ESCAPE 824064

LAPP
Laboratoire d'Annecy de Physique des Particules

Gray Scott Reloaded 2024 : Computing on heterogeneous hardware

Pierre Aubert

ESCAPE
cta cherenkov telescope array
cnrs
UNIVERSITÉ SAVOIE MONT BLANC

Introduction

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New edition of **Gray Scott Battle** school (2023) : **4** days

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Attendees :
- **Students**
- **Researchers**
- **Engineers**

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Gray Scott Reloaded : **12** days

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- More **Technos**
- More **Tools**
- More **Time to practice**

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Free formation

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For French Speakers

Free formation

Reprises

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IN2P3 transverse project

~ **20** people

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Performance tests

Valgrind MAQAO Perf

Precision

Cadna

Container

apptainer.org docker

Fortran

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Xtensor alpaka Kokkos

HPX V1.2 DRAFT

Vulkan 1.2 FORGING AHEAD

NVIDIA CUDA

NVIDIA HPC DEV

OpenVINO

OpenCL OpenACC More Science, Less Programming

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C++ R Fortran

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1.2 FORGING AHEAD

CPU

GPU

FPGA

multi-core
many-core

TERATEC / EuroCC / EuroHPC

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- **Association**
- **Valorisation** / **Dissemination** of Knowledge :
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- **Bridge** between **Academy** and **Industry**

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+33 Countries

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DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT

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supernemo collaboration

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LSST CORPORATION

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LHCb

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VIRGO

ATLAS EXPERIMENT

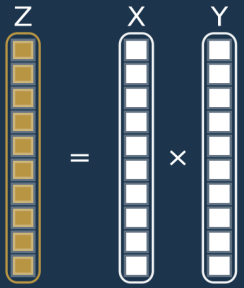
LHCb

LSST CORPORATION

Simple Examples

Simple Examples

Hadamard Product



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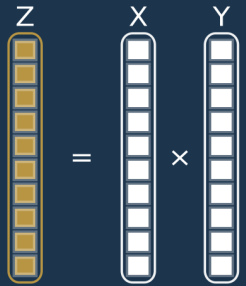

Reduction

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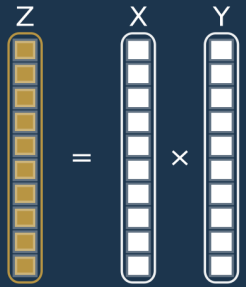
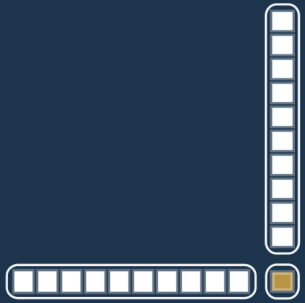


Reduction

Dot Product



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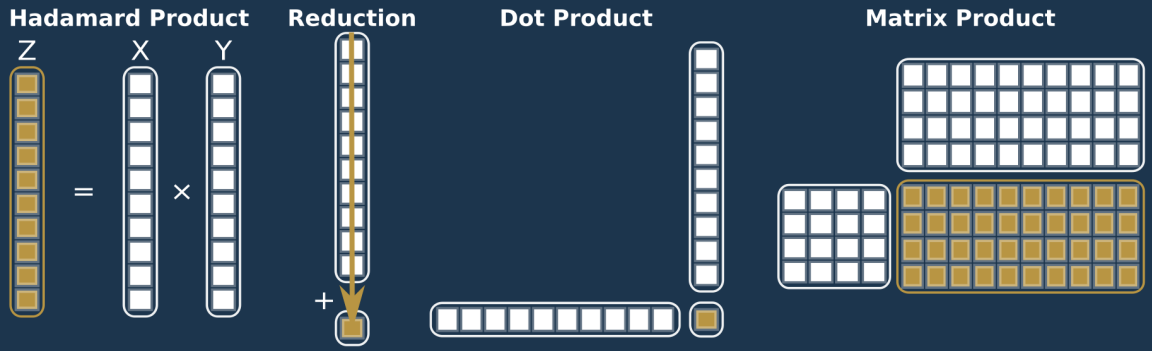

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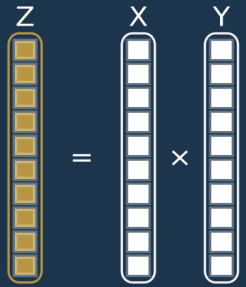

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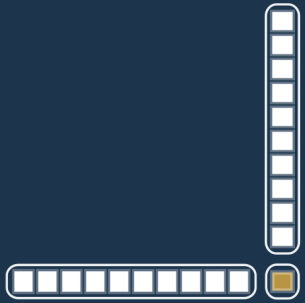

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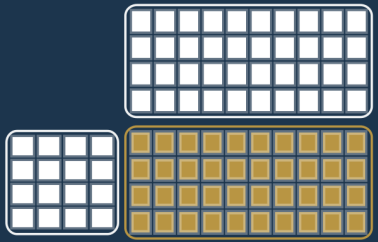

MKL

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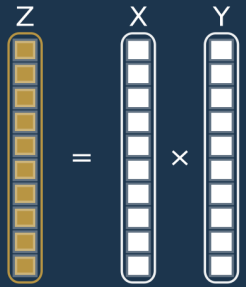

