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Basics of Pencil Code & some philosophy

(Pencil Code School, Geneva/CERN, 20th of September 2025)

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Overview:

* Magneto-Hydrodynamics (MHD)
* Requirements for PC
* Philosophy of the PC
* Getting and Installing PC
* OpenMP and MPI
* Choosing a sample
* Selecting modules and processor layout
* Compiling PC
* Efficient computing strategies
* Changing parameters
* Setting up initial condition (“start”)
* Propagate an existing state (“run”)
* Boundary conditions

Introduction to MHD

Basic equations:

$$c\vec{\nabla}\times\vec{B}=4\pi\vec{j} \qquad c\vec{\nabla}\times\vec{E}=-\frac{\partial\vec{B}}{\partial t} \qquad \vec{\nabla}\cdot\vec{B}=0$$ (Maxwell's equations)

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Basic MHD assumptions:

* $v\ll c$: non-relativistic, quasi-stationary state change, no EM waves
* $\sigma\gg 1$: high conductivity, quasi-neutral plasma, E determined by $\partial B/\partial t$

What follows from MHD assumptions?:

$$c\nabla\times E=-\frac{\partial B}{\partial t}\ \Rightarrow\ c\frac{E}{L}\approx\frac{B}{T}\Rightarrow\frac{E}{B}=\frac{1}{c}\frac{L}{T}\approx\frac{v}{c}\ll 1$$ (*E* less important than B)

$$\frac{\partial E/\partial t}{c\nabla\times B}\approx\frac{E/T}{cB/L}\approx\frac{E\,v}{B\,c}\approx\frac{v^2}{c^2}\ll 1$$ (no displacement current)

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linearized equations => wave propagation, stability

Induction Equation

Example – evolution of ***B*** under influence of given ***v*:**

$$\frac{\partial \vec{B}}{\partial t} = c\vec{\nabla}\times\vec{E} = -c\vec{\nabla}\times\left(\lambda\vec{j} - \frac{1}{c}\vec{v}\times\vec{B}\right) = -c\vec{\nabla}\times\left(\frac{\lambda c}{4\pi}\vec{\nabla}\times\vec{B} - \frac{1}{c}\vec{v}\times\vec{B}\right)$$

$$\Rightarrow \frac{\partial \vec{B}}{\partial t} = \vec{\nabla}\times\left(\vec{v}\times\vec{B}\right) - \vec{\nabla}\times\left(\frac{\lambda c^2}{4\pi}\vec{\nabla}\times\vec{B}\right) = \vec{\nabla}\times\left(\vec{v}\times\vec{B}\right) - \eta\vec{\nabla}\times\vec{\nabla}\times\vec{B}$$

with $\eta = \frac{\lambda c^2}{4\pi} = \frac{1}{\mu_0 \sigma} = \text{const}.$ (magnetic diffusivity)

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$$\Rightarrow \frac{\partial \vec{B}}{\partial t} = \vec{v}\left(\vec{\nabla}\cdot\vec{B}\right) - \vec{B}\left(\vec{\nabla}\cdot\vec{v}\right) + \left(\vec{B}\cdot\vec{\nabla}\right)\vec{v} - \left(\vec{v}\cdot\vec{\nabla}\right)\vec{B} - \eta\,\vec{\nabla}\times\vec{\nabla}\times\vec{B}$$

induction = 0 – expansion/contraction + shear/stretching – advection – diffusion

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* energy balance, if there is viscosity – or for compressible fluids...
  (see also Navier-Stokes equations for viscous media)

Requirements

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Technical requirements:

* Laptop
* Windows or MAC users: VirtualBox or VMware (or dual boot)
* ubuntu 20.04 LTS or newer (or other Linux-oid operating system)
* installed packages (ubuntu DEB package names):
  - mandatory: gcc, gfortran, make
    subversion or git
    libhdf5-openmpi-dev
  - optional: gnuplot, julia, libomp-dev
    jupyter, pluma

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=> Code of Conduct

pencil-code/license/CODE_OF_CONDUCT.md

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OpenMP parallelization

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=> Short overview:
https://cyber.dabamos.de/programming/modernfortran/openmp.html

=> Documentation of version 5, including examples:
https://www.openmp.org/wp-content/uploads/openmp-examples-5.0.0.pdf

