CUDA® C++ in Jupyter: Adding CUDA Runtime Support to Cling

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S. Ehrig[1] and A. Huebl[1,2]

[1] Helmholtz-Zentrum Dresden – Rossendorf, Germany
[2] Lawrence Berkeley National Laboratory, USA

NVIDIA GPU Technology Conference 2020

San Jose, March 26th 2020

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Novel Particle Accelerator Research

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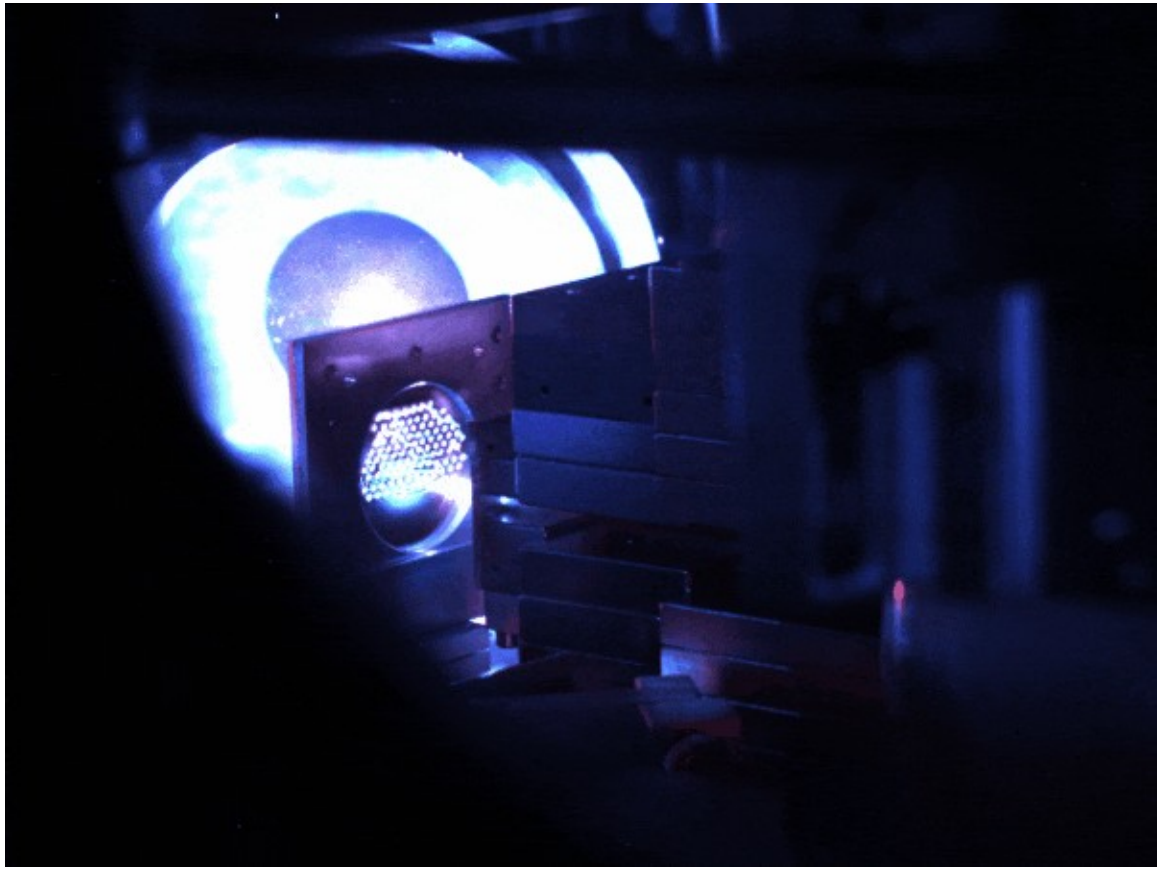

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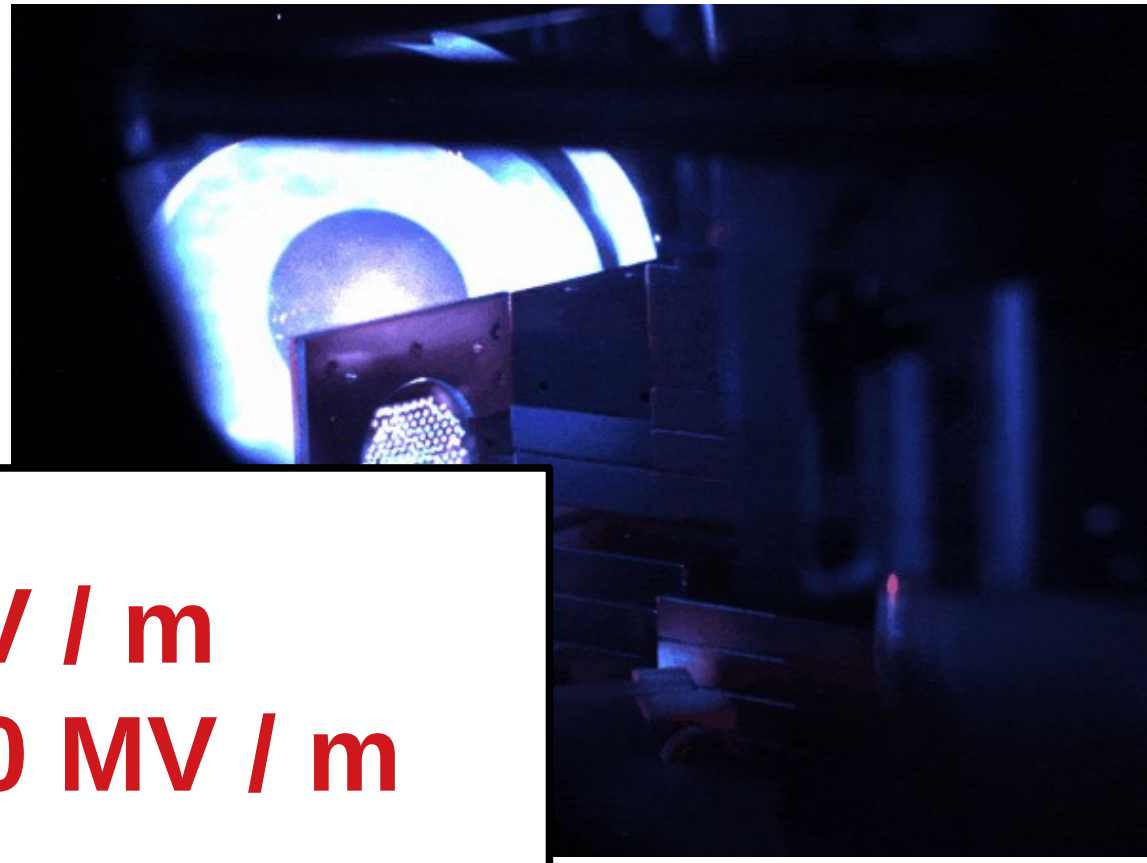

~100 MV / m

→ 1 000 000 MV / m

Laser-Plasma Simulations

Modeling Matter under Extreme Conditions

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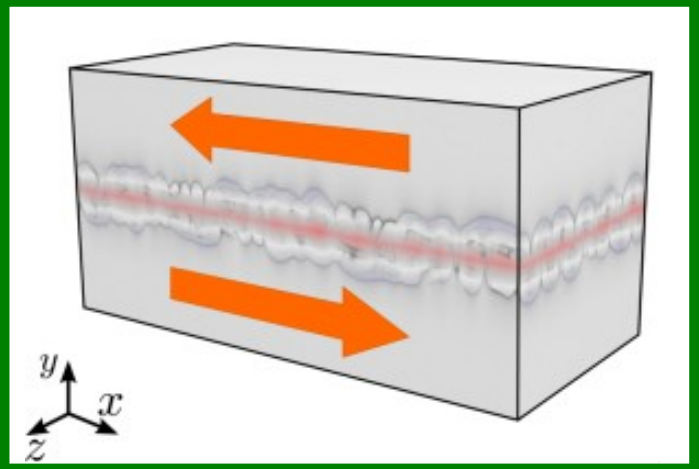
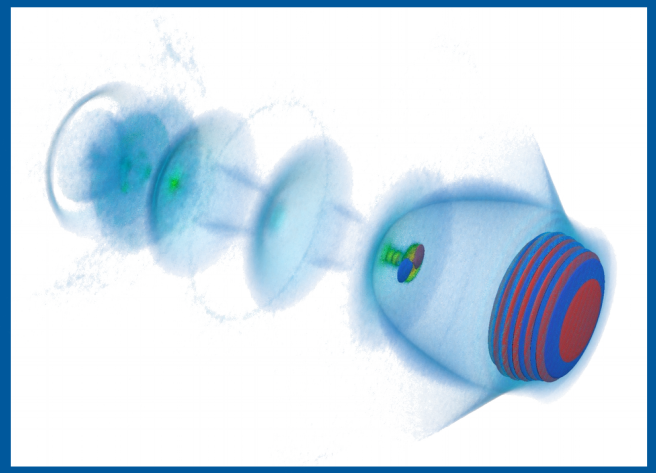
Astrophysics in the Lab

- Astrophysics
- Plasma instabilities



Novel Particle Accelerators

- Compact X-ray, electron and ion beam sources
- Pushing the Energy Frontier
- Matter at extreme conditions



Massively Parallel HPC

- Leadership-scale supercomputing
- Novel algorithms

69 PFlop/s (SP)

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Data Driven Science at Exascale

The Widening Gap between Flop/s and I/O Bandwidth

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SYSTEM SPECS	TITAN	SUMMIT	FRONTIER
Peak Performance	27 PF	200 PF	> 1.5 EF
		1/3x	1/3x
Storage	32 PB, 1 TB/s, Lustre Filesystem	250 PB, 2.5 TB/s, GPFS™	2-4x performance and capacity of Summit's I/O subsystem. Frontier will have near node storage like Summit.