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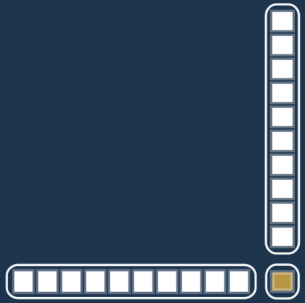

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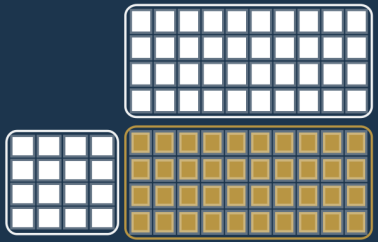

MKL

Eigen

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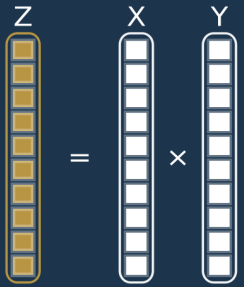

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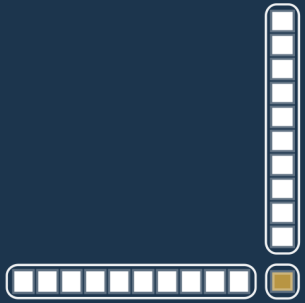

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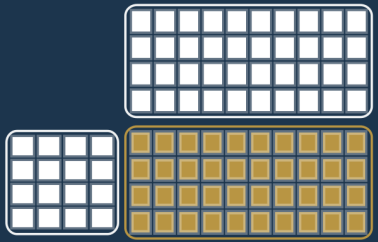

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Armadillo

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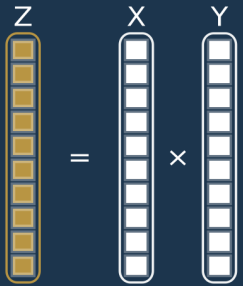

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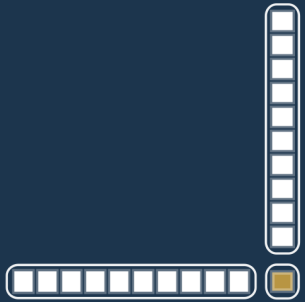

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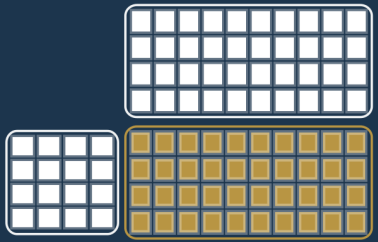

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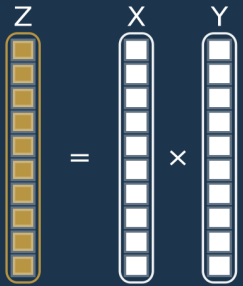

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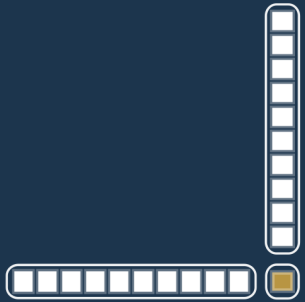

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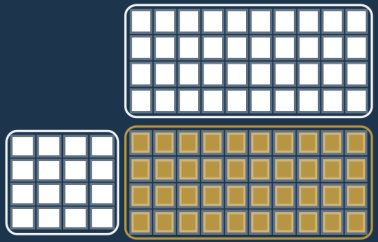

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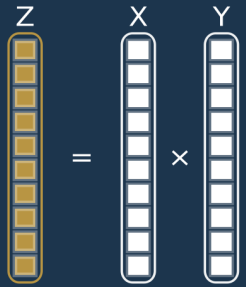

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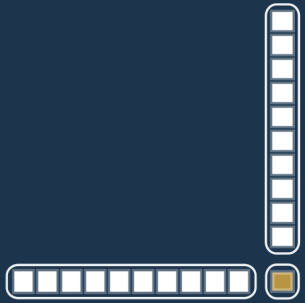

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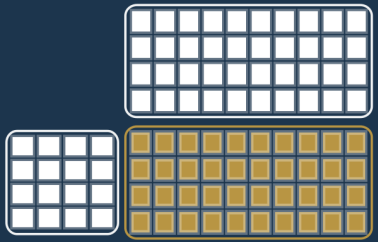

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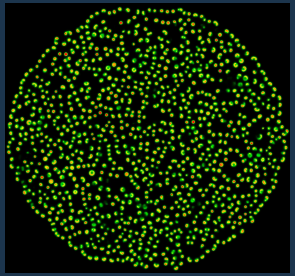
School computing example

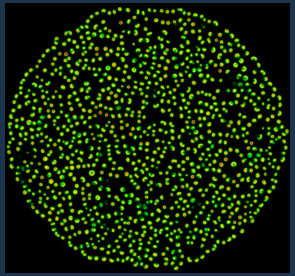
Gray Scott reaction (a chemistry game of life)



School computing example

Gray Scott reaction (a chemistry game of life)

$$
\begin{aligned}
U + 2V &\longrightarrow 3V \\
V &\longrightarrow P
\end{aligned}
$$



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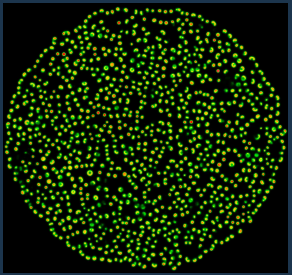