OpenMP parallelization

Implicit parallelization within the code:

```
#define N 100000

int main() {
    int a[N];

#pragma omp parallel for
    for (int i = 0; i < N; ++i)
        a[i] = 2 * i;

    return 0;
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(if code permits parallelization!!!)

MPI parallelization

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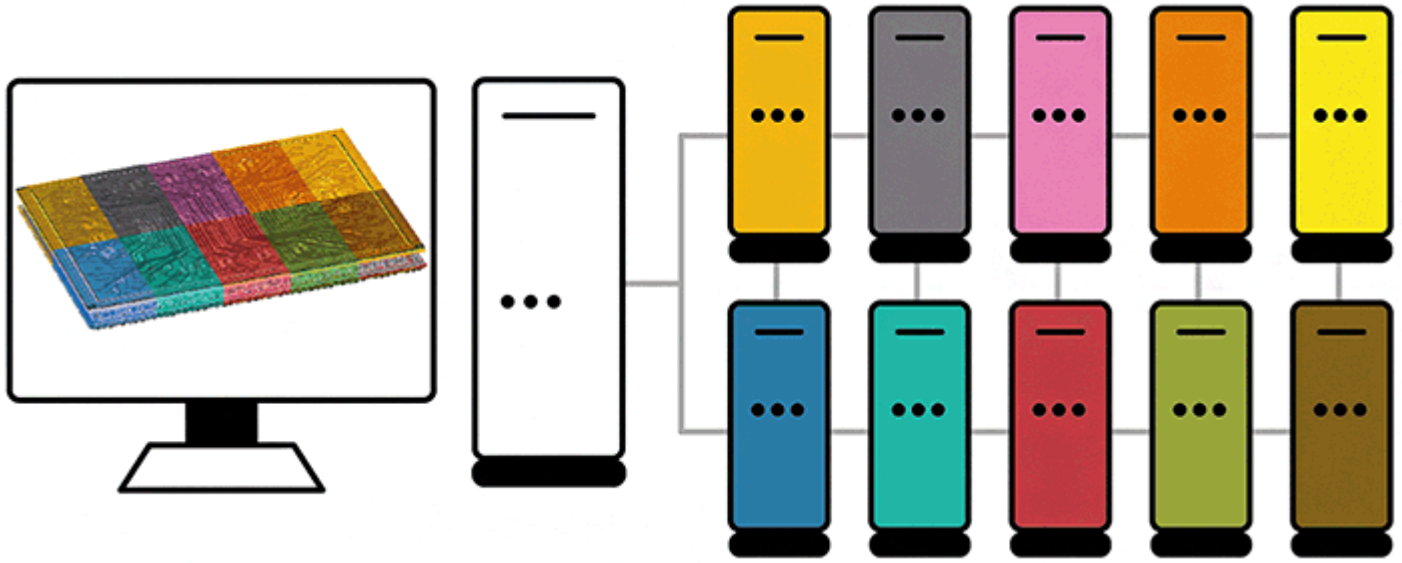

=> typically identical compute nodes

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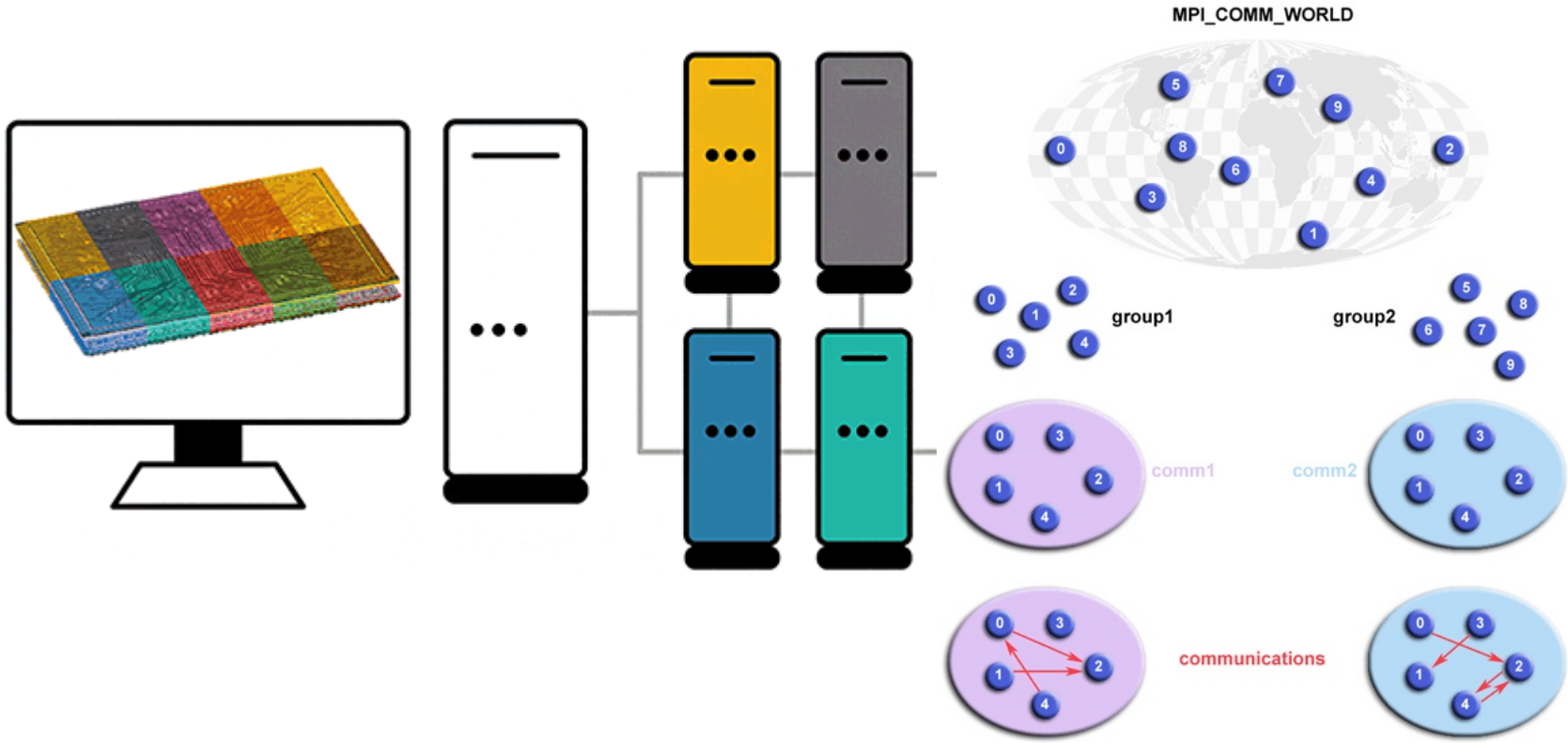

