Workshop on Scalable Physics-Informed Neural Networks

Session 2 – Introduction to JAX

Dr. Ben Moseley

Scalable
Scientific Machine Learning
Lab

IMPERIAL

Poll

Scalability challenges of PINNs

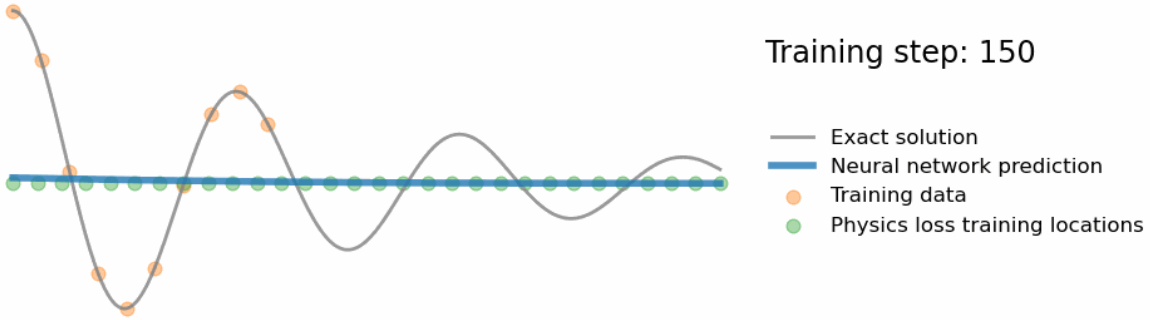
Advantages of PINNs

- **Mesh-free**
- Can solve forward and inverse problems, and seamlessly incorporate **observational data**
- Mostly **unsupervised**
- Can perform well for high-dimensional PDEs

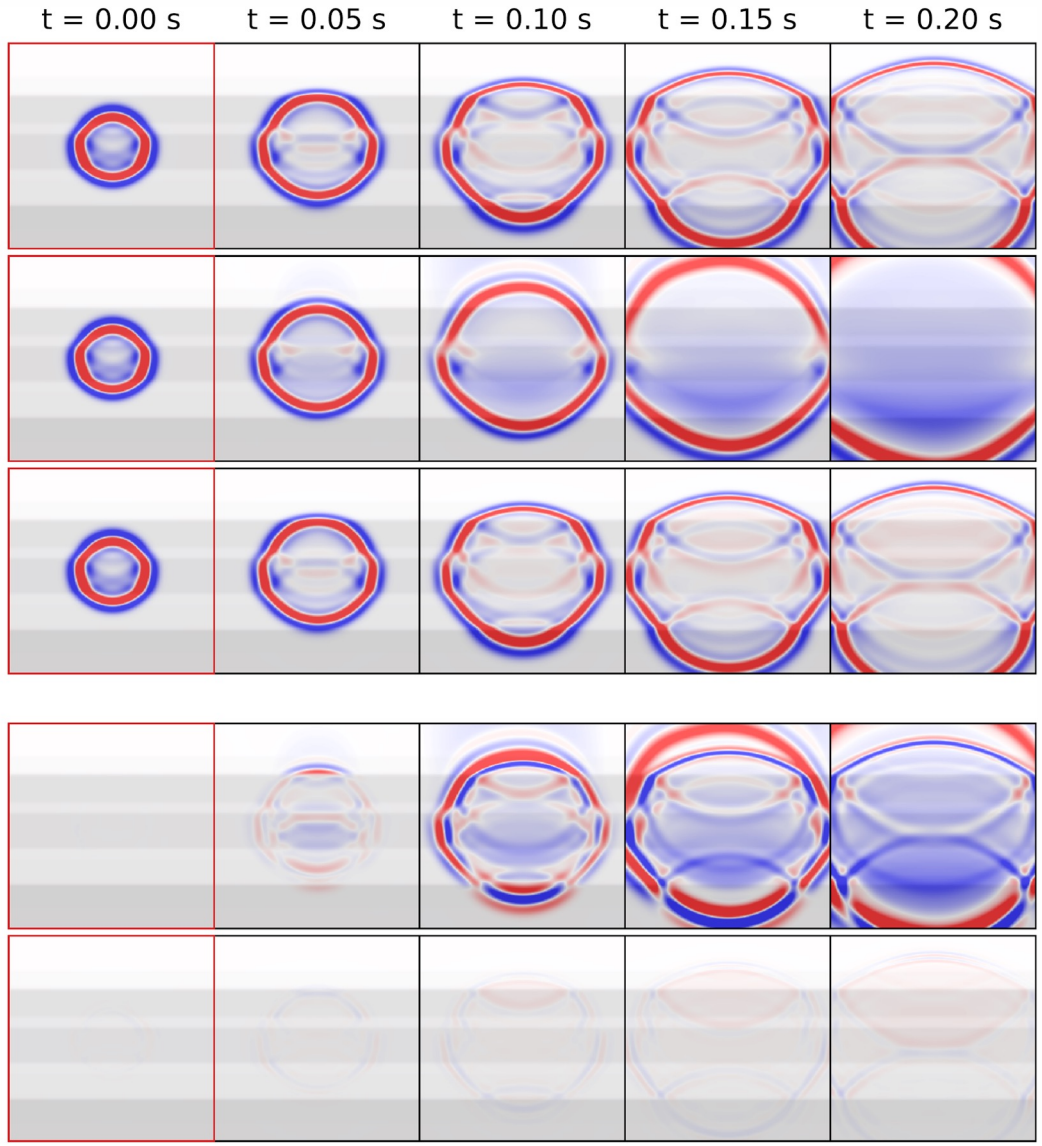
Limitations of PINNs

- **Computational cost** often high (especially for forward-only problems)
- Can be hard to **optimise**
- Challenging to **scale** to high-frequency, multi-scale problems

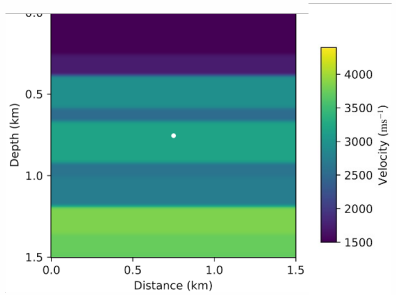
(although many PINN improvements exist!)



PINNs for solving wave equation



Velocity model, $c(x, y)$

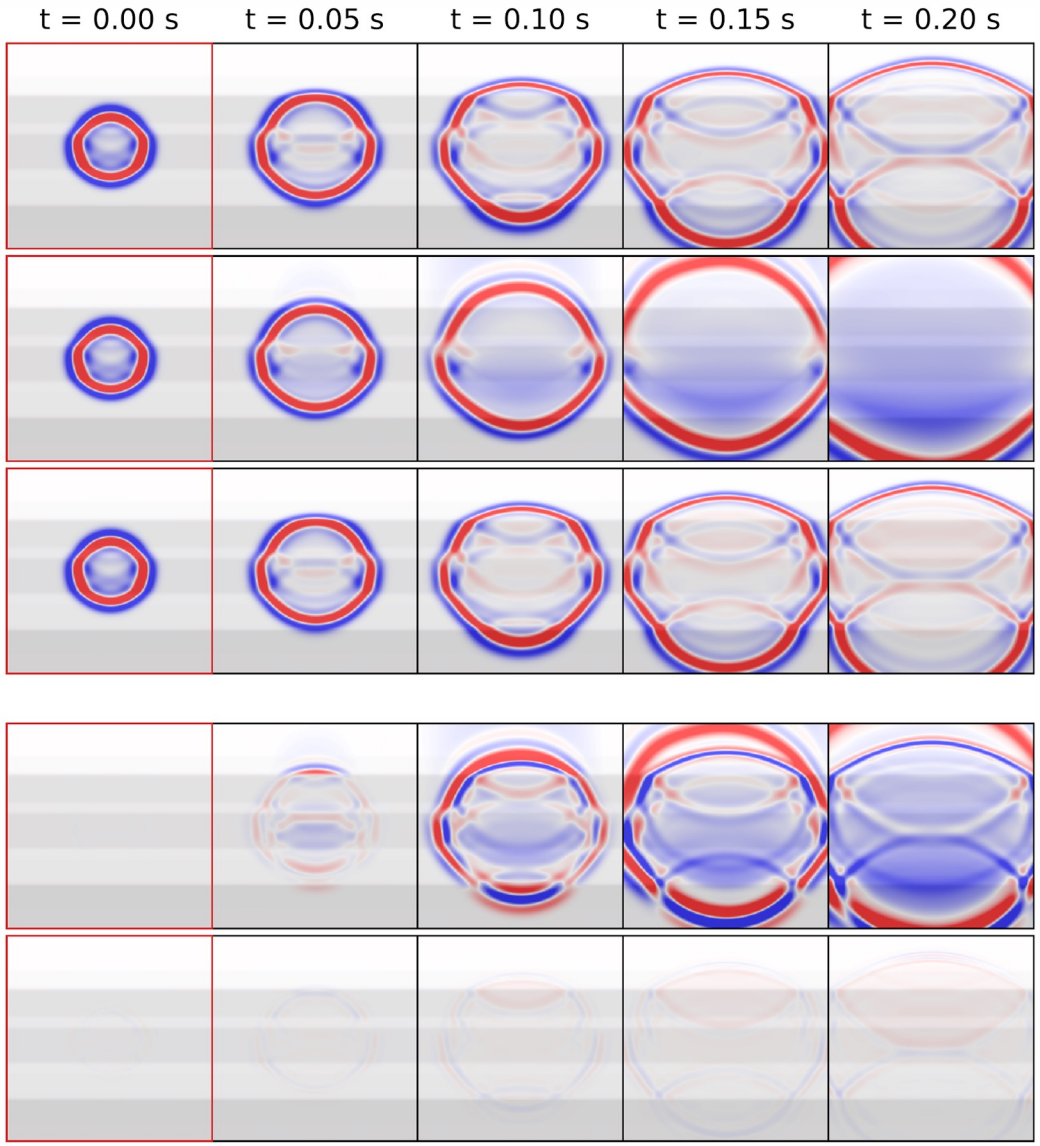


Moseley et al, Solving the wave equation with physics-informed deep learning, ArXiv (2020)