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In situ approaches: **tightly** versus **loosely** coupled workflows

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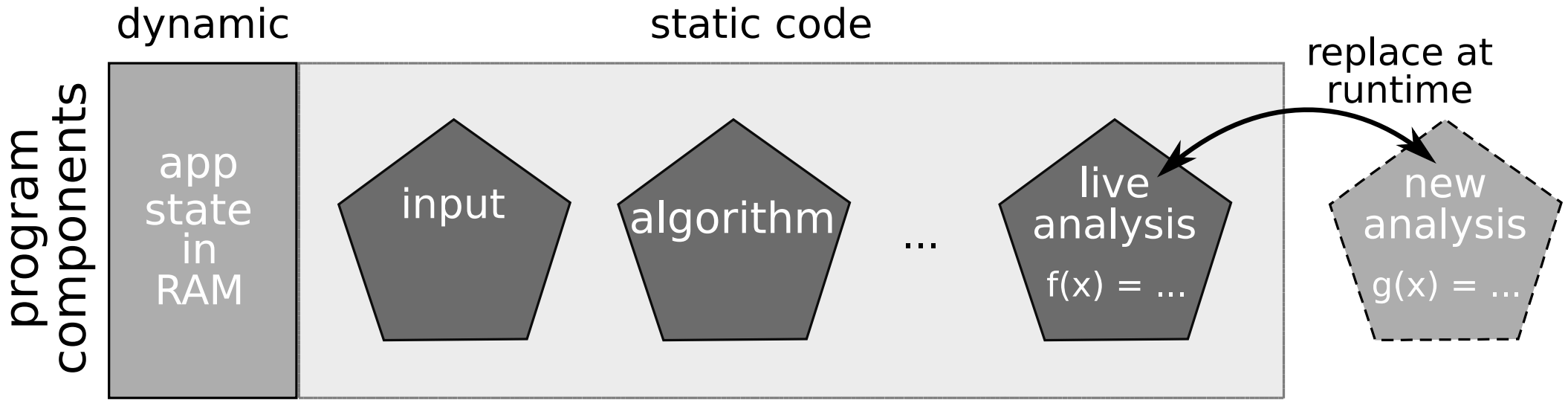
C++ *Feels* too Static

Data is Code is Data



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Interactive C++
An introduction to Cling

How to use Cling

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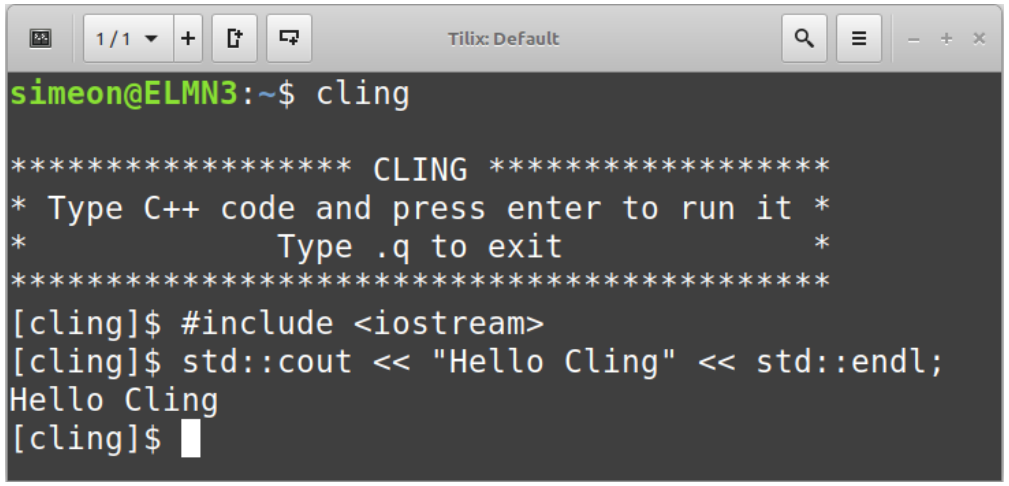
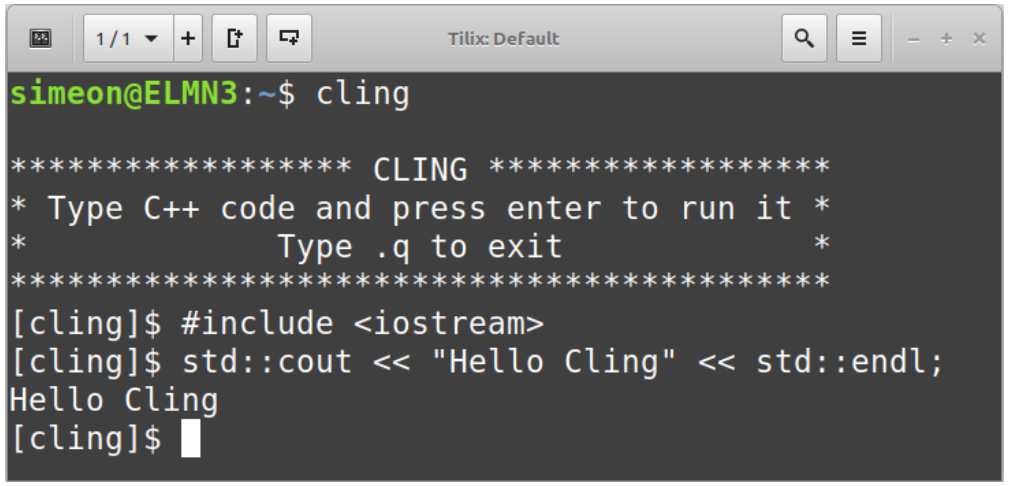


How to use Cling




```
#include "cling/Interpreter/Interpreter.h"

int main(int argc, char *argv){
      auto cling = cling::Interpreter(argc, argv);
      return 0;
}
```

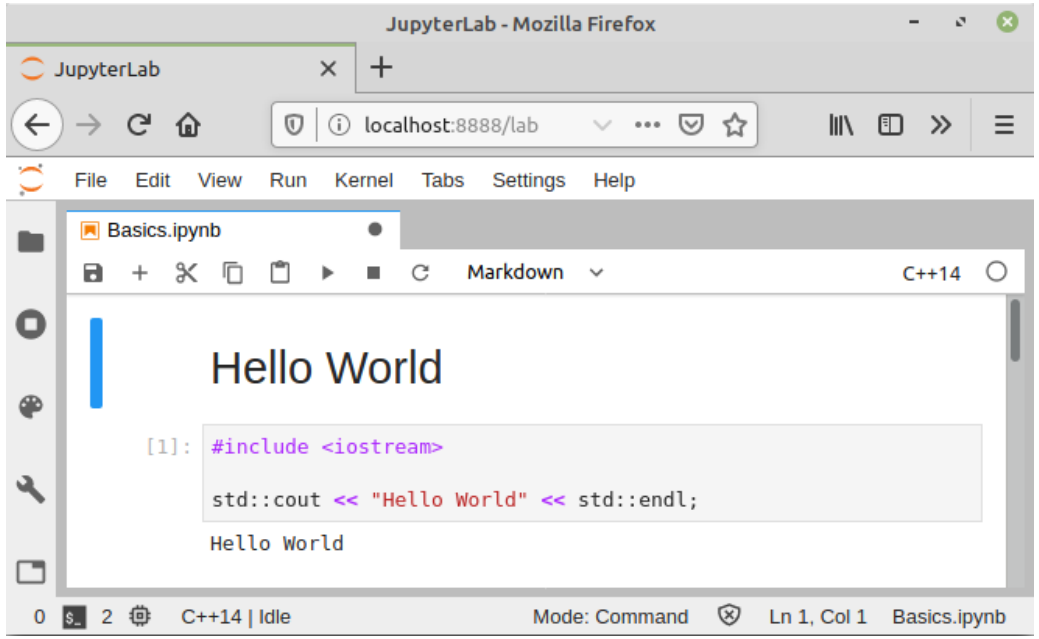
How to use Cling

```
simeon@ELMN3:~$ cling

****************** CLING ******************
* Type C++ code and press enter to run it *
*             Type .q to exit             *
*******************************************
[cling]$ #include <iostream>
[cling]$ std::cout << "Hello Cling" << std::endl;
Hello Cling
[cling]$
```

```
#include "cling/Interpreter/Interpreter.h"

int main(int argc, char *argv){
      auto cling = cling::Interpreter(argc, argv);
      return 0;
}
```



[Jupyter Live Demo]

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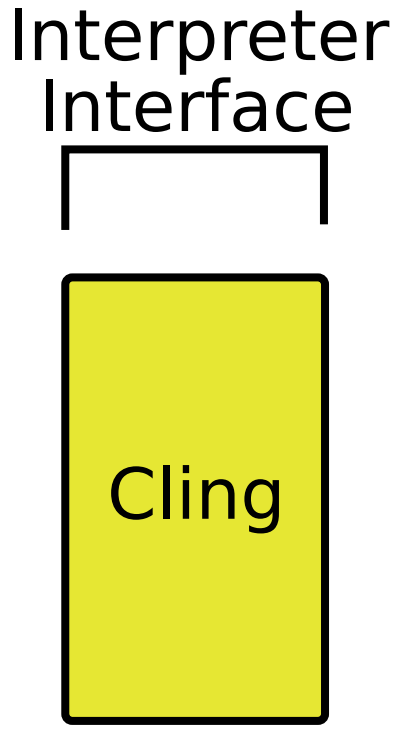
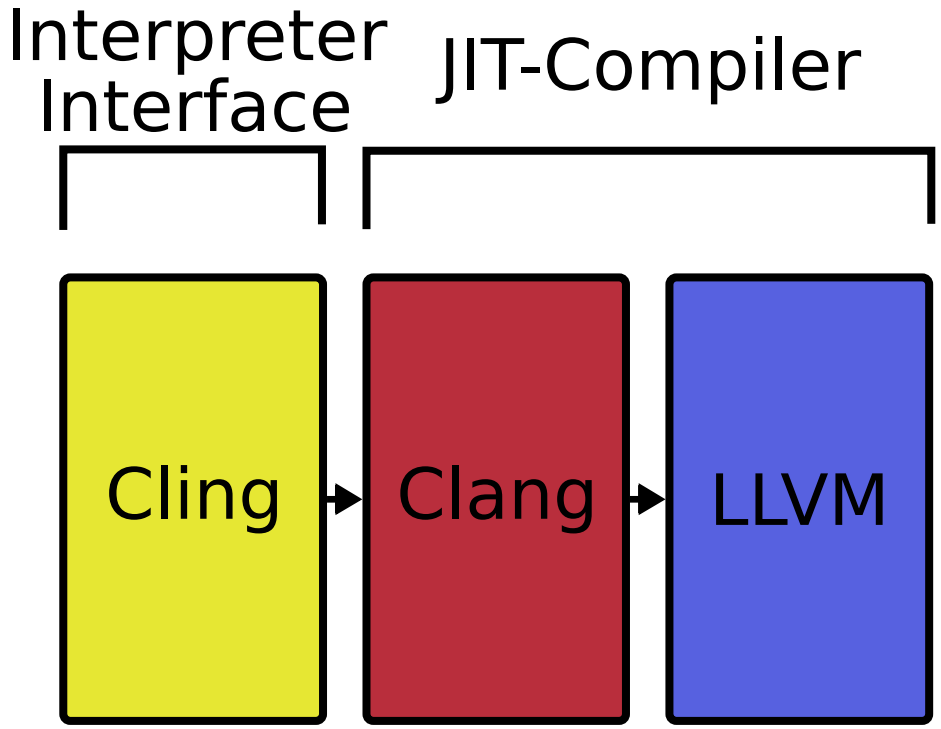
Architecture