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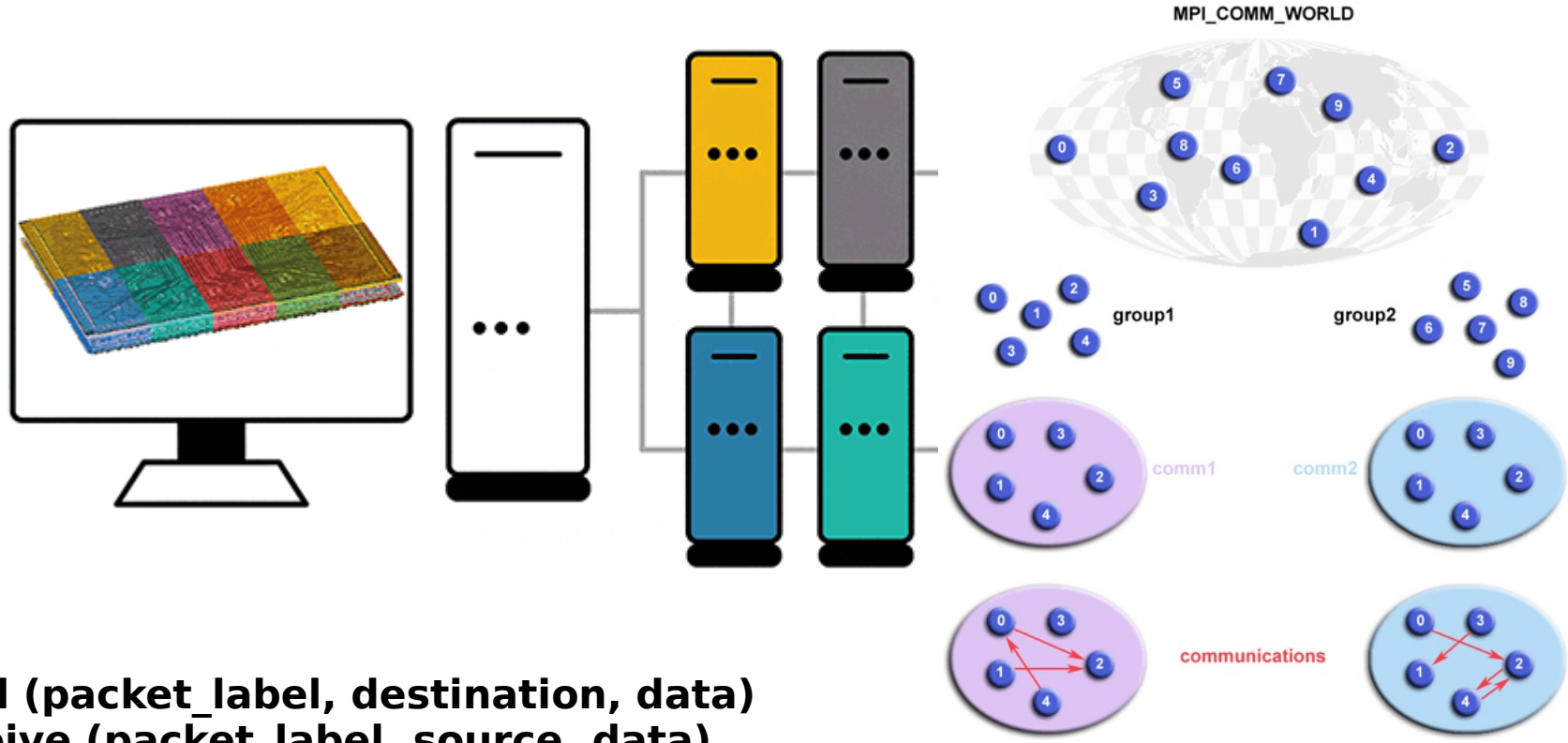

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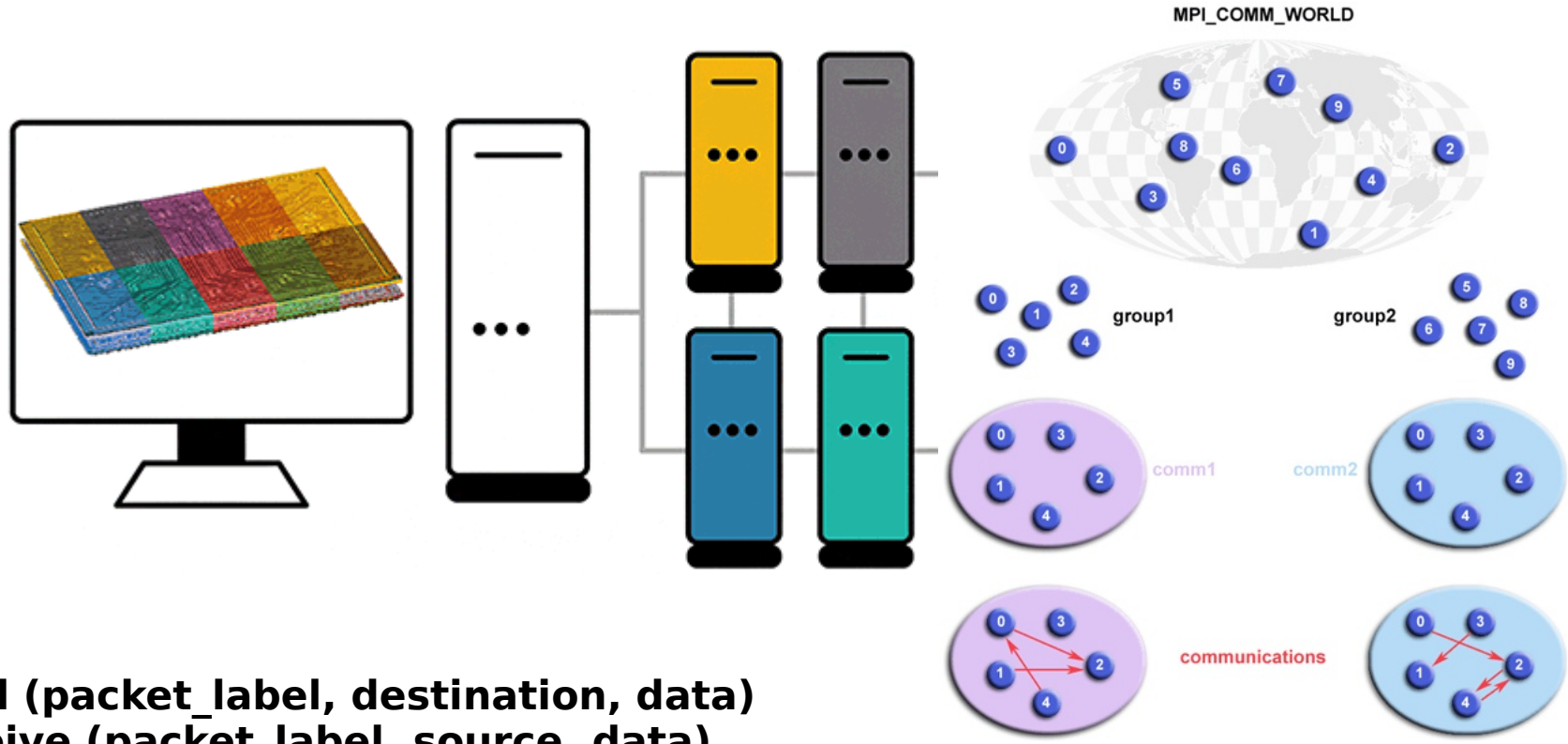

MPI_Send (packet_label, destination, data)
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MPI_ISend (packet_label, destination, data)
MPI_IReceive (packet_label, source, data)
MPI_IWait (packet_label, source)

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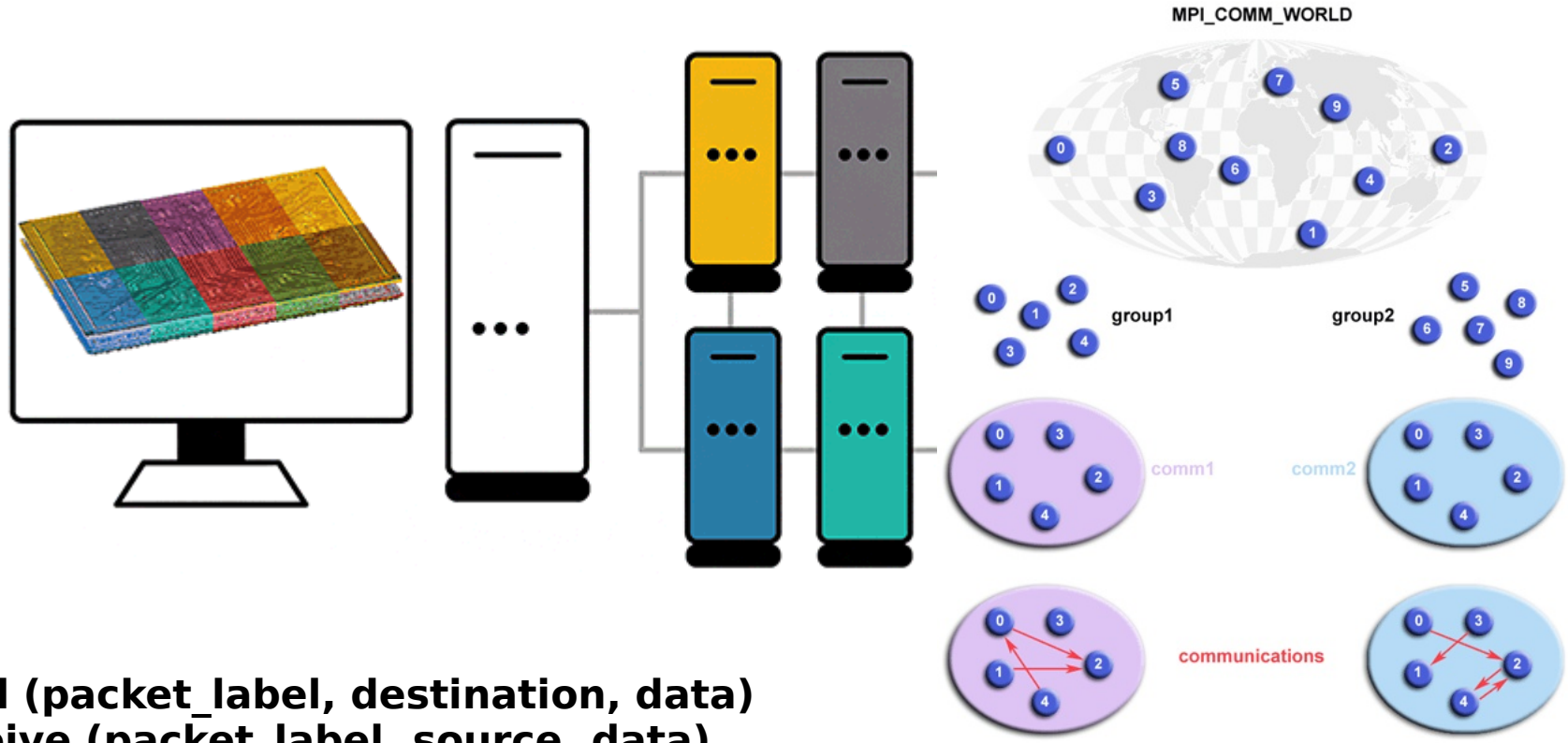

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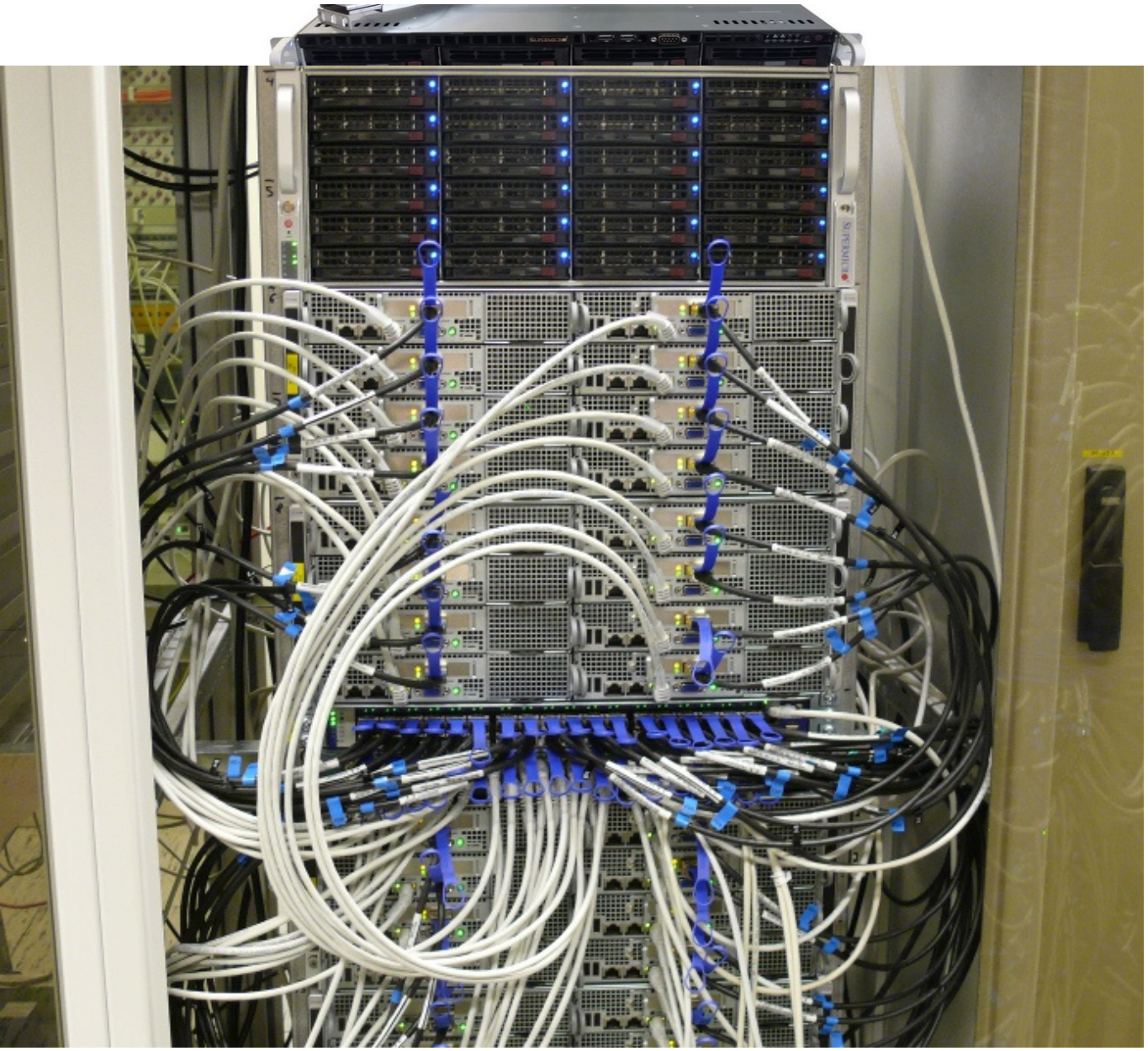
