CSCS
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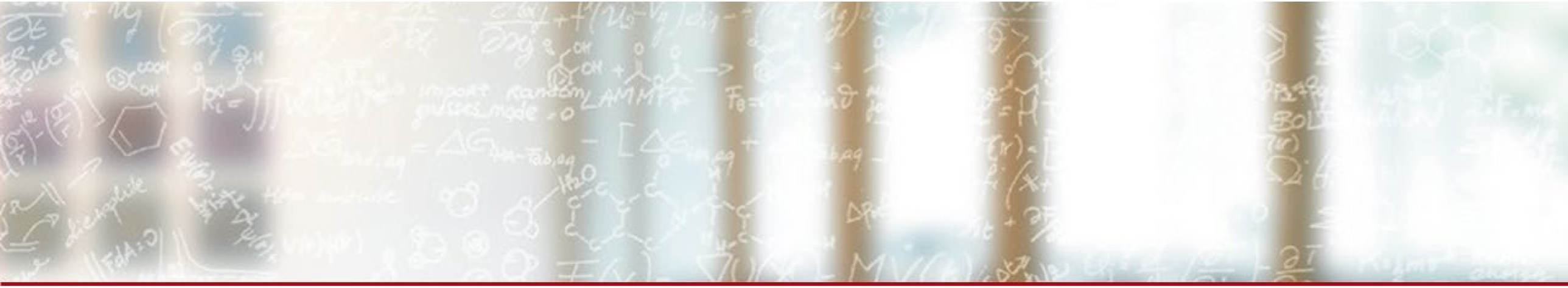
Swiss National Supercomputing Centre

ETH zürich



Interactive Multi-GPU Supercomputing with Julia

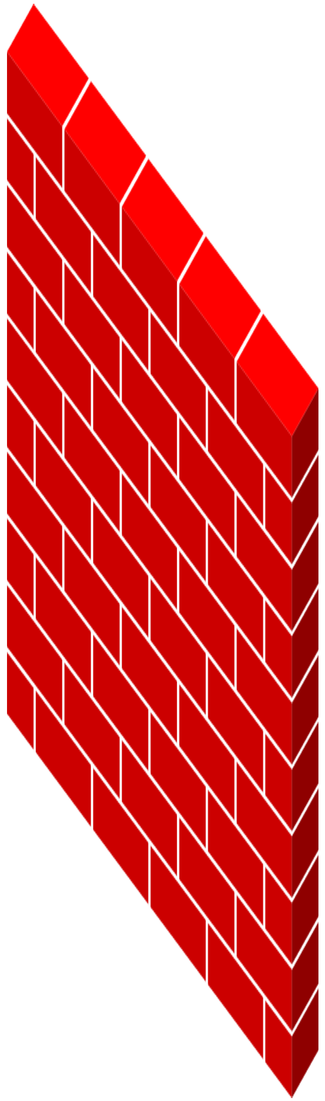
CSCS User Lab Day – Meet the Swiss National Supercomputing Centre

Samuel Omlin

September 9th 2019

Protoype

```
P = rand(4,3)
```



Production code

```
float* P;
P = malloc(…);
rand(P,…);
```

The two language problem

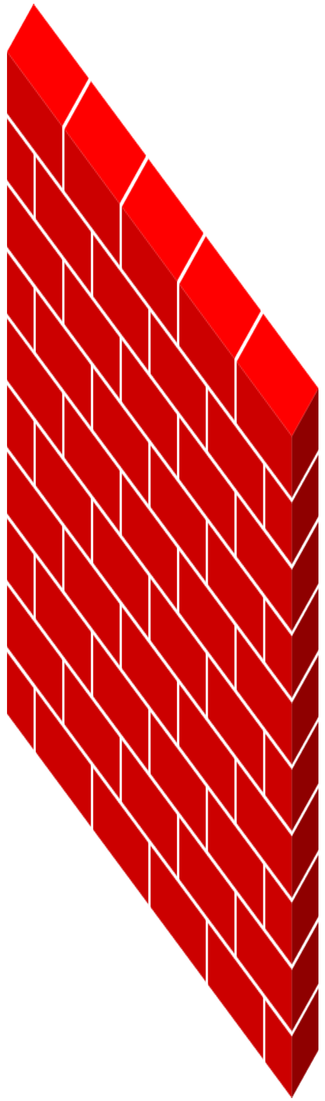
Protoype (MATLAB / Python /...)

simple & high-level

interactive

low development cost

slow



Production code (C / C++ / Fortran / ...)

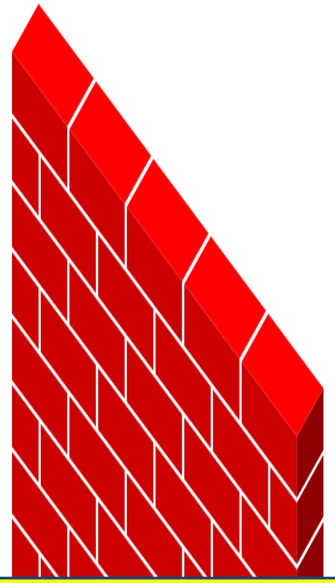
complex & low-level

not interactive

high development cost

fast

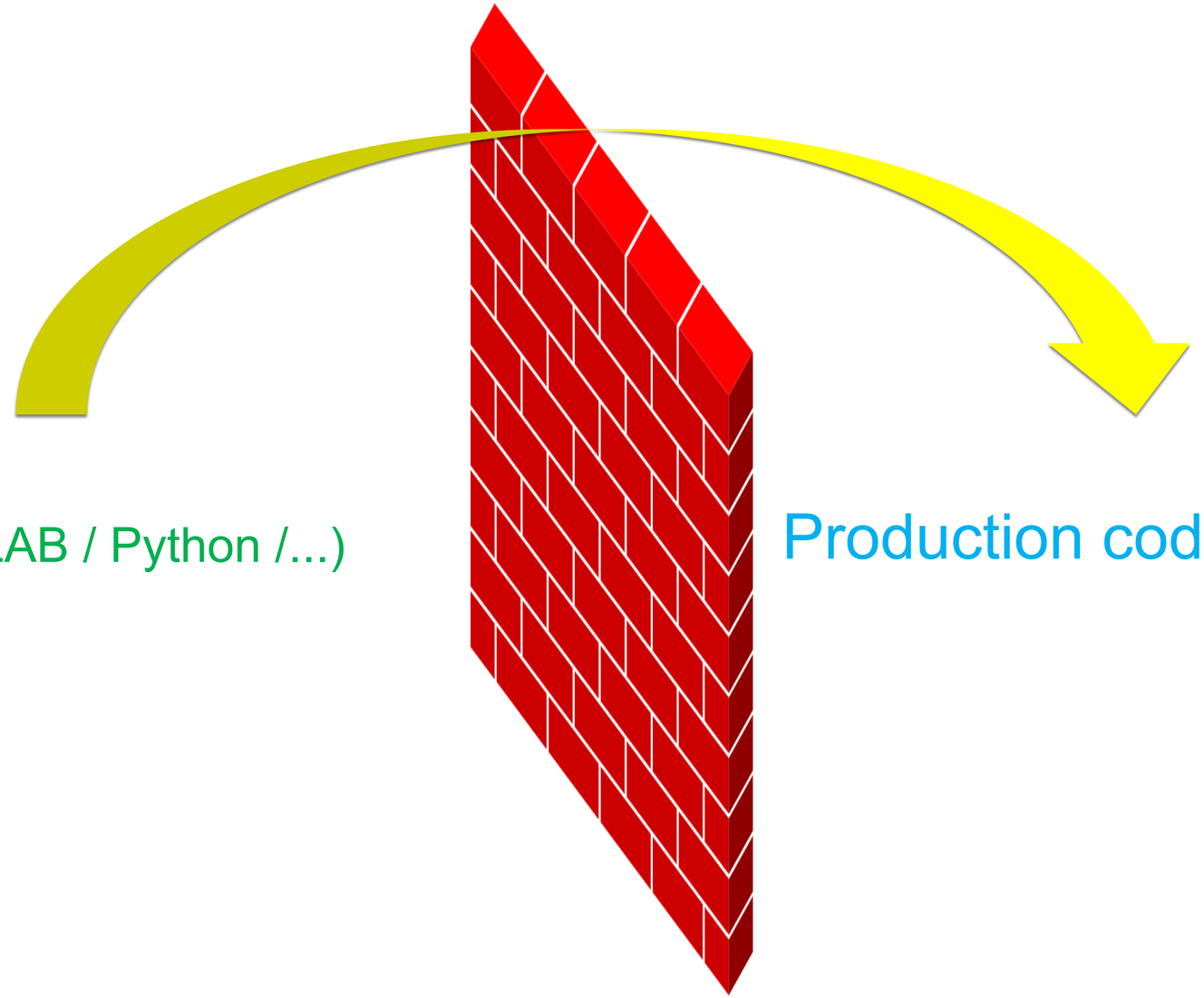
The two language problem



Protoype (MATLAB / Python /...)	Production code (C / C++ / Fortran / ...)
simple & high-level	complex & low-level
interactive	not interactive
low development cost	igh development cost
slow	fast

We really need both languages!

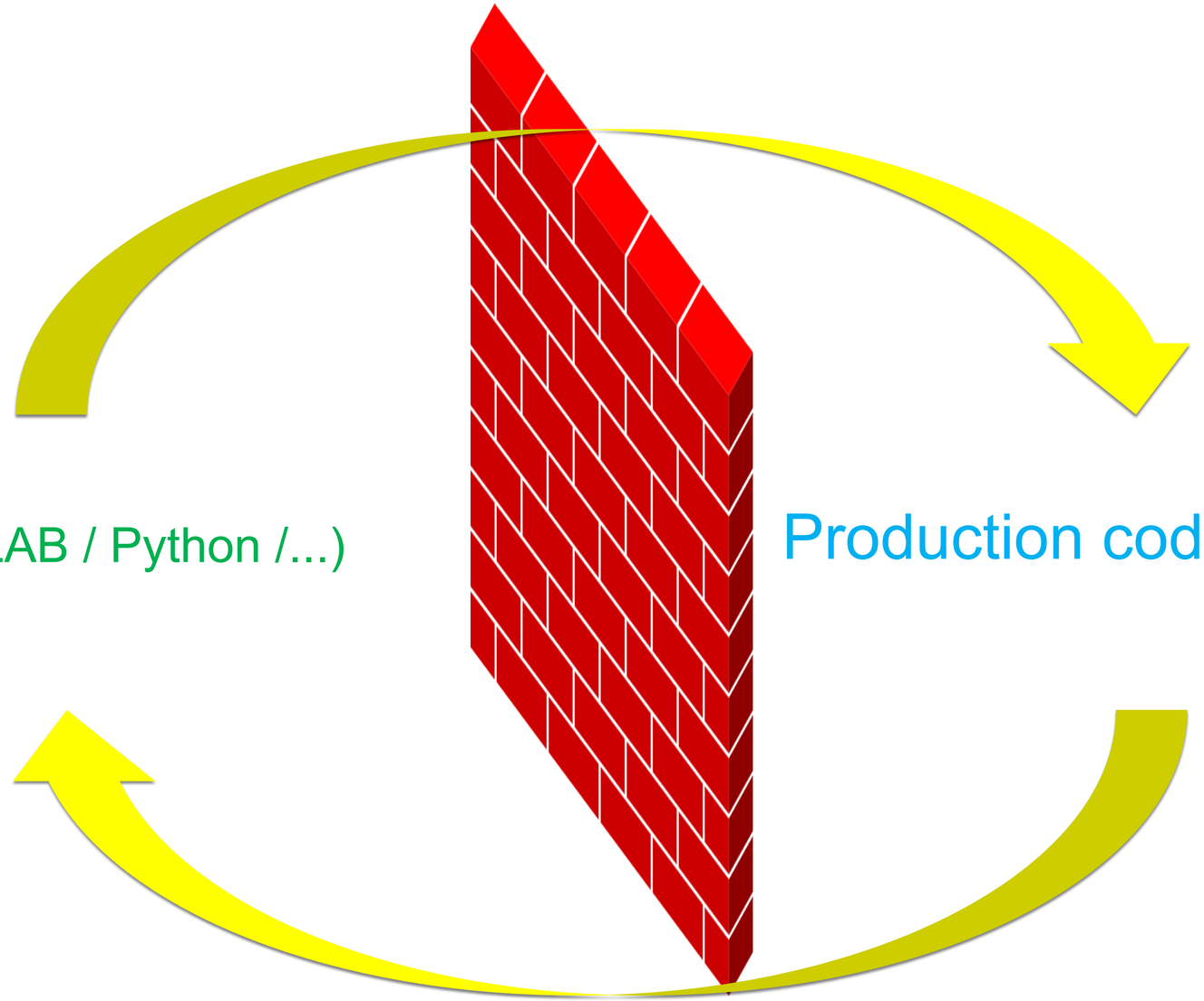
The two language problem



Protoype (MATLAB / Python /...)