Xeus-Cling Jupyter Architecture

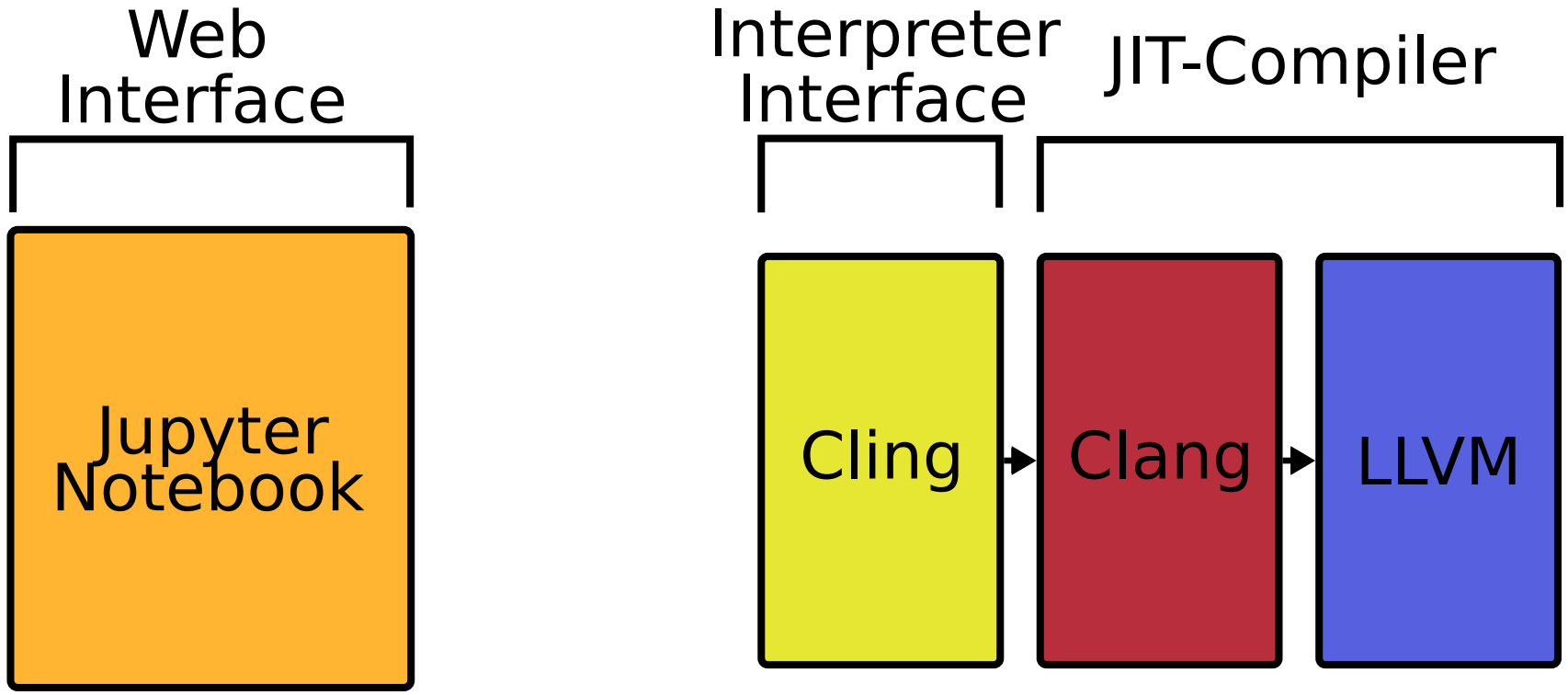
Xeus-Cling Jupyter Architecture



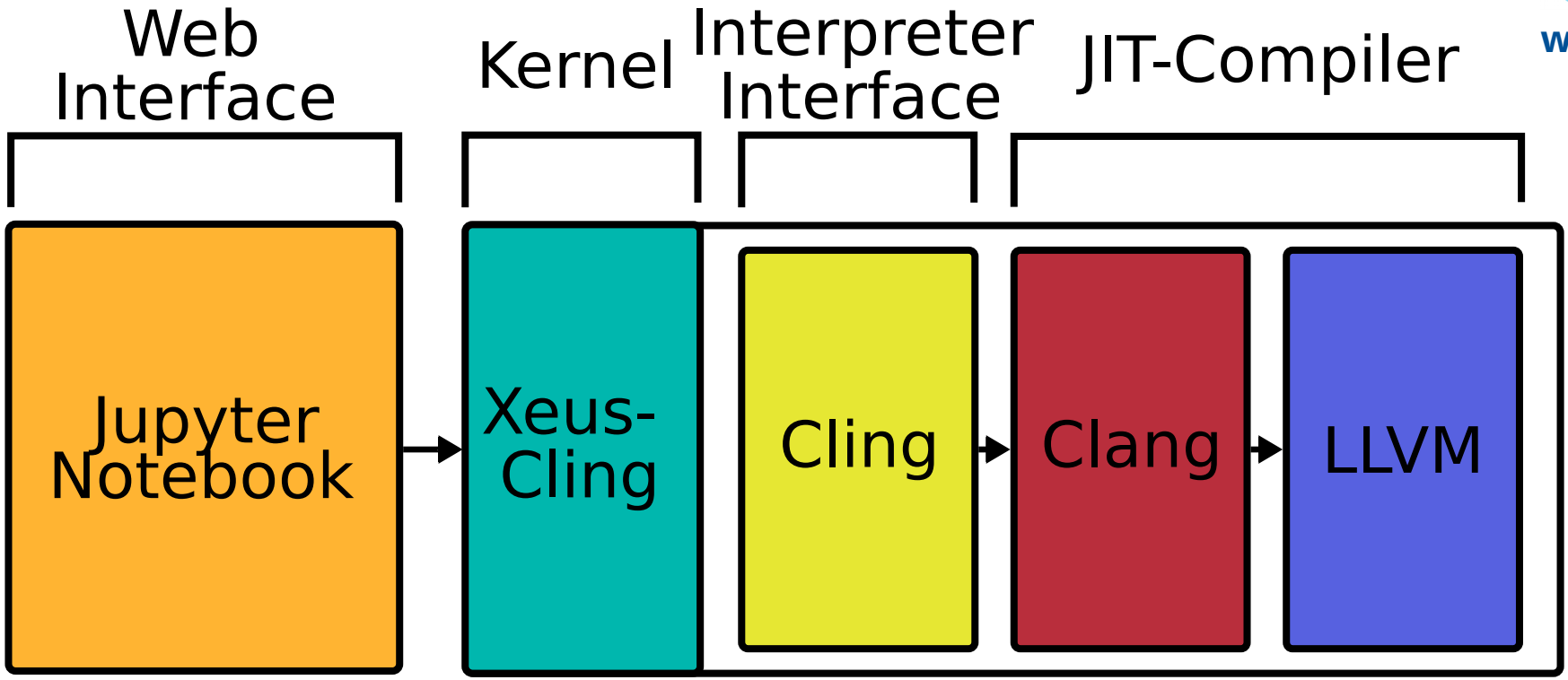
Xeus-Cling Jupyter Architecture



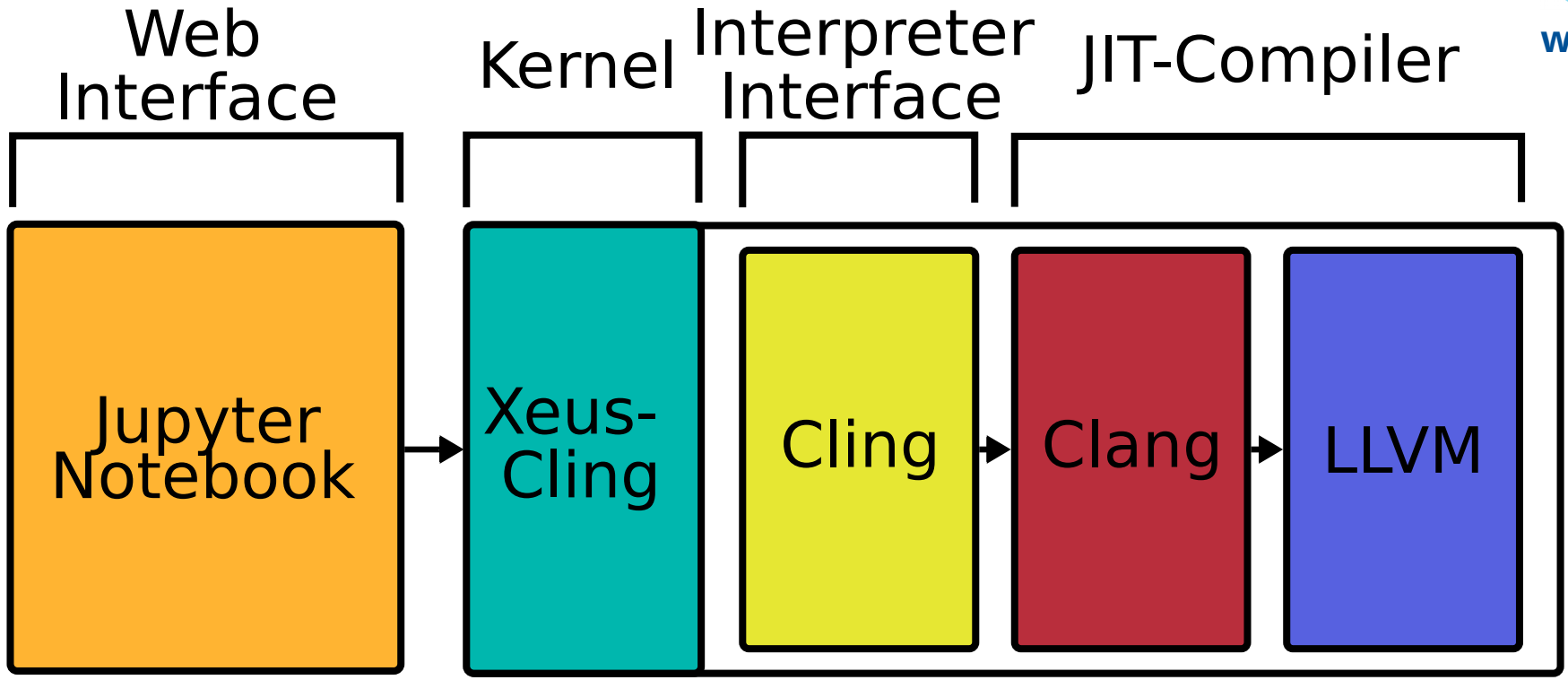
Xeus-Cling Jupyter Architecture



Xeus-Cling Jupyter Architecture



Xeus-Cling Jupyter Architecture



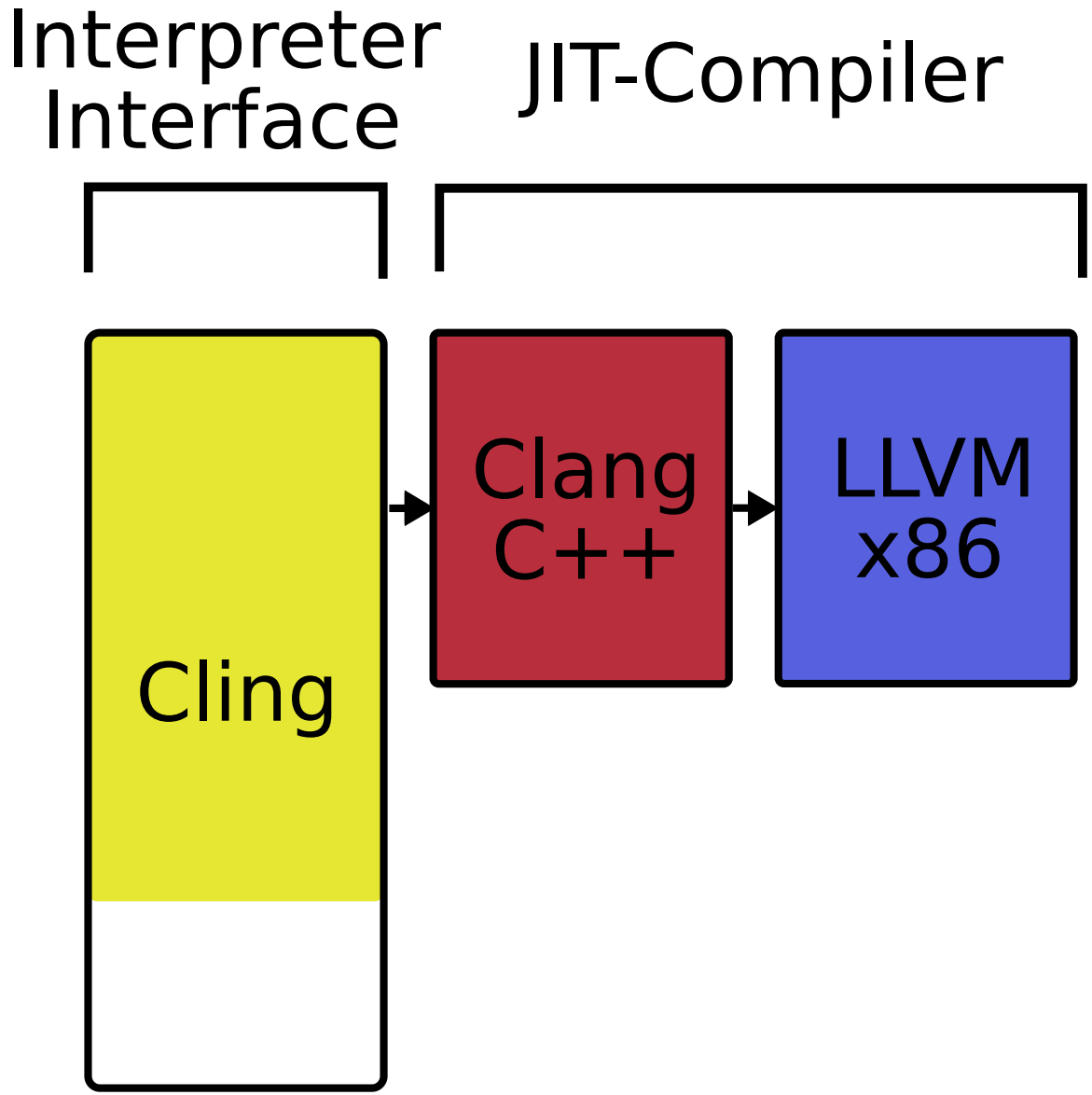