MPI_Broadcast (packet_label, source, data[, target group])
MPI_Barrier ([target group])

LEO high-performance computer:



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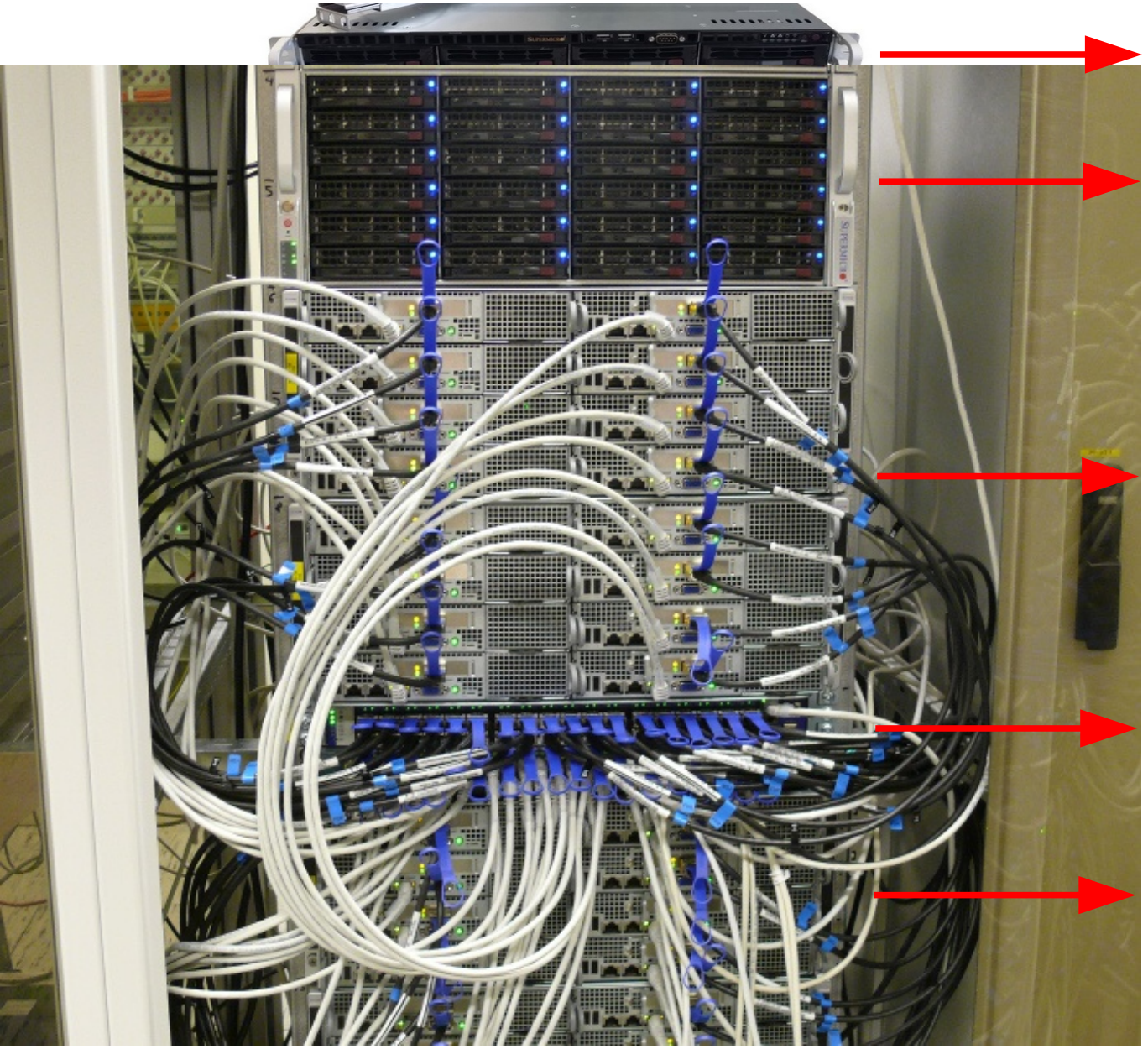

frontend (LEO1 + LEO2)

harddisks (LEONAS1 + 2)

compute nodes (LEONs)

network switches

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* **computation time:**
  > 10 million core-hours per year (~ 250 k€ per year)

LEO high-performance computer:

* **software modules library: “module avail”**