Computing :

$$\begin{aligned} U + 2V &\longrightarrow 3V \\ V &\longrightarrow P \end{aligned}$$

$$\begin{aligned} \frac{\partial u}{\partial t} &= r_u \nabla^2 u - uv^2 + f_r \times (1 - u) \\ \frac{\partial v}{\partial t} &= r_v \nabla^2 v + uv^2 - (f_r + k_r) \times v \end{aligned}$$

- u and v are concentration of product **U** and **V**
- r_u and r_v diffusion rate of **U** and **V**
- k_r (**Kill Rate**), conversion rate from **V** to **P**
- f_r (**Feed Rate**), speed of process which feed **U** and kills **V** and **P**
- $\nabla^2 u$ and $\nabla^2 v$ are différence of space concentration between current cell and its neighbours

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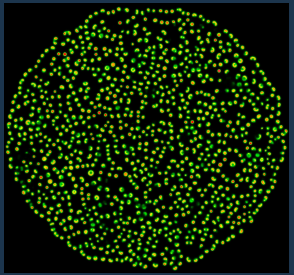

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- Easy to understand
- Not so easy for the compiler
- Possibility of high speed up

Languages / Technos

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Fortran

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Fortran

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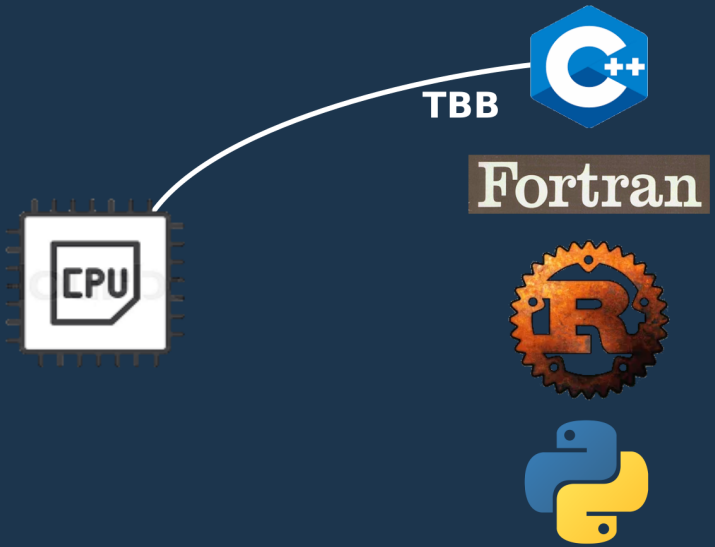

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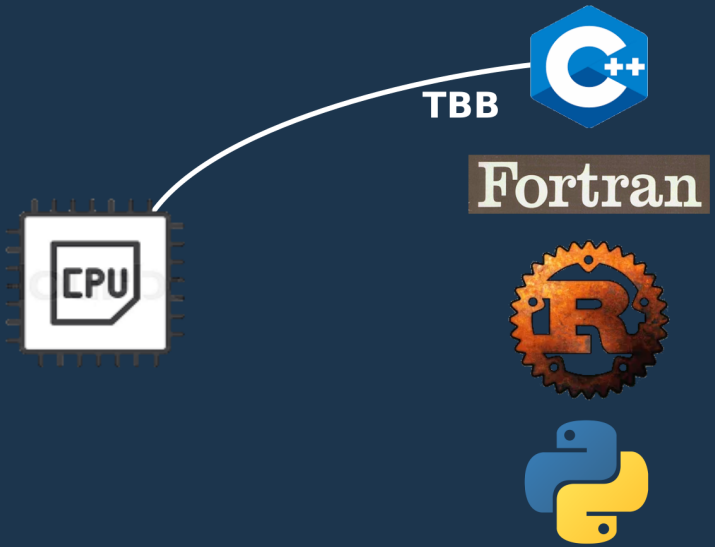

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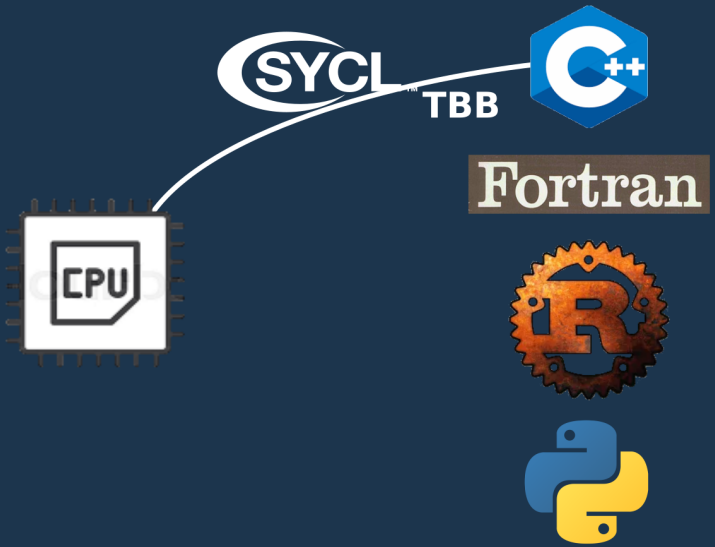