Mini-batch size $N_b = N_p = 500$ (random sampling)
Fully connected network with 10 layers, 1024 hidden units
Softplus activation
Adam optimiser

⚠ **Training time ~1 hr on a GPU!**

PINNs for solving wave equation



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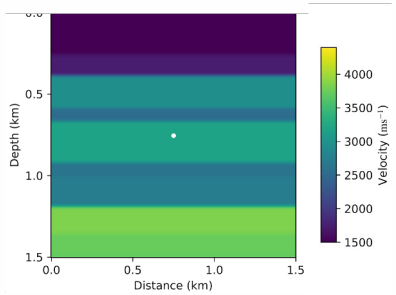

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Mini-batch size $N_b = N_p = 500$ (random sampling)
Fully connected network with 10 layers, 1024 hidden units
Softplus activation
Adam optimiser

⚠ **Training time ~1 hr on a GPU!**

⚠ **PINNs need to be retrained for each new I/BC !**

Can physics-informed neural networks (PINNs) beat finite difference / finite element methods?

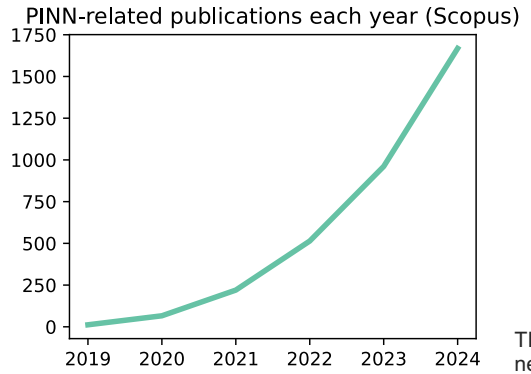
Can physics-informed neural networks beat the finite element method?

Tamara G Grossmann, Urszula Julia Komorowska, Jonas Latz, Carola-Bibiane Schönlieb

IMA Journal of Applied Mathematics, Volume 89, Issue 1, January 2024, Pages 143–174, https://doi.org/10.1093/imamat/hxae011
Published: 23 May 2024 **Article history**

7. Discussion and conclusions

After having investigated each of the PDEs on its own, let us now discuss and draw conclusions from the results as a whole. Considering the solution time and accuracy, PINNs are not able to beat FEM in our study. In all the examples that we have studied, the FEM solutions were faster at the same or at a higher accuracy.



TITLE-ABS-KEY ("physics-informed neural network" OR "physics informed neural network")

Solving inverse problems in physics by optimizing a discrete loss: Fast and accurate learning without neural networks

Petr Karnakov, Sergey Litvinov, Petros Koumoutsakos Author Notes

PNAS Nexus, Volume 3, Issue 1, January 2024, pgae005, https://doi.org/10.1093/pnasnexus/pgae005
Published: 11 January 2024 **Article history**

Conclusion

We introduce the ODIL framework for solving inverse problems for PDEs by casting their discretization as an optimization problem and applying optimization techniques that are widely available in machine-learning software. The concept of casting the PDE as is closely related to the neural network formulations proposed by (15–17) and recently revived as PINNs. However, the fact that we use the discrete approximation of the equations allows for ODIL to be orders of magnitude more efficient in terms of computational cost and accuracy compared to the PINN for which complex flow problems "remain elusive" (71).

Workshop overview

Session 1: **Intro to PINNs**

- *Lecture* (1 hr): Introduction to SciML and PINNs
- *Code-along* (30 min): Training a PINN in PyTorch

Session 2: **Accelerating PINNs with JAX**

- *Lecture* (30 min): Introduction to JAX
- *Practical* (1 hr): Introduction to JAX and coding a PINN from scratch in JAX

Session 3: **Accelerating PINNs with domain decomposition and NLA**

- *Lecture* (30 min): Challenges with PINNs and improving their performance with domain decomposition and numerical linear algebra
- *Practical* (1 hr): Coding finite basis PINNs and extreme learning machine FBPINNs in JAX

Introduction to JAX

What is JAX?

JAX = accelerated array computation + program transformation

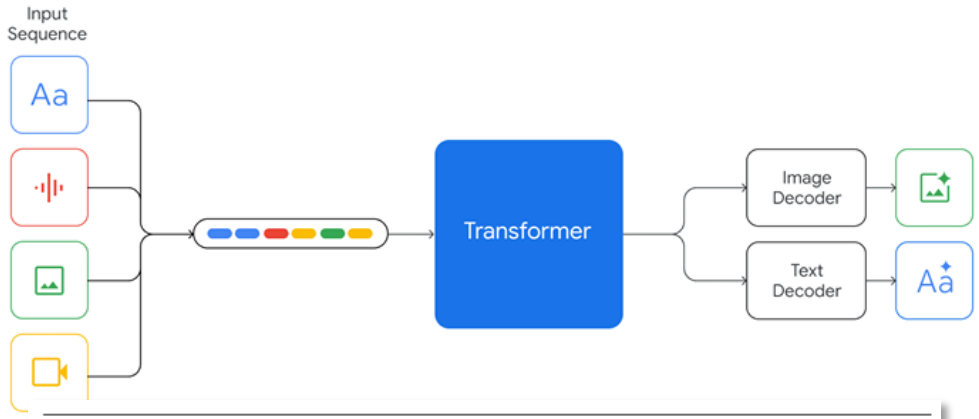
.. Which is incredibly useful for high-performance numerical computing and large-scale (Sci)ML

JAX in ML

Google DeepMind

Gemini: A Family of Highly Capable Multimodal Models

Gemini Team, Google[1]

