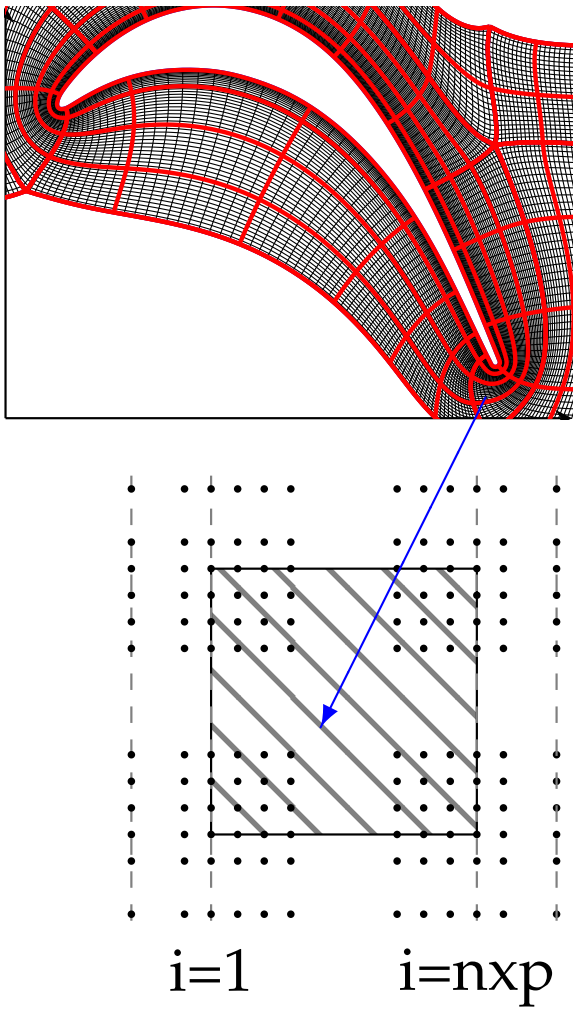

Step 1 - Computationally heavy Part

```
!$acc parallel loop gang
      do k=nzp_start,nzp_end
!$acc loop worker
        do j=jbegwp,jendwp
!$acc loop vector
          do i=ibegwp,iendwp
            ddw4(i,j,k) = qph(i,j,k,2)*r_et(i,j)
          end do
        end do
      end do
!$acc end parallel loop
        call ddxi_all(ddw4(1-xhalo,1-yhalo,1)
     &              ,ddw1(1-xhalo,1-yhalo,1)  ,nzp)
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!$acc loop vector
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          end do
        end do
      end do
!$acc end parallel loop