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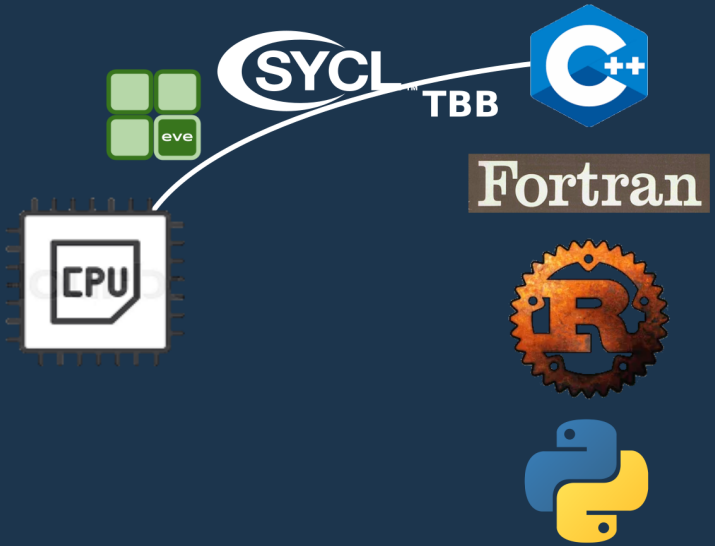

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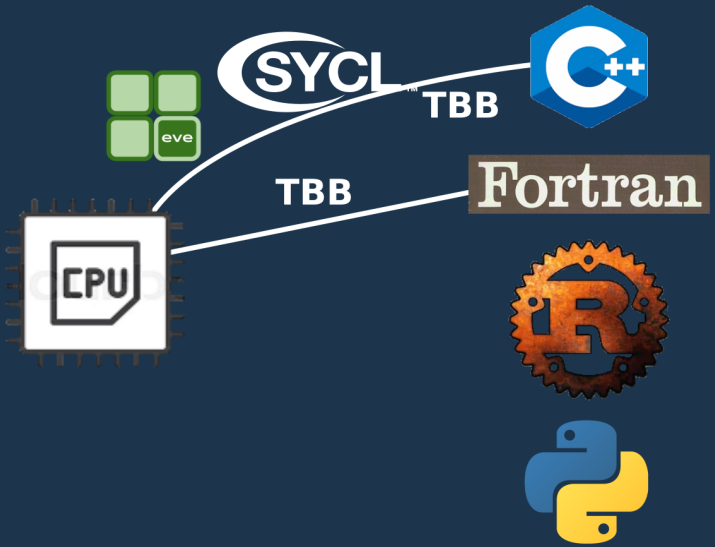

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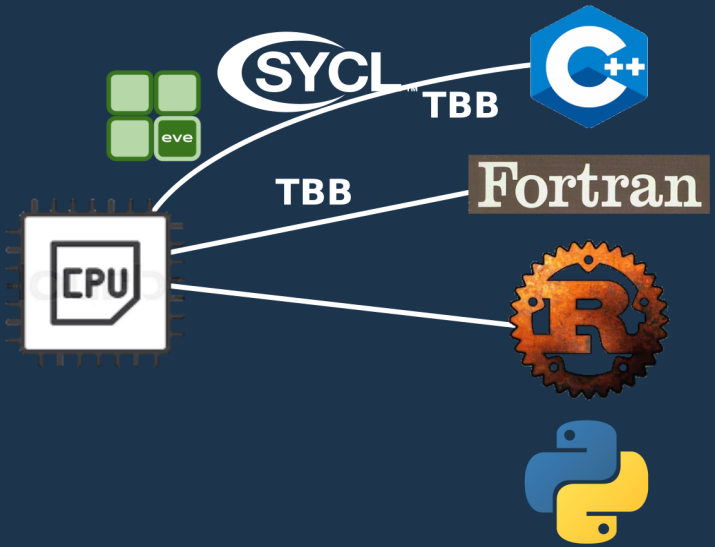

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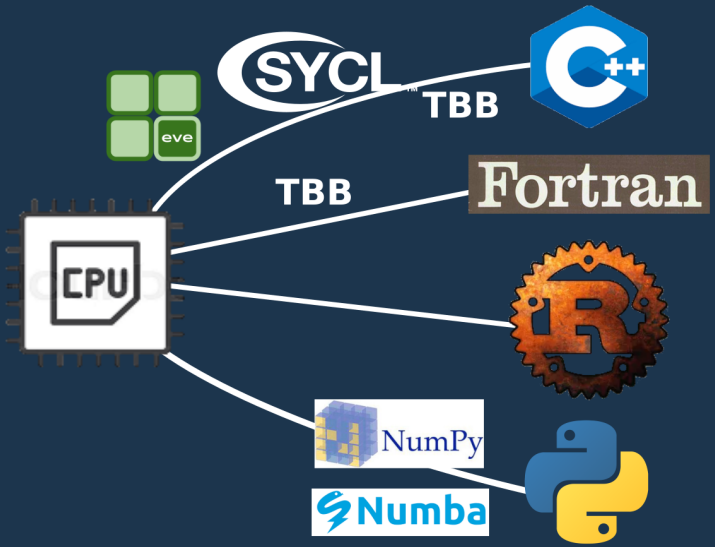