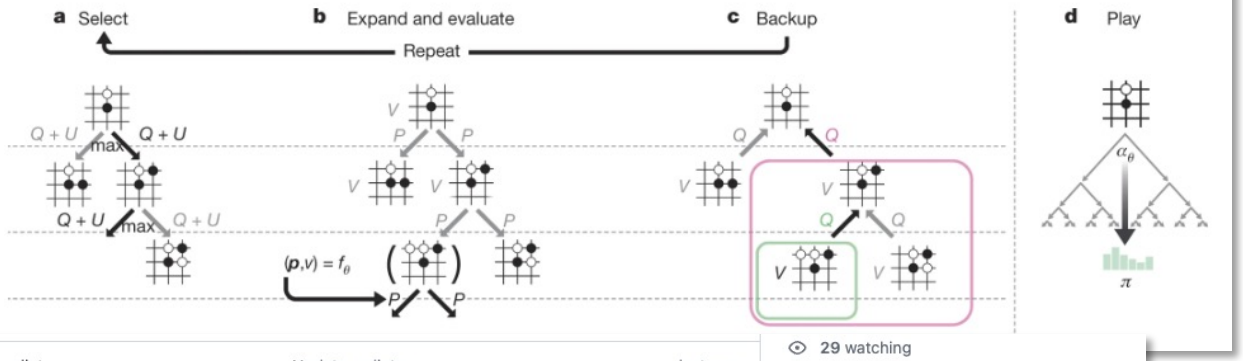


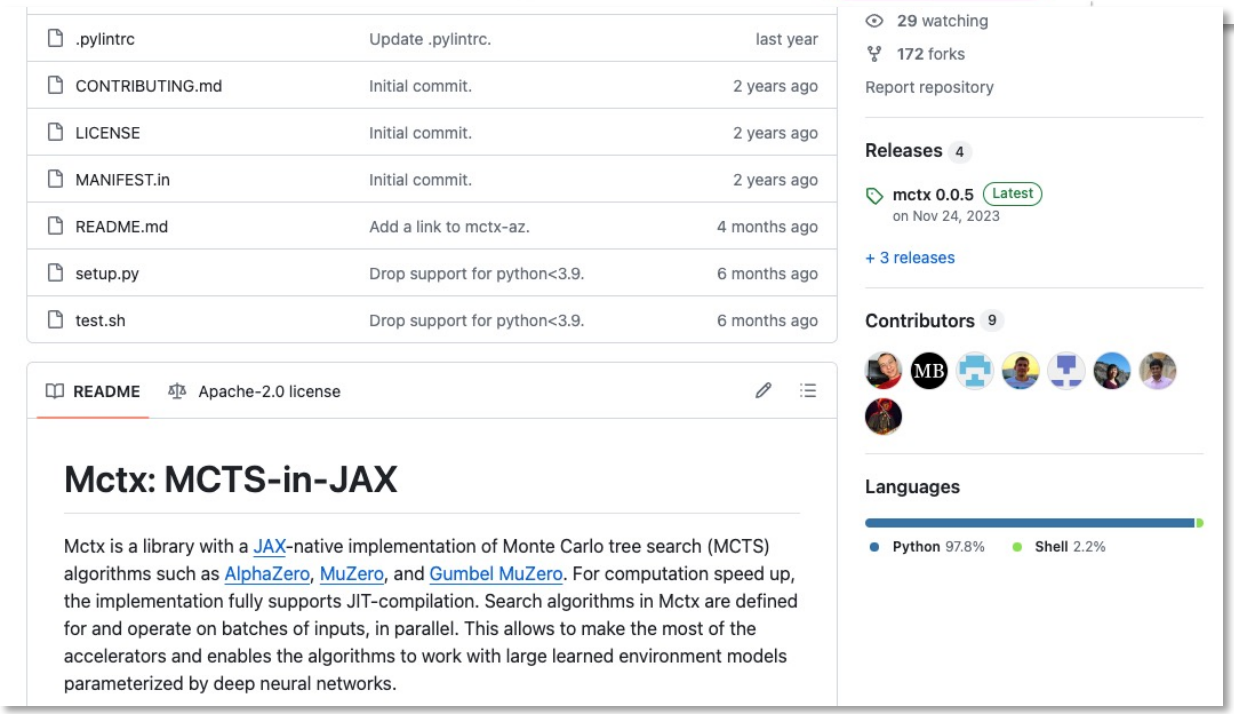
	Implementation Frameworks
Hardware & Software	Hardware: Training was conducted on TPUv4 and TPUv5e (Jouppi et al., 2020, 2023). Software: JAX (Bradbury et al., 2018), ML Pathways (Dean, 2021). JAX allows researchers to leverage the latest generation of hardware, including TPUs, for faster and more efficient training of large models.

Google/ DeepMind, Gemini: A Family of Highly Capable Multimodal Models, ArXiv (2023)

Figure 2: MCTS in AlphaGo Zero.

From: Mastering the game of Go without human knowledge





Silver et al, Mastering the game of Go without human knowledge, Nature (2017)

JAX in scientific computing

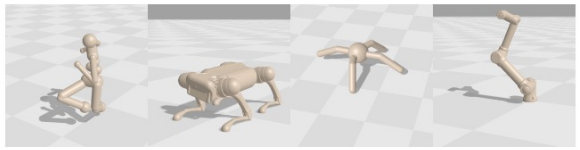
README.md Internal change 2 months ago
setup.py Internal change 2 months ago

README Code of conduct Apache-2.0 license Security

BRAX

Brax is a fast and fully differentiable physics engine used for research and development of robotics, human perception, materials science, reinforcement learning, and other simulation-heavy applications.

Brax is written in JAX and is designed for use on acceleration hardware. It is both efficient for single-device simulation, and scalable to massively parallel simulation on multiple devices, without the need for pesky datacenters.



Brax simulates environments at millions of physics steps per second on TPU, and includes a suite of learning algorithms that train agents in seconds to minutes:

Used by 200 + 192

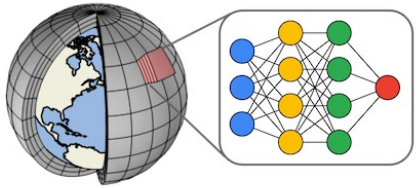
Contributors 33

+ 19 contributors

Languages

Jupyter Notebook 50.4% Python 48.1% JavaScript 1.5%

README Contributing Apache-2.0 license



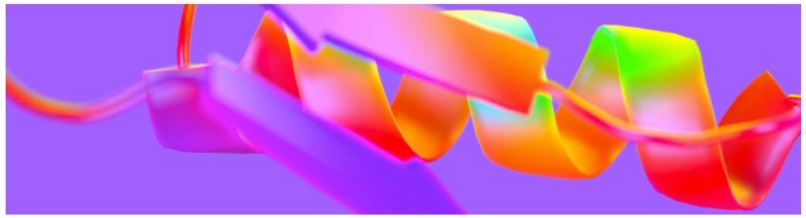
NeuralGCM

Neural General Circulation Models for Weather and Climate

NeuralGCM is a Python library for building hybrid ML/physics atmospheric models for weather and climate simulation.

requirements.txt
run_alphafold.py
run_alphafold_test.py
setup.py

README Apache-2.0 license

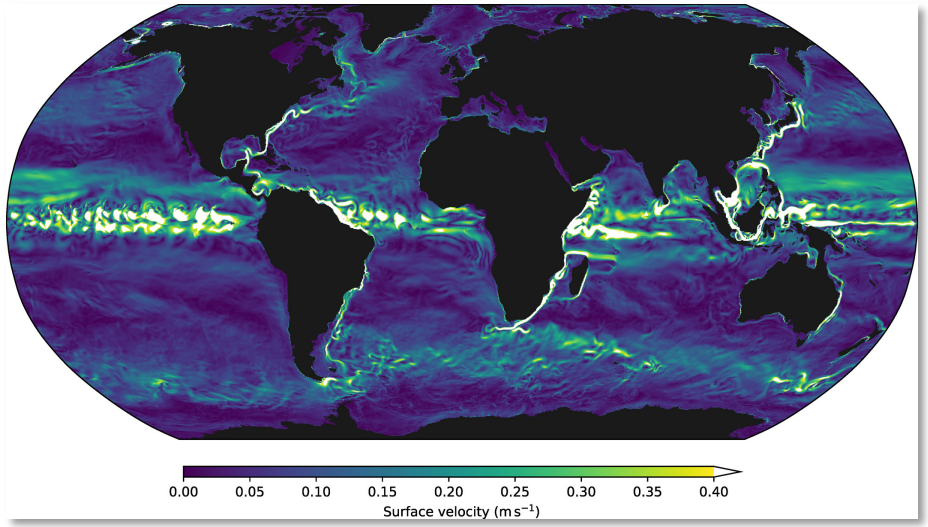


AlphaFold

This package provides an implementation of the inference pipeline of AlphaFold v2. For simplicity, we refer to this model as AlphaFold throughout the rest of this document.

Languages

Python 92.2% Jupyter Notebook 5.4% Shell 2.0% Dockerfile 0.4%



← Ocean surface velocity, simulated in 24 hr using 16 NVIDIA A100 GPUs

Hafner et al, Fast, Cheap, and Turbulent - Global Ocean Modeling With GPU Acceleration in Python, Journal of Advances in Modeling Earth Systems (2021)

What is JAX?

JAX = accelerated array computation + program transformation

```
import jax.numpy as jnp
```

- JAX is NumPy on the CPU and GPU!
- JAX uses XLA (Accelerated Linear Algebra) to compile and run NumPy code, *lightning fast*

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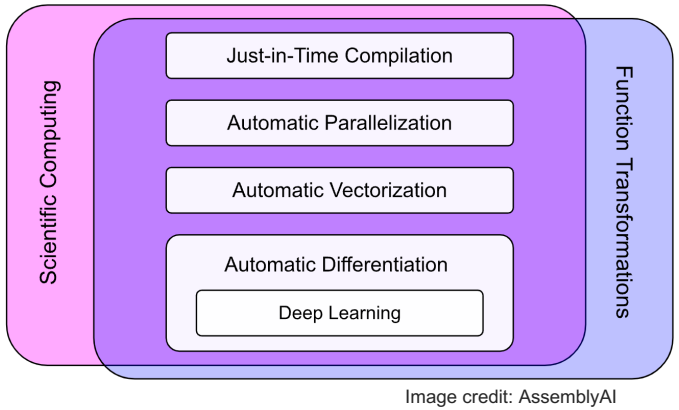

Image credit: AssemblyAI

- JAX can automatically *differentiate* and *parallelise* native Python and NumPy code

JAX = accelerated array computation

JAX is NumPy on the GPU

```python
import numpy as np

A = np.array([[1., 2., 3.],
              [1., 2., 3.],
              [1., 2., 3.],])

x = np.array([4.,5.,6.])

b = A @ x
print(b)
```

```
---
[32. 32. 32.]
```

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(10,000 x 10,000) (10,000 x 10,000)
NumPy on CPU (Apple M1 Max):
7.22 s ± 109 ms

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JAX on GPU (NVIDIA RTX 3090):
56.9 ms ± 222 µs (**126x** faster)

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```

(10,000 x 10,000) (10,000 x 10,000)
JAX on GPU (NVIDIA RTX 3090):
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Why is this operation faster on the GPU?