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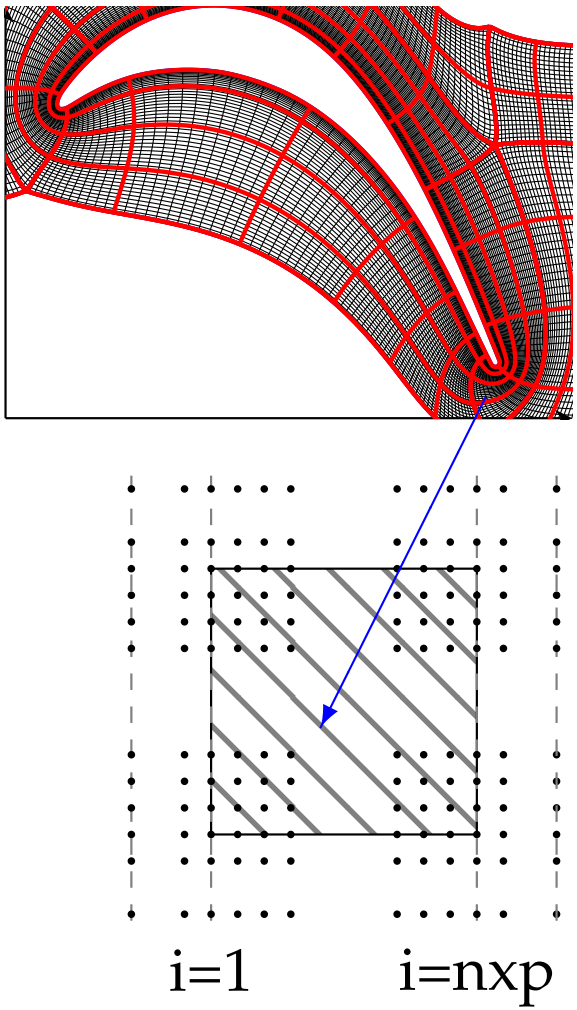

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- compare runtime of
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  - ACC version using 1 MPI rank per node

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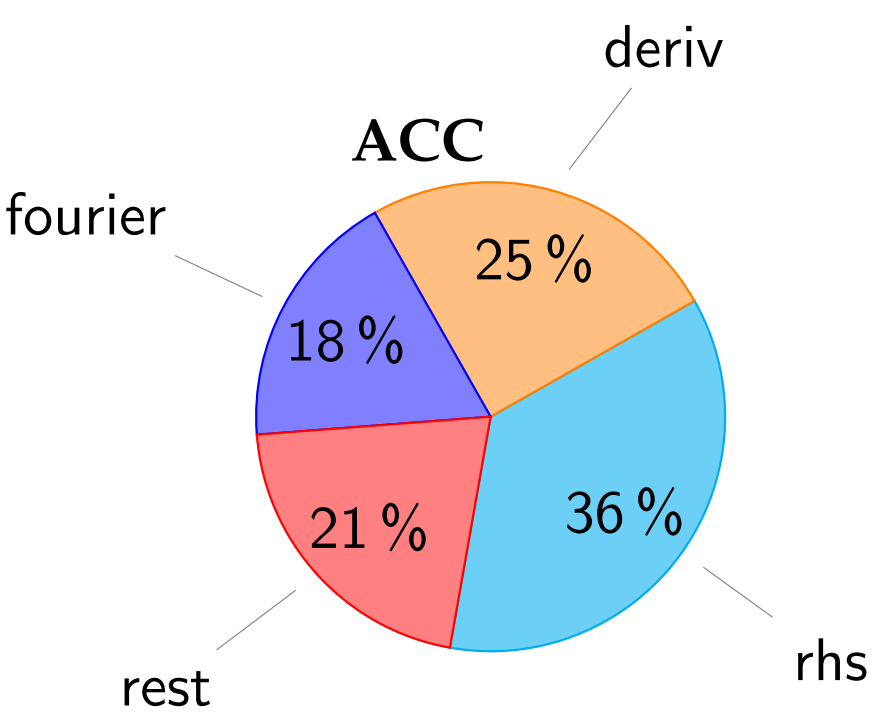
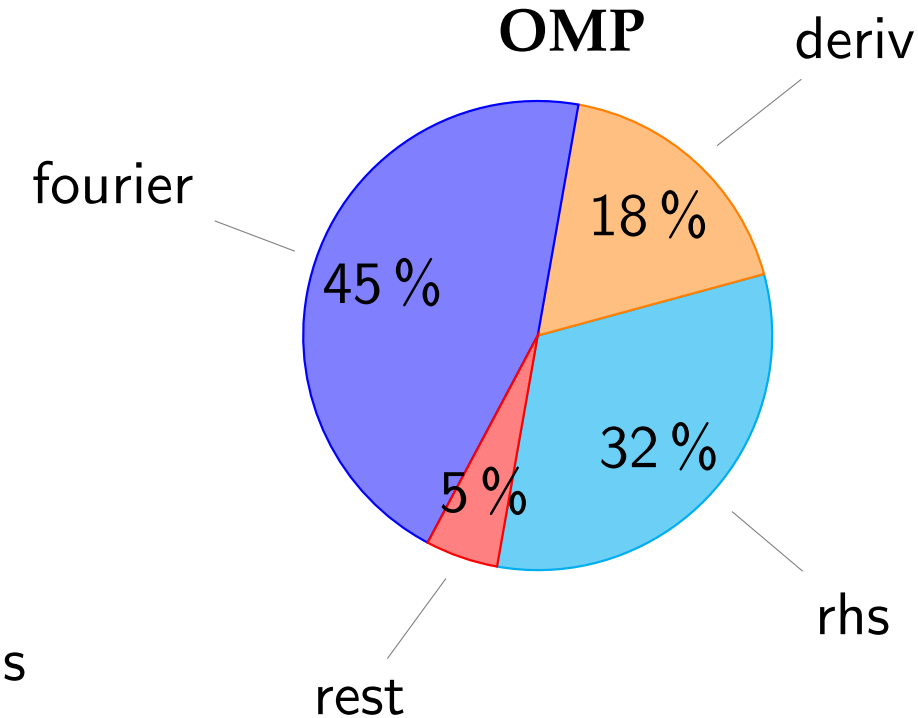
- compare runtime of
  - hybrid open MPI/OMP with 1 MPI rank per node (16 OMP threads)
  - ACC version using 1 MPI rank per node
- overall speedup of 18% (GPU vs. CPU)
- data transfer between GPU and CPU $\approx$ 30% of runtime

Step 1 - Computationally heavy Part