```
---------------------- /software/modules/COMPILER ----------------------
gnu/RHEL-7(default)

------------------------ /software/modules/DATA ------------------------
idl/7.06/32_bit              python/2.7.9+3.4.2(default)
idl/7.06/64_bit              qsas/3.0.1(default)
idl/8.2.3                    spedas/1.00(default)
idl/8.4(default)             spedas/bleeding
julia/0.3.9(default)         spedas/yesterday
julia/0.4.0-dev

------------------------ /software/modules/LIBS ------------------------
fftw/3.3.4(default)              phdf5/1.8.17/mvapich2/2.1/gnu
nasa-cdf/3.6.0.4(default)        phdf5/1.8.17/openmpi/1.10.3/gnu
phdf5/1.8.17/mpich/3.1.4/gnu     solarsoft/2014-12-09(default)

------------------------ /software/modules/MPI -------------------------
mpich/3.1.4/gnu    mvapich2/2.1/gnu   openmpi/1.10.3/gnu

---------------------- /software/modules/TOOLS -----------------------
dislin/10.5.3(default)              valgrind/3.11.0/openmpi/1.10.3/gnu
filezilla/3.10.0.2(default)
```

LEO high-performance computer:

* **MPI job queue:**

Name	maximum Runtime per job	at least Nodes per job	maxium Nodes per job	maximum simultaneously used Nodes by this queue	maximum running Jobs per User	Priority	Default
`short`	20 min	1	2	2	2	20	
`normal`	24 h	1	13	32	4	10	X
`long`	96 h	1	4	4	1	5	
`large`	12 h	17	32	32	1	15	

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4) Compiling PC