JAX is NumPy on the GPU

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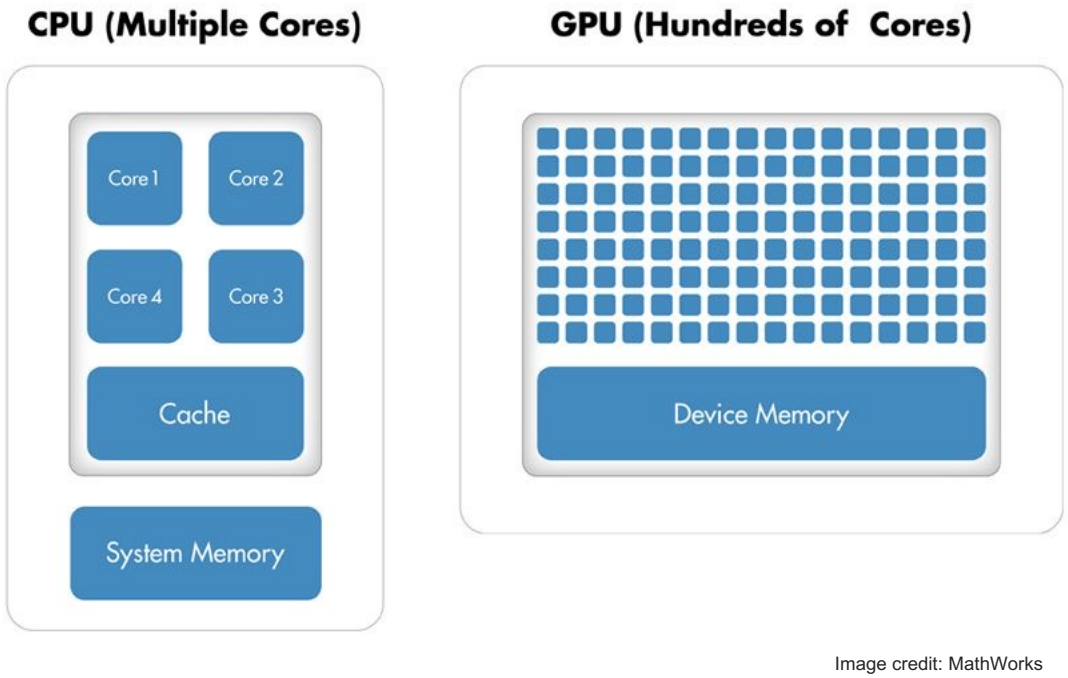

Image credit: MathWorks

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(10,000 x 10,000) (10,000 x 10,000)
JAX on GPU (NVIDIA RTX 3090):
56.9 ms ± 222 µs (**126x** faster)

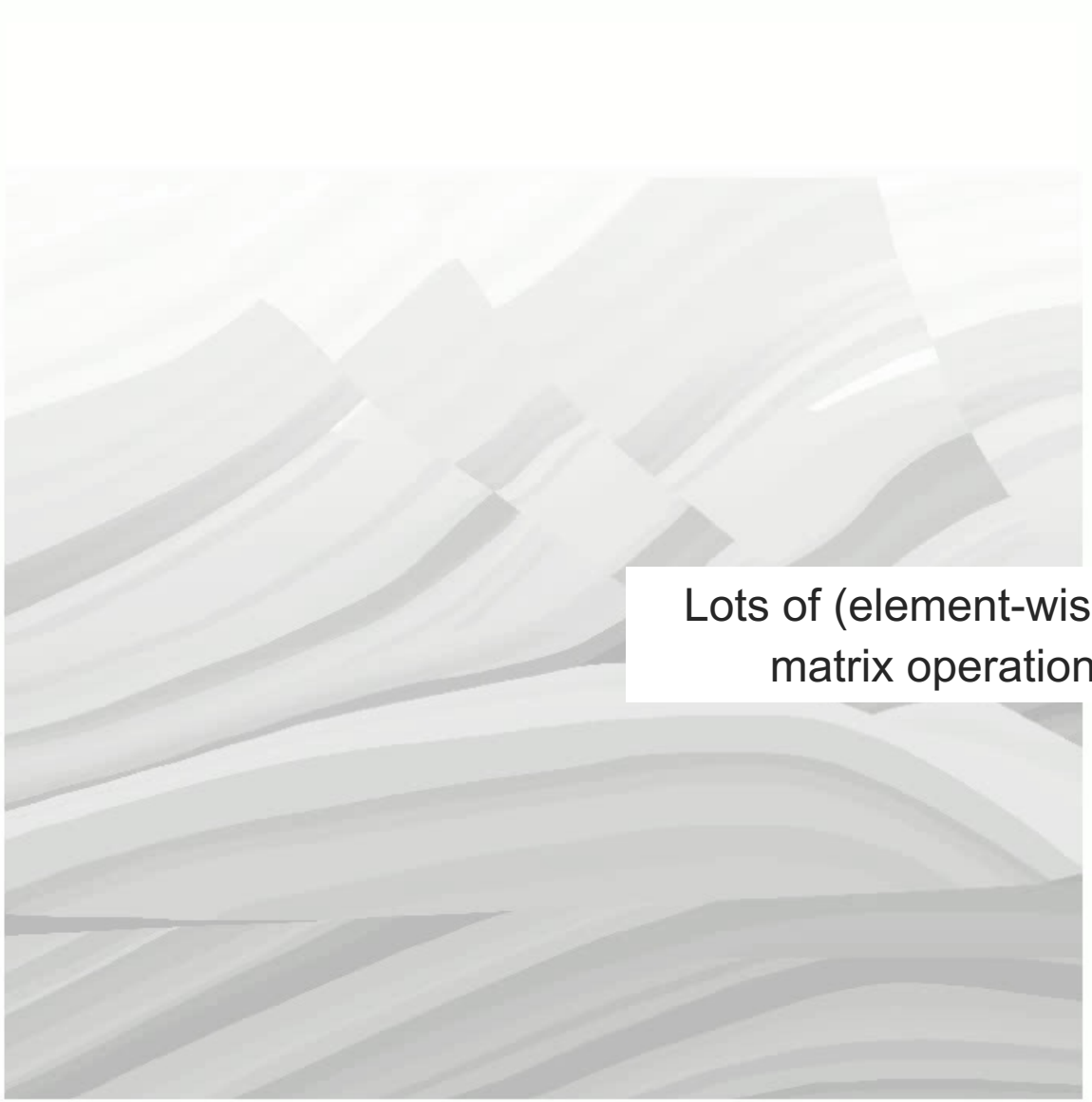
Low latency
Ideal for serial processing

High throughput
Ideal for parallel processing

Wave simulation

```python
import numpy as np


def forward(velocity, density, source_i, f0, NX, NY, NSTEPS, DELTAX, DELTAY, DELTAT):

    assert velocity.shape == density.shape == (NX, NY)
    assert source_i.shape == (2,)

    pressure_present = np.zeros((NX, NY))
    pressure_past = np.zeros((NX, NY))

    kronecker_source = np.zeros((NX, NY))
    kronecker_source[source_i[0], source_i[1]] = 1.

    # precompute some arrays
    t0 = 1.2 / f0
    factor = 1e-3
    kappa = density*(velocity**2)
    density_half_x = np.pad(0.5 * (density[1:NX,:]+density[:NX-1,:]), [[0,1],[0,0]], mode="edge")
    density_half_y = np.pad(0.5 * (density[:,1:NY]+density[:,:NY-1]), [[0,0],[0,1]], mode="edge")

    carry = pressure_past, pressure_present

    def single_step(carry, it):
        pressure_past, pressure_present = carry

        t = it*DELTAT

        # compute the first spatial derivatives divided by density
        value_dpressure_dx = np.pad((pressure_present[1:NX,:]-pressure_present[:NX-1,:]) / DELTAX, [[0,1],[0,0]], mode="constant", constant_values=0.)
        value_dpressure_dy = np.pad((pressure_present[:,1:NY]-pressure_present[:,:NY-1]) / DELTAY, [[0,0],[0,1]], mode="constant", constant_values=0.)

        pressure_xx = value_dpressure_dx / density_half_x
        pressure_yy = value_dpressure_dy / density_half_y

        # compute the second spatial derivatives

        value_dpressurexx_dx = np.pad((pressure_xx[1:NX,:]-pressure_xx[:NX-1,:]) / DELTAX, [[1,0],[0,0]], mode="constant", constant_values=0.)
        value_dpressureyy_dy = np.pad((pressure_yy[:,1:NY]-pressure_yy[:,:NY-1]) / DELTAY, [[0,0],[1,0]], mode="constant", constant_values=0.)

        dpressurexx_dx = value_dpressurexx_dx
        dpressureyy_dy = value_dpressureyy_dy

        # add the source (pressure located at a given grid point)
        a = (np.pi**2)*f0*f0

        # Ricker source time function (second derivative of a Gaussian)
        source_term = factor * (1 - 2*a*(t-t0)**2)*np.exp(-a*(t-t0)**2)

        pressure_future =   - pressure_past \
                            + 2 * pressure_present \
                            + DELTAT*DELTAT*(dpressurexx_dx+dpressureyy_dy)*kappa

        pressure_future += DELTAT*DELTAT*(4*np.pi*(velocity**2)*source_term*kronecker_source)# latest seismicCPML

        wavefield = pressure_future

        # move new values to old values (the present becomes the past, the future becomes the present)
        pressure_past = pressure_present
        pressure_present = pressure_future

        carry = pressure_past, pressure_present
        return carry, wavefield

    wavefields = np.zeros((NSTEPS, NX, NY), dtype=float)
    for it in range(NSTEPS):
        carry, w = single_step(carry, it)
        wavefields[it] = w.copy()

    return wavefields
```

Wave simulation



Lots of (element-wise) matrix operations!