Production code (C / C++ / Fortran / ...)

The two language problem



Protoype (MATLAB / Python /...)

Production code (C / C++ / Fortran / ...)

Solution

A language that can be used for both

Protoype & Production code

Solution

A language that can be used for both

Protoype & Production code

Solution

simple & high-level

interactive

low development cost

fast

Solution

simple & high-level

interactive

low development cost

fast

Fast and interactive???

Julia code is compiled, yet only shortly before you use it the first time.

Solution

Mature?

Is “adult” now:
v1.0.0 released in Aug 2018

simple & high-level

interactive

low development cost

fast

Solution

simple & high-level

interactive

low development cost

fast

1-day fly?

Developed at MIT and by a fast growing open-source community

Solution

Too good to be true!

Solution

Too good to be true!

Let's see!

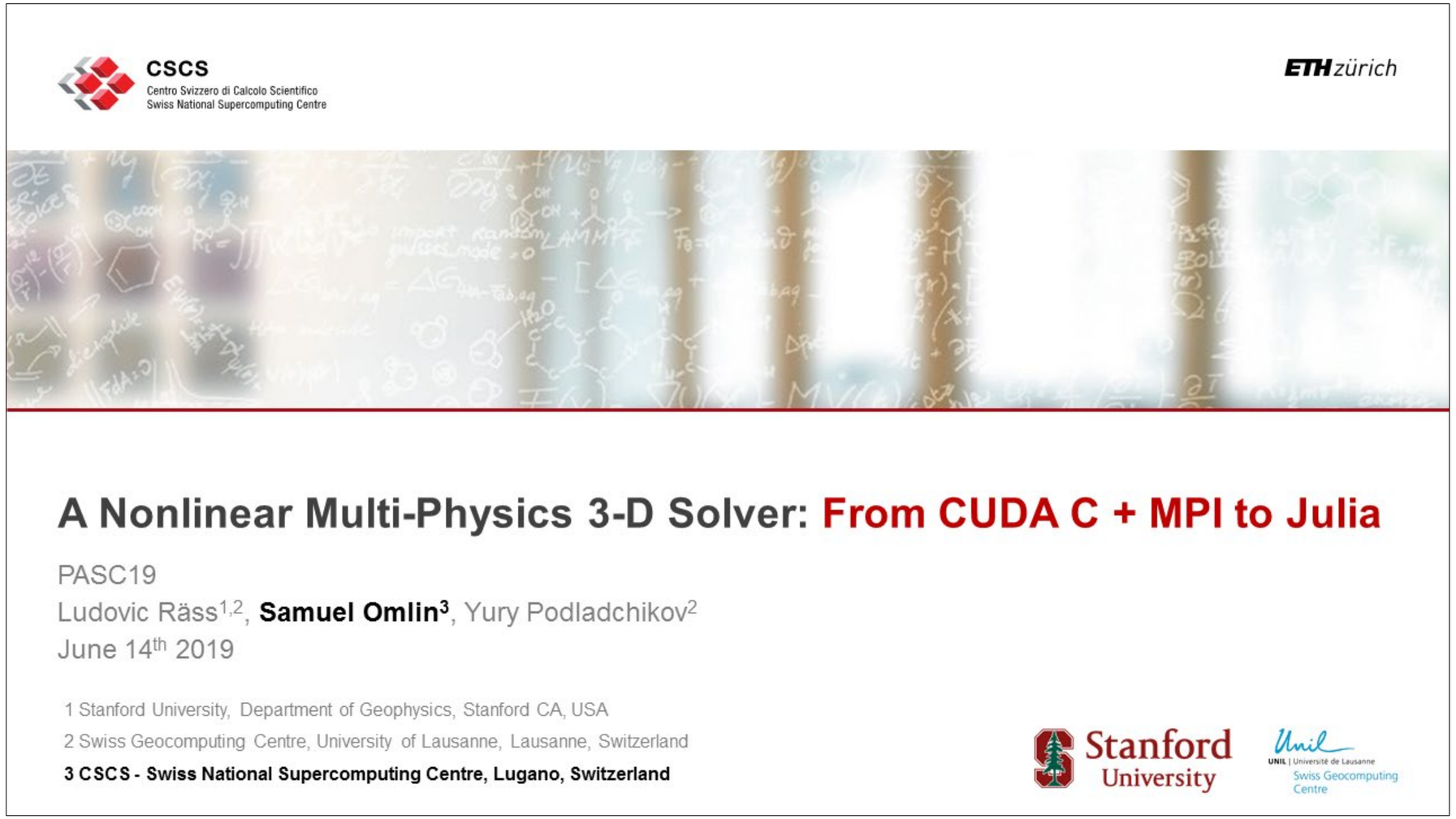
Solution

Too good to be true!

I least I got intrigued…

Let's see!

Case study



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A Nonlinear Multi-Physics 3-D Solver: From CUDA C + MPI to Julia

PASC19

Ludovic Räss[1,2], **Samuel Omlin[3]**, Yury Podladchikov[2]

June 14th 2019

1 Stanford University, Department of Geophysics, Stanford CA, USA
2 Swiss Geocomputing Centre, University of Lausanne, Lausanne, Switzerland
3 CSCS - Swiss National Supercomputing Centre, Lugano, Switzerland

Stanford University

UNIL | Université de Lausanne
Swiss Geocomputing Centre

Case study

Stanford University

PORTING A MASSIVELY PARALLEL MULTI-GPU APPLICATION TO JULIA: A 3-D NONLINEAR MULTI-PHYSICS FLOW SOLVER

Ludovic Räss[1,2], Samuel Omlin[3], Yury Podladchikov[2]

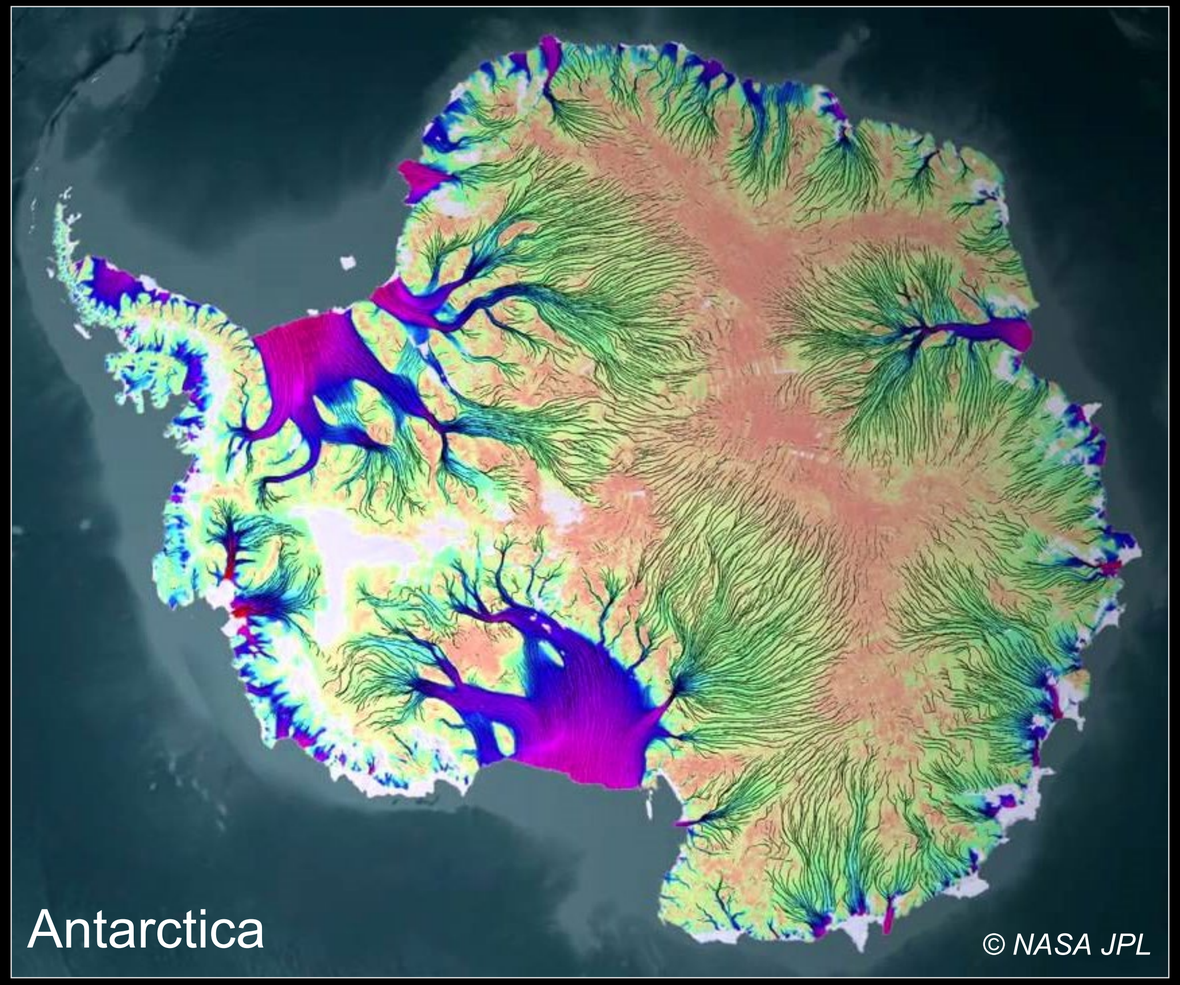
[1] Stanford University, Department of Geophysics, Stanford CA, USA
[2] Swiss Geocomputing Centre, University of Lausanne, Lausanne, Switzerland
[3] CSCS - Swiss National Supercomputing Centre, Lugano, Switzerland

23 July 2019 | JuliaCon 2019 | Baltimore MD

Agenda

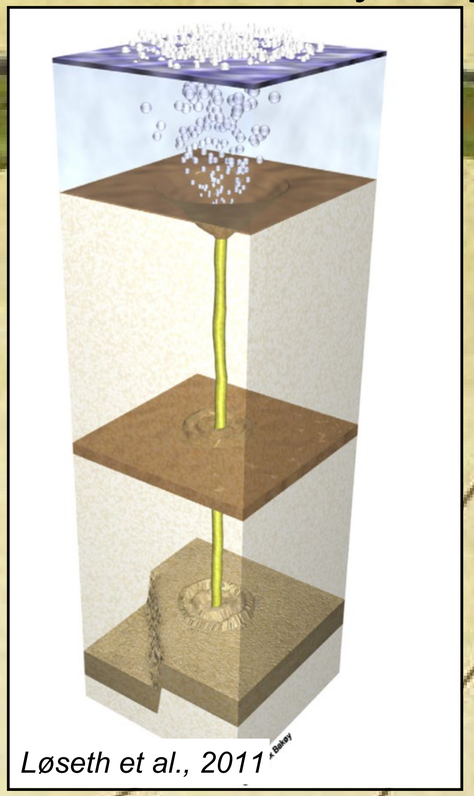
- The two language problem ✓
- Case study: the solver
- Porting to Julia | Multi-GPU Programming in Julia
- Case study: results
- Case study: conclusions
- General conclusions
- Outlook & recommendations