- *rest* $\Rightarrow$ CPU code runs slower (1 vs 16 OMP threads)





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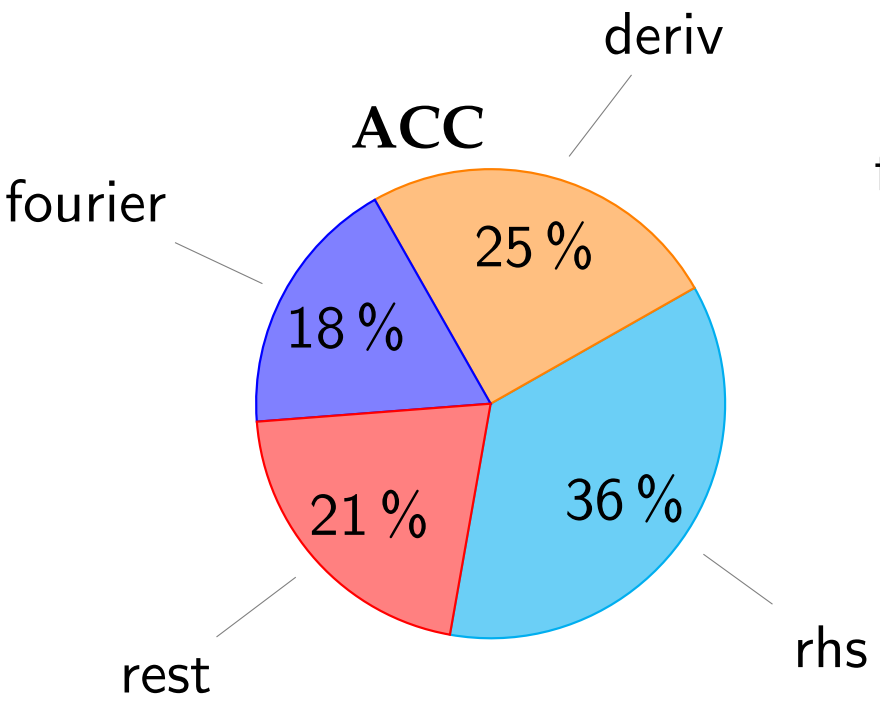
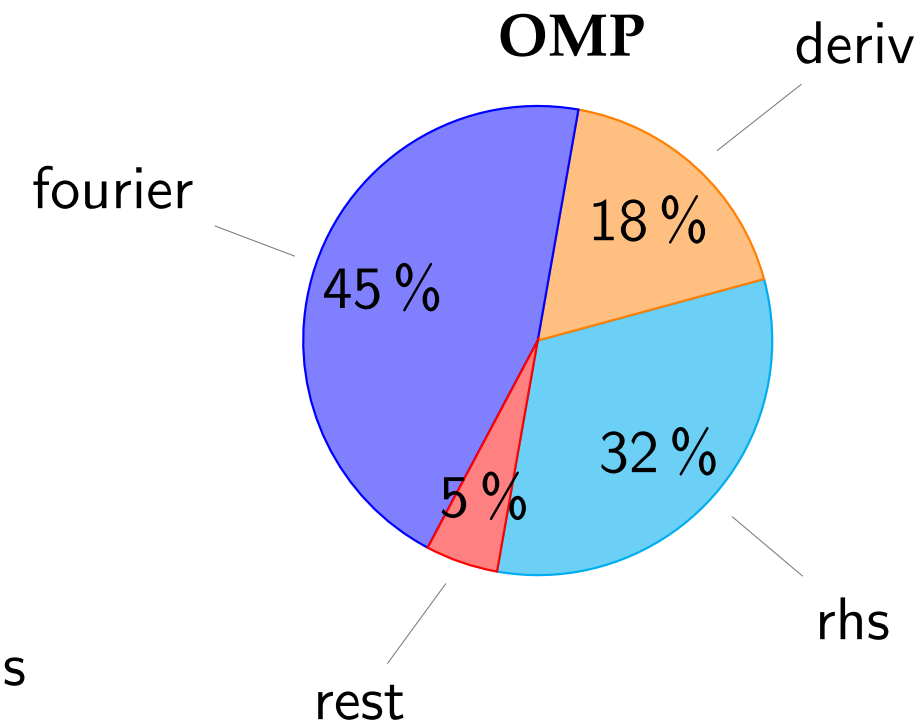
- FFTW (cufft) are significantly faster





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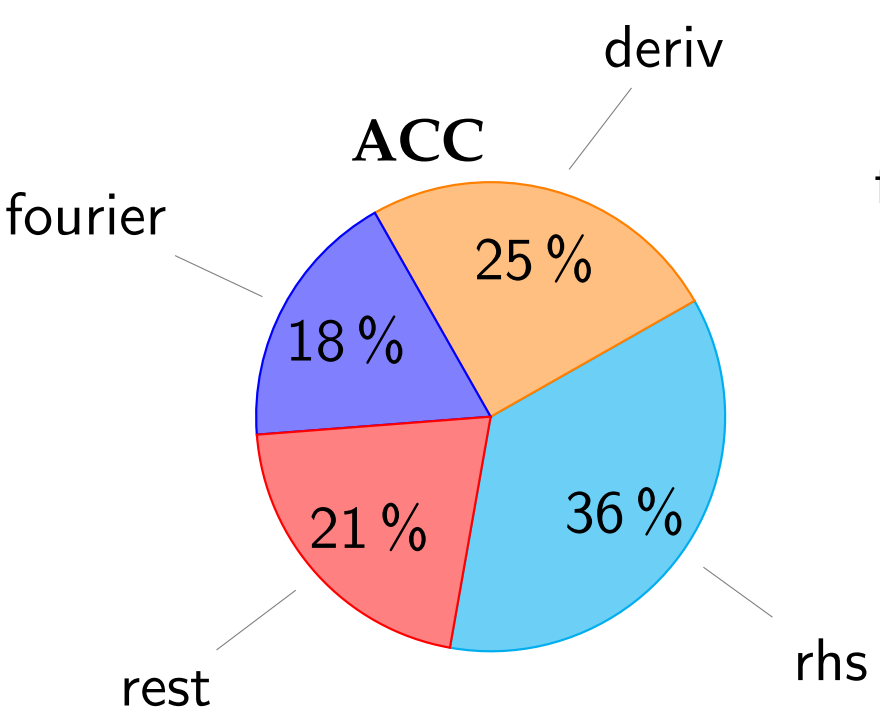
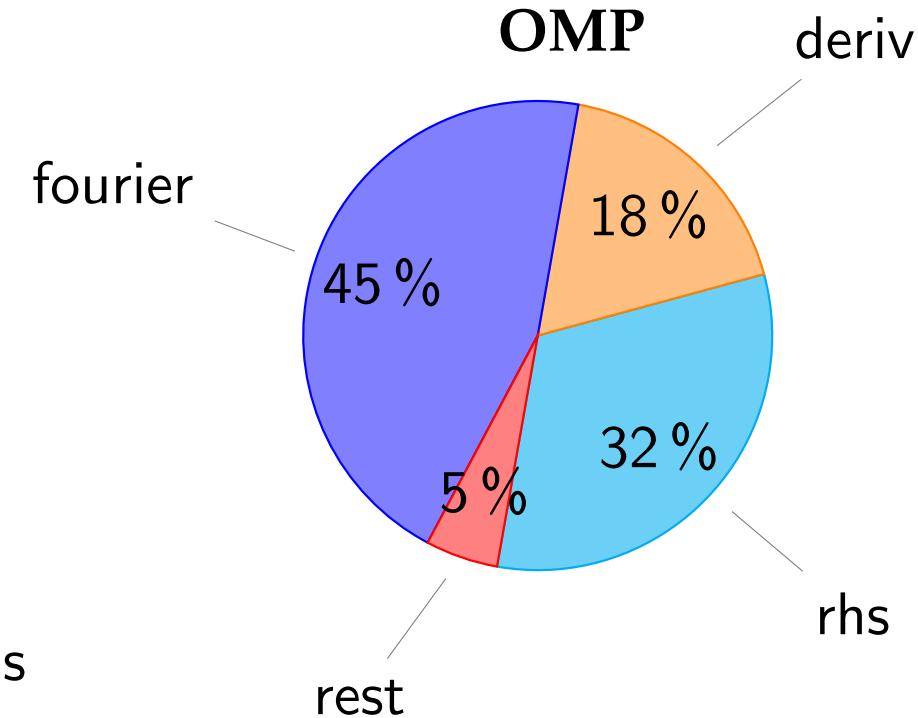
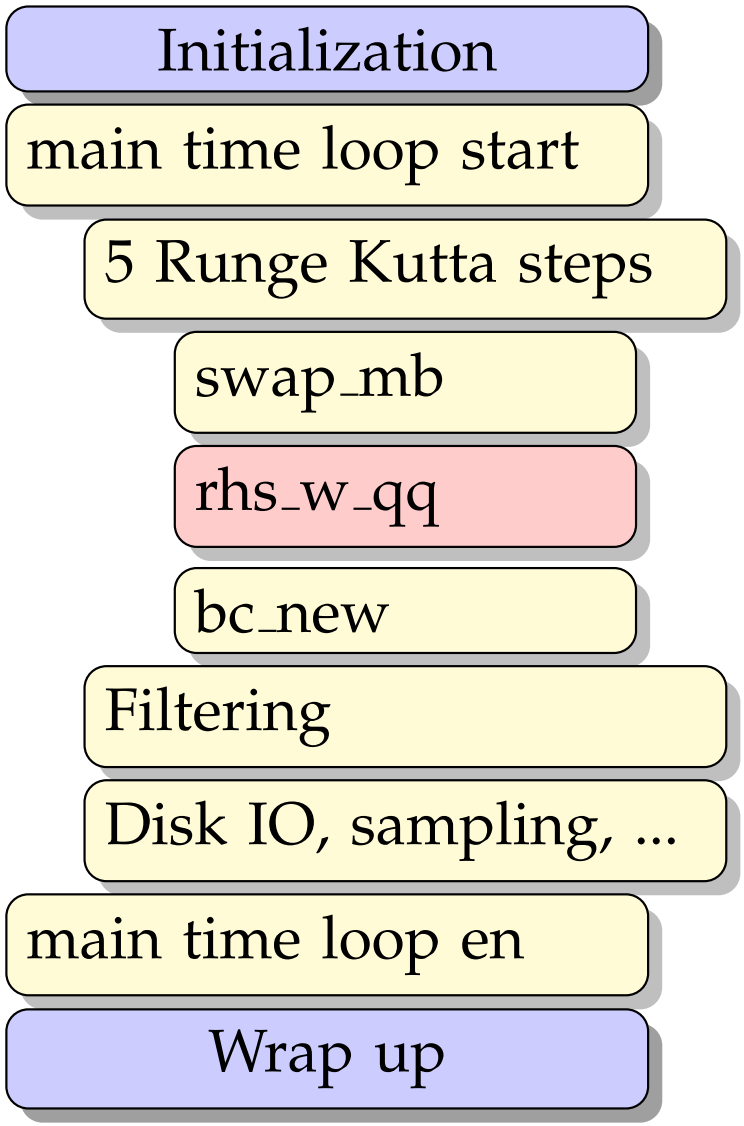
- *rest* $\Rightarrow$ CPU code runs slower (1 vs 16 OMP threads)
- FFTW (cufft) are significantly faster
- *deriv* and *rhs* similar relative fraction





Step 2 - Limitting data transfer



- 30% of walltime spent in CPU-GPU data transfer