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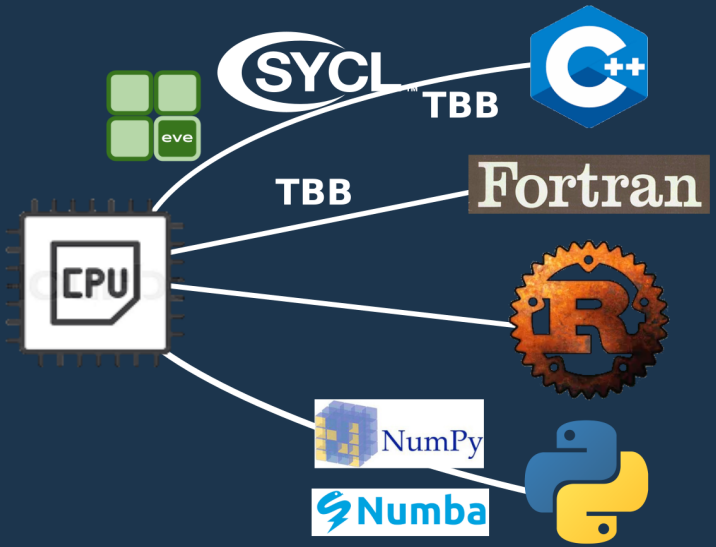

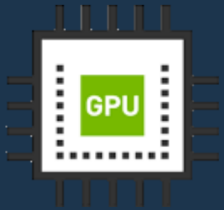

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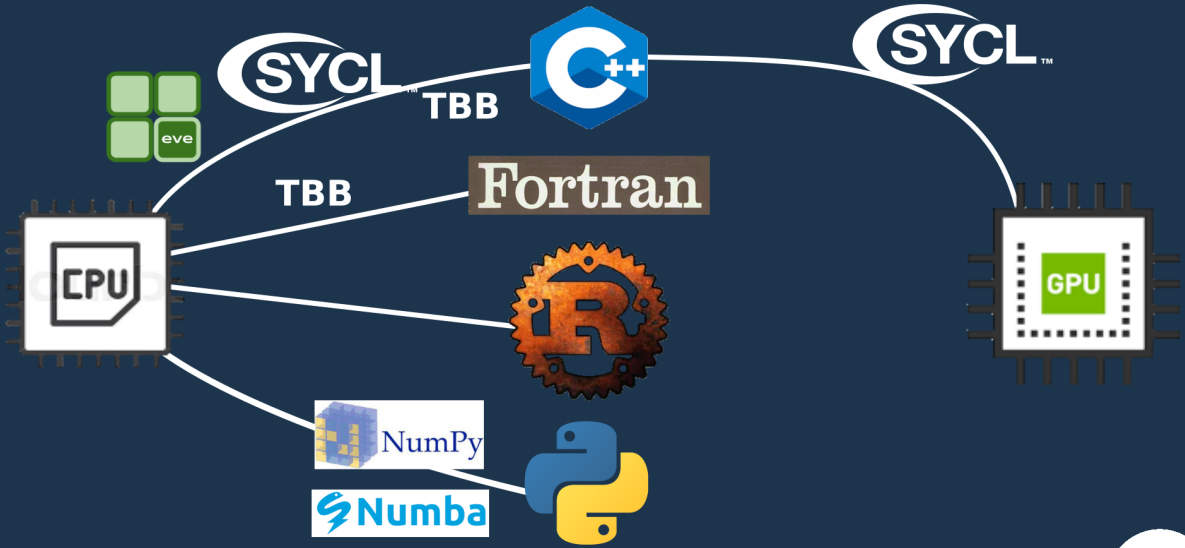