Multi-physics flow localisation

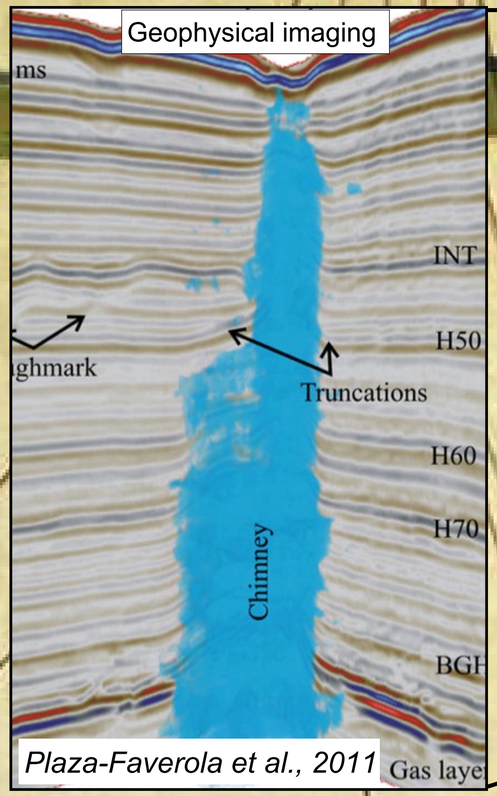


Subsurface reservoirs

Localised buoyancy-driven flow



Løseth et al., 2011



Plaza-Faverola et al., 2011

Extraction and storage

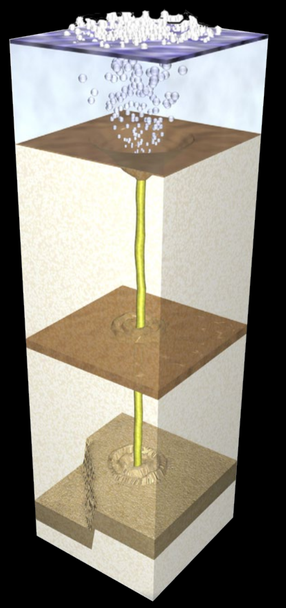
The multiphysics solver

…resolves complex meso-scale dynamics

- includes nonlinear multi-physics feedbacks
- captures *spontaneous* localisation in space + time
- handles highly localised action in large domains
- and is computationally very challenging:

Extremely high-resolution 3-D forward models are mandatory

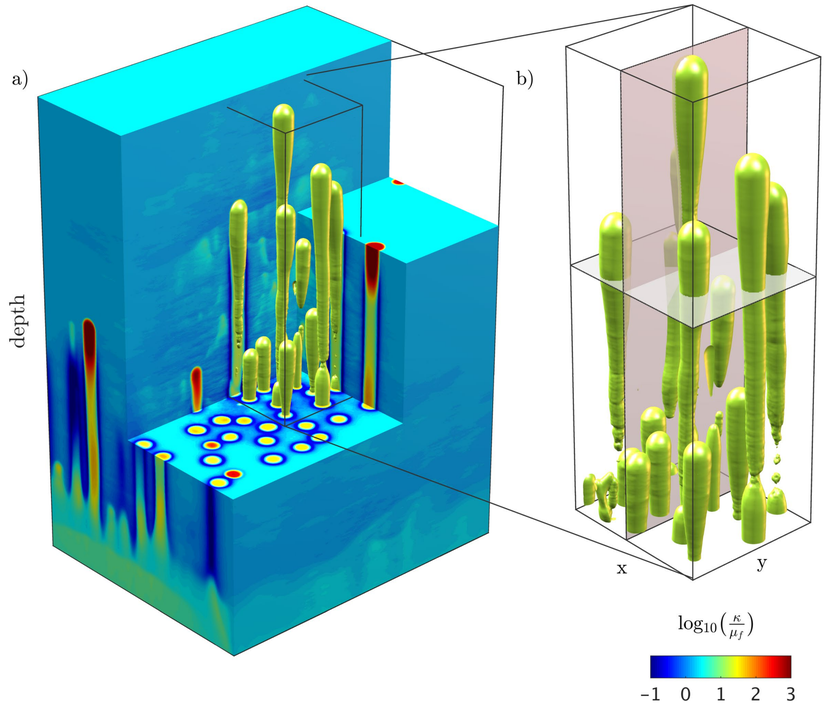
Requires a supercomputing approach



The movie making-of

Resolution:

- space: 1000 x 1000 x 2000 grid points in 3-D
- time: 20’000 implicit time steps



Räss et al., 2018. Nature Scientific Reports

Numerical method & code

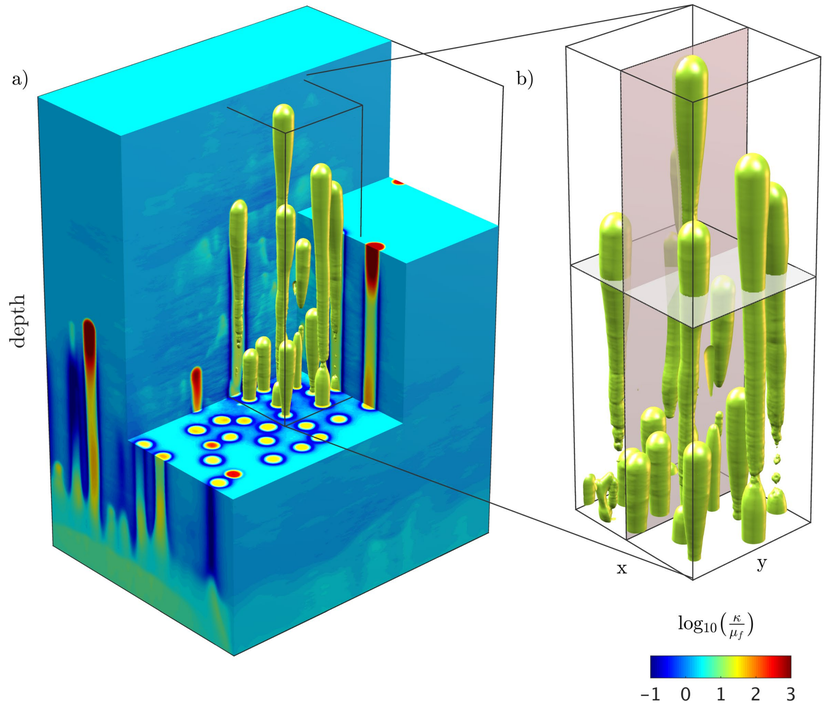
Numerical method:

- Finite-Difference stencils on Cartesian, staggered grid
- Iterative implicit time stepping: pseudo transient method

Code:

- CUDA C + MPI

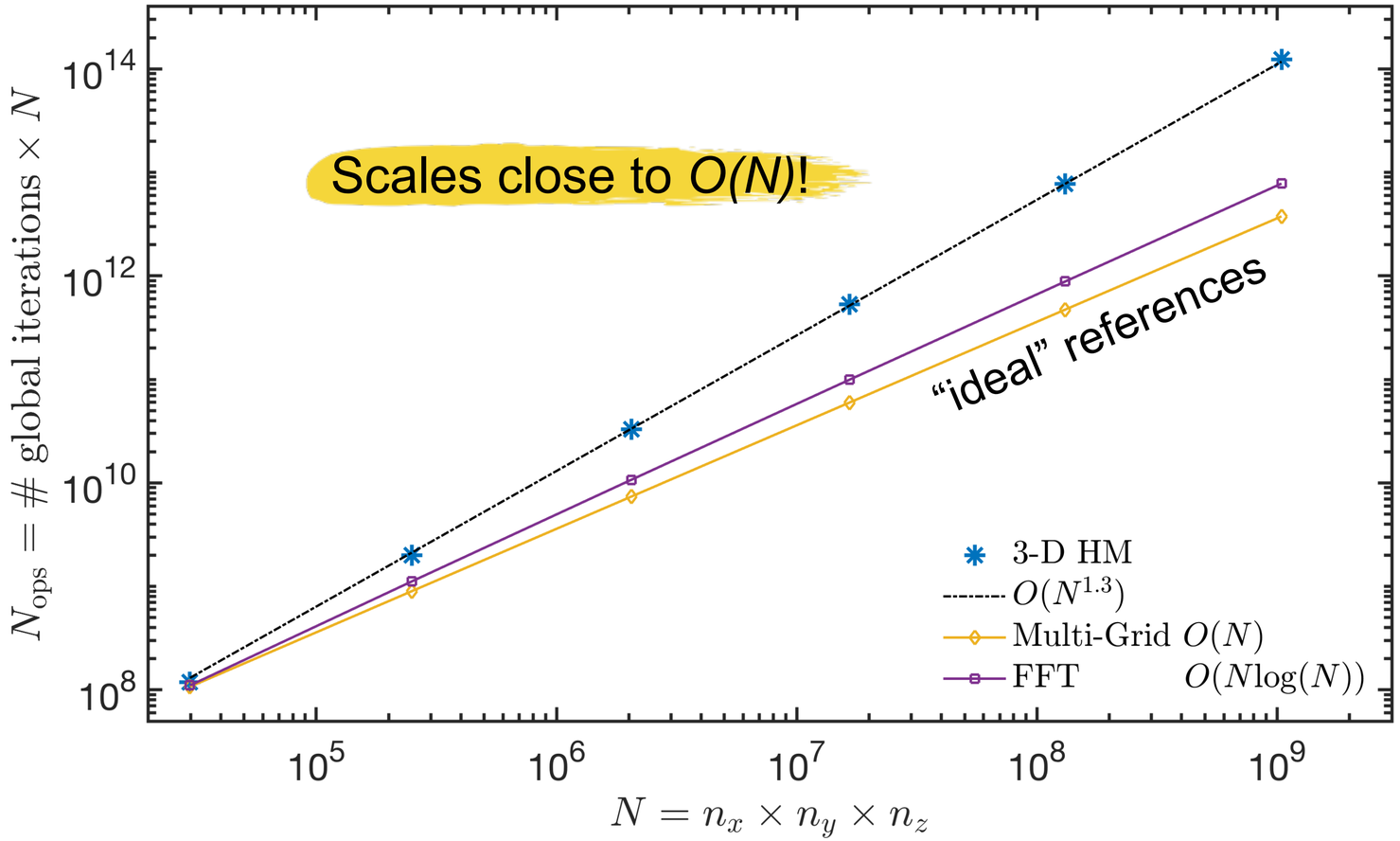
Runs close to hardware limit !