- move everything to GPU except for

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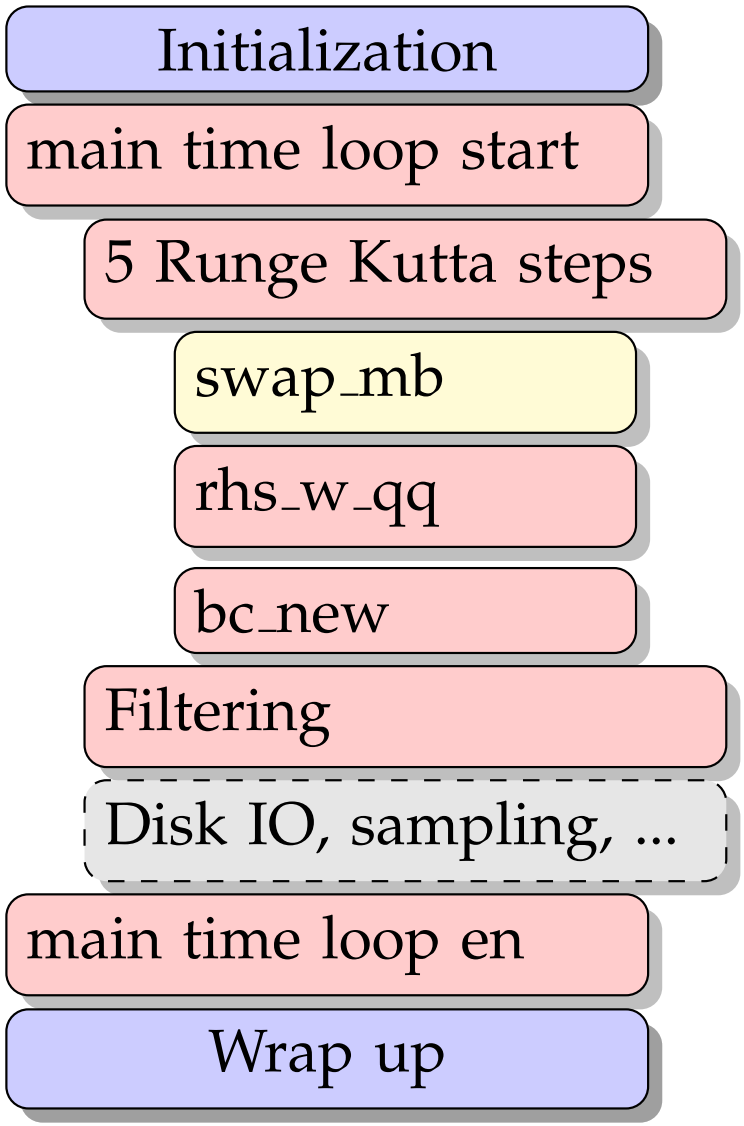
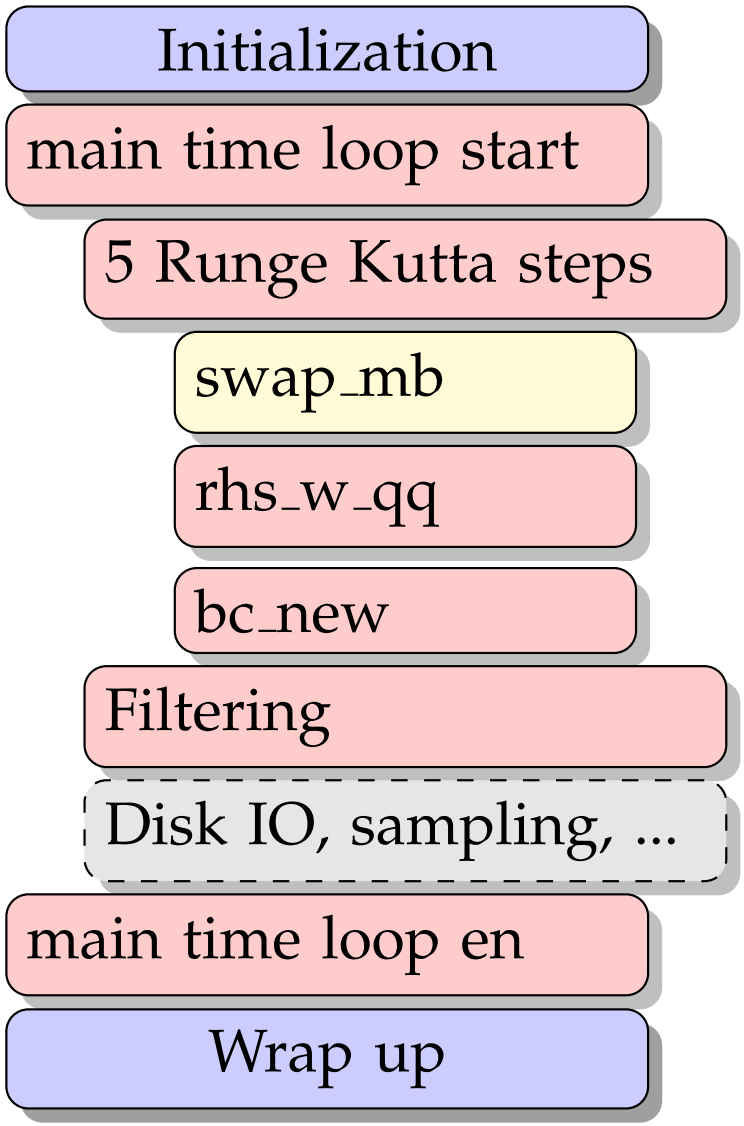


- 30% of walltime spent in CPU-GPU data transfer
- move everything to GPU except for
  - swapping - MPI communication

Step 2 - Limitting data transfer



- 30% of walltime spent in CPU-GPU data transfer
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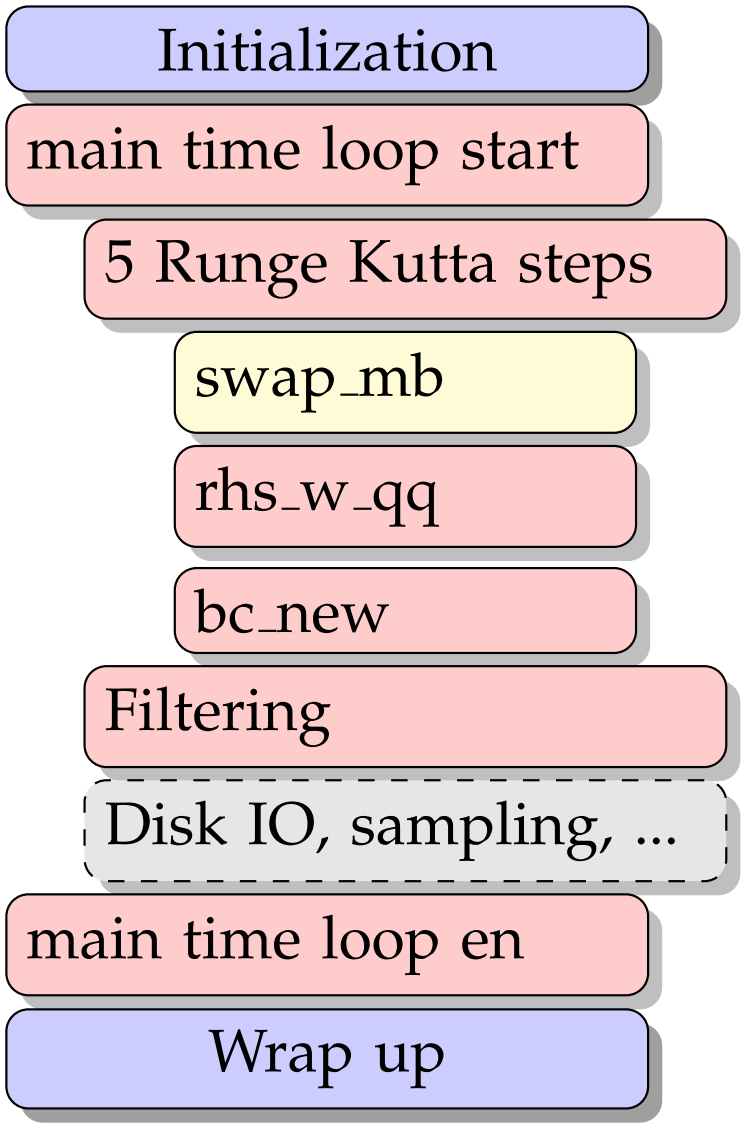

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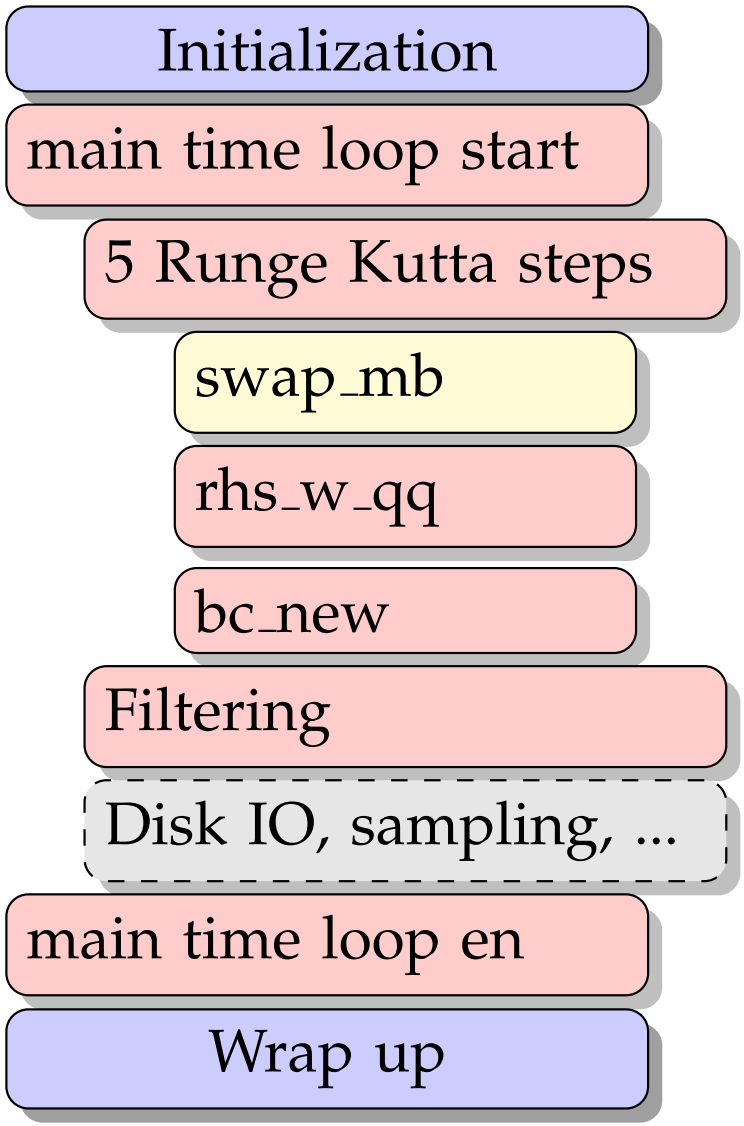

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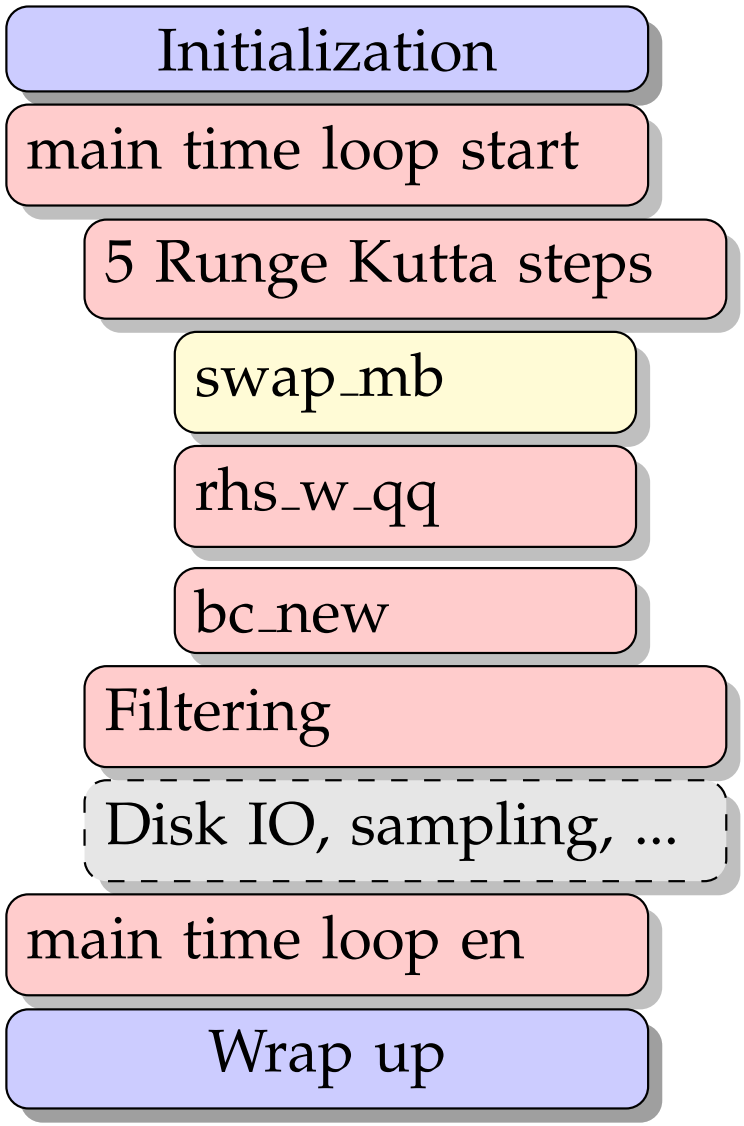