Jupyter

Quant-stack

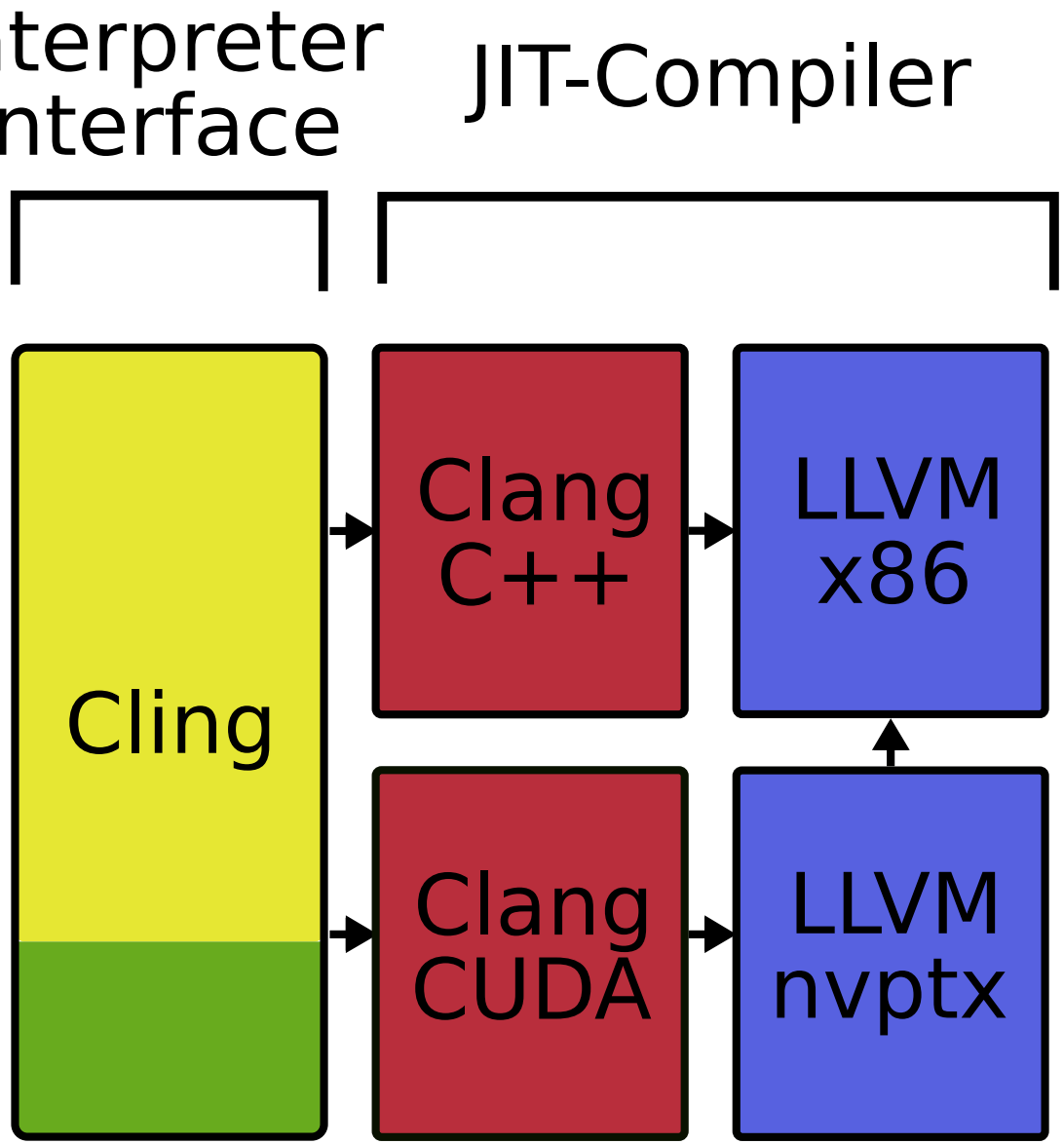
CERN

LLVM

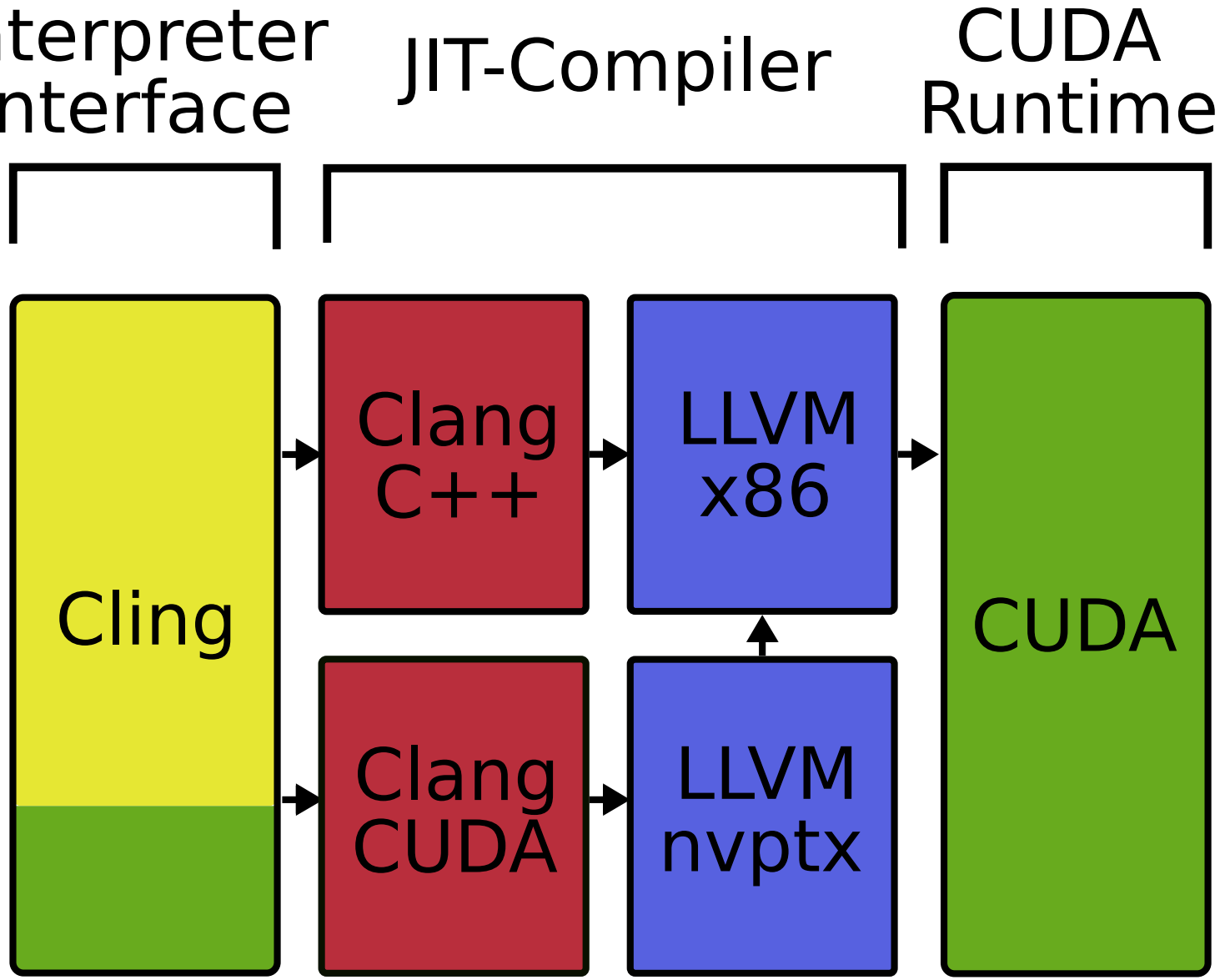
CUDA Extension



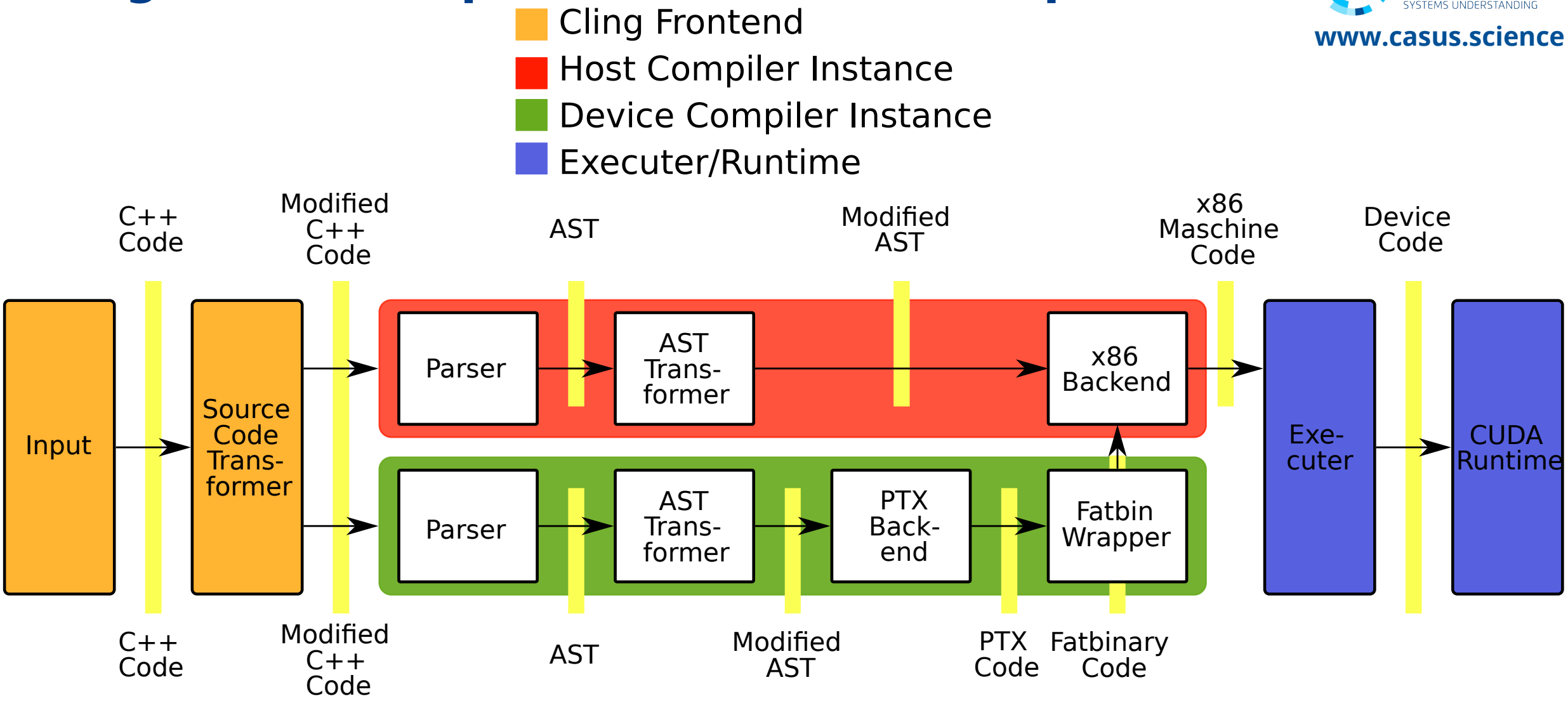
CUDA Extension



CUDA Extension



Cling-CUDA Compiler and Execution Pipeline



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Our Vision for Interactive, GPU-driven Supercomputing