Räss et al., 2018. Nature Scientific Reports

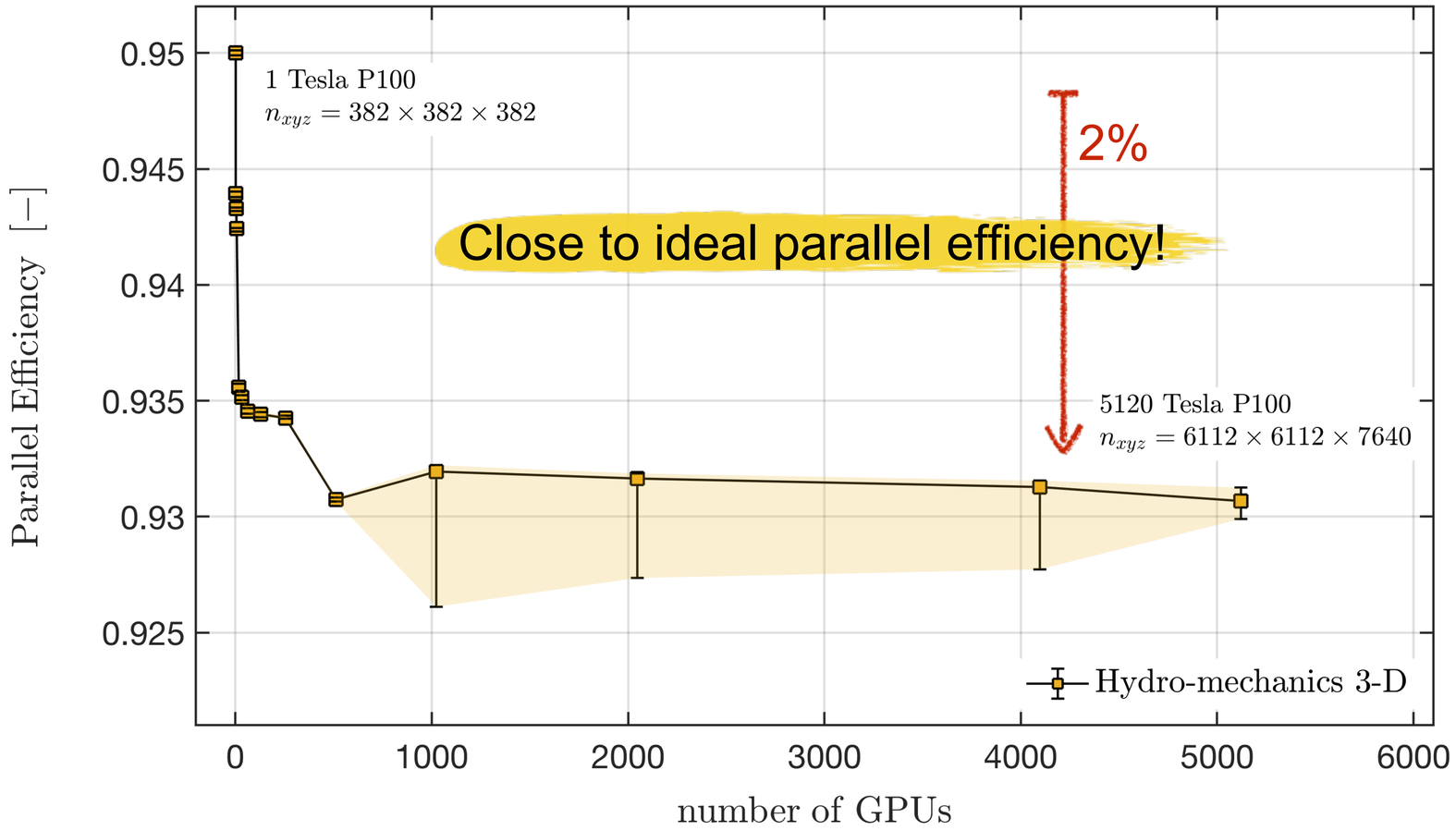
Pseudo-Transient solver

Scaling of our iterative GPU solver with numerical grid resolution N



Hide MPI communication

Weak scaling on Cray XC50 “Piz Daint” @ CSCS | 5120 Nvidia P100 GPUs



Agenda

- The two language problem ✓
- Case study: the solver ✓
- Porting to Julia | Multi-GPU Programming in Julia
- Case study: results
- Case study: conclusions
- General conclusions
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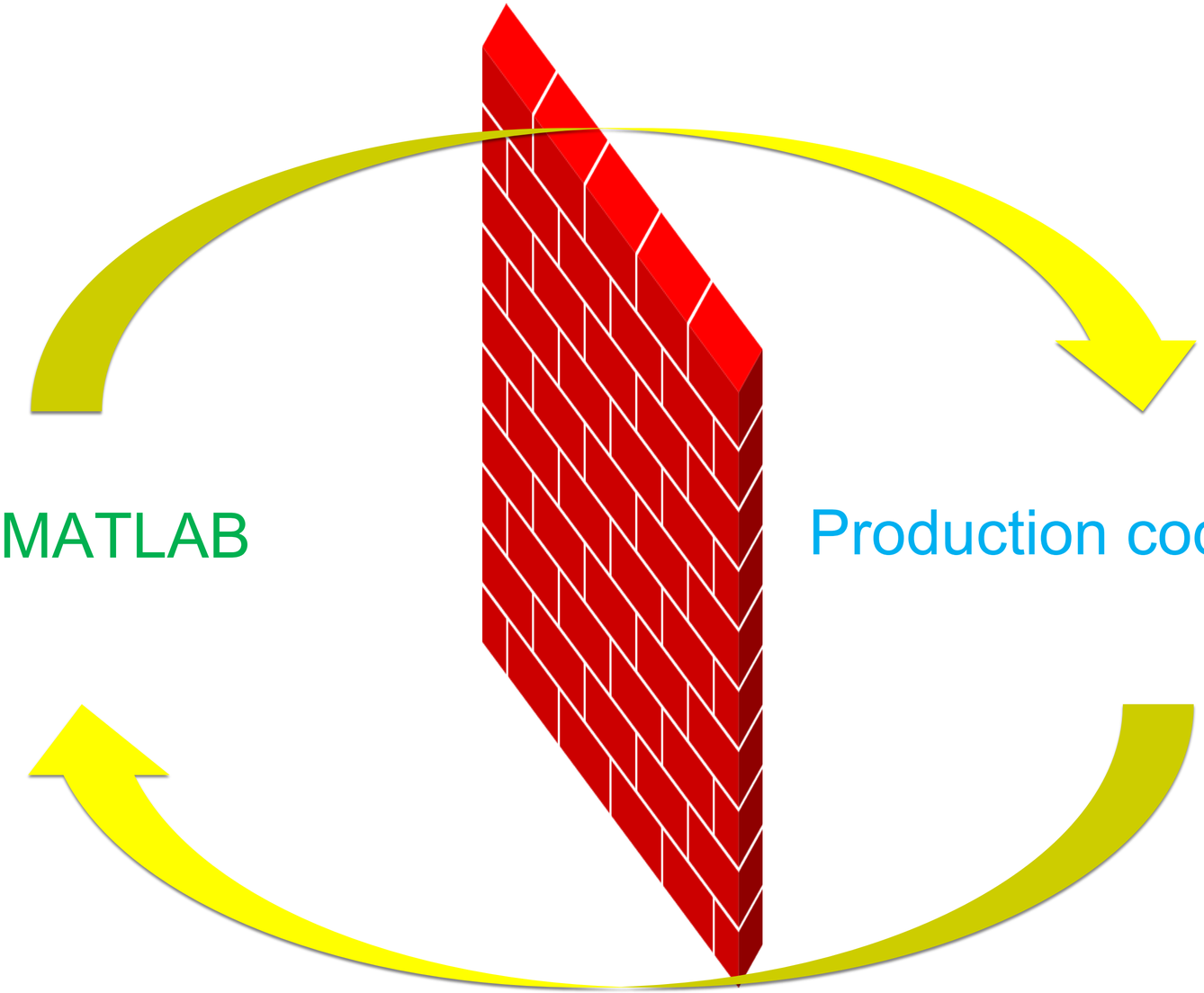
The two language problem for our solver

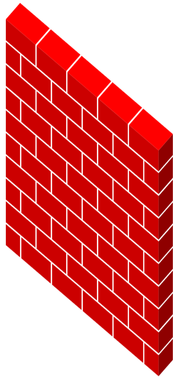


Protoype: MATLAB

Production code: CUDA C + MPI

Porting approach

Protoype: MATLAB



Production code: CUDA C + MPI

julia

Code structure

```
# physical and numerical parameters


# initializations of fields

# time loop

  # nonlinear iterations


     # convergence check


  # postprocessing & visualization
```

the julia code

Protoype
MATLAB

```
# physical and numerical parameters

# initializations of fields

# time loop

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```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
nx   = 128
# initializations of fields

# time loop

  # nonlinear iterations


    # convergence check


  # postprocessing & visualization
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
nx   = 128
# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop

  # nonlinear iterations


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  # postprocessing & visualization
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
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# time loop
for it = 1:nt
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    # convergence check


  # postprocessing & visualization

end
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

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  while (err > eps)
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     # convergence check

  end
  # postprocessing & visualization

end
```

Production
code
CUDA C
(+ MPI)

the julia code

CUDA kernel example (1-D heat diffusion)

```
function diffusion1D_kernel!(Te2, Te, Ci, lam, dt, dx)
        ix = (blockIdx().x-1) * blockDim().x + threadIdx().x # thread ID
        if ix>1 && ix<size(Te2,1)
            Te2[ix] = Te[ix] + dt*(Ci[ix]*(- (  (-lam*(Te[ix+1] - Te[ix  ])/dx)
                                              - (-lam*(Te[ix  ] - Te[ix-1])/dx)
                                             )/dx
                                       )
                                  )
        end

        return nothing
end
```

the julia code

Versus normal CPU function (1-D heat diffusion)

```
function diffusion1D_kernel!(Te2, Te, Ci, lam, dt, dx)
    for ix = 1:size(Te,1)
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                                              - (-lam*(Te[ix  ] - Te[ix-1])/dx)
                                             )/dx
                                   )
                                  )
        end
    end
    return nothing
end
```

the julia code

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                                   )
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the julia code

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                                             )/dx
                                   )
                              )
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Fourier's law of heat conduction:

$$\mathbf{q}_x = -\lambda \frac{\partial T}{\partial x}$$

the julia code

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                                              - (-lam*(Te[ix  ] - Te[ix-1])/dx)
                                            )/dx
                                   )
                                  )

        end

        return nothing
end
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Fourier's law of heat conduction:

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Conservation of energy: $\frac{\partial T}{\partial t} = \frac{1}{C_p}\left(-\frac{\partial q_x}{\partial x}\right)$

the julia code

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                                            )/dx
                                  )
                                  )
        end

        return nothing
end
```

Fourier's law of heat conduction:

$$\mathbf{q_x} = -\lambda \frac{\partial T}{\partial x}$$

Conservation of energy: $\frac{\partial T}{\partial t} = \frac{1}{C_p}\left(-\frac{\partial q_x}{\partial x}\right)$

Update of Temperature: $\mathbf{T_{t+1}} = \mathbf{T_t} + \mathbf{dt}\frac{dT_t}{dt}$

the julia code

CUDA kernel example (1-D heat diffusion)

```
function diffusion1D_kernel!(Te2, Te, Ci, lam, dt, dx)
        ix = (blockIdx().x-1) * blockDim().x + threadIdx().x # thread ID
        if ix>1 && ix<size(Te2,1)
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                                             )/dx
                                   )
                                  )
        end

        return nothing
end
```

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
nx   = 128
# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
for it = 1:nt
  # nonlinear iterations
  while (err > eps)
     @cuda … compute_phi_etc(…)
     # convergence check

  end
  # postprocessing & visualization

end
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
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# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
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  while (err > eps)
     @cuda … compute_phi_etc(…)
     # convergence check
     if mod(iter,10)==0 err = …; end
  end
  # postprocessing & visualization

end
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
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# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
for it = 1:nt
  # nonlinear iterations
  while (err > eps)
     @cuda … compute_phi_etc(…)
     # convergence check
     if mod(iter,10)==0 err = …; end
  end
  # postprocessing & visualization
  heatmap(phi[:,ny/2,:])
end
```

Production
code
CUDA C
(+ MPI)

the julia code

Protoype
MATLAB

```
# physical and numerical parameters
phi0 = 1e-2
nx   = 128
# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
for it = 1:nt
  # nonlinear iterations
  # postprocessing & visualization
  phi_change .= phi .- phi_init
end
```

Computed automatically on the GPU!
(assuming that phi_change and phi_init were allocated with cuzeros() / cuones())

Production
code
CUDA C
(+ MPI)

Multi-GPU – implicit domain decomposition

We created a small Julia module for Cartesian **staggered** grids:

GG: implicit **G**lobal **G**rid

Multi-GPU – implicit domain decomposition

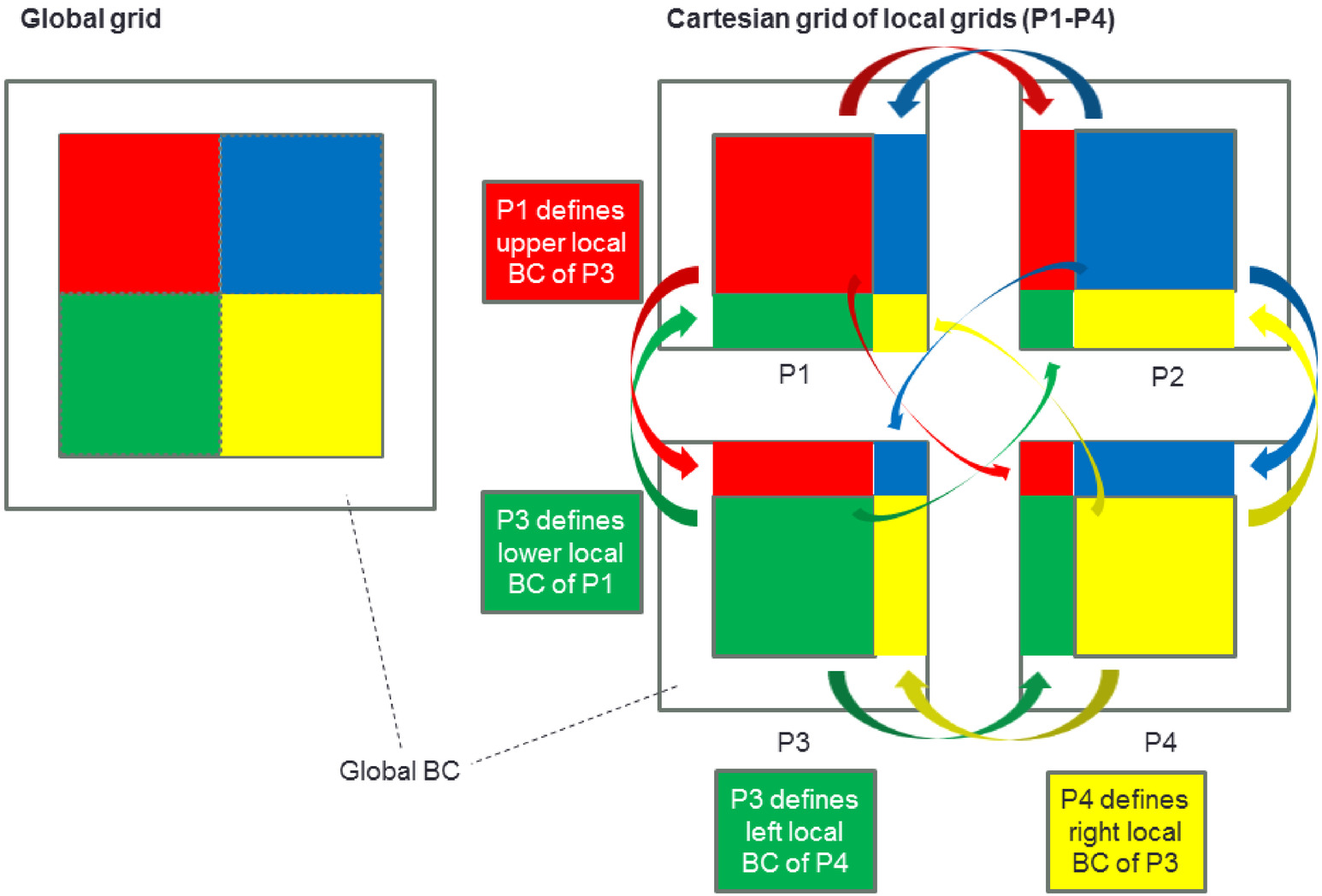
We created a small Julia module for Cartesian **staggered** grids:

GG: implicit **G**lobal **G**rid

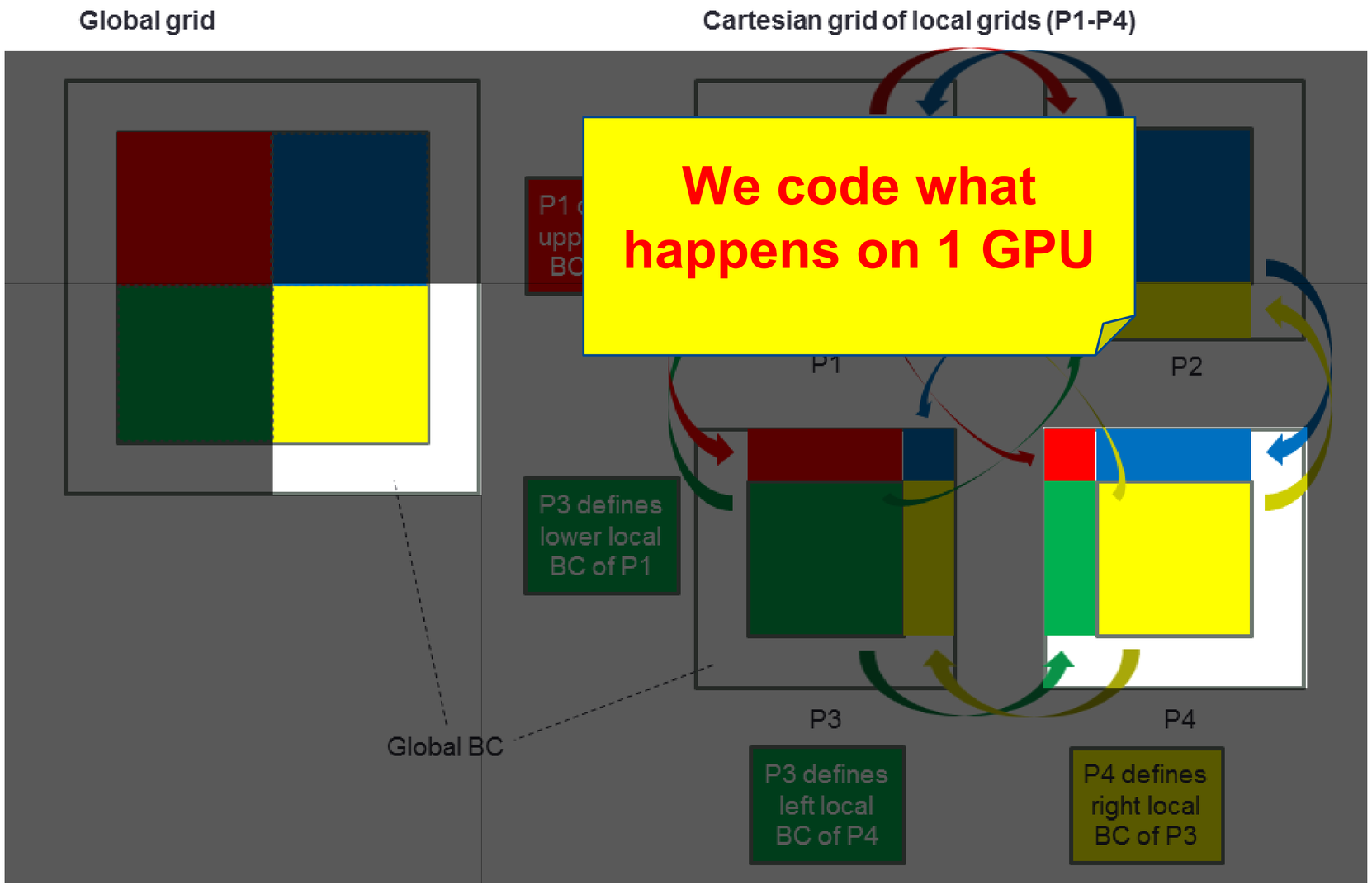
Uses MPI[1]!

[1] https://github.com/JuliaParallel/MPI.jl

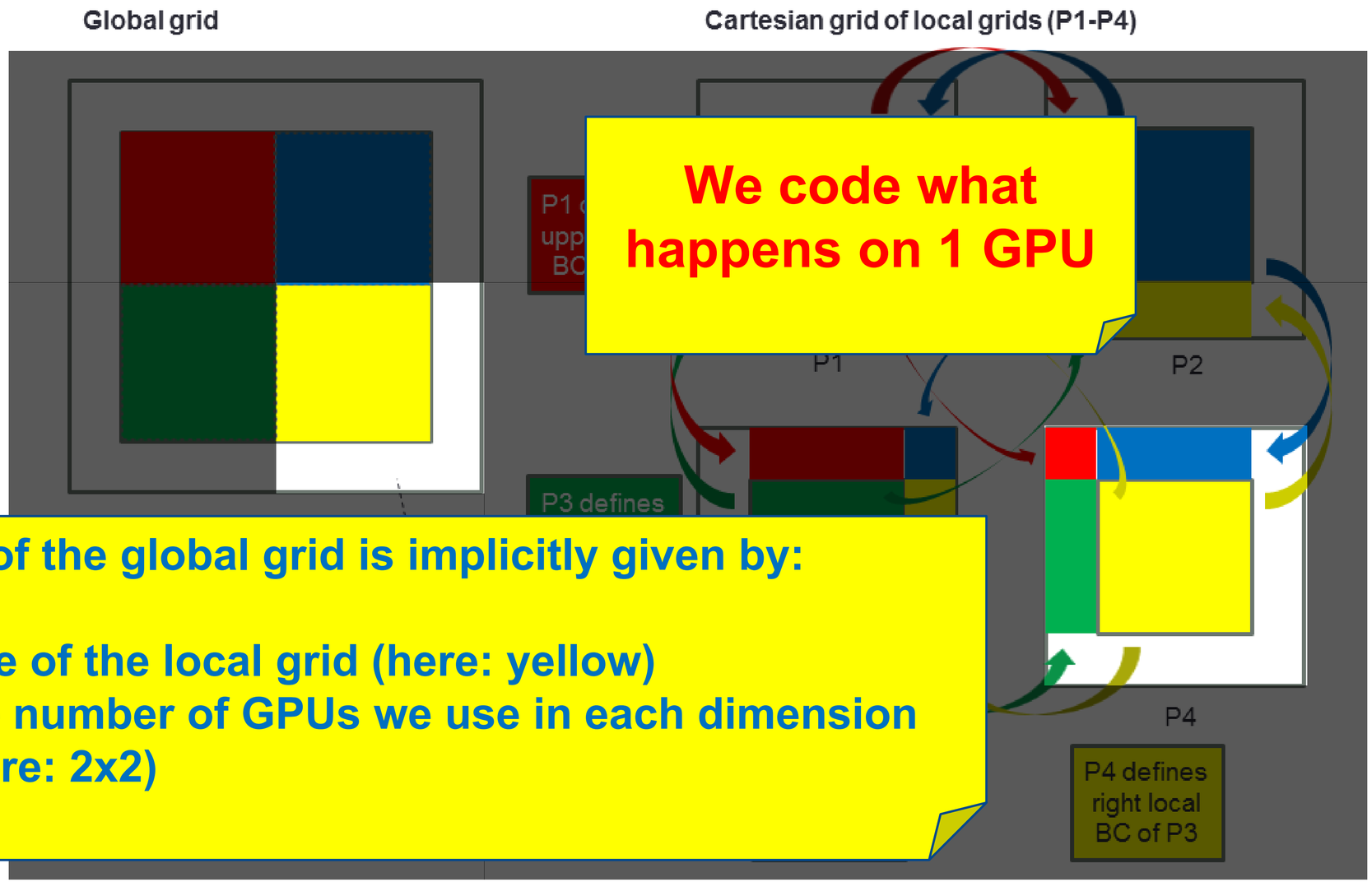
Multi-GPU – implicit domain decomposition?



Multi-GPU – implicit domain decomposition?



Multi-GPU – implicit domain decomposition?



Size of the global grid is implicitly given by:

- size of the local grid (here: yellow)
- the number of GPUs we use in each dimension (here: 2x2)

GG: implicit Global Grid

Multi-GPU parallelization with only 3 “buttons”!

- init_global_grid()
- update_halo!()
- finalize_global_grid()

GG: implicit Global Grid

Multi-GPU parallelization with only 3 “buttons”!

- init_global_grid()
- update_halo!()
- finalize_global_grid()

…and functions providing **global coordinates (x_g(), y_g(), z_g())**…

GG: implicit **G**lobal **G**rid

Multi-GPU parallelization with only 3 “buttons”!

- init_global_grid()
- update_halo!()
- finalize_global_grid()

Keeps the logic for Multi-GPU parallelization separate from your numerical algorithm!
=
No “IT noise” in your numerical algorithm!

…and functions providing **global coordinates (x_g(), y_g(), z_g())**…

the julia code

Protoype
MATLAB

```
init_global_grid(nx,ny,nz)
# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
for it = 1:nt
  # nonlinear iterations
  while (err > eps)
     @cuda … compute_phi_etc(…)
     update_halo(phi,Vx,Vy,Vz,…)
  # convergence check
     if mod(iter,10)==0 err = …; end
  end
  # postprocessing & visualization
  …
end
finalize_global_grid()
```

Production
code
CUDA C
(+ **MPI**)

the julia code

Protoype
MATLAB

```
init_global_grid(nx,ny,nz)
# initializations of fields
phi = phi0*cuones(nx,ny,nz)
# time loop
for it = 1:nt
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  while (err > eps)
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     update_halo(phi,Vx,Vy,Vz,…)
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     if mod(iter,10)==0 err = …; end
  end
  # postprocessing & visualization
  …
end
finalize_global_grid()
```

+ some initializations using x_g(), y_g(), z_g()

Production
code
CUDA C
(+ **MPI**)

A single code for single-thread CPU to Multi-GPU?