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- runtime increase by 7x

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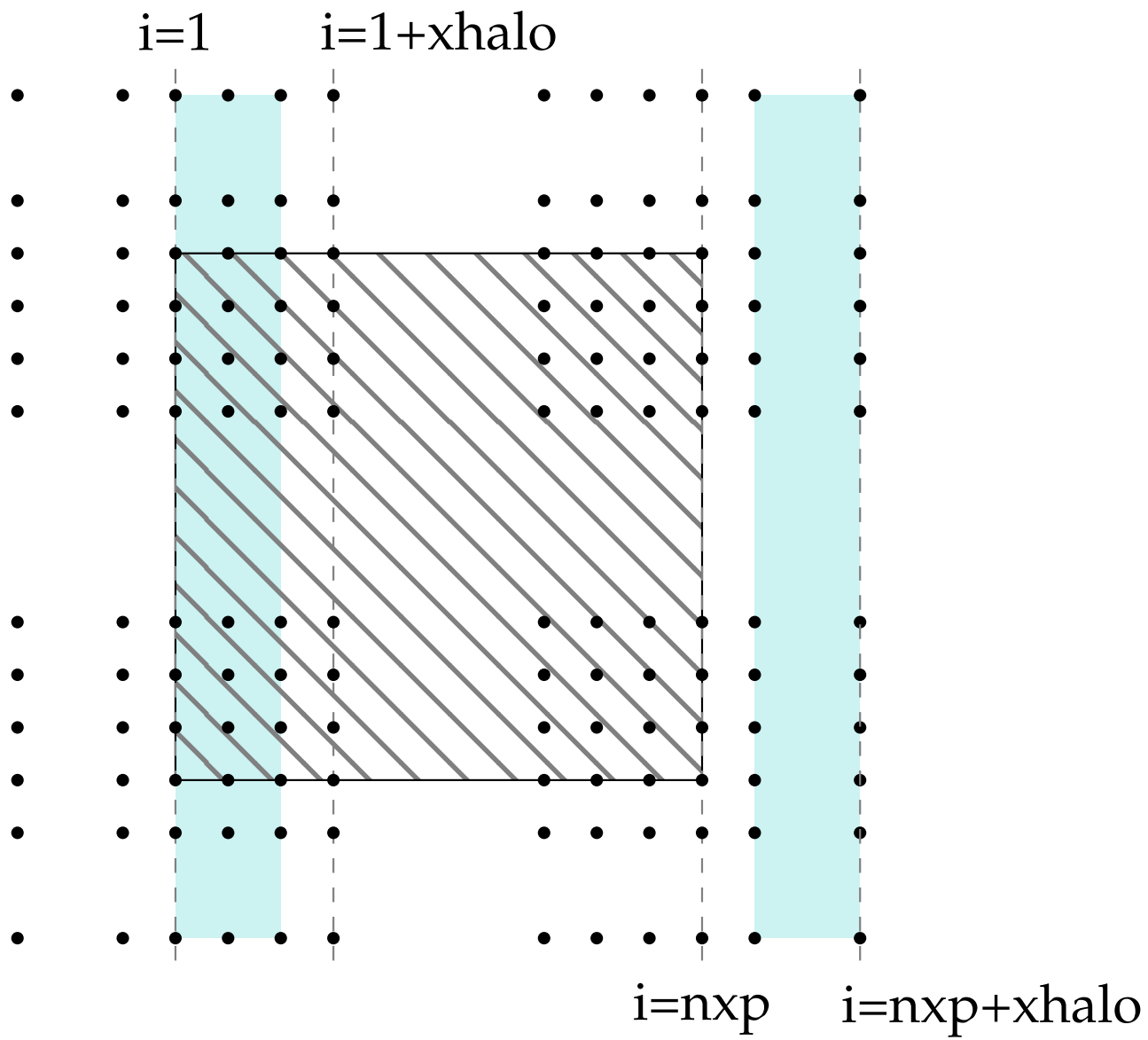

STEP 2 - LIMITING DATA TRANSFER

```
!$acc parallel loop private(l)
        do n=1,nv
          do k=1,kpoints
           do j=1-yhalo,nyp+yhalo
             do i=1,xhalo
                l = i + (j+yhalo-1)*xhalo
     &            + (k-1)*(nyp+2*yhalo)*xhalo
     &            + (n-1)*(kpoints)*(nyp+2*yhalo)*xhalo
               ahoxm(l) = a(i,j,k,n)
             enddo
           enddo
         enddo
       enddo
```

- base version: $> 1600s$