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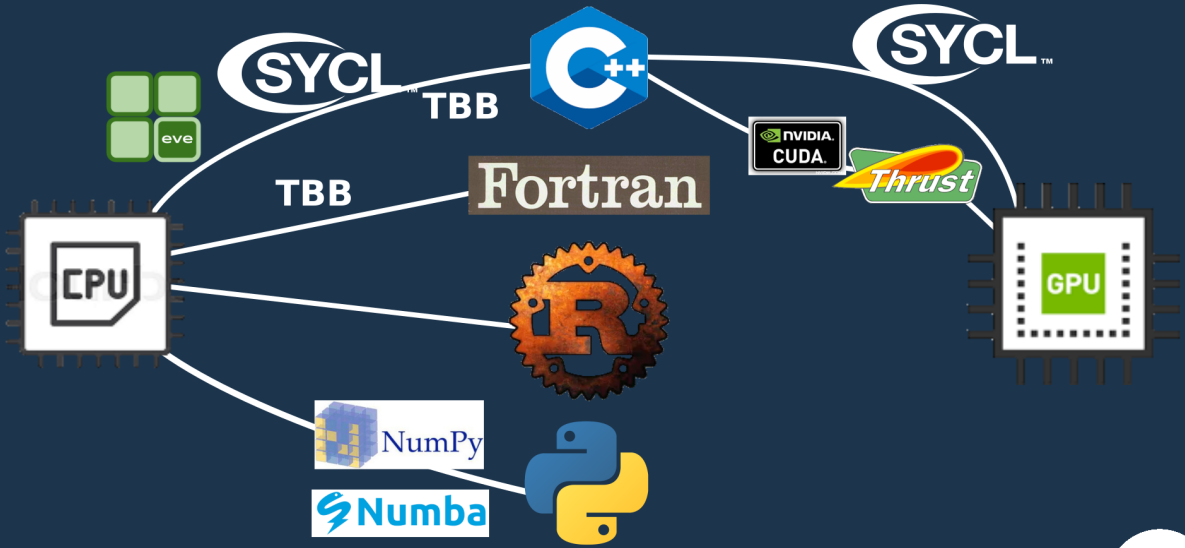
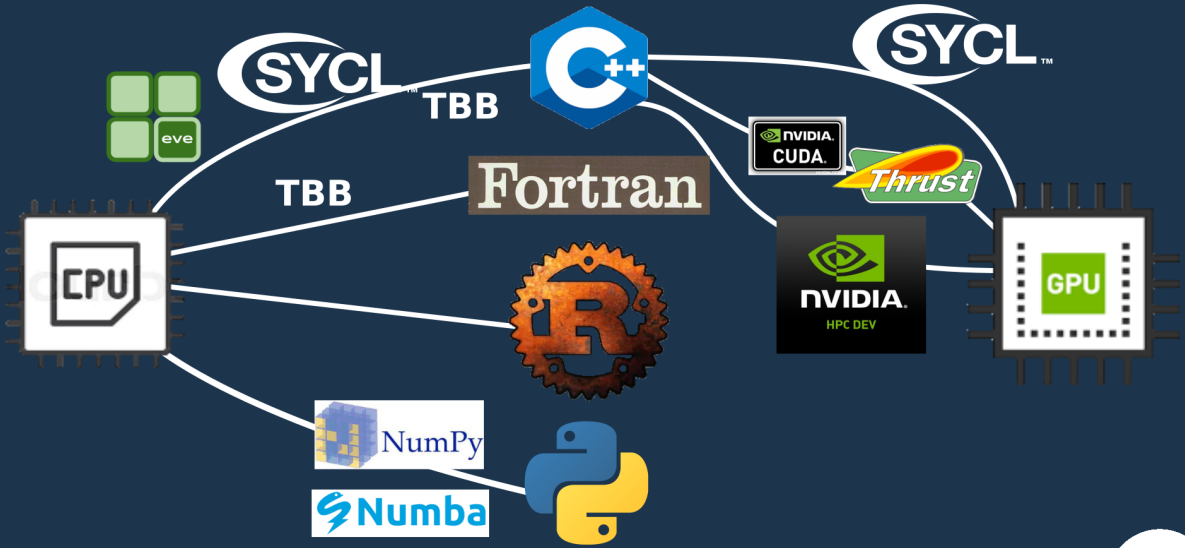
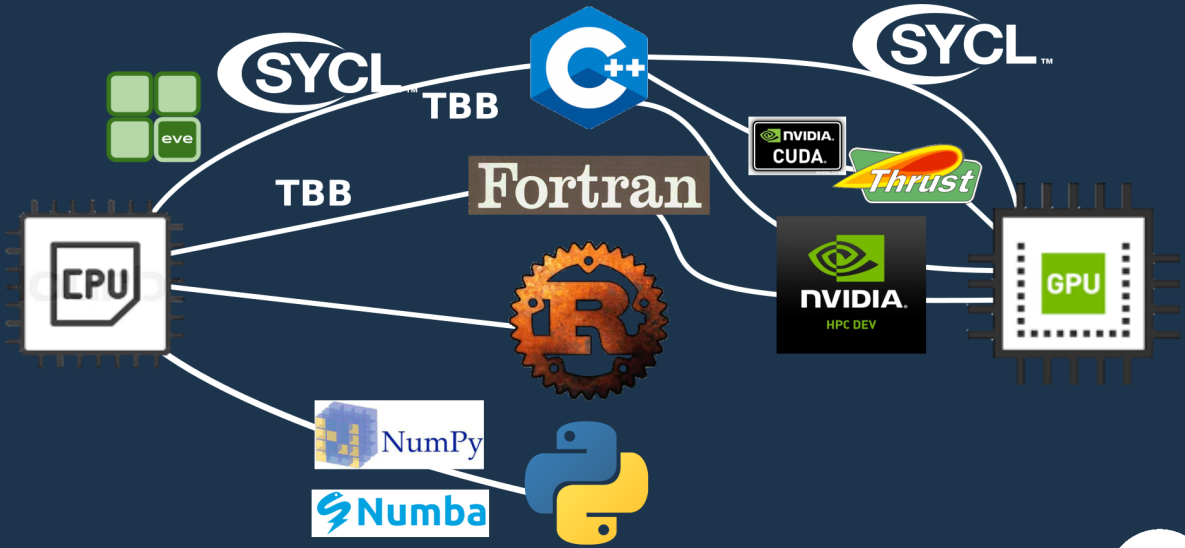