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PIConGPU

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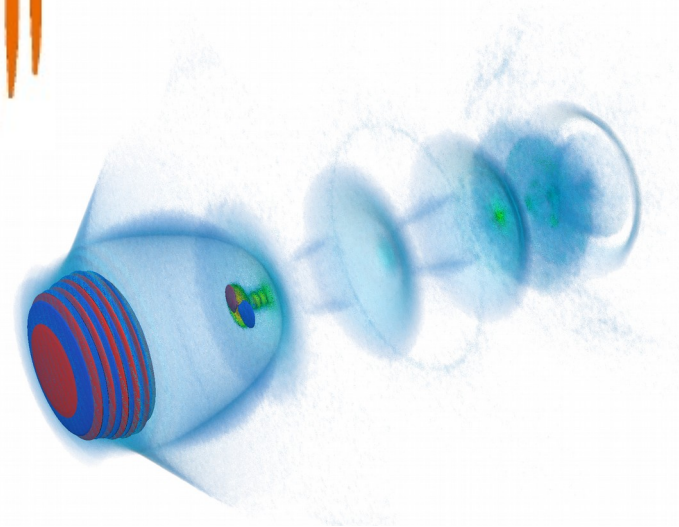

A. Huebl et al., ISC High Performance, pp. 15-29 (2017)
DOI:10.1007/978-3-319-67630-2_2

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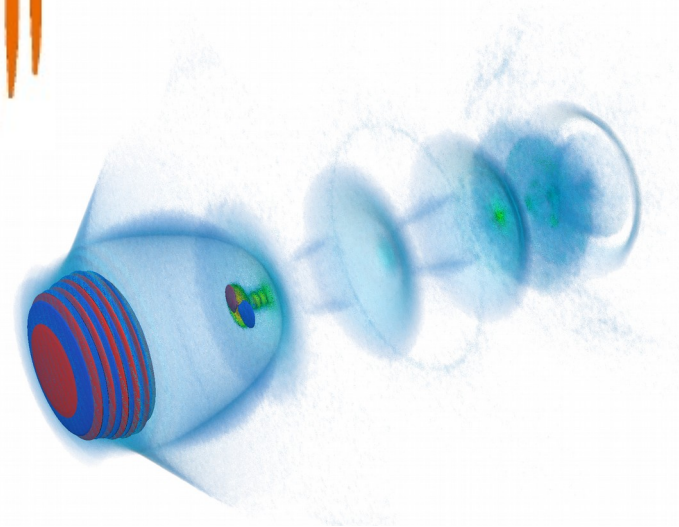