Step 2 - Limiting data transfer

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!$acc parallel loop private(l) collapse(2)
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!dir$ unroll
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- final version: $\approx 12s$

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- base version: $> 1600s$
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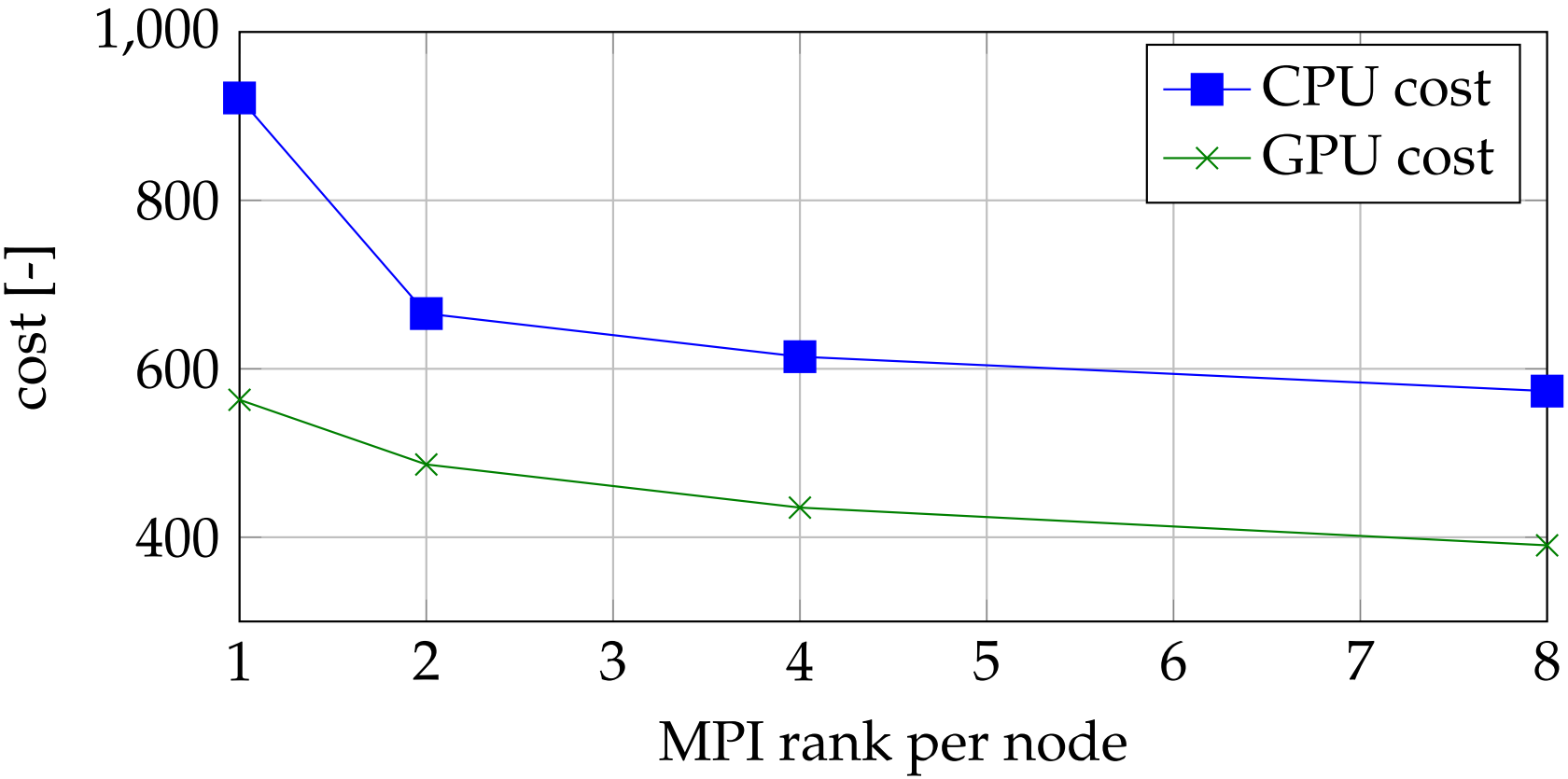
- $\approx 30 - 40\%$ speed up w.r.t. CPU version
- packing on CPU fastest if using l=l+1
- GPU faster as CPU

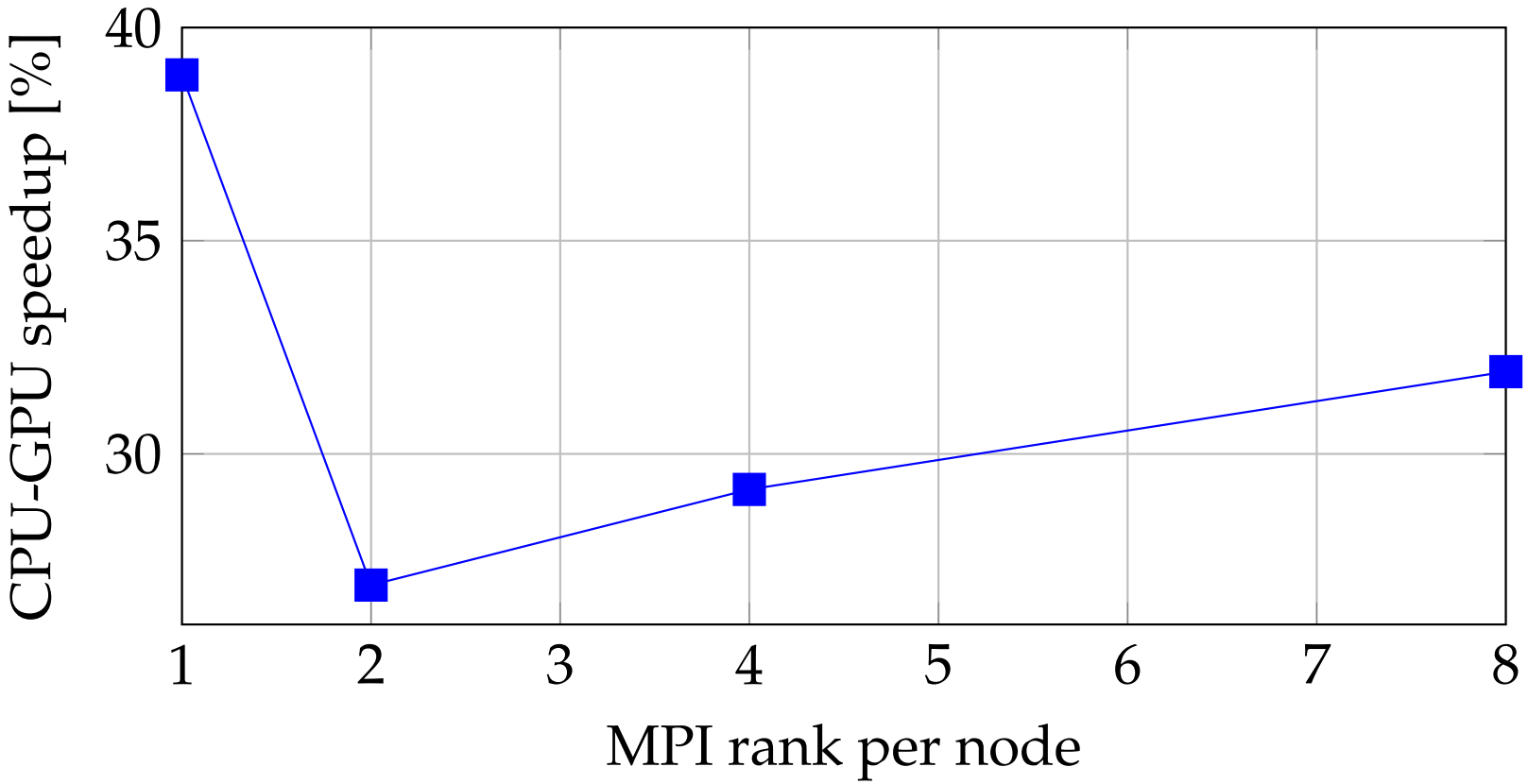
Step 2 - Speed-up

- strong scaling
- Using 64 - 512 nodes