   => **pc_build**

Memory alignment and cache efficiency

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Alignment of data in memory:

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C(2,1)	D(2,2)
E(3,1)	F(3,2)

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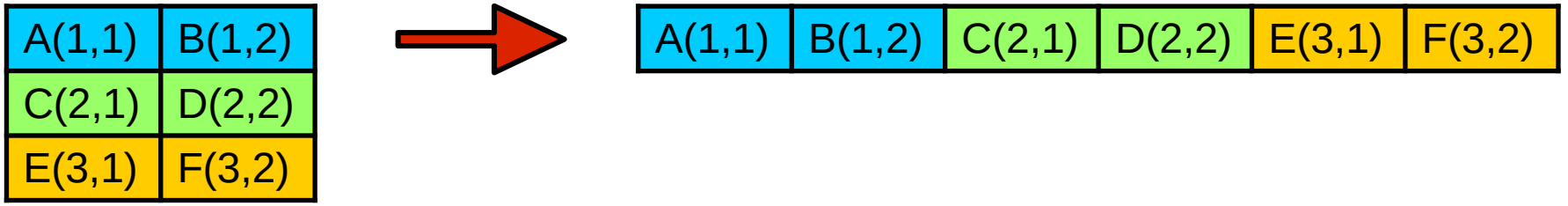

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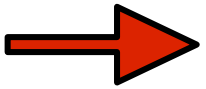

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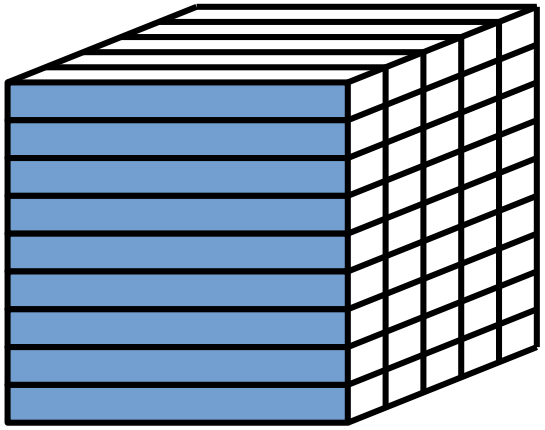
Cache efficiency:



Memory alignment and cache efficiency

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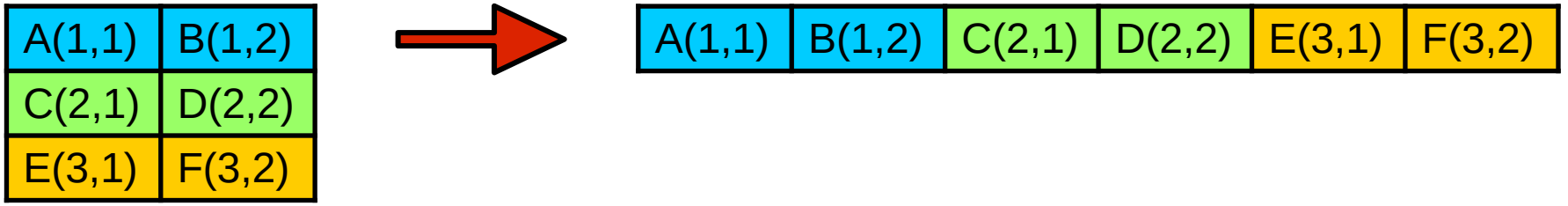

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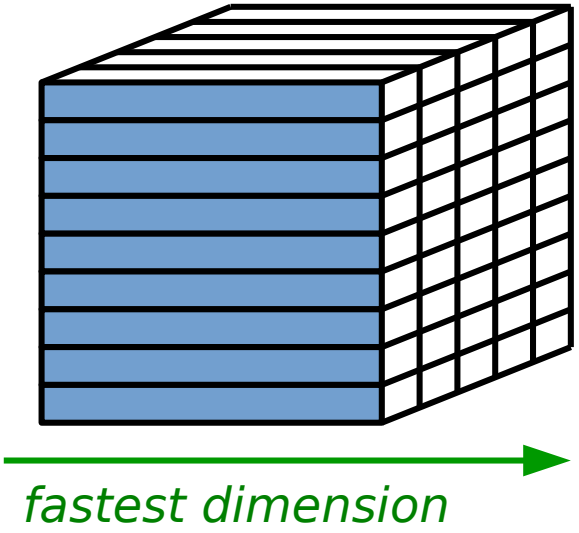

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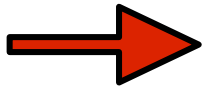

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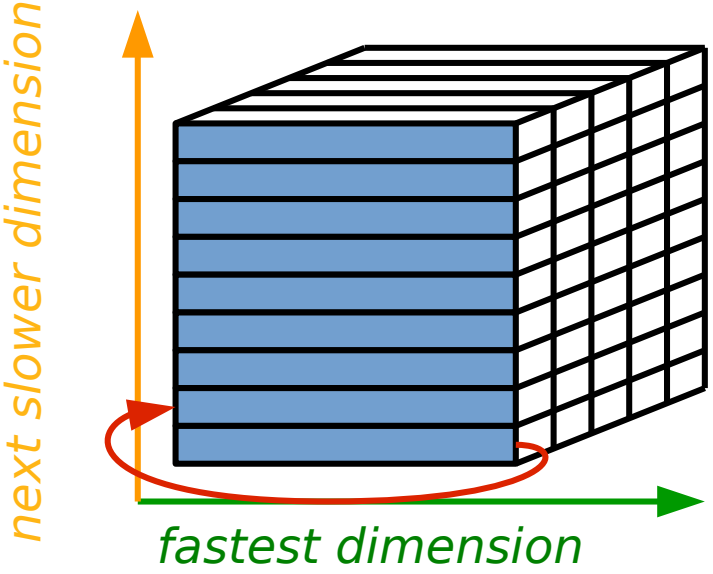

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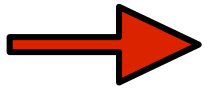

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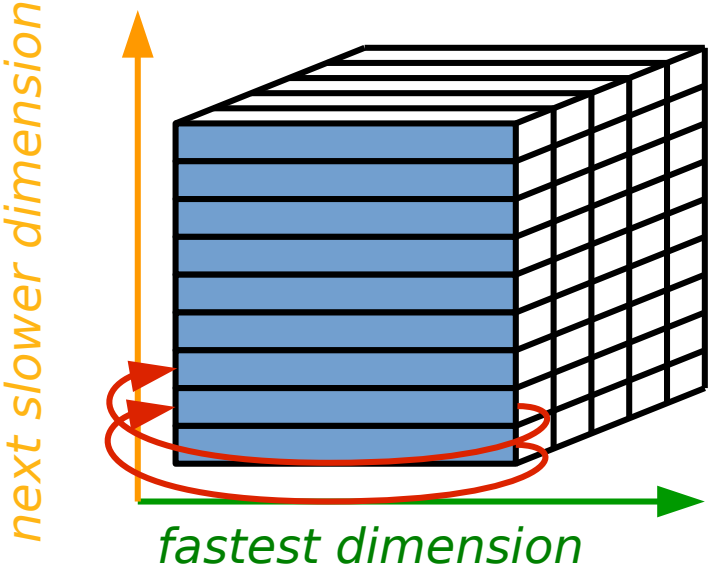

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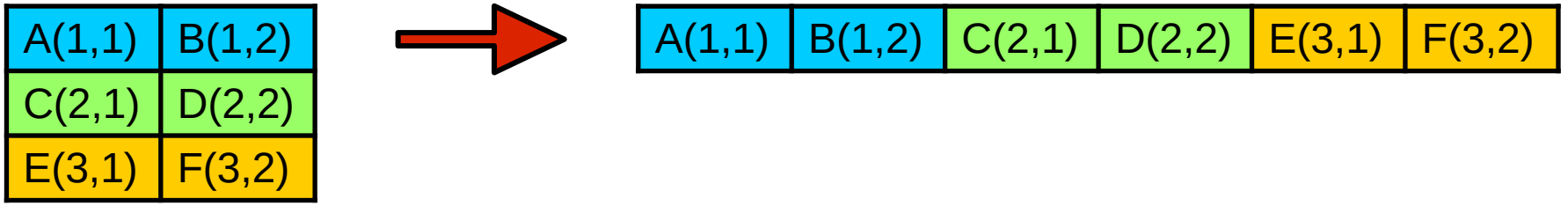

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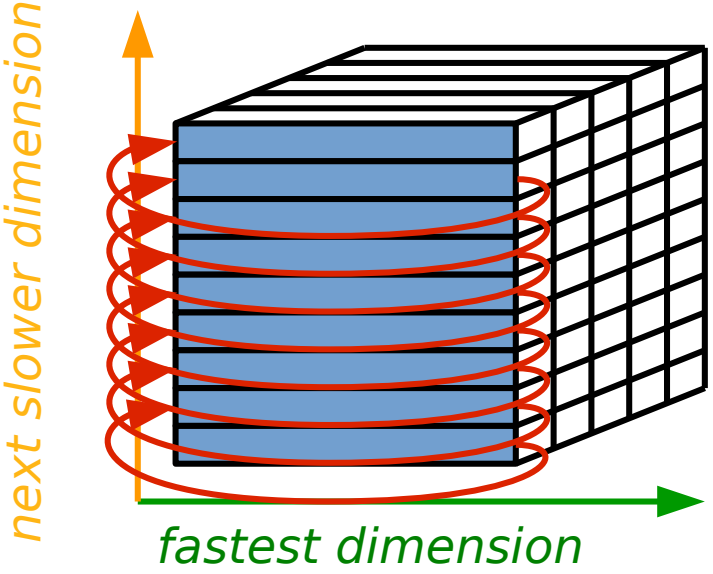

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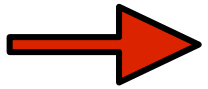