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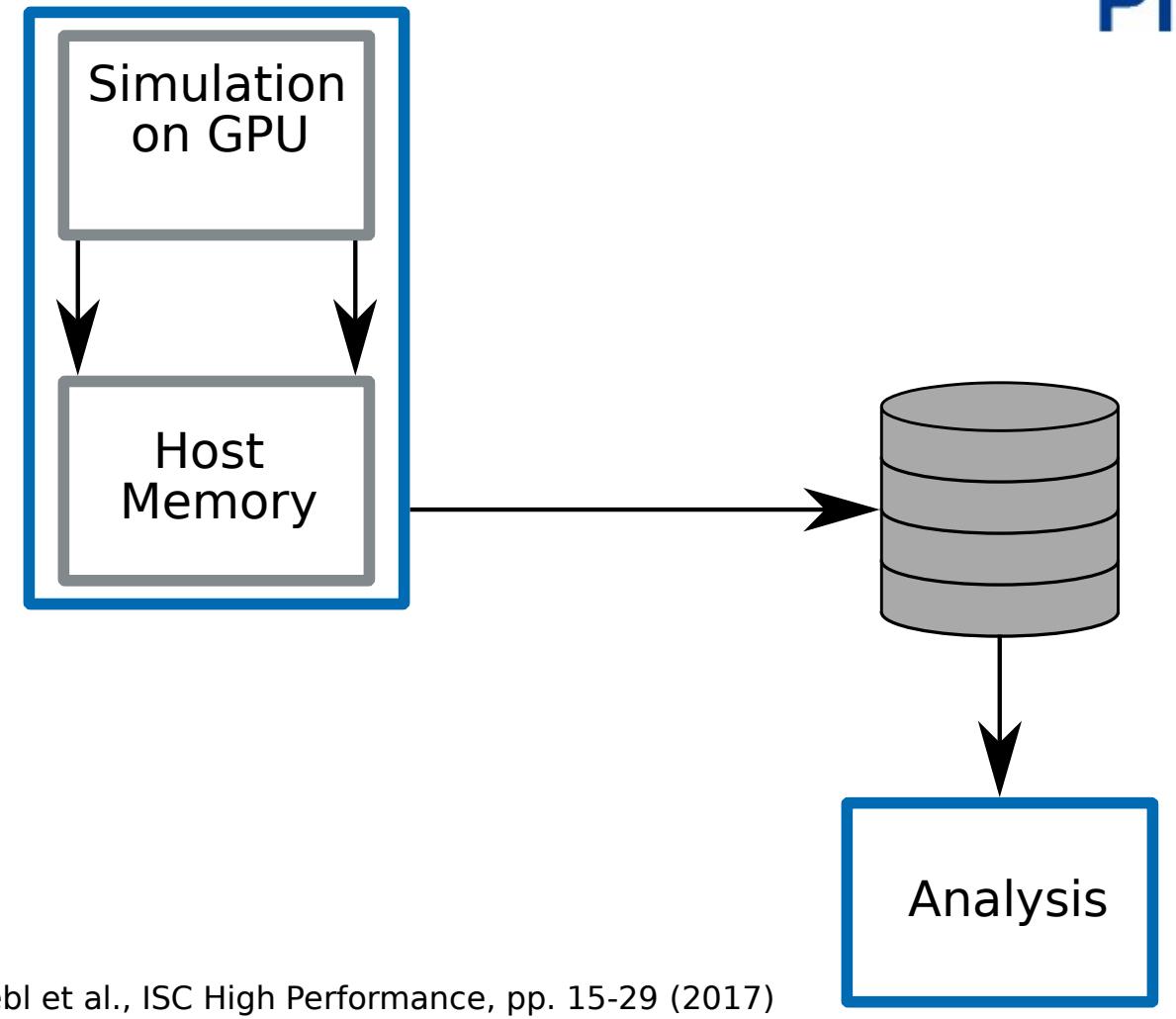

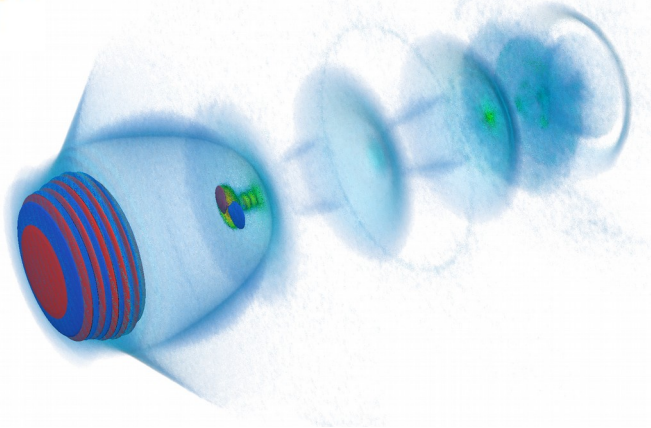

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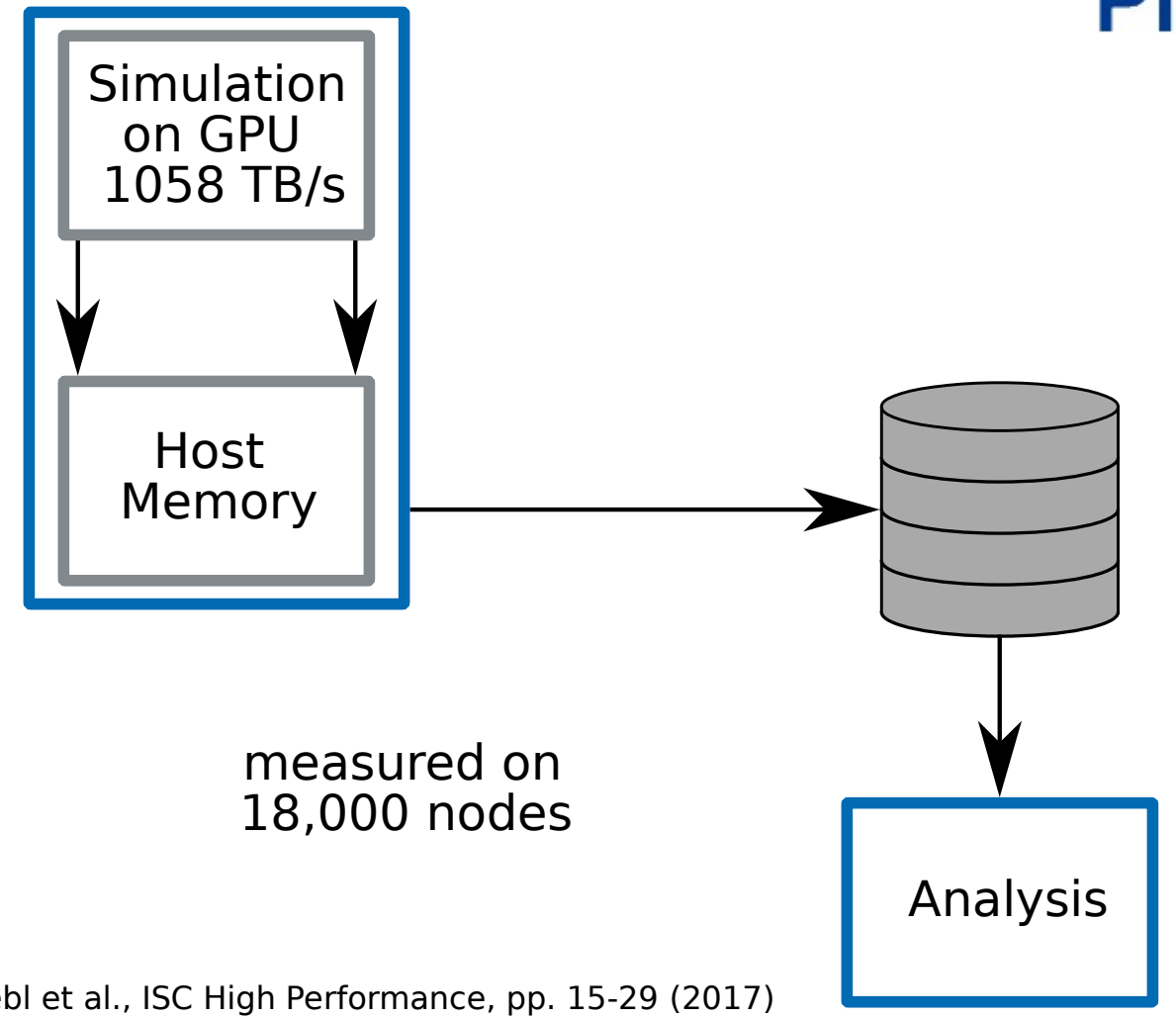
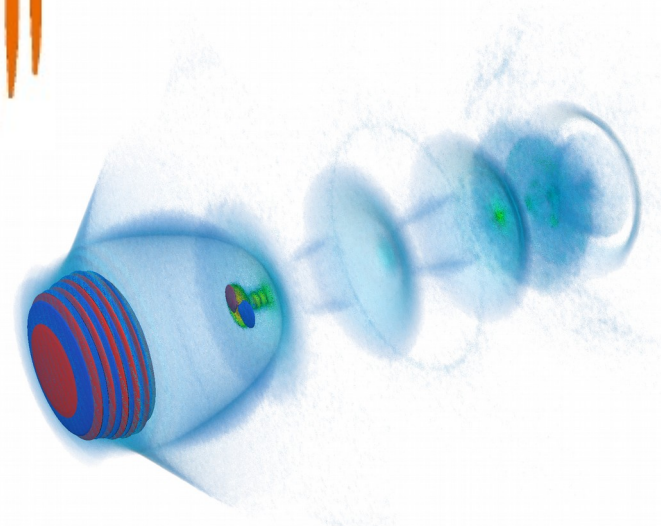