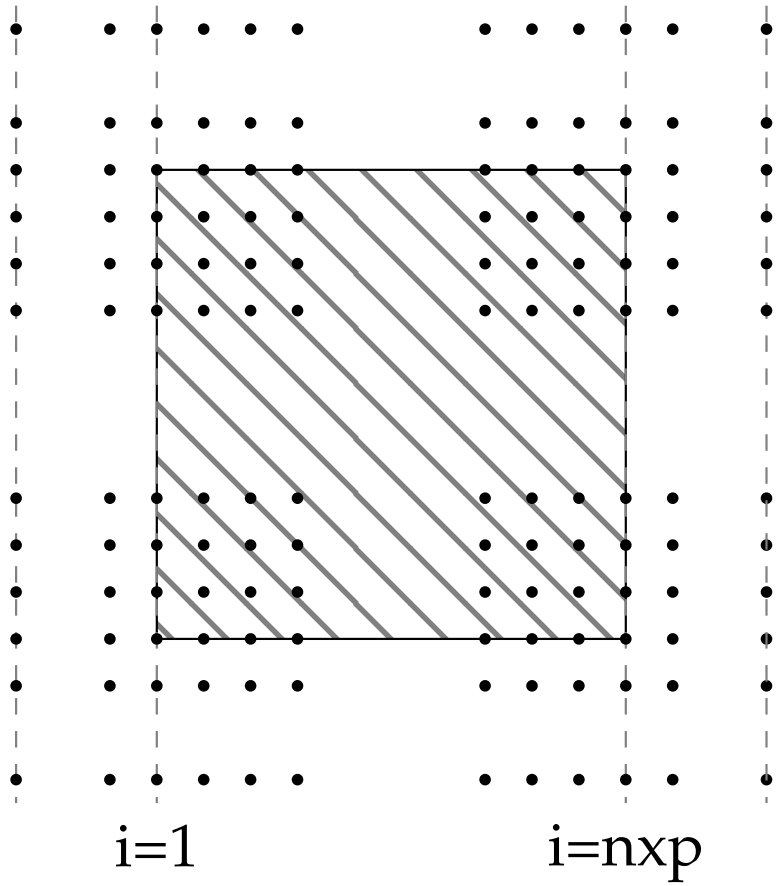
Step 2 - Speed-up

- strong scaling
- Using 64 - 512 nodes
- speed up around 30%



Step 3 - Additional tweaks

- mostly innermost loop length: nxp+2×xhalo
- generate grid such that innermost loop length is 32,64 or 128



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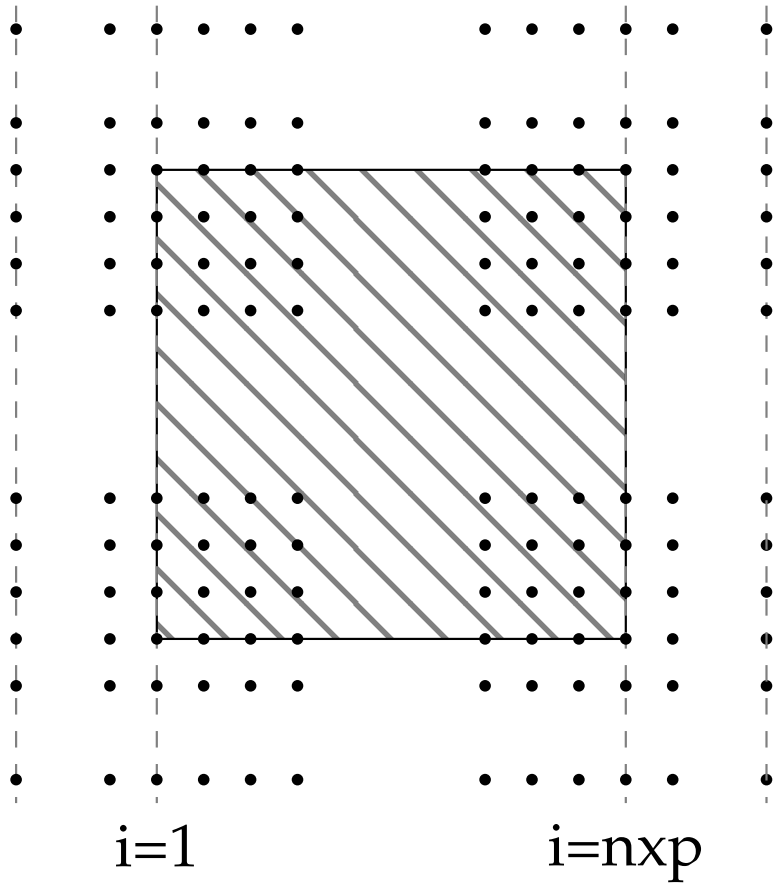

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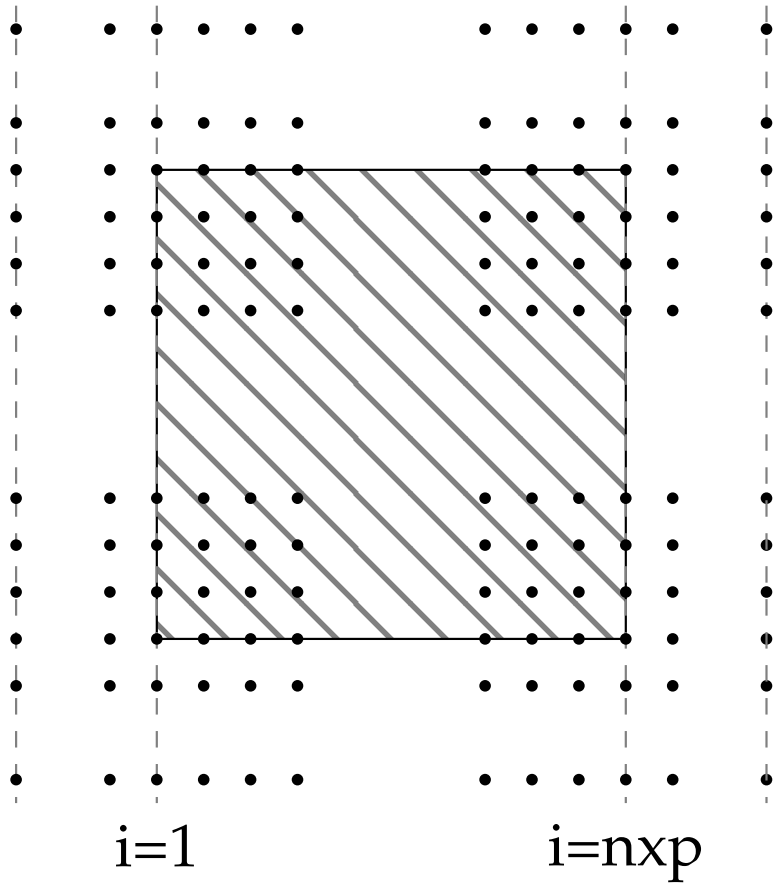
- less flexible but significant performance improvement



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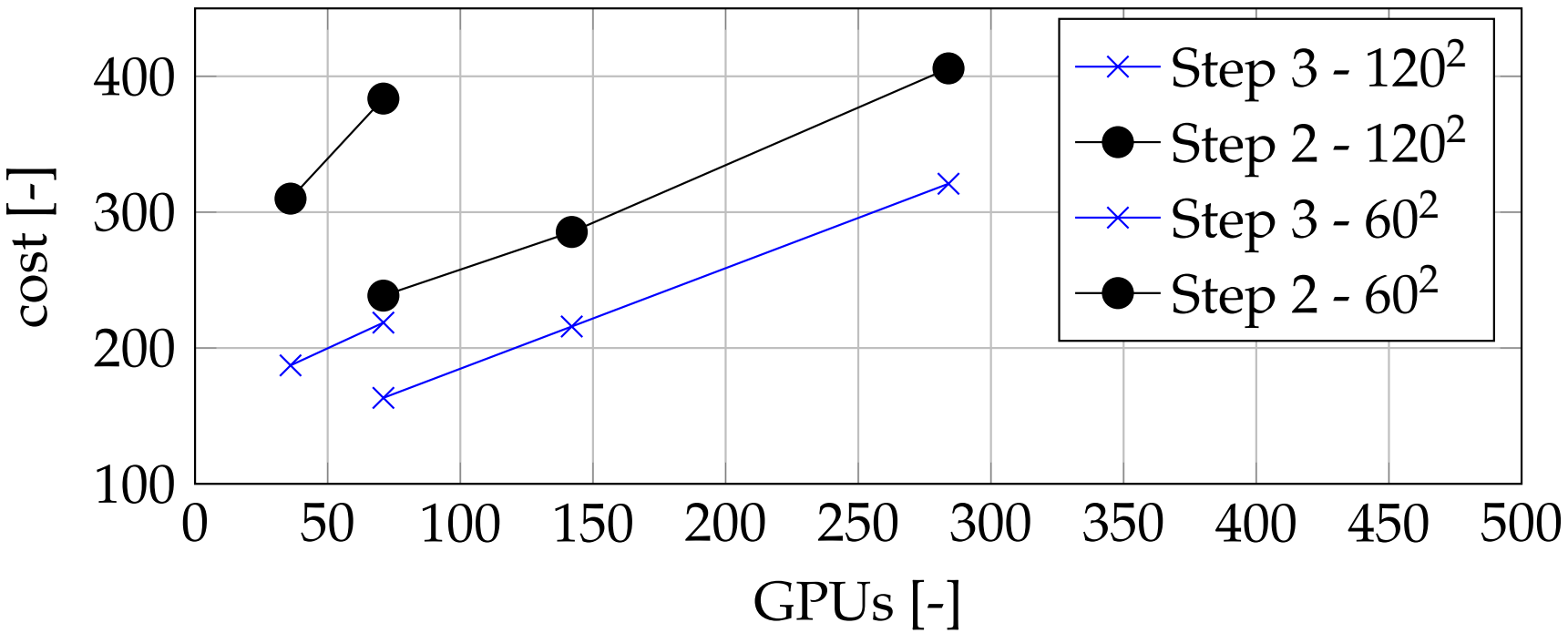

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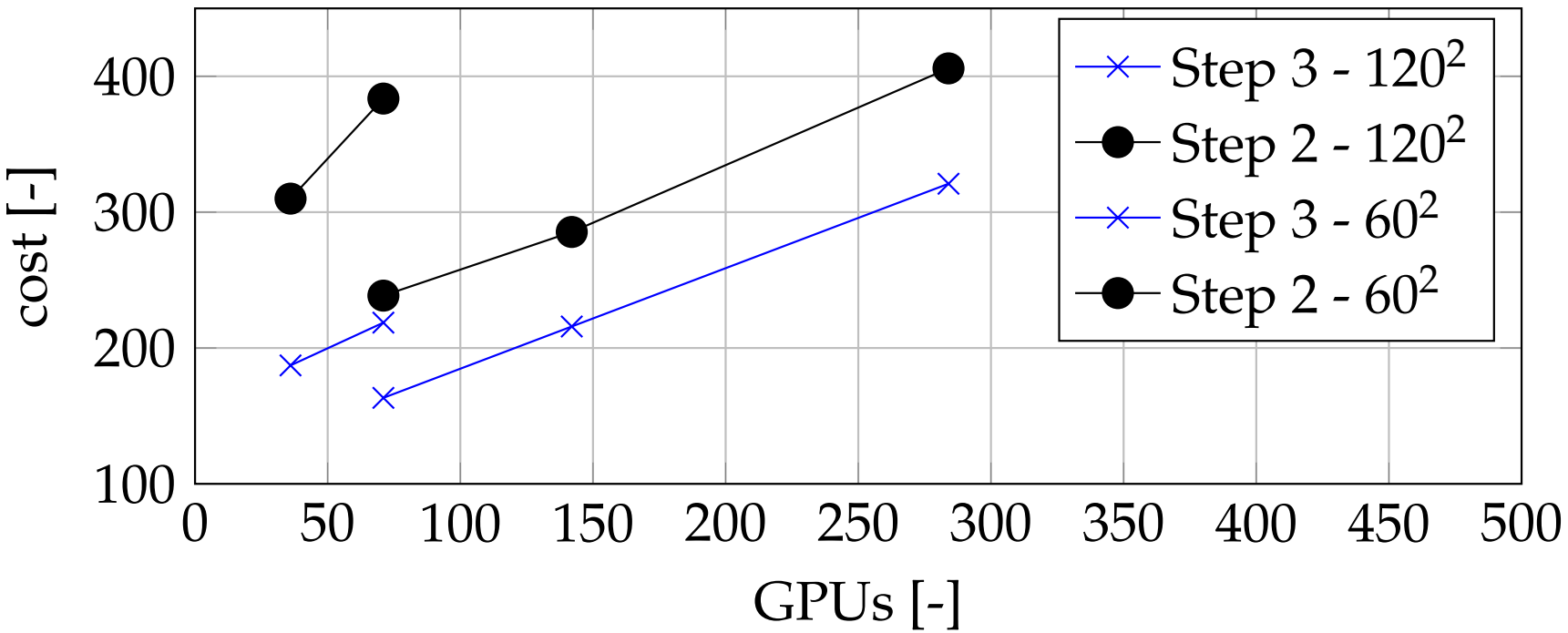