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        # add the source (pressure located at a given grid point)
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        pressure_future += DELTAT*DELTAT*(4*np.pi*(velocity**2)*source_term*kronecker_source)# latest seismicCPML

        wavefield = pressure_future

        # move new values to old values (the present becomes the past, the future becomes the present)
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        carry = pressure_past, pressure_present
        return carry, wavefield

    wavefields = np.zeros((NSTEPS, NX, NY), dtype=float)
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        wavefields[it] = w.copy()

    return wavefields
```

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import jax


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    pressure_past = jnp.zeros((NX, NY))

    kronecker_source = jnp.zeros((NX, NY))
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    t0 = 1.2 / f0
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    def single_step(carry, it):
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        # compute the second spatial derivatives

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        # add the source (pressure located at a given grid point)
        a = (jnp.pi**2)*f0*f0

        # Ricker source time function (second derivative of a Gaussian)
        source_term = factor * (1 - 2*a*(t-t0)**2)*jnp.exp(-a*(t-t0)**2)

        pressure_future =   - pressure_past \
                          + 2 * pressure_present \
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        pressure_future += DELTAT*DELTAT*(4*jnp.pi*(velocity**2)*source_term*kronecker_source)# latest seismicCPML

        wavefield = pressure_future

        # move new values to old values (the present becomes the past, the future becomes the present)
        pressure_past = pressure_present
        pressure_present = pressure_future

        carry = pressure_past, pressure_present
        return carry, wavefield

    _, wavefields = jax.lax.scan(single_step, carry, jnp.arange(NSTEPS))

    return wavefields
```

```python
import numpy as np


def forward(velocity, density, source_i, f0, NX, NY, NSTEPS, DELTAX, DELTAY, DELTAT):

    assert velocity.shape == density.shape == (NX, NY)
    assert source_i.shape == (2,)

    pressure_present = np.zeros((NX, NY))
    pressure_past = np.zeros((NX, NY))

    kronecker_source = np.zeros((NX, NY))
    kronecker_source[source_i[0], source_i[1]] = 1.

    # precompute some arrays
    t0 = 1.2 / f0
    factor = 1e-3
    kappa = density*(velocity**2)
    density_half_x = np.pad(0.5 * (density[1:NX,:]+density[:NX-1,:]), [[0,1],[0,0]], mode="edge")
    density_half_y = np.pad(0.5 * (density[:,1:NY]+density[:,:NY-1]), [[0,0],[0,1]], mode="edge")

    carry = pressure_past, pressure_present

    def single_step(carry, it):
        pressure_past, pressure_present = carry

        t = it*DELTAT

        # compute the first spatial derivatives divided by density
        value_dpressure_dx = np.pad((pressure_present[1:NX,:]-pressure_present[:NX-1,:]) / DELTAX, [[0,1],[0,0]], mode="constant", constant_values=0.)
        value_dpressure_dy = np.pad((pressure_present[:,1:NY]-pressure_present[:,:NY-1]) / DELTAY, [[0,0],[0,1]], mode="constant", constant_values=0.)

        pressure_xx = value_dpressure_dx / density_half_x
        pressure_yy = value_dpressure_dy / density_half_y

        # compute the second spatial derivatives

        value_dpressurexx_dx = np.pad((pressure_xx[1:NX,:]-pressure_xx[:NX-1,:]) / DELTAX, [[1,0],[0,0]], mode="constant", constant_values=0.)
        value_dpressureyy_dy = np.pad((pressure_yy[:,1:NY]-pressure_yy[:,:NY-1]) / DELTAY, [[0,0],[1,0]], mode="constant", constant_values=0.)

        dpressurexx_dx = value_dpressurexx_dx
        dpressureyy_dy = value_dpressureyy_dy

        # add the source (pressure located at a given grid point)
        a = (np.pi**2)*f0*f0

        # Ricker source time function (second derivative of a Gaussian)
        source_term = factor * (1 - 2*a*(t-t0)**2)*np.exp(-a*(t-t0)**2)

        pressure_future =   - pressure_past \
                          + 2 * pressure_present \
                          + DELTAT*DELTAT*(dpressurexx_dx+dpressureyy_dy)*kappa

        pressure_future += DELTAT*DELTAT*(4*np.pi*(velocity**2)*source_term*kronecker_source)# latest seismicCPML

        wavefield = pressure_future

        # move new values to old values (the present becomes the past, the future becomes the present)
        pressure_past = pressure_present
        pressure_present = pressure_future

        carry = pressure_past, pressure_present
        return carry, wavefield

    wavefields = np.zeros((NSTEPS, NX, NY), dtype=float)
    for it in range(NSTEPS):
        carry, w = single_step(carry, it)
        wavefields[it] = w.copy()

    return wavefields
```

Wave simulation

NumPy on **CPU** (Apple M1 Max): 8.06 s ± 54.7 ms

JAX (jit compiled) on **CPU** (Apple M1 Max): 1.58 s ± 11.6 ms (**5x** faster)

JAX (jit compiled) on **GPU** (NVIDIA RTX 3090): 65.5 ms ± 30.2 µs (**123x** faster)

Code along – Introduction to JAX

Follow along here:

github.com/**benmoseley/scalable-pinns-workshop**

What is JAX?

JAX = accelerated array computation + program transformation

```
import jax.numpy as jnp
```

- JAX is NumPy on the CPU and GPU!
- JAX uses XLA (Accelerated Linear Algebra) to compile and run NumPy code, *lightning fast*

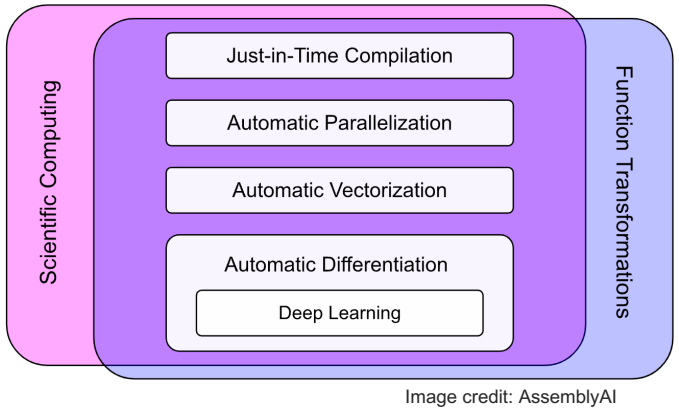

Image credit: AssemblyAI

- JAX can automatically *differentiate* and *parallelise* native Python and NumPy code

JAX = program transformation

What is a program transformation?

```python
import jax
import jax.numpy as jnp

def f(x):
    return x**2
```

What is a program transformation?

```python
import jax
import jax.numpy as jnp

def f(x):
    return x**2

dfdx = jax.grad(f)# this returns a python function!
```

What is a program transformation?

```python
import jax
import jax.numpy as jnp

def f(x):
    return x**2

dfdx = jax.grad(f)# this returns a python function!

x = jnp.array(10.)

print(x)
print(dfdx(x))

---
10.0
20.0
```

What is a program transformation?

```python
import jax
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def f(x):
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print(x)
print(dfdx(x))

---
10.0
20.0
```

Step 1: convert Python function into a simple intermediate language (jaxpr)

```
print(jax.make_jaxpr(f)(x))

---
{ lambda ; a:f32[]. let b:f32[] = integer_pow[y=2] a in (b,) }
```

What is a program transformation?

```python
import jax
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def f(x):
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---
10.0
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```

Step 1: convert Python function into a simple intermediate language (jaxpr)

```
print(jax.make_jaxpr(f)(x))

---
{ lambda ; a:f32[]. let b:f32[] = integer_pow[y=2] a in (b,) }
```

Step 2: apply transformation (e.g. return the corresponding gradient function)

```
print(jax.make_jaxpr(dfdx)(x))

---
{ lambda ; a:f32[]. let
    _:f32[] = integer_pow[y=2] a
    b:f32[] = integer_pow[y=1] a
    c:f32[] = mul 2.0 b
    d:f32[] = mul 1.0 c
  in (d,) }
```

What is a program transformation?

```python
import jax
import jax.numpy as jnp

def f(x):
    return x**2

dfdx = jax.grad(f)# this returns a python function!

x = jnp.array(10.)

print(x)
print(dfdx(x))

---
10.0
20.0
```

Program transformation = 

Transform one **program** to another **program**

- Treats programs as **data**
- Aka **meta-programming**

Program transformations are composable

```
import jax
import jax.numpy as jnp

def f(x):
    return x**2

dfdx = jax.grad(f)# this returns a python function!

d2fdx2 = jax.grad(dfdx)# transformations are composable!

x = jnp.array(10.)

print(x)
print(d2fdx2(x))

---
10.0
2.0
```

- We can **arbitrarily compose** program transformations in JAX!

- This allows highly **sophisticated** workflows to be developed

Autodifferentiation in JAX

```python
import jax
import jax.numpy as jnp

def f(x):
    return jnp.sum(x**2)

x = jnp.arange(5.)

g = jax.grad(f)# returns function which computes gradient
j = jax.jacfwd(f)# returns function which computes Jacobian
j = jax.jacrev(f)# returns function which computes Jacobian
h = jax.hessian(f)# returns function which computes Hessian

print(g(x))
print(h(x))

# vector-Jacobian product
fval, vjp = jax.vjp(f, x)# returns function output and function which computes vjp at x
vjp_val = vjp(1.)

# Jacobian-vector product
v = jnp.ones_like(x)
fval, jvp_val = jax.jvp(f, (x,), (v,))# returns function output and jvp at x

---
[0. 2. 4. 6. 8.]