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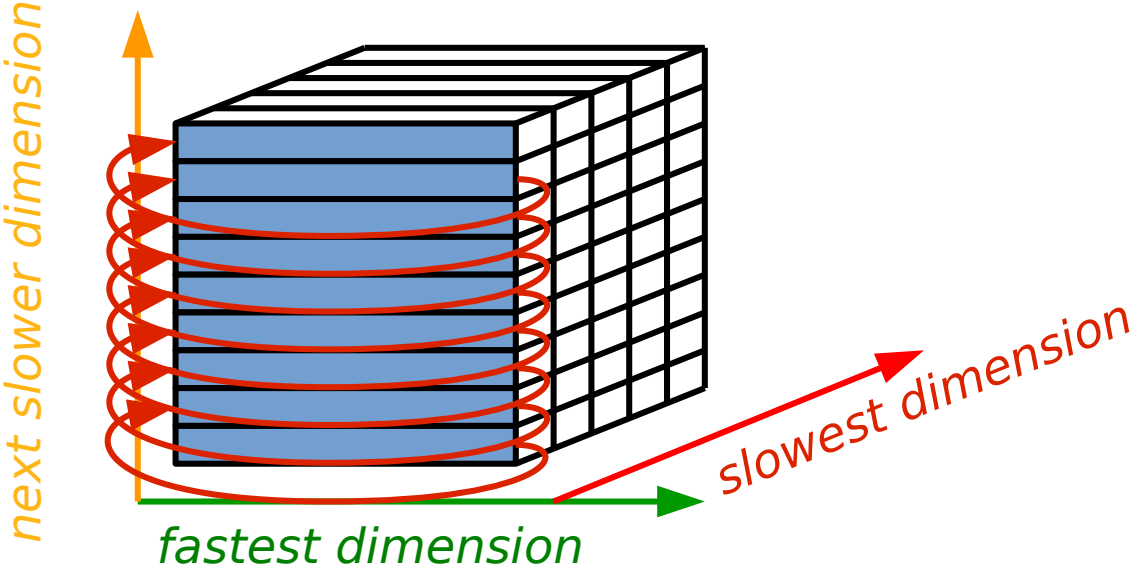
Cache efficiency:

=> both is achieved by elongated subdomains and optimal data access



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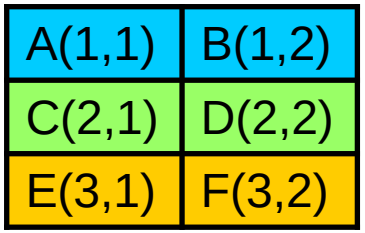

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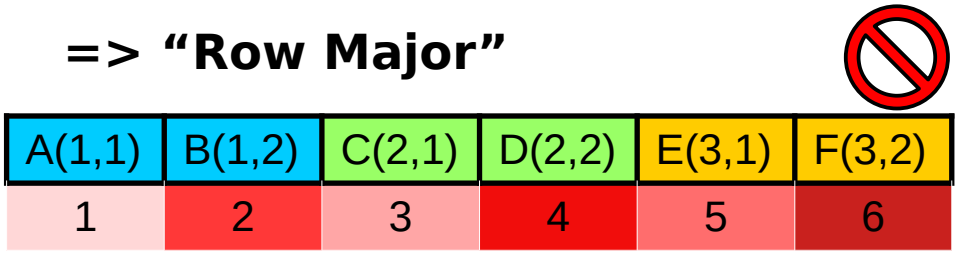

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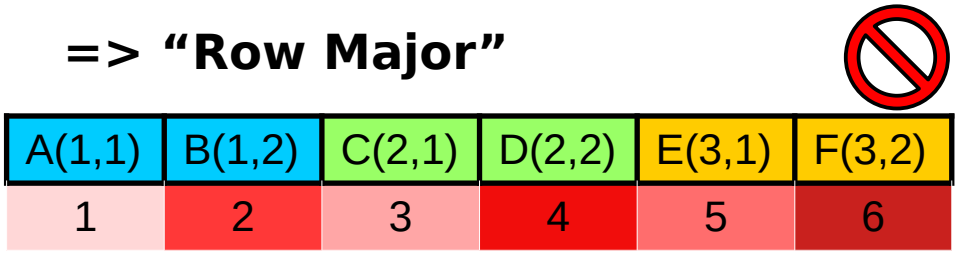

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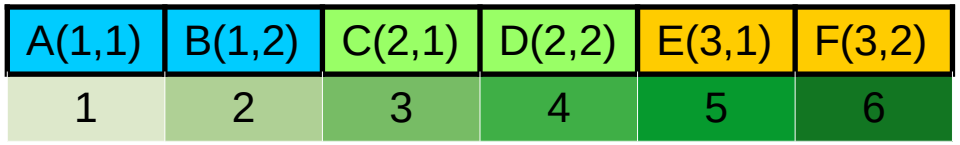

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Vectorization and SIMD

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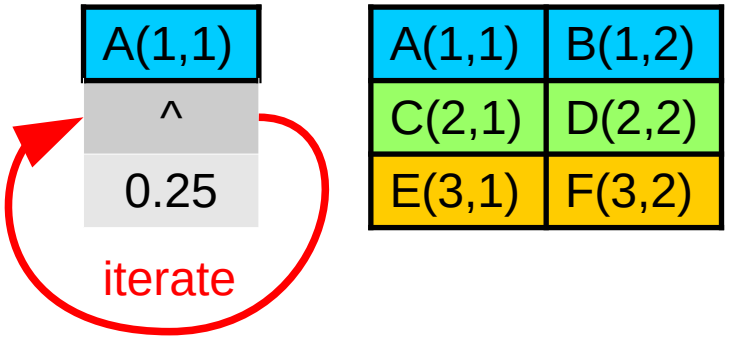
Explicit iteration:



A(1,1)	B(1,2)
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A,B,C,D,E,F

needed CPU instructions:

* 6 times loop overhead
* up to 6 times memory load
* 6 times mathematics
* 6 times memory store

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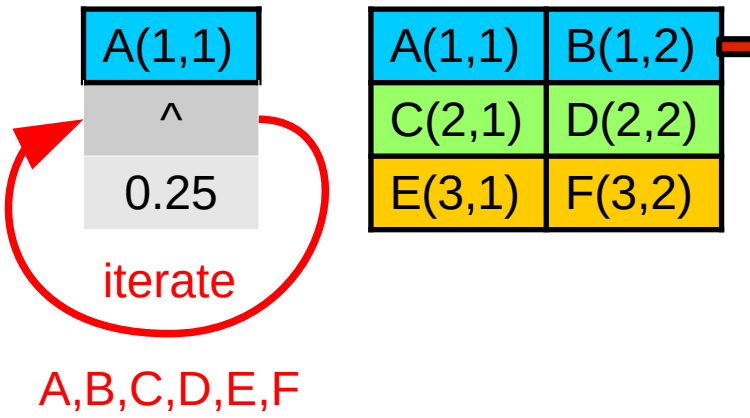

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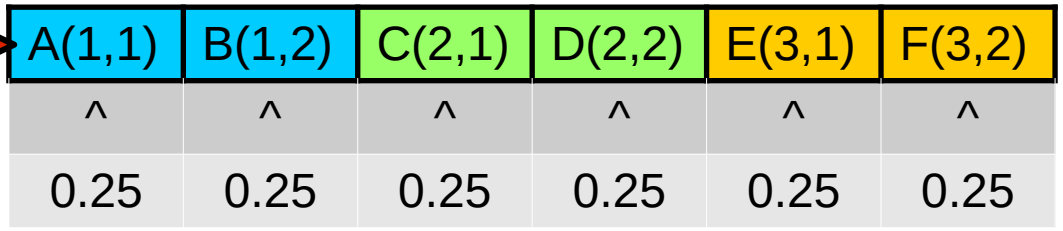

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SIMD case:

* no loop overhead
* 1 memory load (L2-cache line!)
* 1 mathematics
* 1 memory store

  => up to 1000 times faster!

Abuse of mathematics