Would be fantastic for development and debugging…

…and decrease development and maintenance costs.

Solution (part 1)

```
USE_GPU = true

@static if USE_GPU
    using CuArrays, CUDAnative, CUDAdrv [1]
    myzeros(dims...) = cuzeros(dims...)
    myones(dims...)  = cuones(dims...);
else
    myzeros(dims...) = zeros(dims...)
    myones(dims...)  = ones(dims...)
end

macro kernel(cublocks, cuthreads, kernel)
    @static if USE_GPU
       esc(:( @cuda blocks=$cublocks threads=$cuthreads $kernel ))
    else
        esc(:( $kernel ))
    end
end
```

@static: evaluated at parse time – no if statement in the final code!

[1] https://github.com/JuliaGPU/

the julia code

Protoype
MATLAB

```
init_global_grid(nx,ny,nz)
# initializations of fields
phi = phi0*myones(nx,ny,nz)
# time loop
for it = 1:nt
  # nonlinear iterations
  while (err > eps)
     @kernel … compute_phi_etc(…)
     update_halo(phi,Vx,Vy,Vz,…)
  # convergence check
     if mod(iter,10)==0 err = …; end
  end
  # postprocessing & visualization
  …
end
finalize_global_grid()
```

Production
code
CUDA C
(+ MPI)

Solution (part 2)

```
macro threadids_or_loop(sizemax, block)
    @static if USE_GPU
       esc(quote
             ix = (blockIdx().x-1) * blockDim().x + threadIdx().x
             iy = (blockIdx().y-1) * blockDim().y + threadIdx().y
             iz = (blockIdx().z-1) * blockDim().z + threadIdx().z
             $block
       end)
    else
       esc(quote
             for iz=1:$sizemax[3]
                for iy=1:$sizemax[2], ix=1:$sizemax[1]
                   $block
                end
             end
       end)
    end
end
```

Solution (part 2)

```
macro threadids_or_loop(sizemax, block)
    @static if USE_GPU
       esc(quote
             ix = (blockIdx().x-1) * blockDim().x + threadIdx().x
             iy = (blockIdx().y-1) * blockDim().y + threadIdx().y
             iz = (blockIdx().z-1) * blockDim().z + threadIdx().z
             $block
       end)
    else
       esc(quote
             @threads for iz=1:$sizemax[3]
                for iy=1:$sizemax[2], ix=1:$sizemax[1]
                   $block
                end
             end
       end)
    end
end
```

@threads: activates multithreading if JULIA_NUM_THREADS > 1

the julia code

CUDA kernel example (1-D heat diffusion)

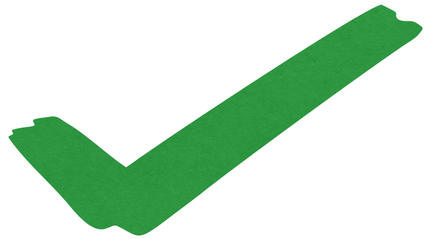
```
function diffusion1D_kernel!(Te2, Te, Ci, lam, dt, dx)
        ix = (blockIdx().x-1) * blockDim().x + threadIdx().x # thread ID
        if ix>1 && ix<size(Te2,1)
            Te2[ix] = Te[ix] + dt*(Ci[ix]*(- (  (-lam*(Te[ix+1] - Te[ix  ])/dx)
                                              - (-lam*(Te[ix  ] - Te[ix-1])/dx)
                                             )/dx
                                   )
                                  )
        end

        return nothing
end
```

the julia code

CUDA kernel example (1-D heat diffusion)

```
function diffusion1D_kernel!(Te2, Te, Ci, lam, dt, dx)
   @threadids_or_loop size(Te2) begin  # (asuming 1D version of macro)
        if ix>1 && ix<size(Te2,1)
            Te2[ix] = Te[ix] + dt*(Ci[ix]*(- (  (-lam*(Te[ix+1] - Te[ix  ])/dx)
                                              - (-lam*(Te[ix  ] - Te[ix-1])/dx)
                                             )/dx
                                   )
                                )
        end
    end
    return nothing
end
```

A single code for single-thread CPU to Multi-GPU?



GPU: USE_GPU = **true | false**

CPU threads: export JULIA_NUM_THREADS = **12**

MPI: srun -n **5120** … julia … PoroVP3D.jl

Simple in-situ visualization?

Wouldn’t it be great to see the results while computing on multiple GPUs?

the julia code

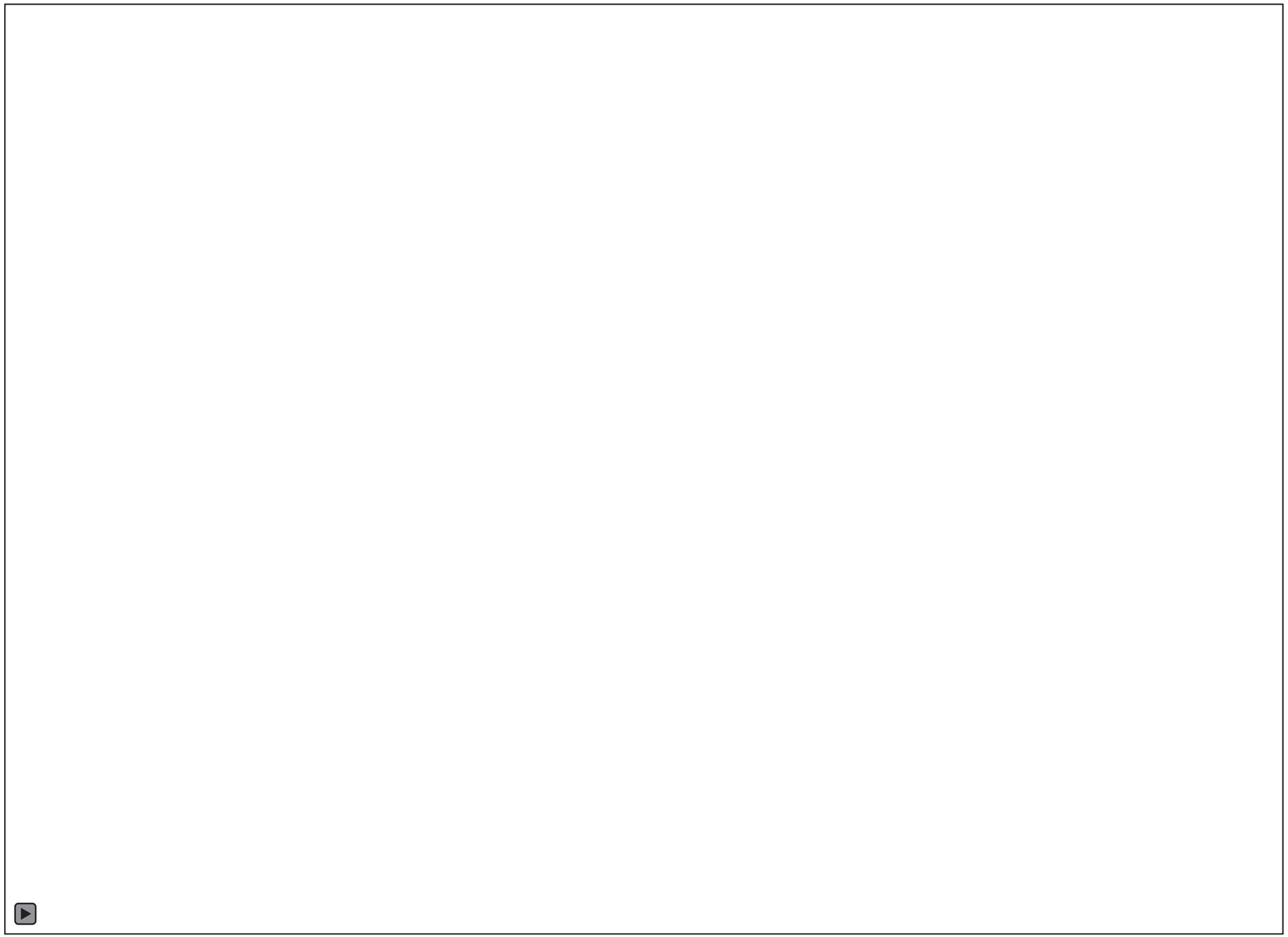
Protoype
MATLAB

```
init_global_grid(nx,ny,nz)
# initializations of fields
phi = phi0*myones(nx,ny,nz)
# time loop
for it = 1:nt
  # postprocessing & visualization
  gather!(phi, phi_v)
  if me==0 heatmap(phi_v[:,ny/2,:]) end
end
finalize_global_grid()
```

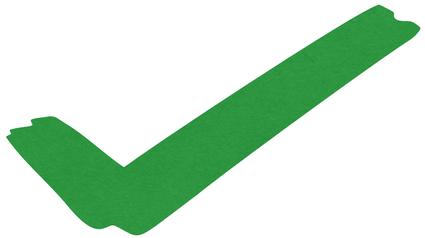
Gather (reduced size) data on MPI rank 0 and visualize it!

Production
code
CUDA C
(+ MPI)

Simple in-situ visualization?



Simple in-situ visualization?



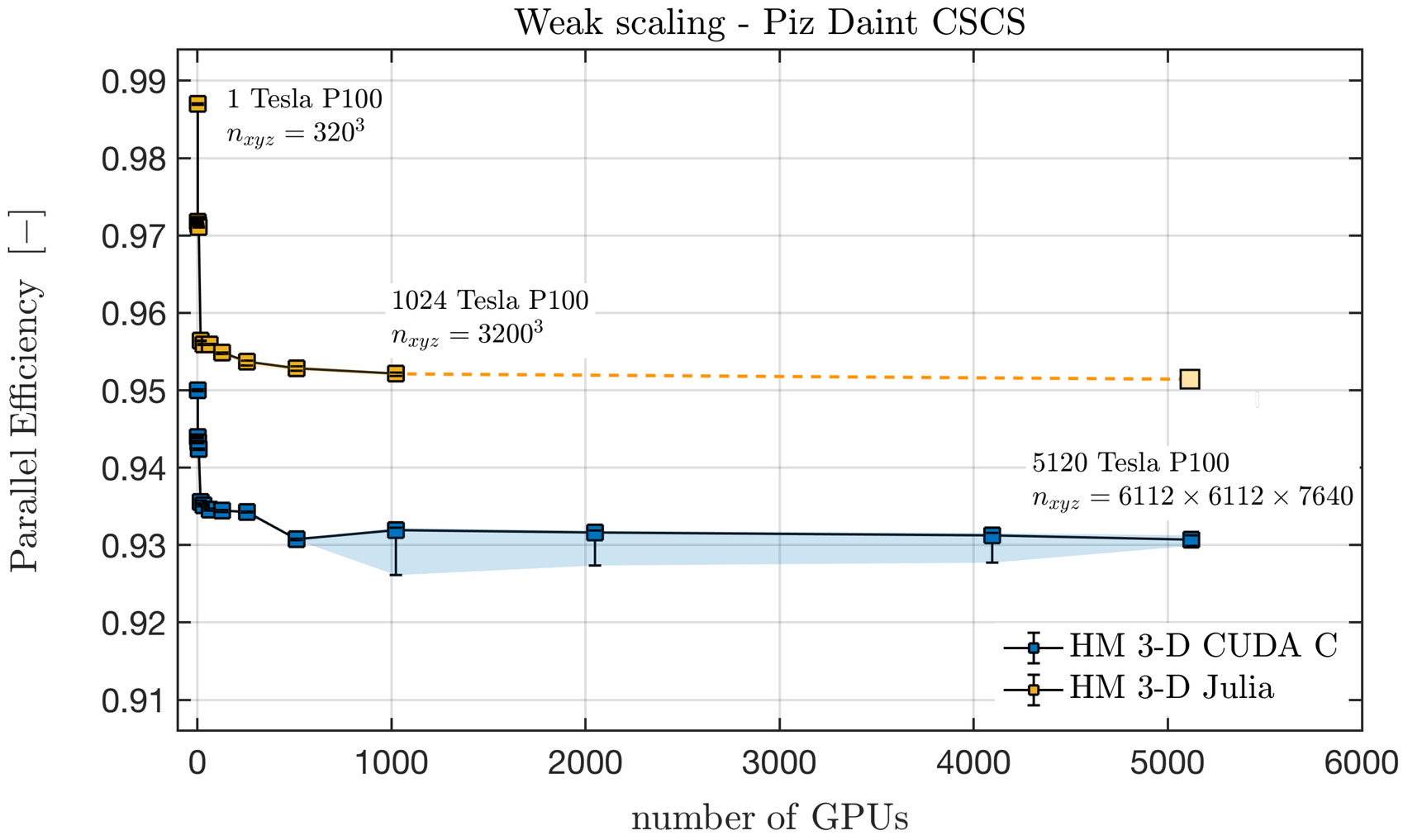
Agenda

- The two language problem ✓
- Case study: the solver ✓
- Porting to Julia | Multi-GPU Programming in Julia ✓
- Case study: results
- Case study: conclusions
- General conclusions
- Outlook & recommendations