[[2. 0. 0. 0. 0.]
 [0. 2. 0. 0. 0.]
 [0. 0. 2. 0. 0.]
 [0. 0. 0. 2. 0.]
 [0. 0. 0. 0. 2.]]
```

- JAX has many autodifferentiation capabilities
- **all** are based on compositions of **vjp** and **jvp** (i.e. reverse- and forward- mode autodiff)

Other function transformations

f(x) → dfdx(x) is not the only function transformation we could make!

- What **other** function transformations can you imagine?

Automatic vectorisation

```python
import jax
import jax.numpy as jnp

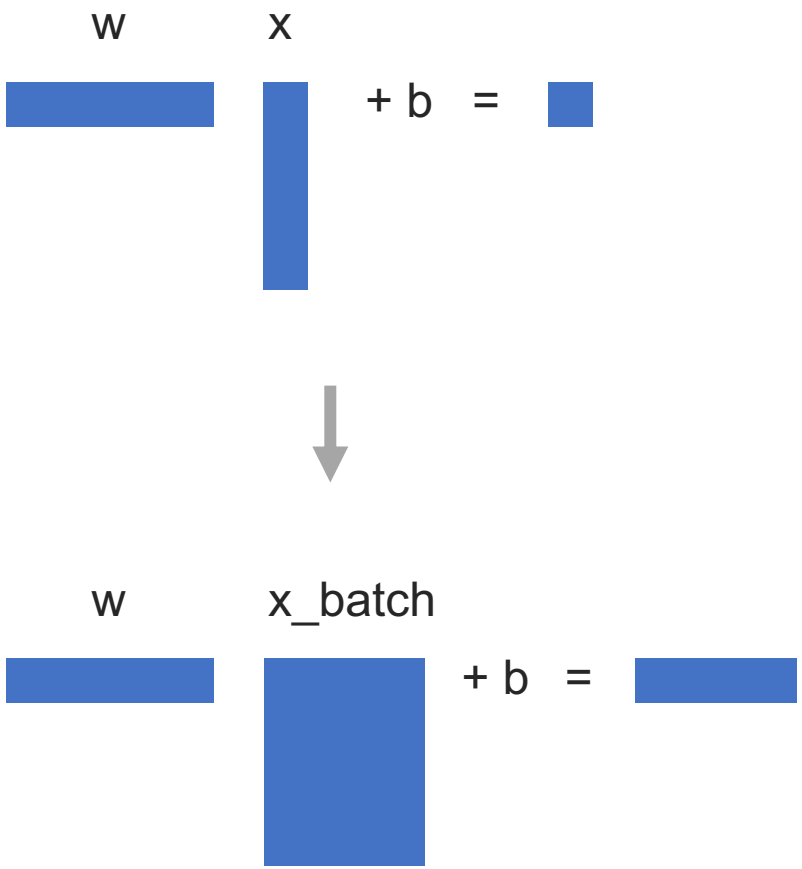
def f(w, b, x):
    y = jnp.dot(w, x) + b
    return y

x = jnp.array([1., 2.])
w = jnp.array([2., 4.])
b = jnp.array(1.)

print(f(w, b, x))
```

- **Vectorisation** is another type of function transformation

  = parallelise the function across many inputs (on a single CPU or GPU)



Automatic vectorisation

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def f(w, b, x):
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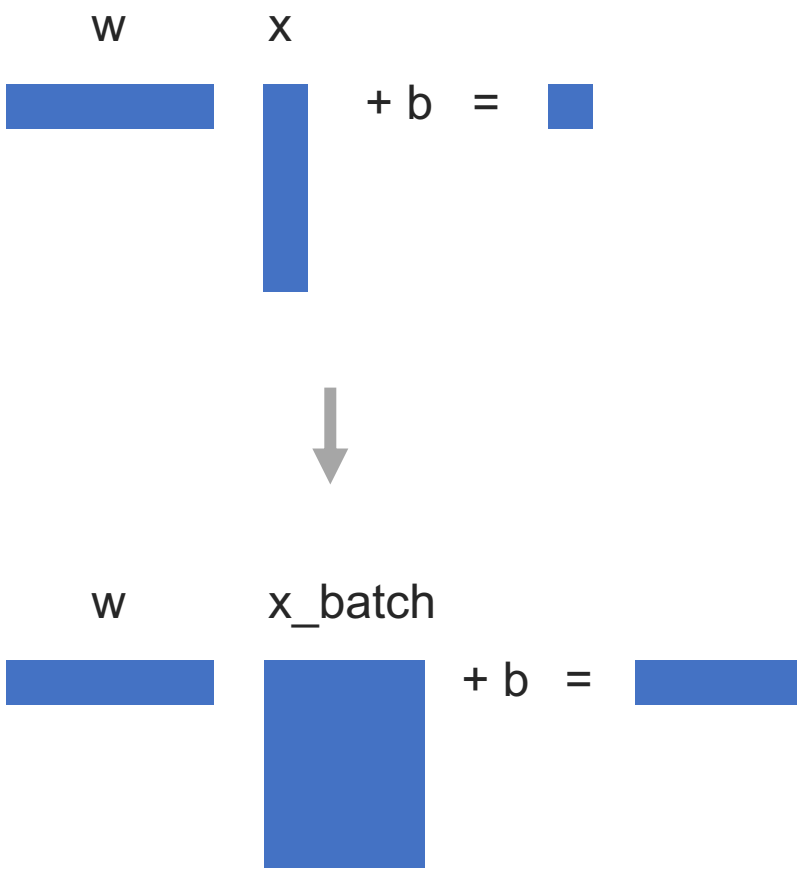
    return y

x = jnp.array([1., 2.])
w = jnp.array([2., 4.])
b = jnp.array(1.)

print(f(w, b, x))

# vectorise function across first dimension of x
f_batch = jax.vmap(f, in_axes=(None, None, 0))
```



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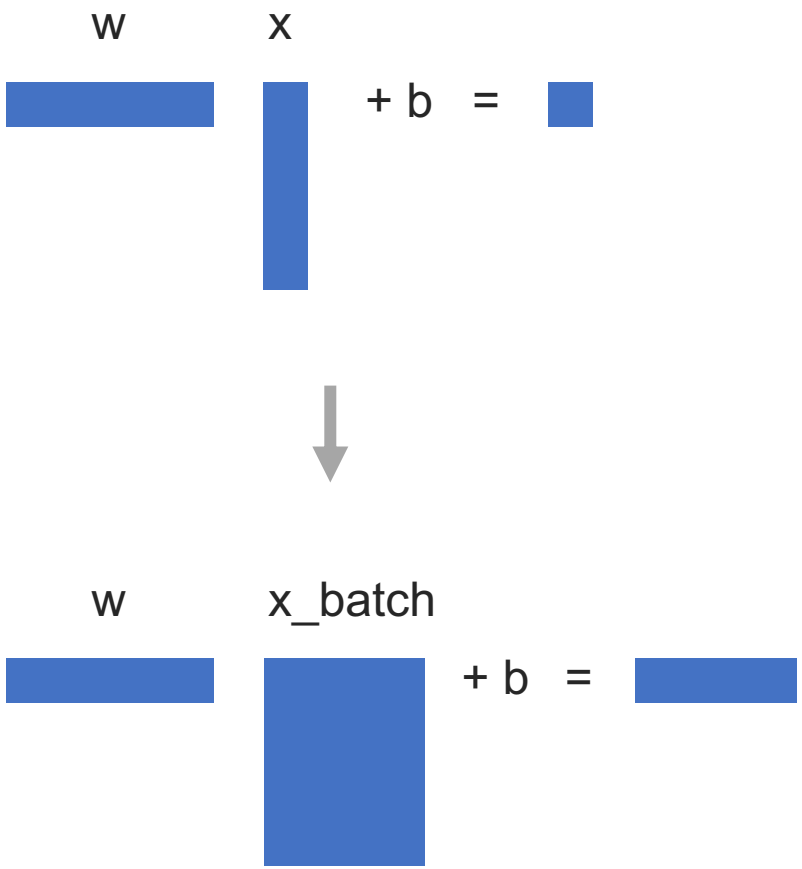
# vectorise function across first dimension of x
f_batch = jax.vmap(f, in_axes=(None, None, 0))

x_batch = jnp.array([[1., 2.],
                     [3., 4.],
                     [5., 6.]])
print(f_batch(w, b, x_batch))

---
11.0
[11. 23. 35.]
```



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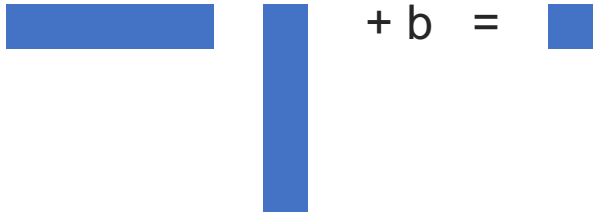
---
11.0
[11. 23. 35.]
```

```
{ lambda ; a:f32[2] b:f32[] c:f32[2]. let
    d:f32[] = dot_general[
      dimension_numbers=(([0], [0]), ([], []))
      preferred_element_type=float32
    ] a c
    e:f32[] = convert_element_type[new_dtype=float32 weak_type=False] b
    f:f32[] = add d e
  in (f,) }
```




```
{ lambda ; a:f32[2] b:f32[] c:f32[3,2]. let
    d:f32[3] = dot_general[
      dimension_numbers=(([0], [1]), ([], []))
      preferred_element_type=float32
    ] a c
    e:f32[] = convert_element_type[new_dtype=float32 weak_type=False] b
    f:f32[3] = add d e
  in (f,) }
```

Automatic vectorisation

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import jax.numpy as jnp

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w = jnp.array([2., 4.])
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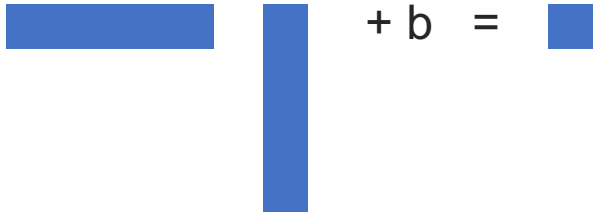


```
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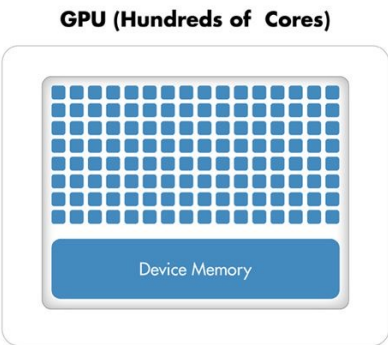
    d:f32[3] = dot_general[
      dimension_numbers=(([0], [1]), ([], []))
      preferred_element_type=float32
    ] a c
    e:f32[] = convert_element_type[new_dtype=float32 weak_type=False] b
    f:f32[3] = add d e
  in (f,) }
```



Much faster than a Python for loop!