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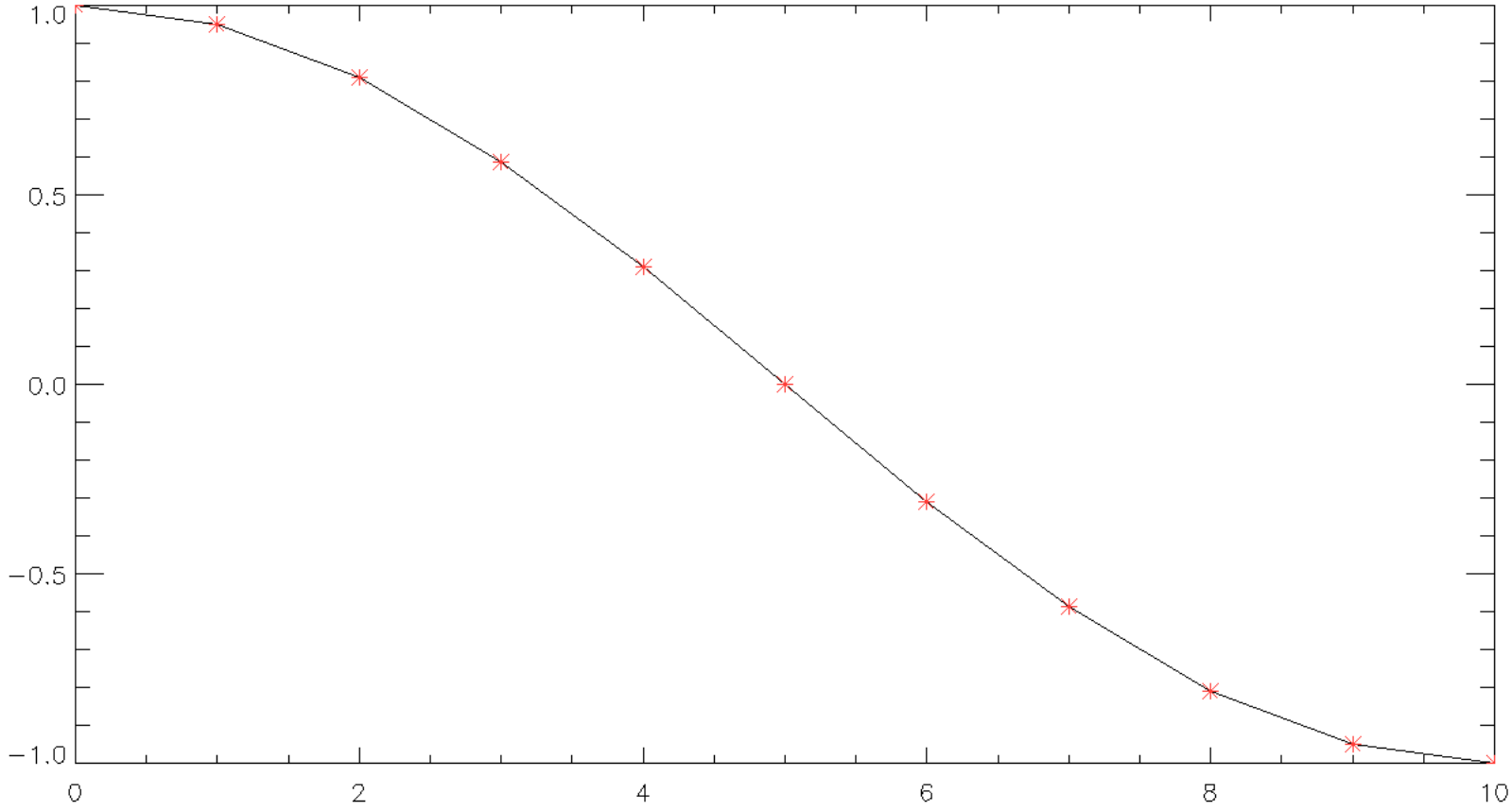
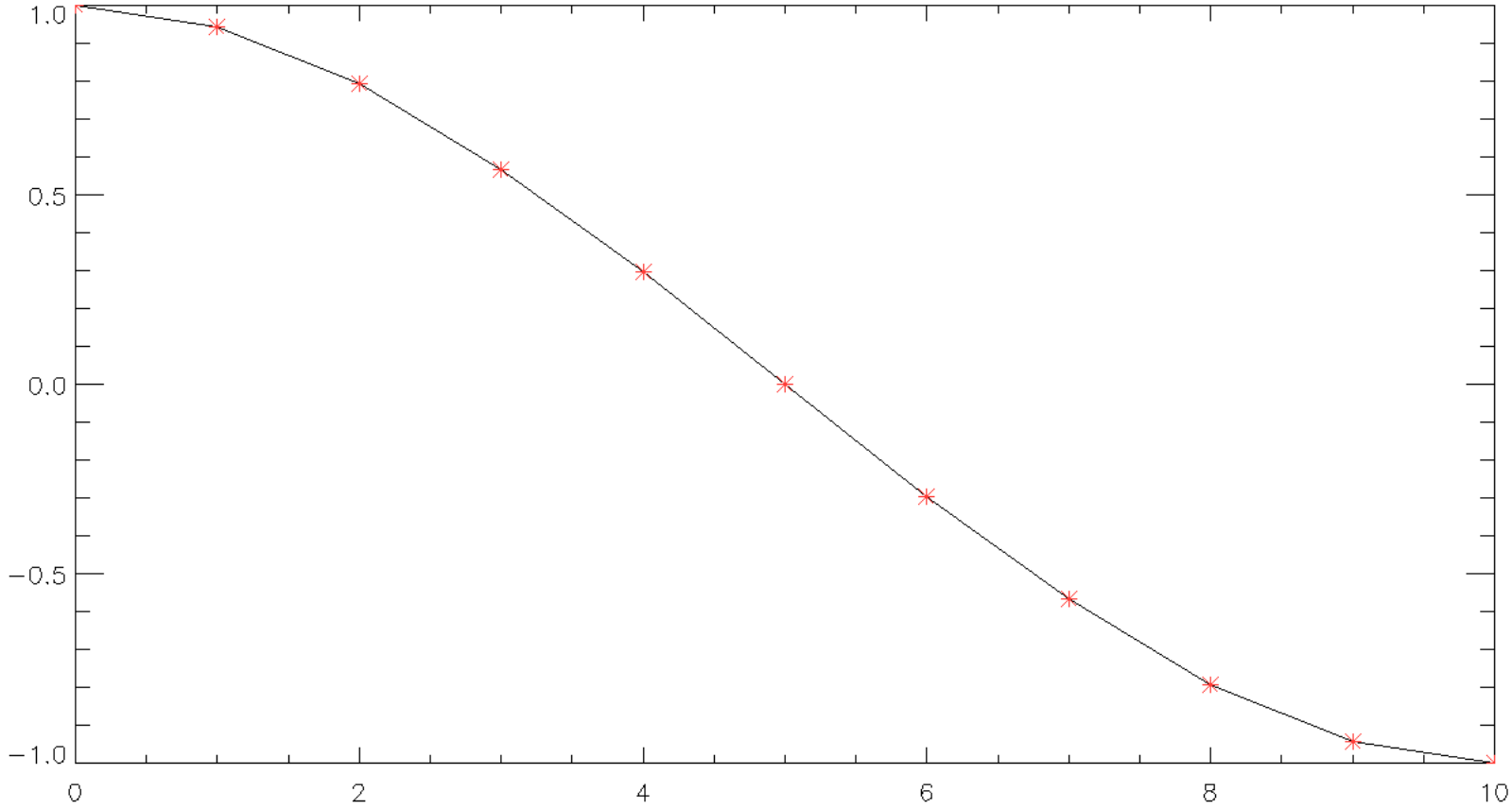


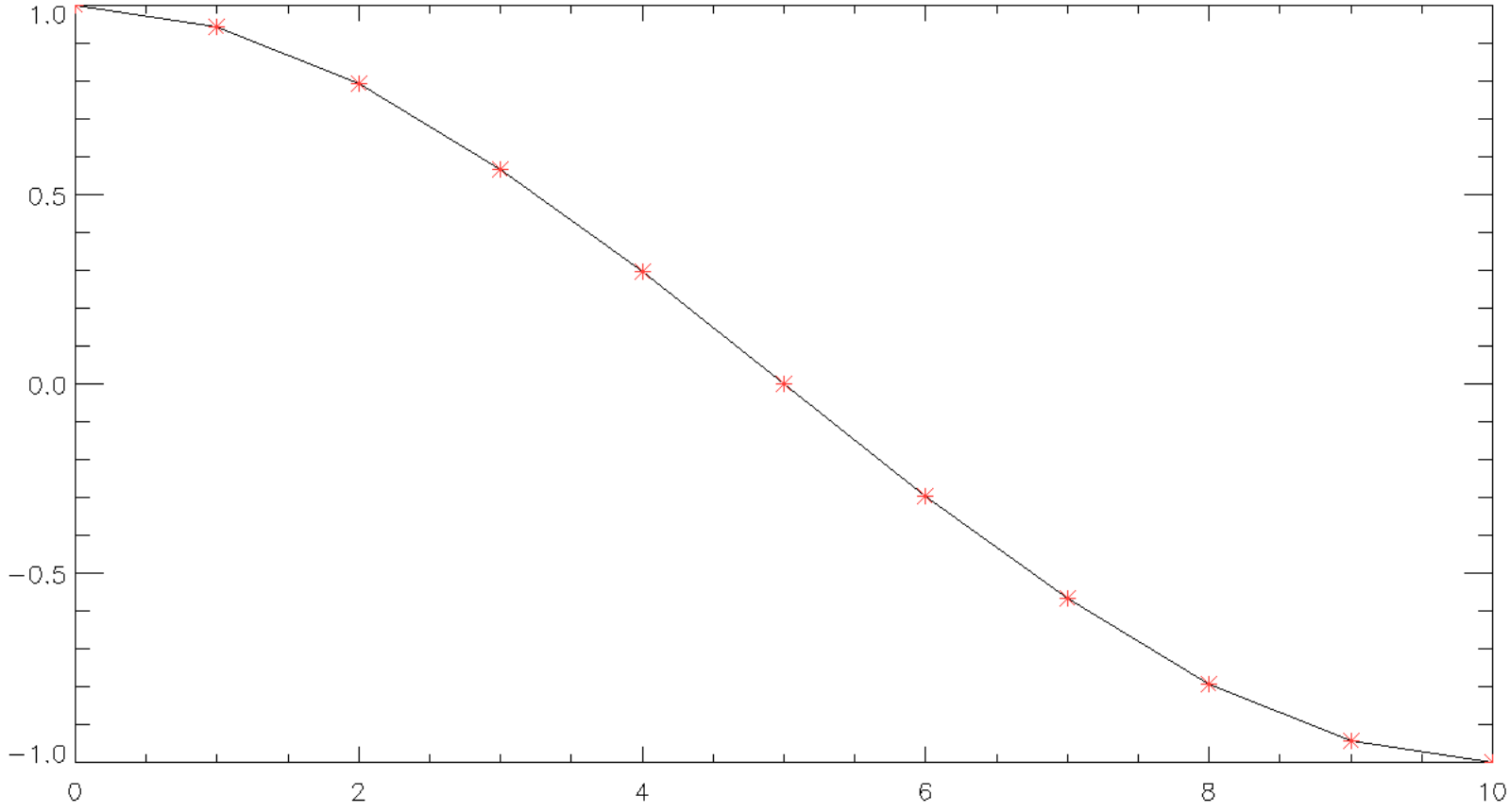
$$f(x)=\cos\left(\frac{\pi}{10}x\right)$$

Abuse of mathematics



$$f(x) = \ldots ?$$

Abuse of mathematics



$$\xi = \left(x - x_0 \right) / \Delta$$

$$f\left(\xi\right) = \frac{1}{2} + \xi\left(\frac{3}{4} - \frac{1}{4}\xi^2\right)$$

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1) Changing parameters

   => edit **start.in**, **run.in**, **print.in**, …

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3) Propagate an existing state (“run”)

   => **pc_run**

Boundary conditions

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Problem: boundary condition is an assumption on the outside area

* ideas?

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* Fixed Boundary $f(x_{B-j}) = f(x_B)$ or $f(x_{B-j}) = const.$
* Ignore Outside (= Mirroring)
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* Periodic $f(x_{B-j}) = f(x_{B+(N-1)-j})$
* Antisymmetric $f(x_{B-j}) = -f(x_{B+j})$ or $f(x_{B-j}) = f(x_B) - f(x_{B+j})$
* Wavelet (= extrapolation with set of pre-defined wave functions)
* and many other possibilities...

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* and many other possibilities...

=> Be aware of the physical meaning of a boundary condition!