

Teaching Automatic Differentiation with Interactive C++ Jupyter Notebooks

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PRINCETON
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High-level interactive programming languages
like Python simplify differentiable programming

No long edit-compile-run cycles

Simple language syntax

Easy to teach



Jupyter Notebooks are great!

```
[1]: import jax.numpy as jnp
from jax import grad, jit, vmap
from jax import random

key = random.key(0)

[6]: grad_tanh = grad(jnp.tanh)
print(grad_tanh(2.0))
print(grad(grad(grad(jnp.tanh)))(2.0))

0.070650816
0.25265465

[14]: def sigmoid(x):
    return 0.5 * (jnp.tanh(x / 2) + 1)

# Outputs probability of a label being true.
def predict(W, b, inputs):
    return sigmoid(jnp.dot(inputs, W) + b)

# Build a toy dataset.
inputs = jnp.array([[0.52, 1.12, 0.77],
                   [0.88, -1.08, 0.15],
                   [0.52, 0.06, -1.30],
                   [0.74, -2.49, 1.39]])
targets = jnp.array([True, True, False, True])

# Training loss is the negative log-likelihood of the training examples.
def loss(W, b):
    preds = predict(W, b, inputs)
    label_probs = preds * targets + (1 - preds) * (1 - targets)
    return -jnp.sum(jnp.log(label_probs))

# Initial
key, W_ke
[5]: # Differentiate 'loss' with respect to the first positional argument:
W_grad = grad(loss, argnum=0)(W, b)
print('W_grad', W_grad)

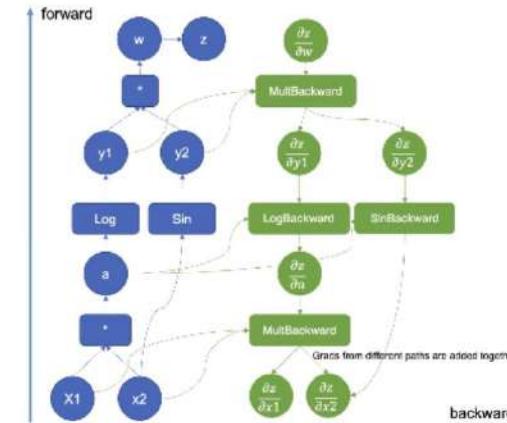
# Since argnum=0 is the default, this does the same thing:
W_grad = grad(loss)(W, b)
print('W_grad', W_grad)

# But we can choose different values too, and drop the keyword:
b_grad = grad(loss, 1)(W, b)
print('b_grad', b_grad)

# Including tuple values
W_grad, b_grad = grad(loss, (0, 1))(W, b)
print('W_grad', W_grad)
print('b_grad', b_grad)

W_grad [-0.433146 -0.7354665 -1.2598922]
W_grad [-0.433146 -0.7354665 -1.2598922]
b_grad -0.6901776
W_grad [-0.433146 -0.7354665 -1.2598922]
b_grad -0.6901776
```

```
[1]: import torch
```



```
[2]: x = torch.tensor([0.5, 0.75], requires_grad=True)
y = torch.log(x[0] * x[1]) * torch.sin(x[1])
y.backward()
x.grad
```

```
[2]: tensor([1.3633, 0.1912])
```

Sources:

<https://docs.jax.dev/en/latest/jax-101.html>

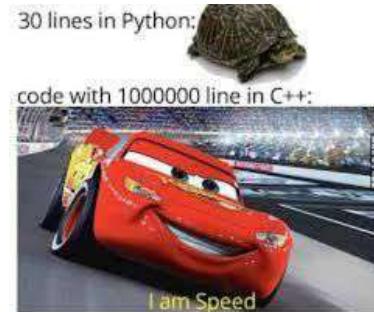
<https://pytorch.org/blog/overview-of-pytorch-autograd-engine/>

C++ still (mostly) the language of choice for performance-oriented scientific software

Long edit-compile-run cycles

Complex language syntax

Not interactive



CoDiPack



clad

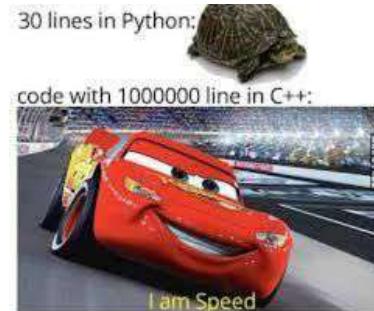


C++ still (mostly) the language of choice for performance-oriented scientific software