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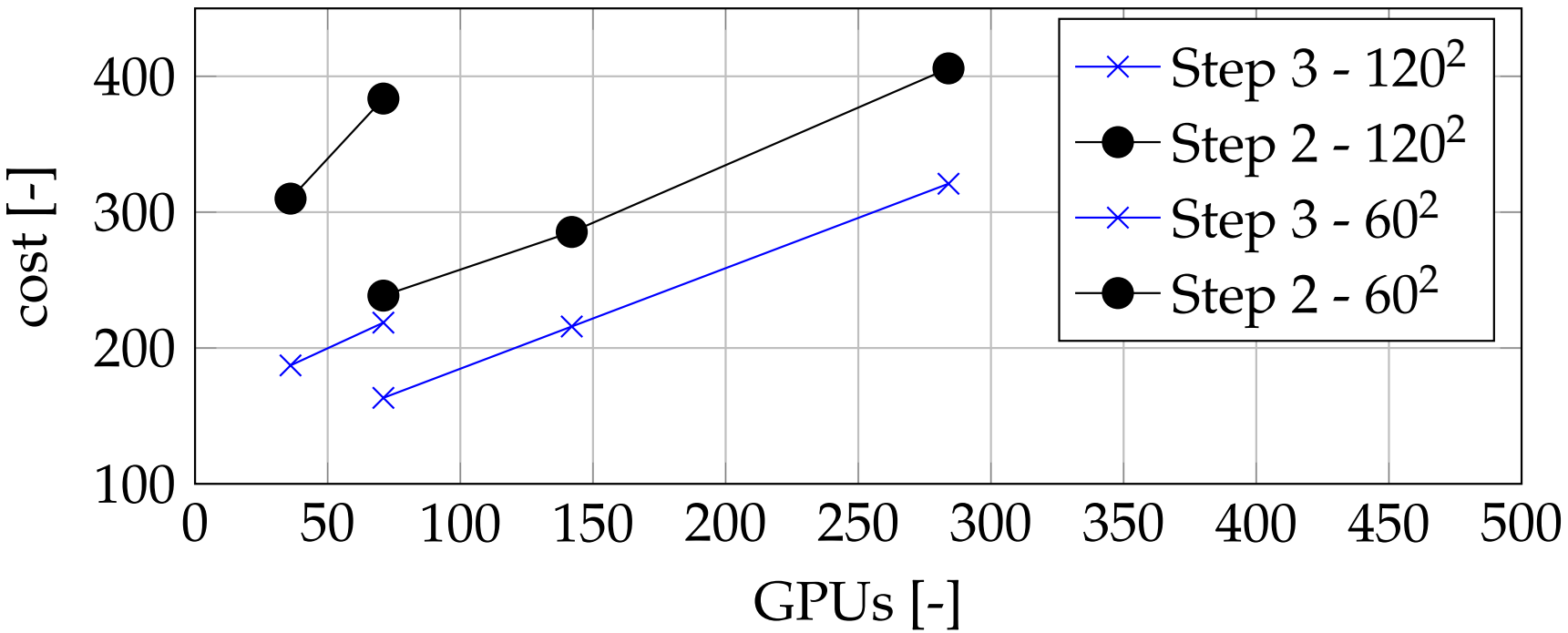
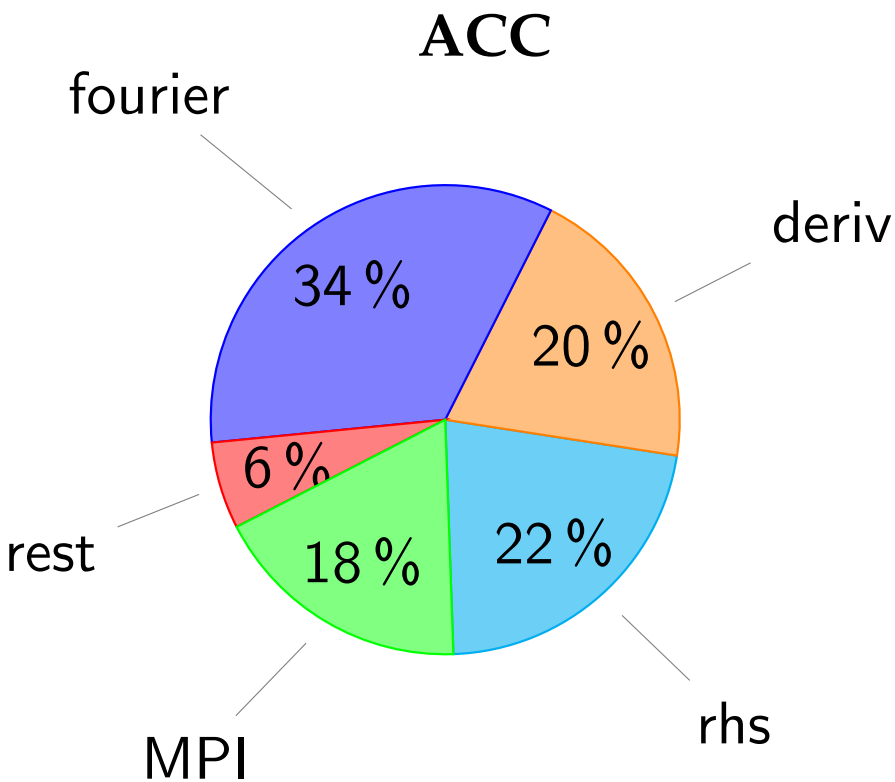
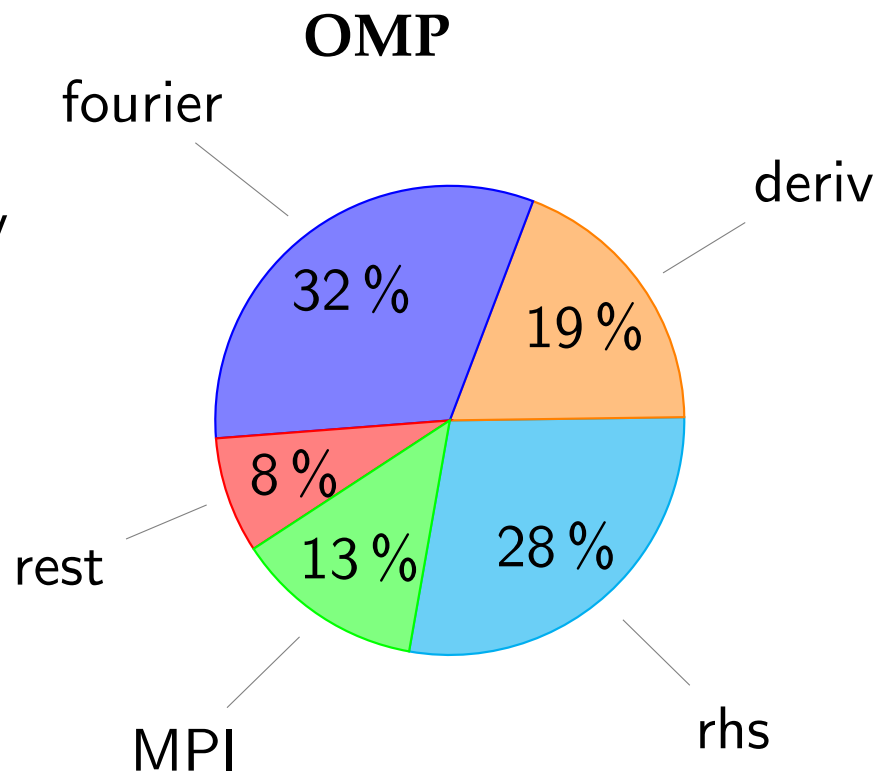
- “best performance” by placing 4 MPI ranks
- try 28^2 (vector_length(32))
- speed up w.r.t. CPU $\approx$ 2x



Step 3 - Profiles

- Piz Daint
- CrayPAT only works for 1 MPI rank per node
- similar distribution of work according to routines





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Longer term (Summit)

- Multi GPU environment - which route to go?
- Are the algorithms optimized for CPU as well the best ones for GPU?