measured on
18,000 nodes



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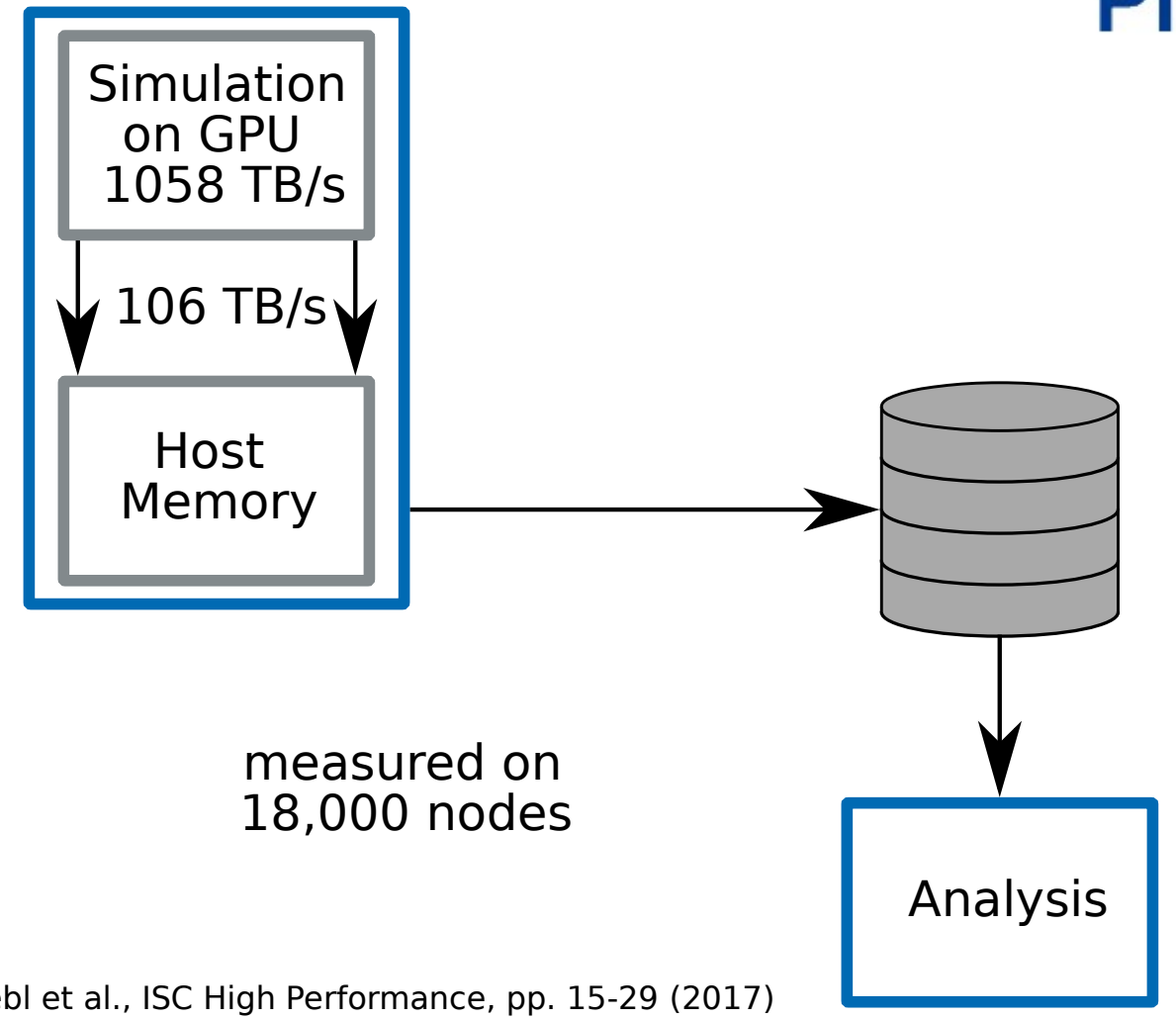

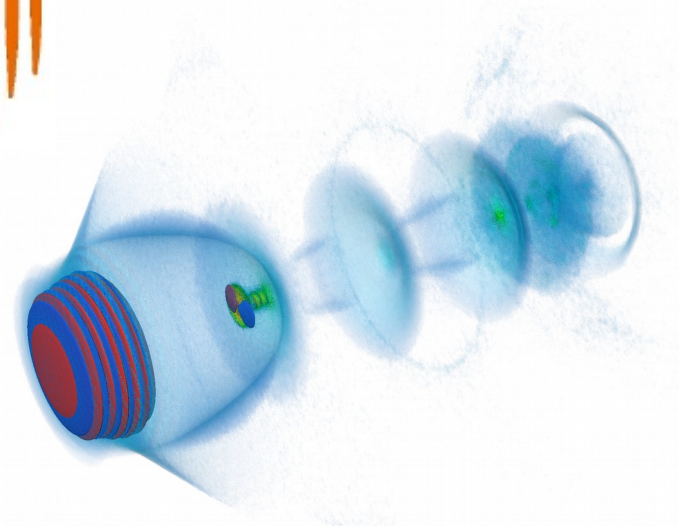

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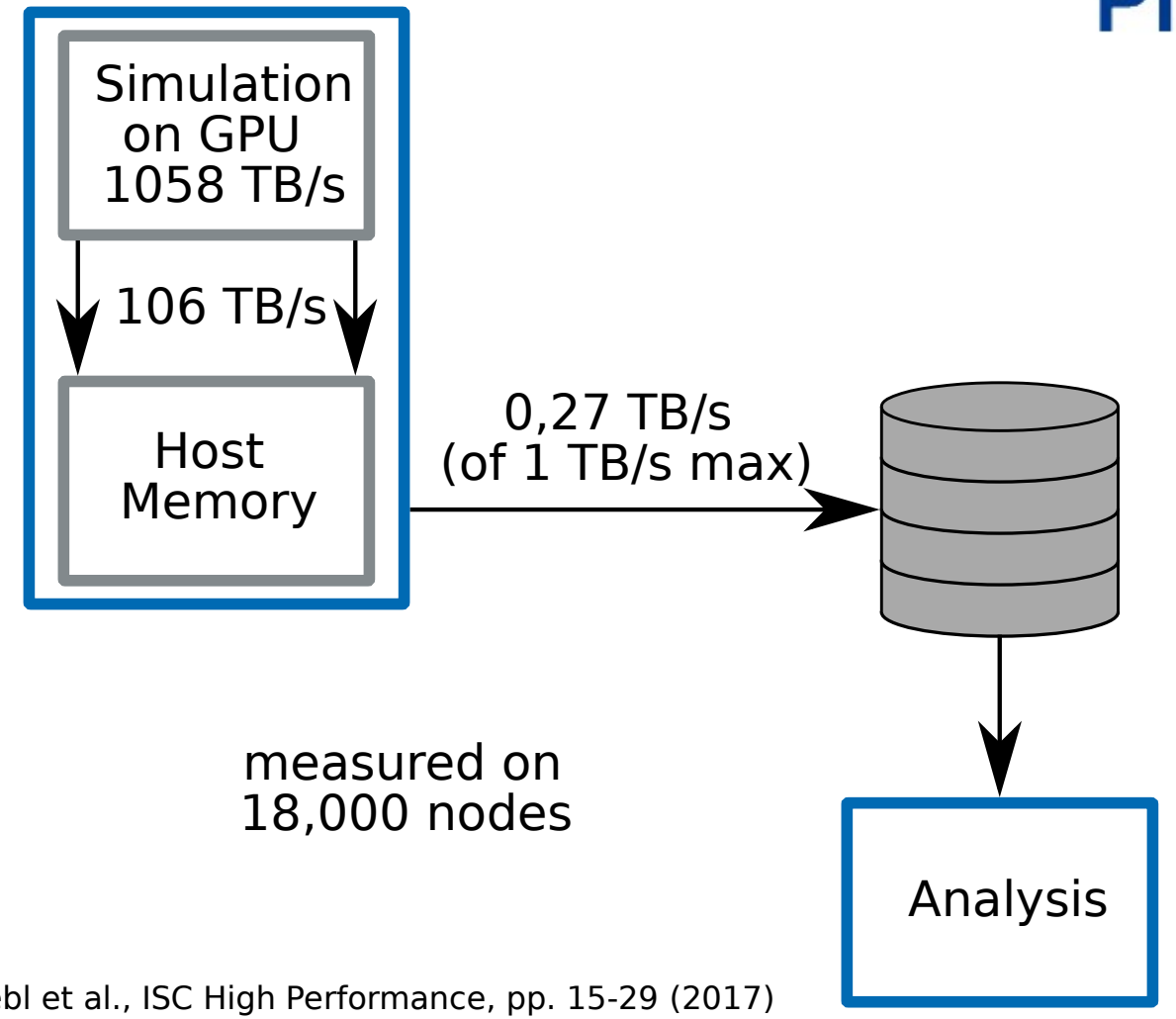

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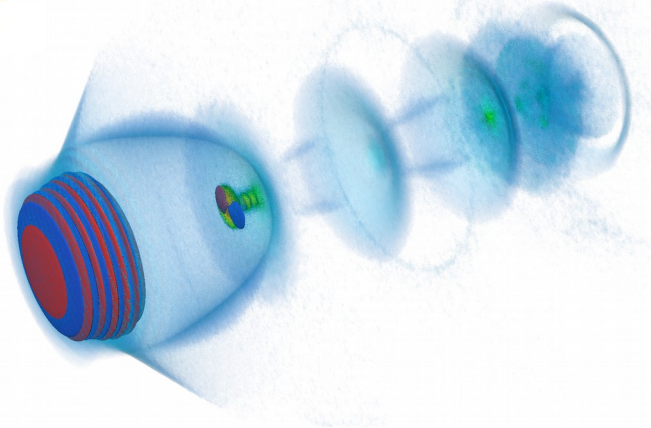

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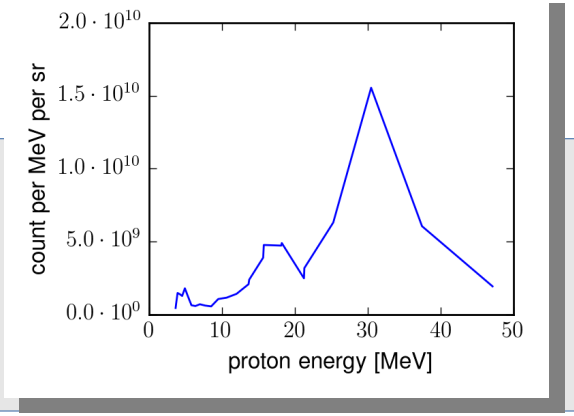
In Situ Data Analysis

Binning of a **spectrogram**
Creation of a **phase space image**



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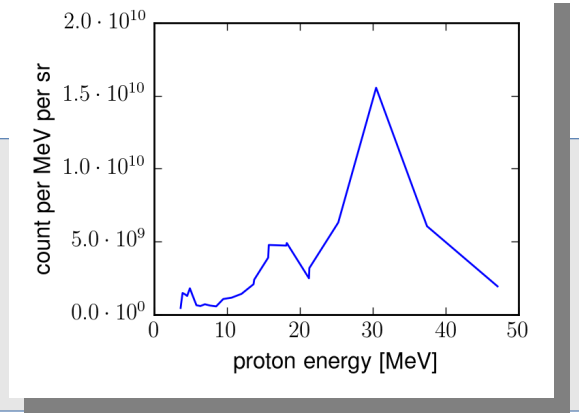
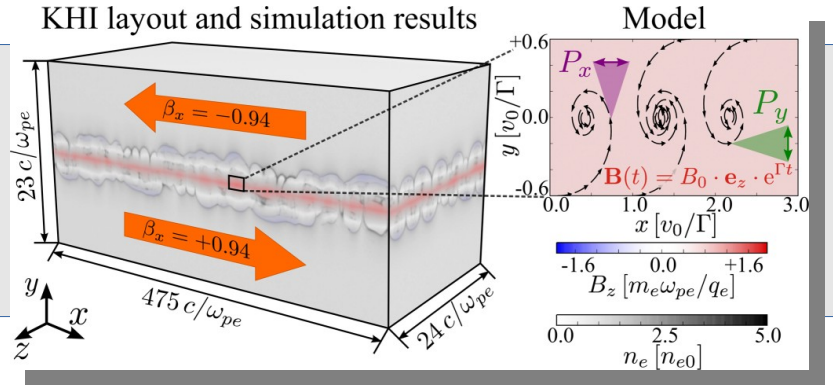