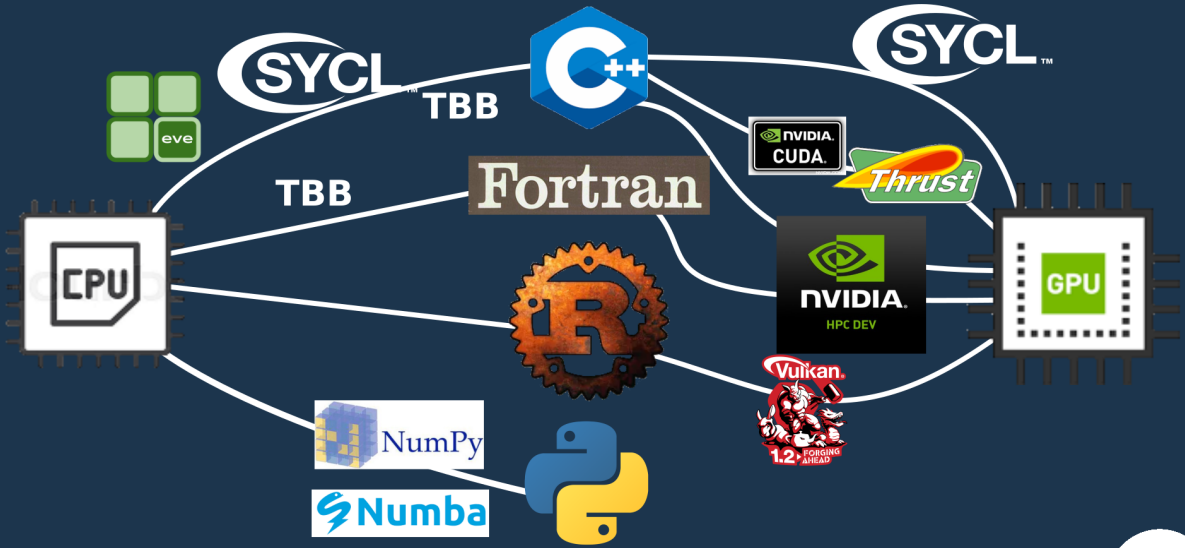
Languages / Technos



Languages / Technos



Languages / Technos



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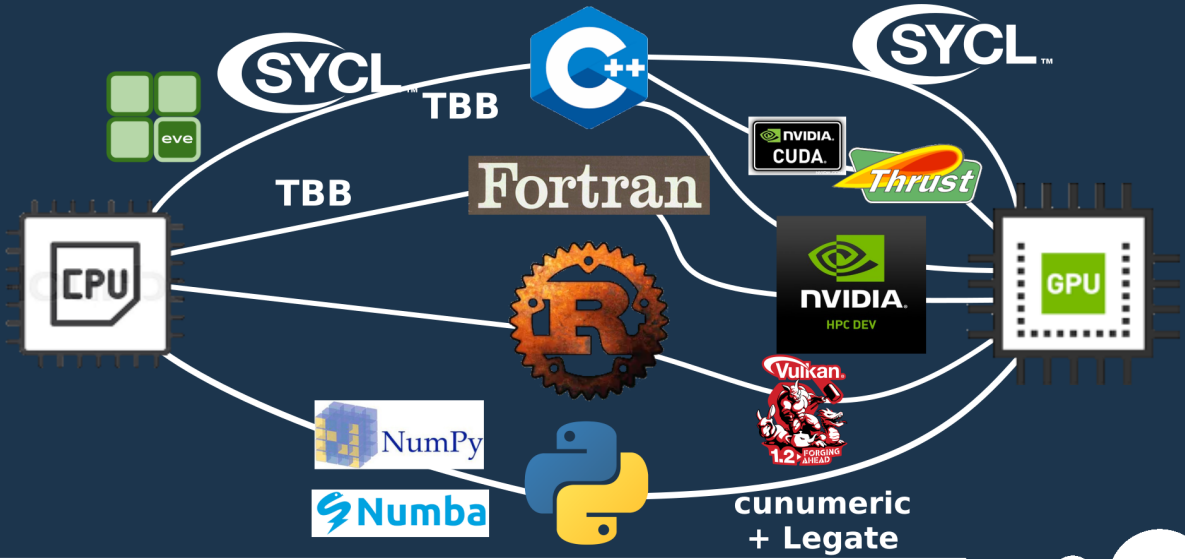

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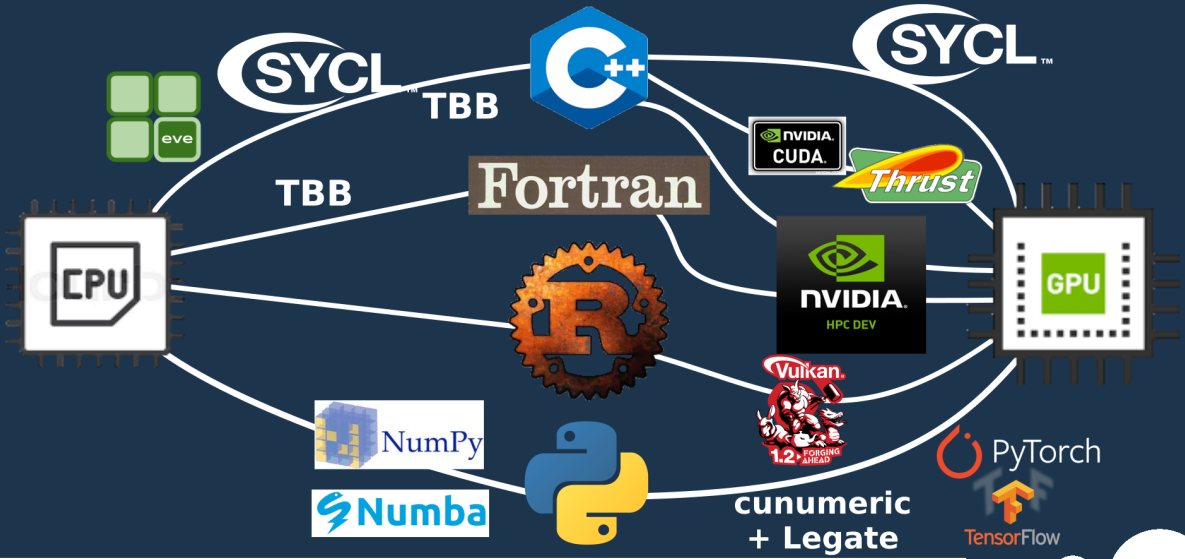