Results

Single GPU performance:

93% of the the CUDA C code



Results

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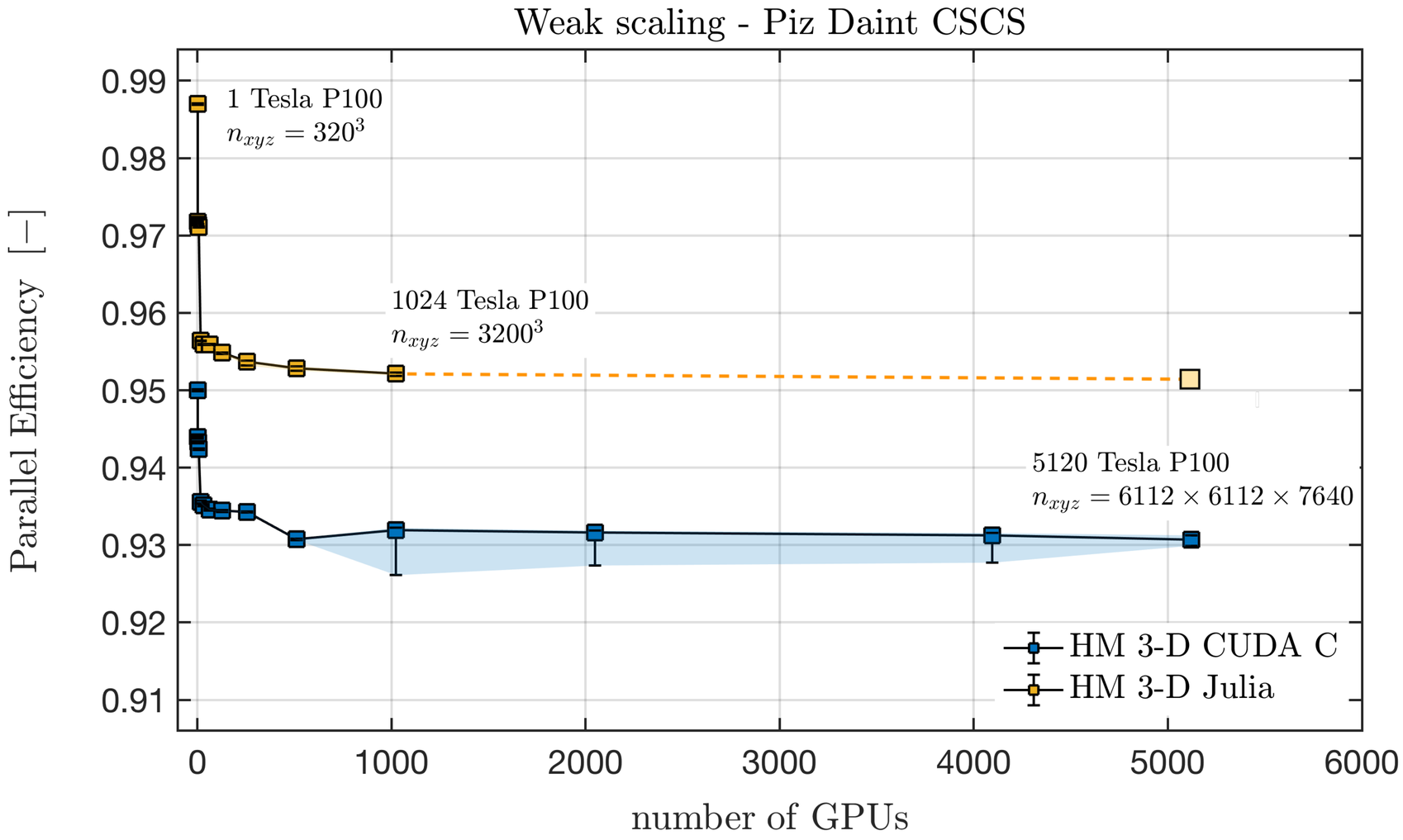
93% of the the CUDA C code

Difference to be analysed



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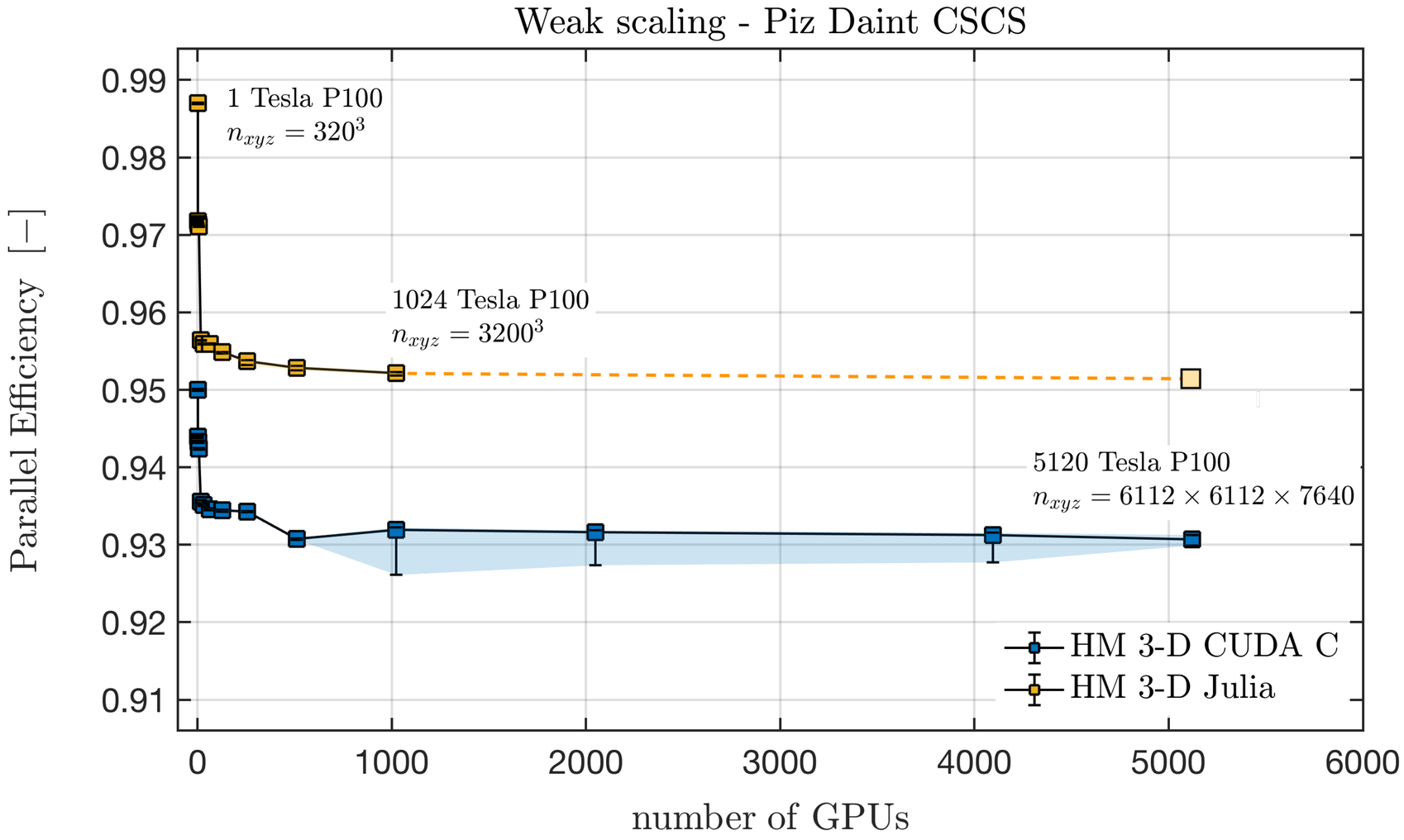

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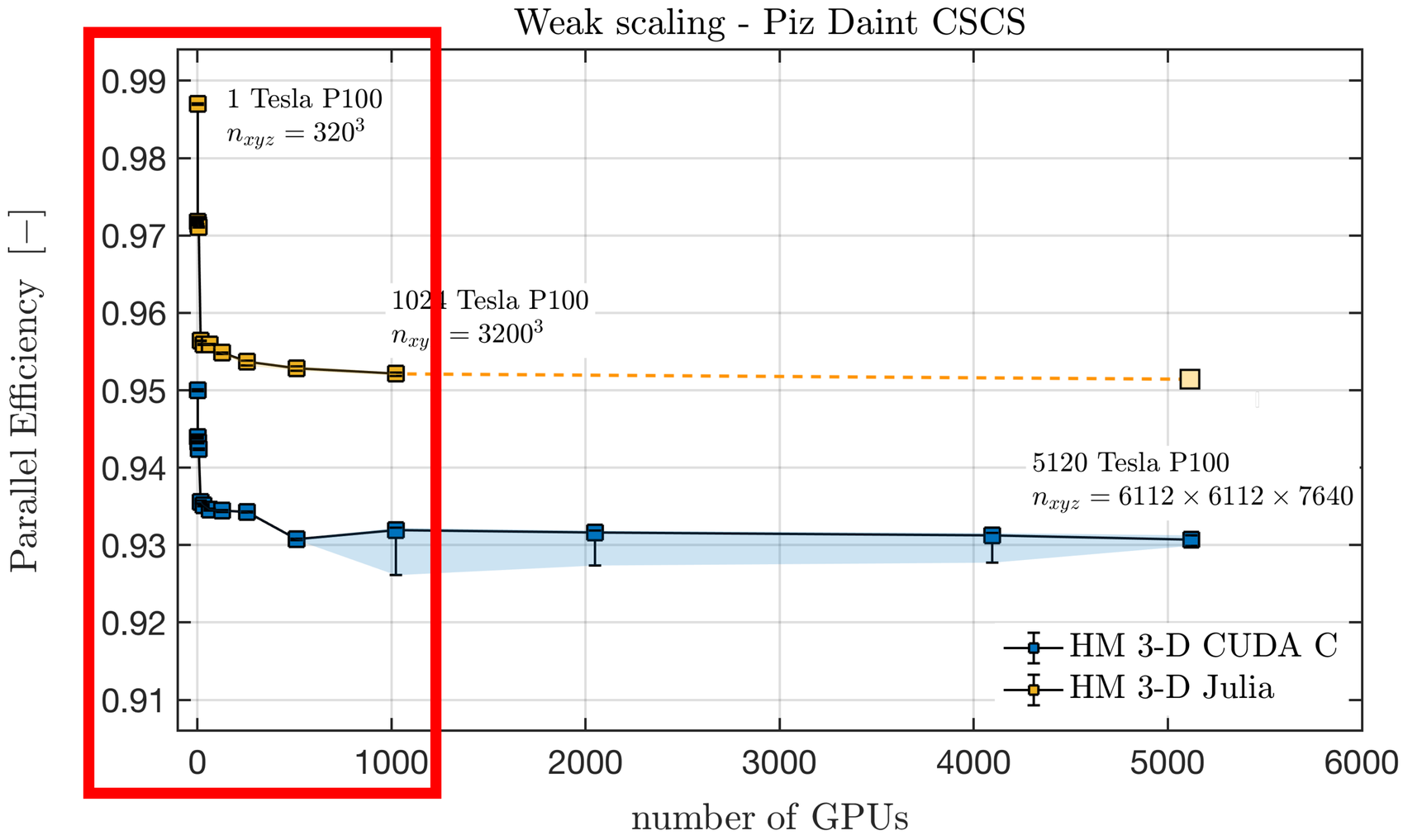