Just-in-time compilation

```python
import jax

def f(x):
    return x + x*x + x*x*x
```

- **Compilation** is another type of function transformation

  = rewrite your code to be faster

Just-in-time compilation

```python
import jax

def f(x):
    return x + x*x + x*x*x
```

- **Compilation** is another type of function transformation

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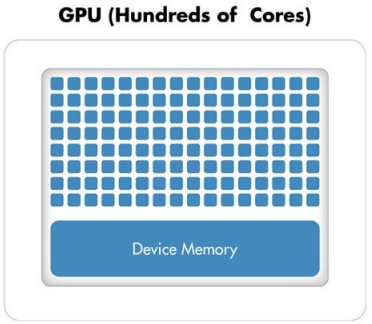

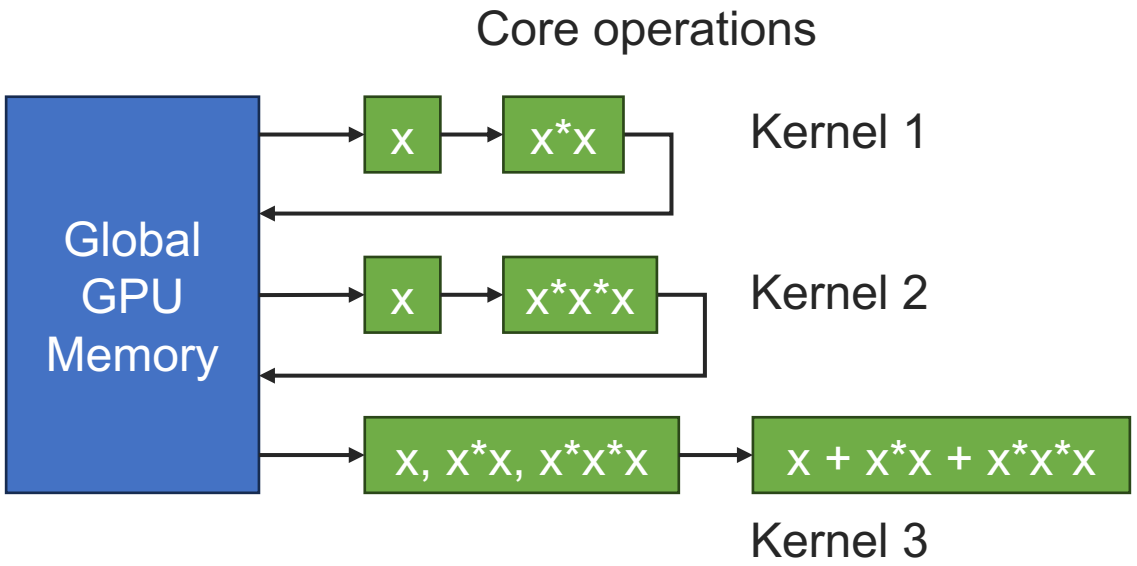

Just-in-time compilation

```python
import jax

def f(x):
    return x + x*x + x*x*x

jit_f = jax.jit(f)# compile function
```

- **Compilation** is another type of function transformation

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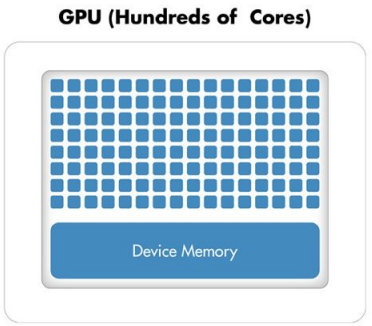
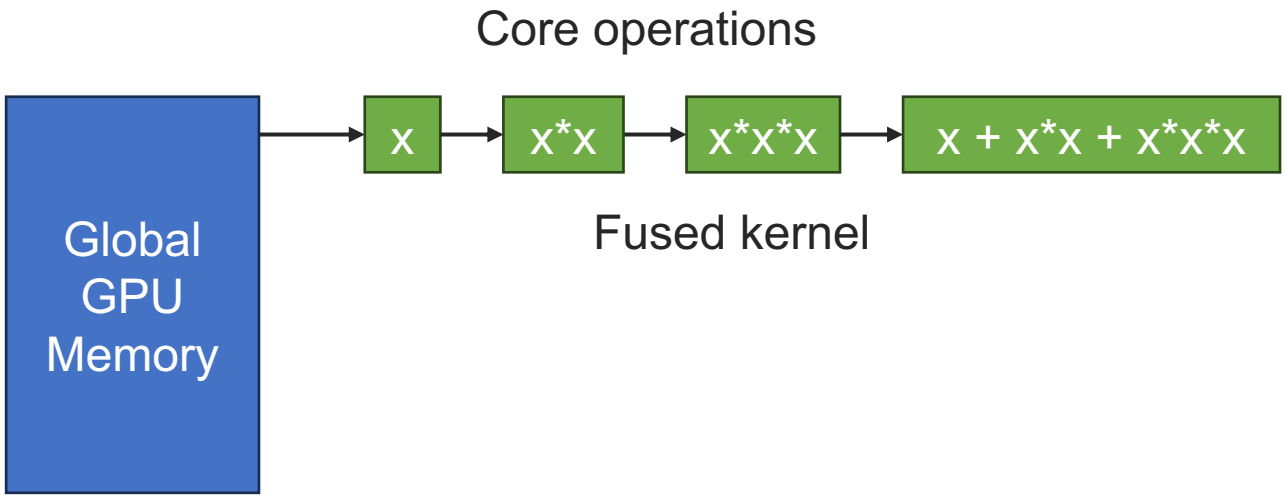




Just-in-time compilation

```
import jax

def f(x):
    return x + x*x + x*x*x

jit_f = jax.jit(f)# compile function

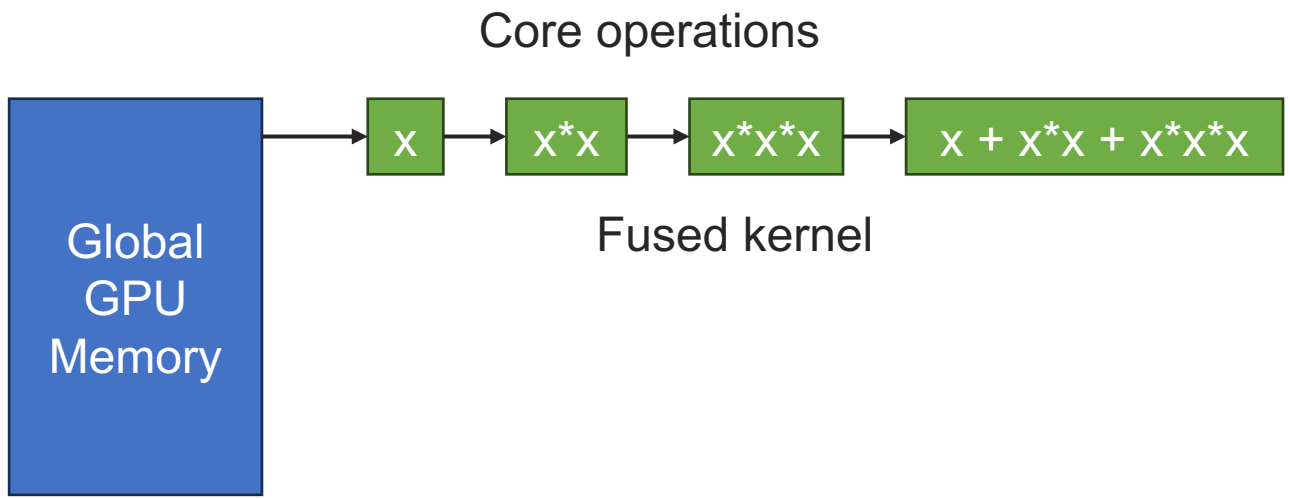
key = jax.random.key(0)
x = jax.random.normal(key, (1000,1000))
%timeit f(x).block_until_ready()
%timeit jit_f(x).block_until_ready()

---
870 µs ± 19.7 µs per loop
117 µs ± 253 ns per loop
```

8x faster!