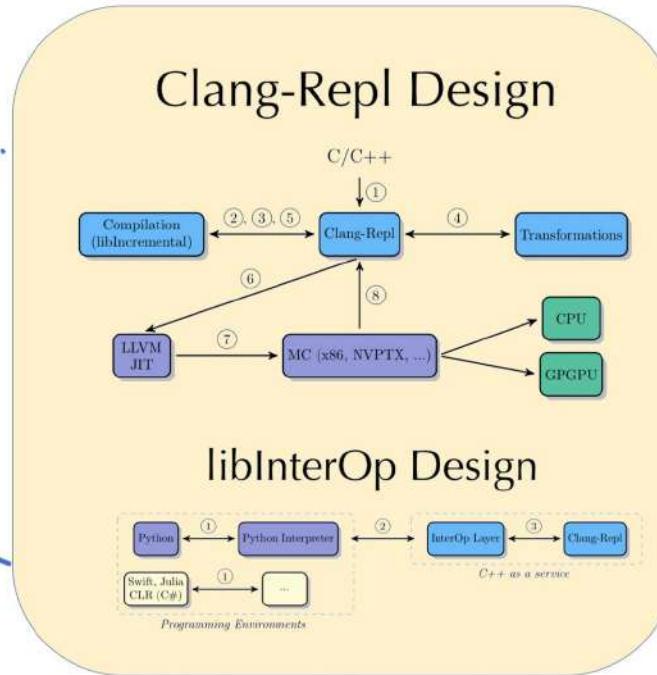
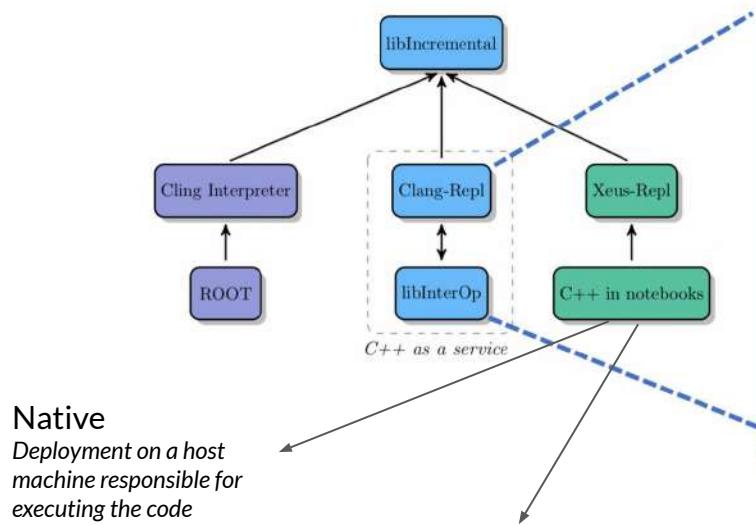
~~Long edit compile run cycles~~

Complex language syntax

~~Not interactive~~



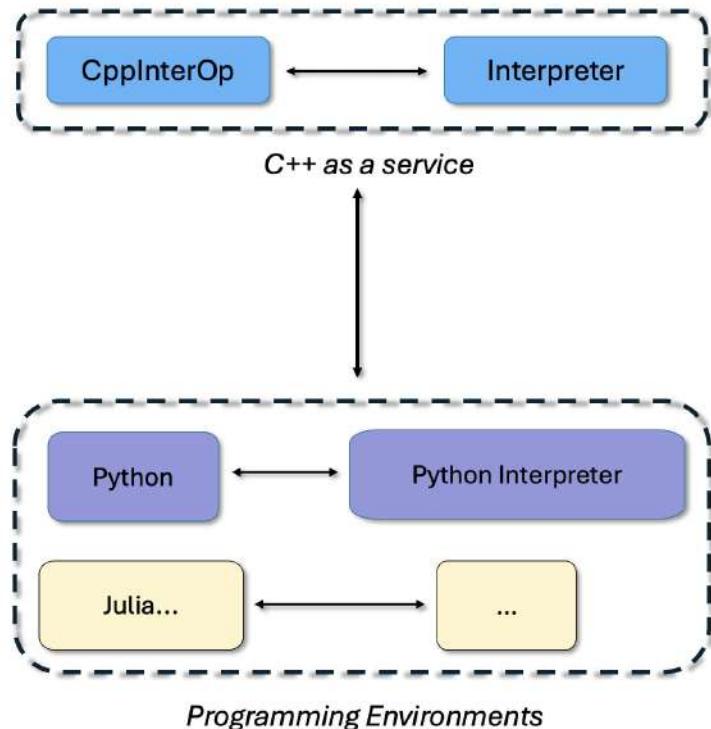
<https://xeus-cpp.readthedocs.io/en/latest/>
<https://clang.llvm.org/docs/ClangRepl.html>



A lightweight layer on top of LLVM that provides efficient, on-demand reflection and a JIT compiler

Easily embeds Clang and LLVM as a libraries in your framework

Supports downstream tools that utilize interactive C++ by using the compiler as a service.