Tools

Tools

Performance tests

Valgrind

Perf

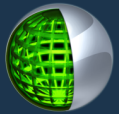
MAQAO

NSight

Tools

Performance tests

Perf



NSight

Memory Profiler

MATL

NUMA Prof

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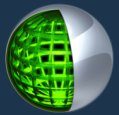
Perf



NSight

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LLVM : CLang / CLang ++ / FLang

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CMake Cross-platform Make

Multi-site diffusion

Multi-site diffusion

Multi-site diffusion

LAPP

~ 40 people

Multi-site diffusion

LAPP

~ 40 people

Teachers : 8

Multi-site diffusion

LAPP

~ 40 people

Teachers : 8

Live Streaming

Multi-site diffusion

LAPP

~ 40 people

Teachers : 8

Live Streaming

Industry

Multi-site diffusion

LAPP

~ 40 people

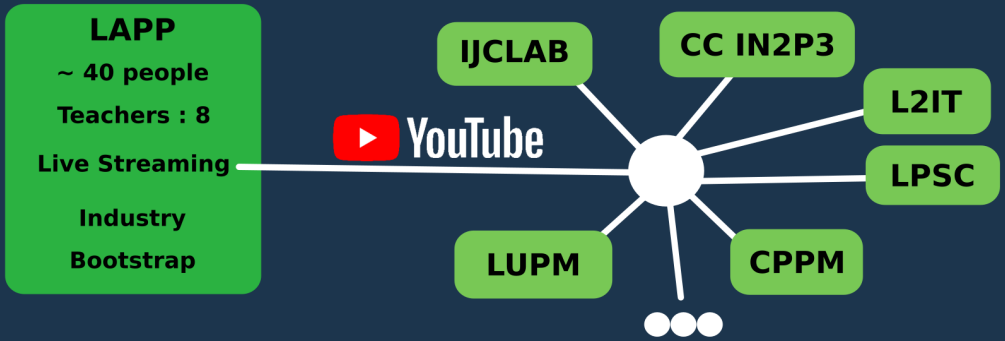
Teachers : 8

Live Streaming

Industry

Bootstrap

Multi-site diffusion



Following Lectures

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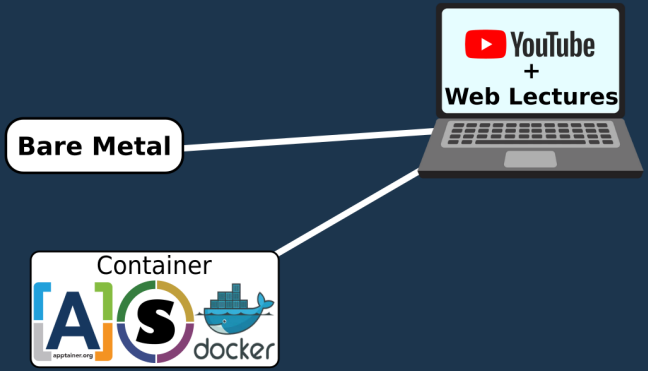

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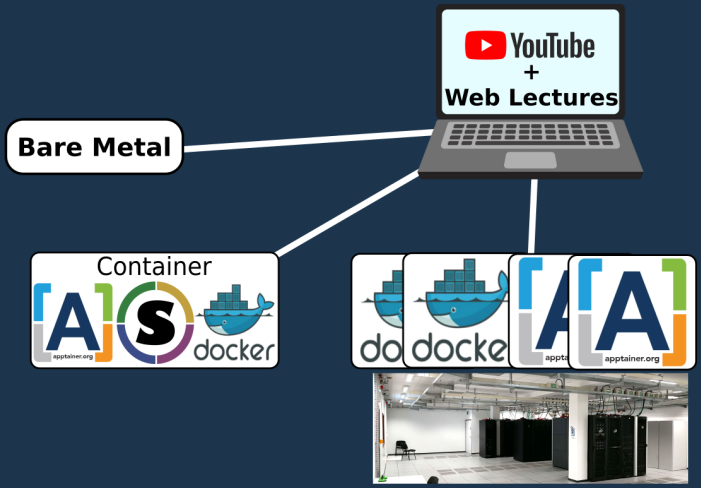

Following Lectures

Following Lectures

Hardware :
- **CPU : Intel, AMD**
- **GPU : NVidia** CC >= 6, **AMD**

Bare Metal

Container

MUST

CERFACS

ROMEO

CRIANN

Conclusion

Gray Scott Reloaded School : **1-12/07/2024 @ LAPP** (Annecy)

- **French speakers**
- For : **Students**, **Researchers**, **Engineers**

School : `https://indico.in2p3.fr/event/30939/overview`

Timetable : `https://indico.in2p3.fr/event/30939/timetable/#all.detailed`

Webinars : `https://indico.in2p3.fr/event/30939/page/3642-les-jeudis-gray-scott`

Registration : from **01/04/2024** to **01/06/2024**