- **Compilation** is another type of function transformation

  = rewrite your code to be faster



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---
870 µs ± 19.7 µs per loop
117 µs ± 253 ns per loop
```

8x faster!

- **Compilation** is another type of function transformation

  = rewrite your code to be faster

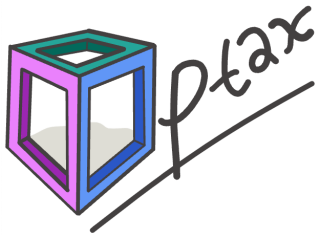
- XLA (accelerated linear algebra) is used for CPU / GPU compilation

- Function is compiled **first time it is called** (i.e. “just-in-time”)

  = upfront cost!

JAX ecosystem

Optimisation



Optax

JAXopt

Optimistix

Neural networks

Flax

Trax

Equinox

Jraph

ML

MaxText (LLMs)

EasyLM

RLax

Scenic

NumPyro

Scientific computing + ML

JAX-MD

Diffrax

Lineax

jax.scipy

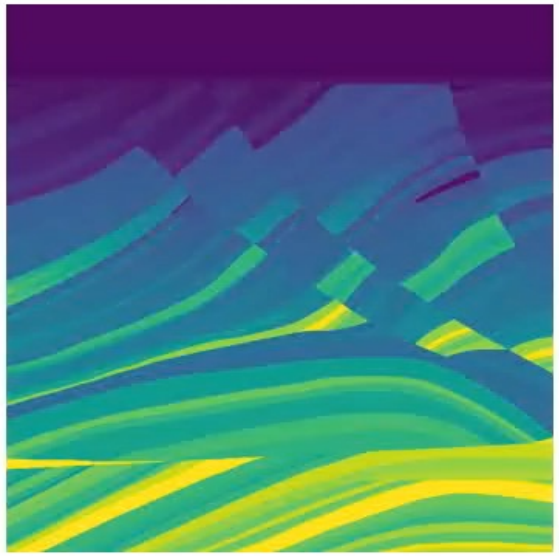
JAX-CFD

DeepXDE

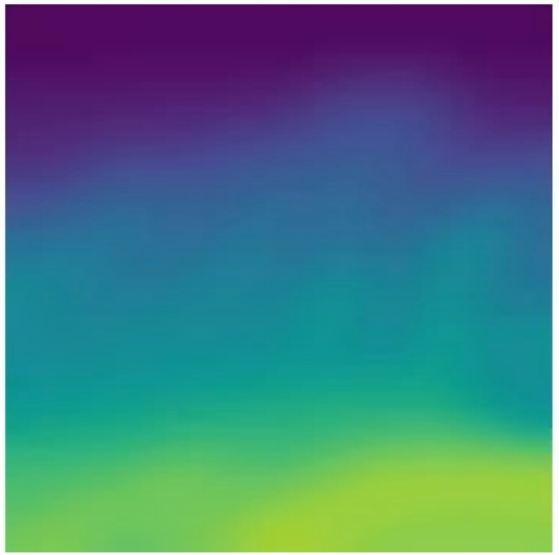
For more: github.com/n2cholas/awesome-jax

Optimisation with Optax

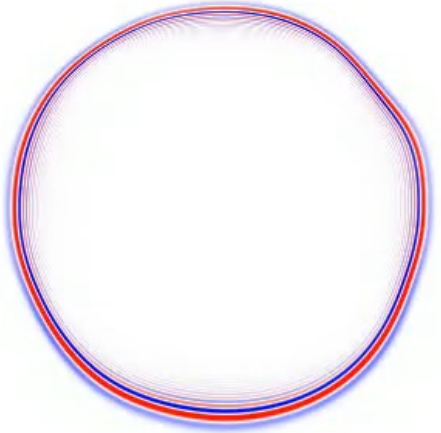
True velocity



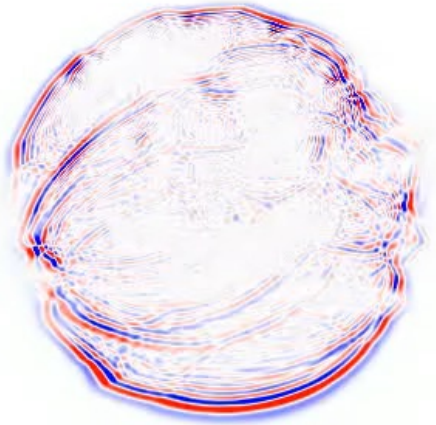
Estimated velocity



Estimated wavefield



True wavefield



```python
def loss(velocity, true_wavefield):
    estimated_wavefield = forward(velocity)
    return jnp.mean((estimated_wavefield-true_wavefield)**2)

# Initialize optimizer.
optimizer = optax.adam(learning_rate=1e-1)
opt_state = optimizer.init(velocity)

# A simple gradient descent loop.
for _ in range(10000):
    grads = jax.grad(loss)(velocity, true_wavefield)
    updates, opt_state = optimizer.update(grads, opt_state)
    velocity = optax.apply_updates(velocity, updates)
```

JAX - the sharp bits 🔪

🔪 **Pure functions**: JAX transforms are designed to work on pure functions

🔪🔪 **Static shapes**: JAX transforms require all shapes to be known **in advance**

🔪 **Out-of-place updates**: JAX only allows out-of-place array updates

🔪 **Random numbers**: JAX requires us to handle RNG explicitly

https://docs.jax.dev/en/latest/notebooks/Common_Gotchas_in_JAX.html

Workshop overview

Session 1: **Intro to PINNs**

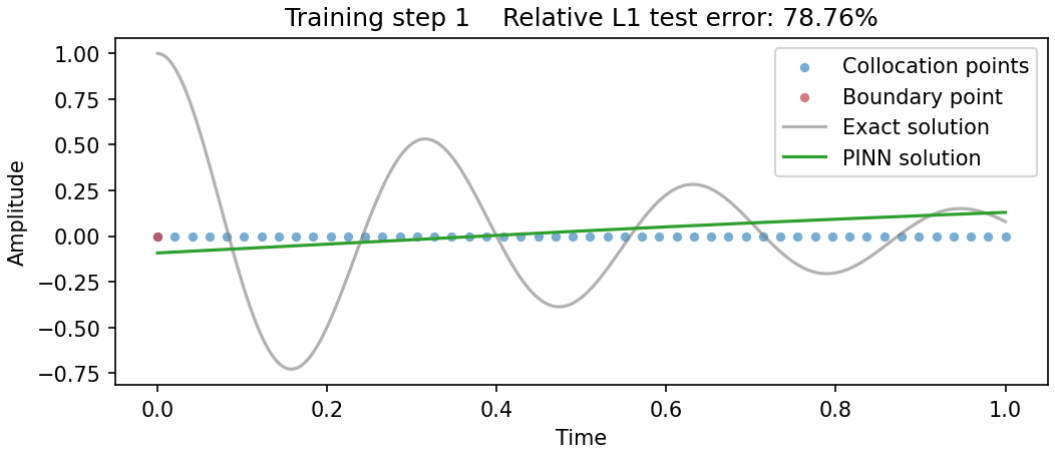
- *Lecture* (1 hr): Introduction to SciML and PINNs
- *Code-along* (30 min): Training a PINN in PyTorch

Session 2: **Accelerating PINNs with JAX**

- *Lecture* (30 min): Introduction to JAX
- *Practical* (1 hr): Introduction to JAX and coding a PINN from scratch in JAX

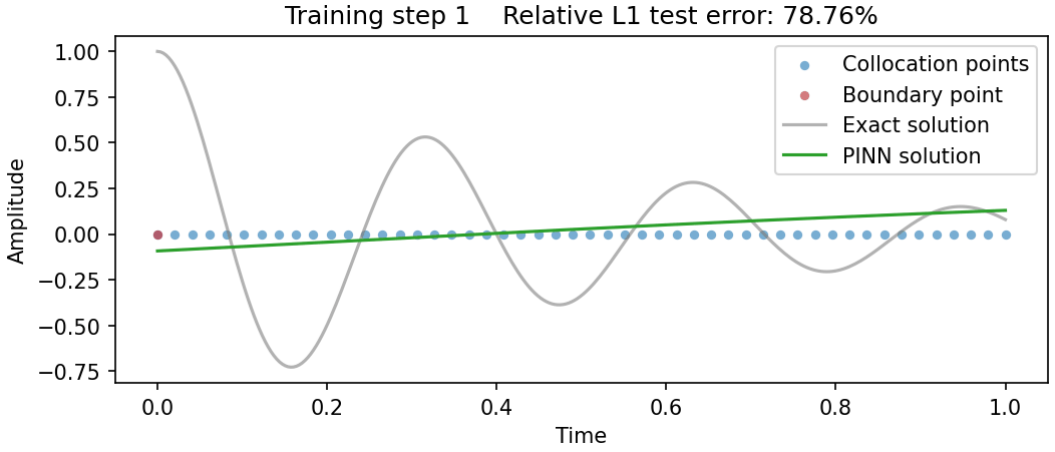
Session 3: **Accelerating PINNs with domain decomposition and NLA**

- *Lecture* (30 min): Challenges with PINNs and improving their performance with domain decomposition and numerical linear algebra
- *Practical* (1 hr): Coding finite basis PINNs and extreme learning machine FBPINNs in JAX



PINN (PyTorch) baseline

82 seconds



PINN **(JAX)**

11 seconds