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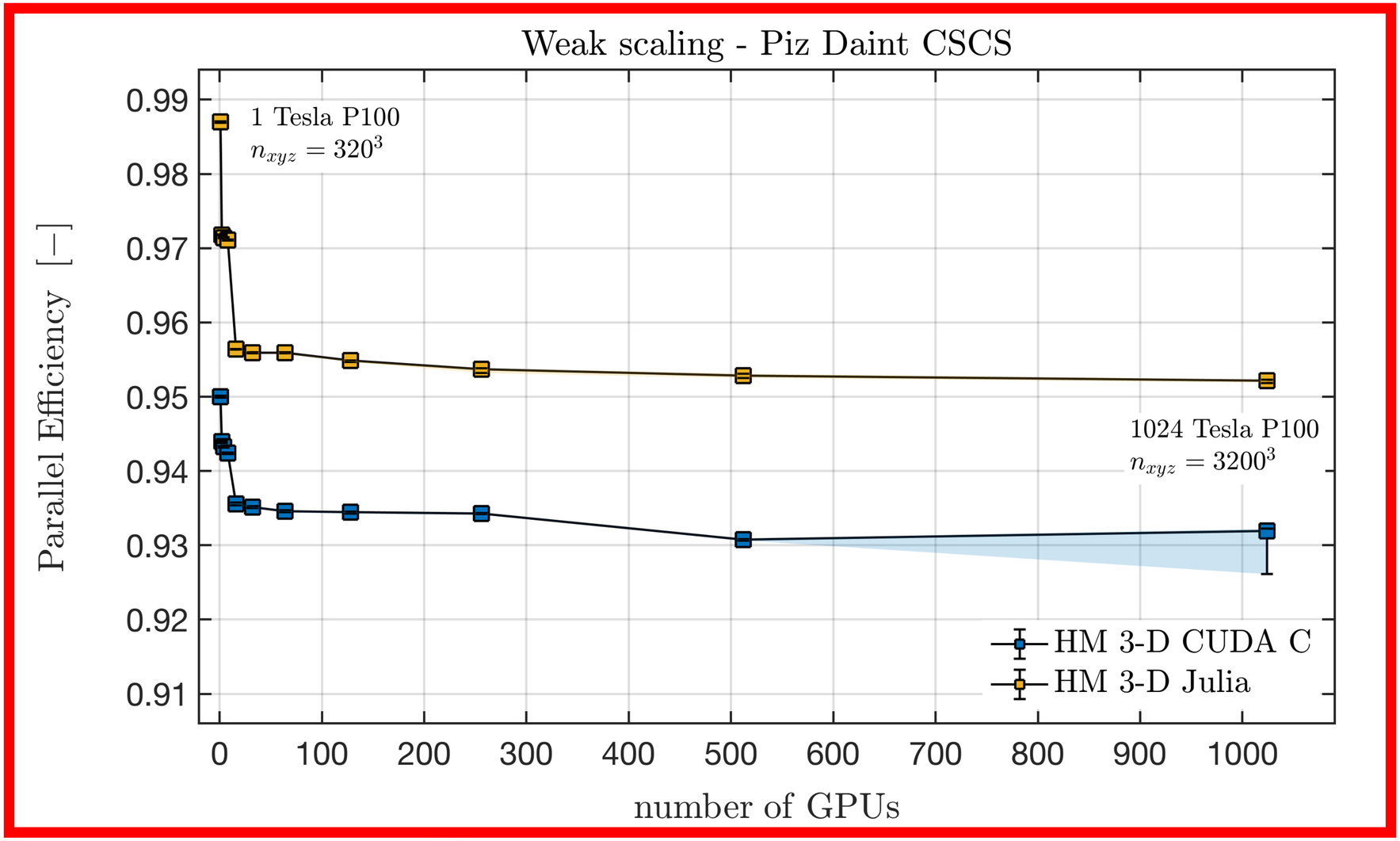

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Kernels can be written also very nice with macros/functions - not shown here…

Case study: conclusions

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GG is reusable for other staggered grid applications!

So easy…
it can be used for teaching Earth Science Bachelors!

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- Performance is nearly as good as with CUDA C after straightforward port to Julia (93%)!

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- A single code for all: from single-thread CPU to Multi-GPU!
- Super simple in-situ visualization!
- Performance is nearly as good as with CUDA C after straightforward port to Julia (90%)!
- >95% parallel efficiency was shown on up to 1024 GPUs.

Case study: conclusions

We solved our two language problem!

Agenda

- The two language problem ✓
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General conclusions

With Julia we can:

- write nice and high-level Multi-GPU code.
- write explicit CUDA kernels to get optimal performance in performance critical parts.
- use MPI efficiently without adding a lot of “IT noise” with an approach as taken with the GG module.
- write a single code for all: from single-thread CPU to Multi-GPU.
- do super simple in-situ visualization.
- get similar performance as with CUDA C.
- scale nearly ideally on the fastest Supercomputers in the world.

General conclusions

With Julia we can solve the two language problem!

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- The two language problem ✓
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Today's news: Julia in production on Piz Daint

Julia modules:

```
$> module load daint-gpu (or daint-mc)
$> module load Julia                          <- includes MPI + CUDA packages
$> module load JuliaExtensions                <- Plots, PyCall & HDF5 packages
                                                 (more to come)
```

Available packages:

```
julia> versioninfo()
```

Note on the Julia package manager manager:

`julia> Pkg.status()` **shows only the packages installed by the user by default, but you can load the above packages normally, e.g.:**

```
julia> using MPI
```

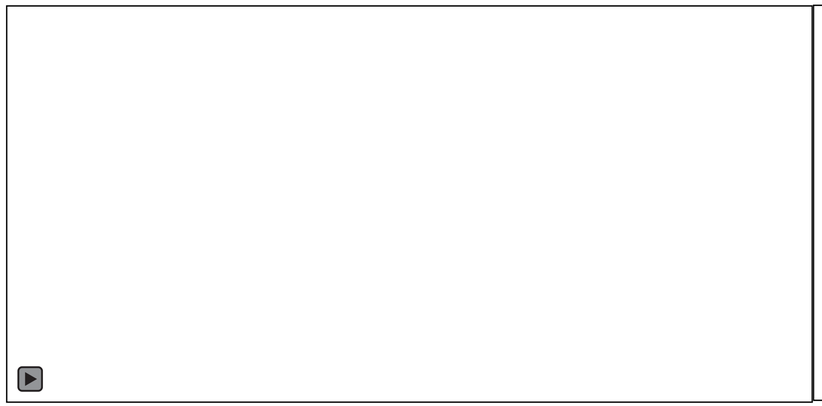
Start an interactive Julia session with GPU:

```
$> srun -C gpu --time=04:00:00 --pty bash
$> julia
```

Solving other PDEs in Julia leveraging a GPU supercomputer

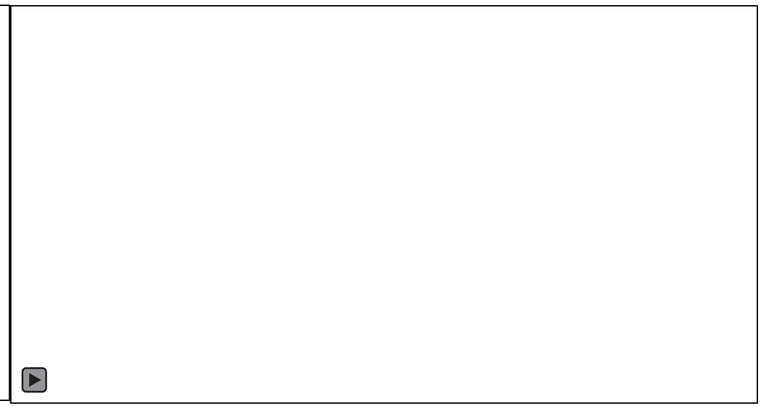
Other multi-GPU PDE solvers created with the presented numerical methods (during PhD):

Shallow water (20 462 x 10 354)

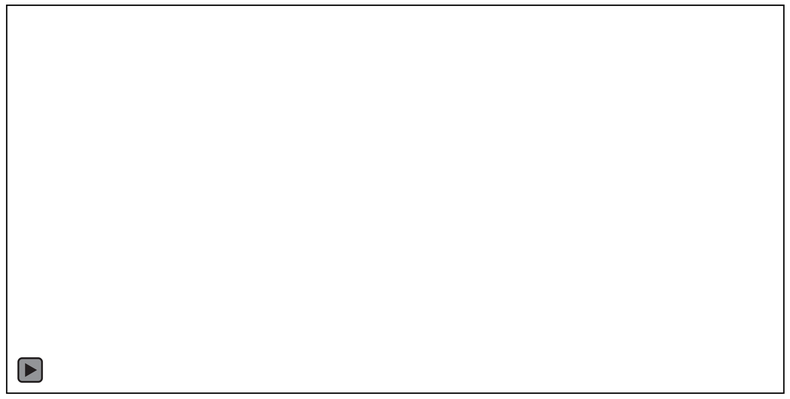


Shear heating (16 378 x 16 378)

Reactive porosity waves (506 x 506 x 2042)



Glacier Flow (20 462 x 10 354)



Cover all types of PDEs! (elliptic, hyperbolic, and parabolic)

Simulations used 80 GPUs

Thermal convection (32 762 x 16 378)

Solving other problems in Julia leveraging a GPU supercomputer

- **General advice:** for best intra and inter-GPU parallelization and scalability, **use local algorithms** (doing most the computations with data stored close in memory; e.g. stencil algorithms)!

Thank you!

Thank you!

You have a Julia project or a project Idea?
Talk to me or write me an E-Mail!
(Samuel.Omlin@cscs.ch)

References

Räss, L., Omlin, S., & Podladchikov, Y. Y. (2019). A Nonlinear Multi-Physics 3-D Solver: From CUDA C + MPI to Julia. PASC19 Conference, Zurich, Switzerland.

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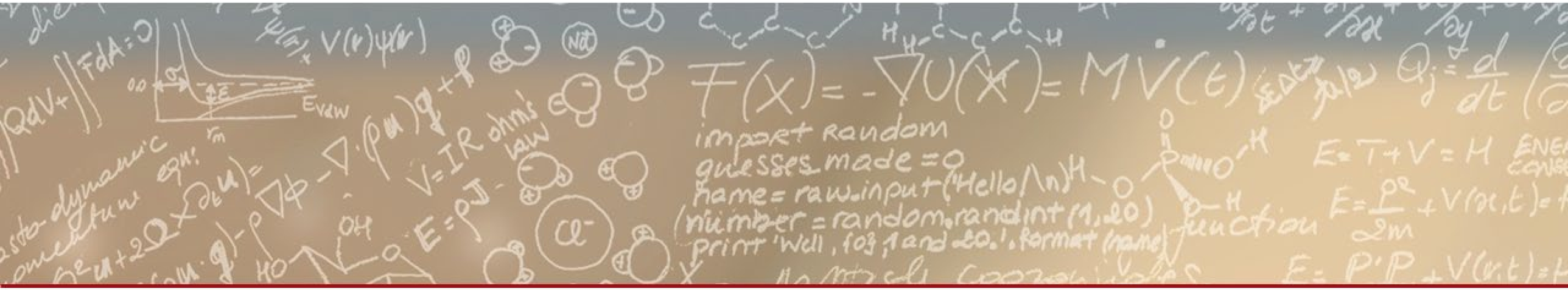

Thank you for your kind attention