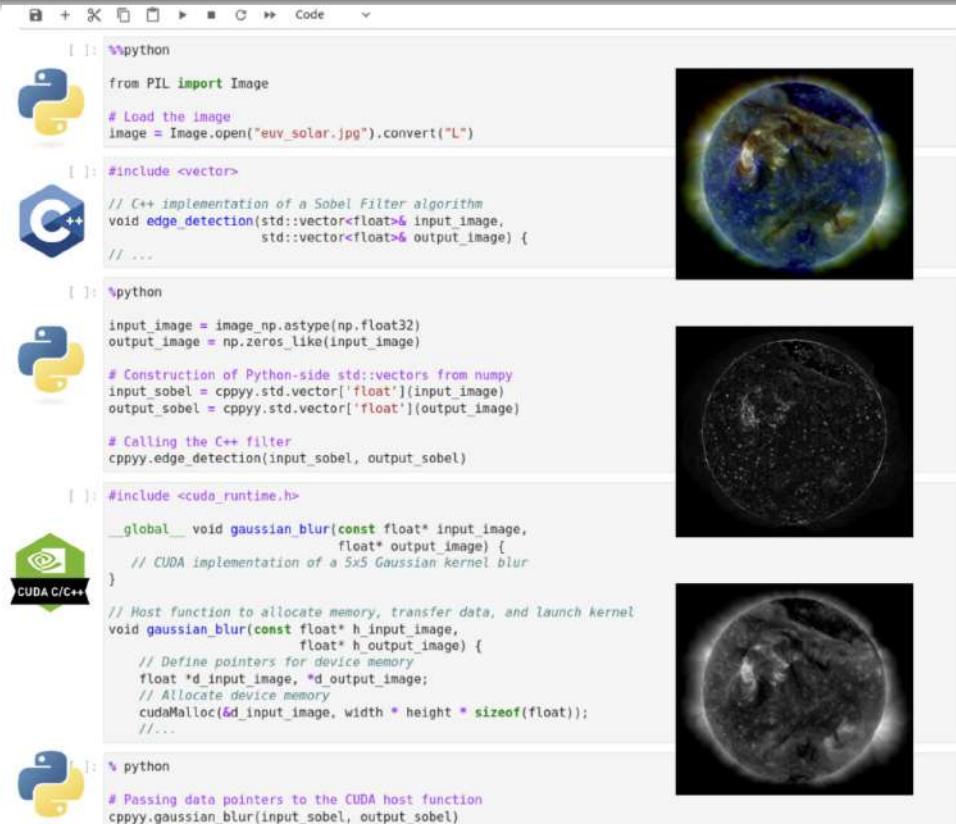
<https://github.com/compiler-research/CppInterOp>

Rudimentary WebAssembly version (no included AD libraries)
here: <https://compiler-research.org/CppInterOp/lab/index.html>

Please reach out for a reproducible docker container of the
demo shown today

- Integration of Python plugin based on `cppyy`
- Allows you to hop between the optimal language for each task
- Script host and device code on the fly
- Automatically bound to Python runtime

Possible, currently not in mainline



The screenshot shows a Jupyter Notebook interface with three code cells. The first cell is Python code using the PIL library to open an image and convert it to grayscale. The second cell is C++ code for edge detection using the `edge_detection` function from `cppyy`. The third cell is Python code that calls the C++ function and then applies a Gaussian blur using CUDA. To the right of the notebook are three images: a color image of the Earth, a grayscale image of a celestial body, and a grayscale image of a complex structure.

```
%python
from PIL import Image
# Load the image
image = Image.open("euv_solar.jpg").convert("L")

%include <vector>
// C++ implementation of a Sobel Filter algorithm
void edge_detection(std::vector<float>& input_image,
                     std::vector<float>& output_image) {
    // ...
}

%python
input_image = image_np.astype(np.float32)
output_image = np.zeros_like(input_image)

# Construction of Python-side std::vectors from numpy
input_sobel = cppyy.std.vector['float'](input_image)
output_sobel = cppyy.std.vector['float'](output_image)

# Calling the C++ filter
cppyy.edge_detection(input_sobel, output_sobel)

%include <cuda_runtime.h>
__global__ void gaussian_blur(const float* input_image,
                             float* output_image) {
    // CUDA implementation of a 5x5 Gaussian kernel blur
}

// Host function to allocate memory, transfer data, and launch kernel
void gaussian_blur(const float* h_input_image,
                    float* h_output_image) {
    // Define pointers for device memory
    float *d_input_image, *d_output_image;
    // Allocate device memory
    cudaMalloc(&d_input_image, width * height * sizeof(float));
    //...
```

A. Jomy, B. Kundu et al, CppInterOp: Advancing Interactive C++ for High Energy Physics, <https://doi.org/10.1051/epiconf/202533701165>

Thank You!