In situ **radiation diagnostics**



A. Huebl et al. (2014), DOI:10.1109/TPS.2014.2327392
R. Pausch et al. (2014, 2017, 2018), DOI:10.1103/PhysRevE.96.013316

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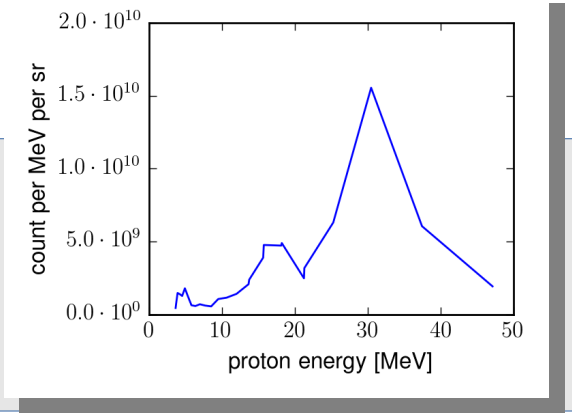
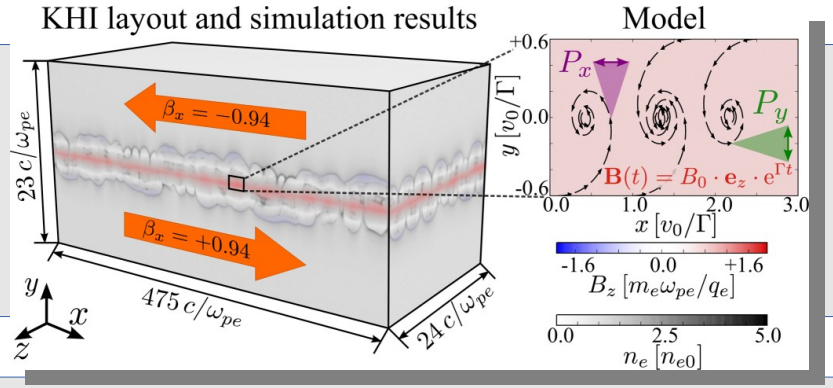
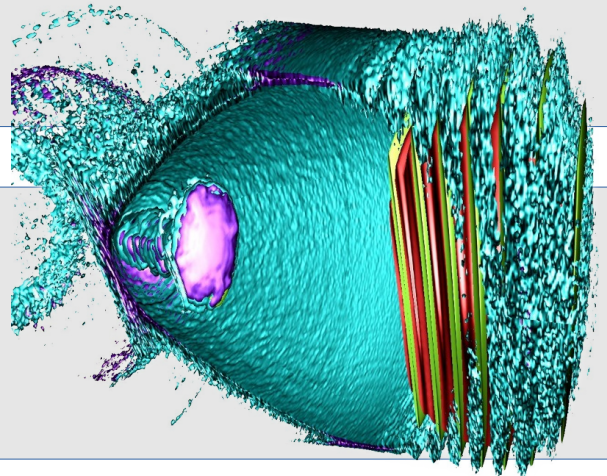


In situ **radiation diagnostics**





Ray-cast or photo-realistic ray-trace
Lossy data **compression**

A. Huebl et al. (2014), DOI:10.1109/TPS.2014.2327392
R. Pausch et al. (2014, 2017, 2018), DOI:10.1103/PhysRevE.96.013316
A. Matthes, A. Huebl et al., ISC'16 (2016), DOI:10.14529/jsfi160403
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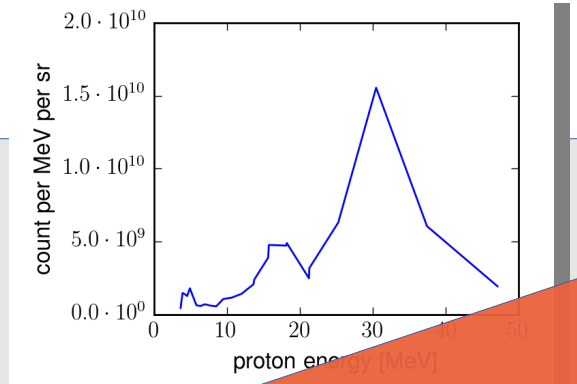
Binning of a **spectrogram**
Creation of a **phase space image**



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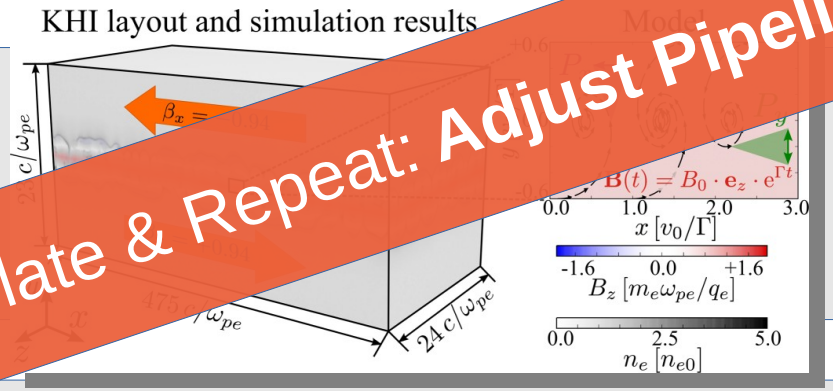
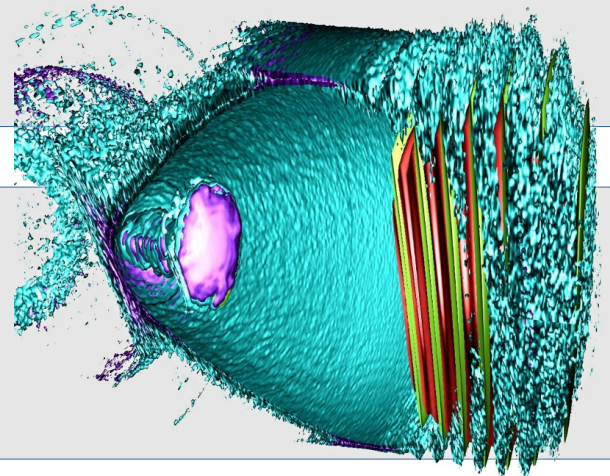


Observe, Correlate & Repeat: Adjust Pipeline

Ray-cast or photo-realistic ray-trace
Lossy data **compression**



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A. Huebl et al., ISC'17 (2017), DOI:10.1007/978-3-319-67630-2_2

Restriction of Analysis

- **I/O bandwidth** limits available data for analysis
- Analysis must be **integrated** into the simulation in-situ

- If you know **what to look** for: pre-configured, fixed analysis
- **Explorative** studies: require **feedback** to the simulation
  - **runtime-dependent** data analysis **kernels**
  - **optimize** kernels on runtime parameters
  - avoid explosion of **parameter space** at compile-time

[Game of Life Demo]

Current development

Cling-CUDA & Jupyter Extension Features

Feature	Status
CUDA Runtime support	✔ (see next slide)
Non-linear program flow	✔
Persistent memory	✔
Template specialization	✔
Includes and linking	✔
REPL Object Representation “`_repr_html_`”	✔
Reflection	✔
Redefinition of kernels	✘
Interaction with web elements	(✔)

Current Development

- Support additional CUDA features
  - `__constant__` device memory
  - global `__device__` variables
  - capture `printf` from kernels

- **Upstream**: features **merged**, follow-up patches submitted
- Implement **redefinition** support for **kernels**
- Support sophisticated C++ libraries in CUDA mode, e.g.
  - **xwidgets**: HTML buttons, sliders ...
  - **Alpaka**: our performance portability layer

Portable programming with Alpaka

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- Alpaka is a C++14 header-only library, providing a GPU/CPU performance-portability layer

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alpaka

```
using Acc1 = alpaka::acc::AccCpuOmp2Blocks<Dim, Idx>;
using Acc2 = alpaka::acc::AccGpuCudaRt<Dim, Idx>;
// ...
auto func = [ ] ALPAKA_FN_ACC ( Acc const & acc) -> void {
                  printf("Hello World\n");
                };

// run Hello World parallel on CPU
alpaka::kernel::exec<Acc1>(queue, workDiv1, func);
// run Hello World parallel on GPU
alpaka::kernel::exec<Acc2>(queue, workDiv2, func);
```

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF
TECHNISCHE UNIVERSITÄT DRESDEN
CBG Max Planck Institute of Molecular Cell Biology and Genetics
HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH – UFZ
Uniwersytet Wrocławski
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Getting started

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  - Linux
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  - Singularity > 3.3, see https://sylabs.io/guides/3.5/user-guide/
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- Nvidia Parallel For All blog post with details and example is work in progress

Source Code

- Cling:
  https://github.com/root-project/cling
- experimental Cling-CUDA features:
  https://github.com/SimeonEhrig/cling
- example notebook and container:
  https://github.com/ComputationalRadiationPhysics/Xeus-Cling-CUDA-Example/tree/master/GOL-function-presentation
- PIConGPU:
  https://github.com/ComputationalRadiationPhysics/picongpu
- Alpaka:
  https://github.com/ComputationalRadiationPhysics/alpaka
- Cling-CUDA diploma thesis (in German)
  https://doi.org/10.5281/zenodo.3713682

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HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

QuantStack
Scientific Computing

CERN

Group: M. Bussmann

S. Corlay, J. Mabille et al., *Jupyter-Xeus*

A. Naumann, et al. *Cling (ROOT)*

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TECHNISCHE UNIVERSITÄT DRESDEN
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