Advanced Methods for Scientific Computing

Analysis and Implementation of L-BFGS methods in Neural Networks

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Doxygen link

Agenda

Challenges in Neural Network Training

Training is a high-dimensional, non convex optimization problem.

- **State of the Art (SGD):**
  - Computationally efficient per iteration ($O(d)$).
  - **Drawback:** Relies only on first-order information (gradient). Slow convergence on ill-conditioned problems.
- **Second-Order Methods (Newton/BFGS):**
  - Incorporate curvature (Hessian). Quadratic or super-linear convergence.
  - **Drawback:** Prohibitive computational cost on large datasets.

LBFGS

Goal: Approximate Newton's direction using limited curvature information.

Two-Loop Recursion:

1. Backward Pass
2. Scaling
3. Forward pass

Line-Search: Strong Wolfe Line Search to ensure sufficient decrease and stable convergence

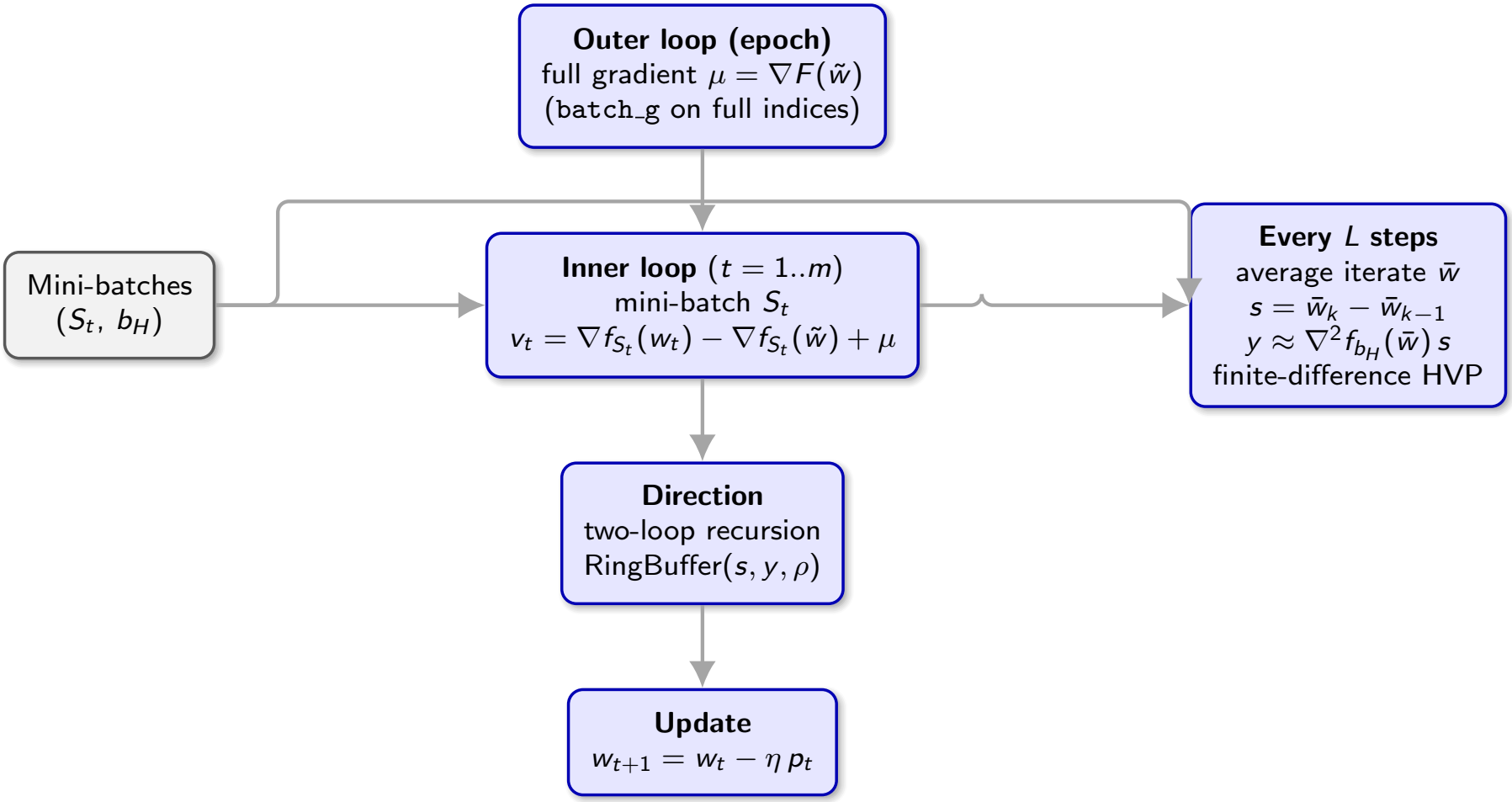
S-LBFGS

Goal: Combine the computational efficiency of stochastic methods with the convergence speed of Quasi-Newton methods.

Our implementation relies on two pillars for stability and efficiency:

1. **Variance Reduction (SVRG):**
   - Reduces the "noise" of the stochastic gradient as the solution is approached.
   - Allows for more stable steps compared to standard GD.
2. **Stable Curvature Updates:**
   - Curvature pairs (s, y) are computed from averaged iterates.
   - Hessian-vector products are computed on mini-batches.

S-LBFGS: Control Flow (CPU Implementation)



Implemented in `src/minimizer/s_lbfgs.hpp`: variance reduction + stable curvature updates are CPU-only.

Dual Backend Architecture (High-Level)

We developed a modular C++ framework with **two concrete backends** sharing the same high-level API.

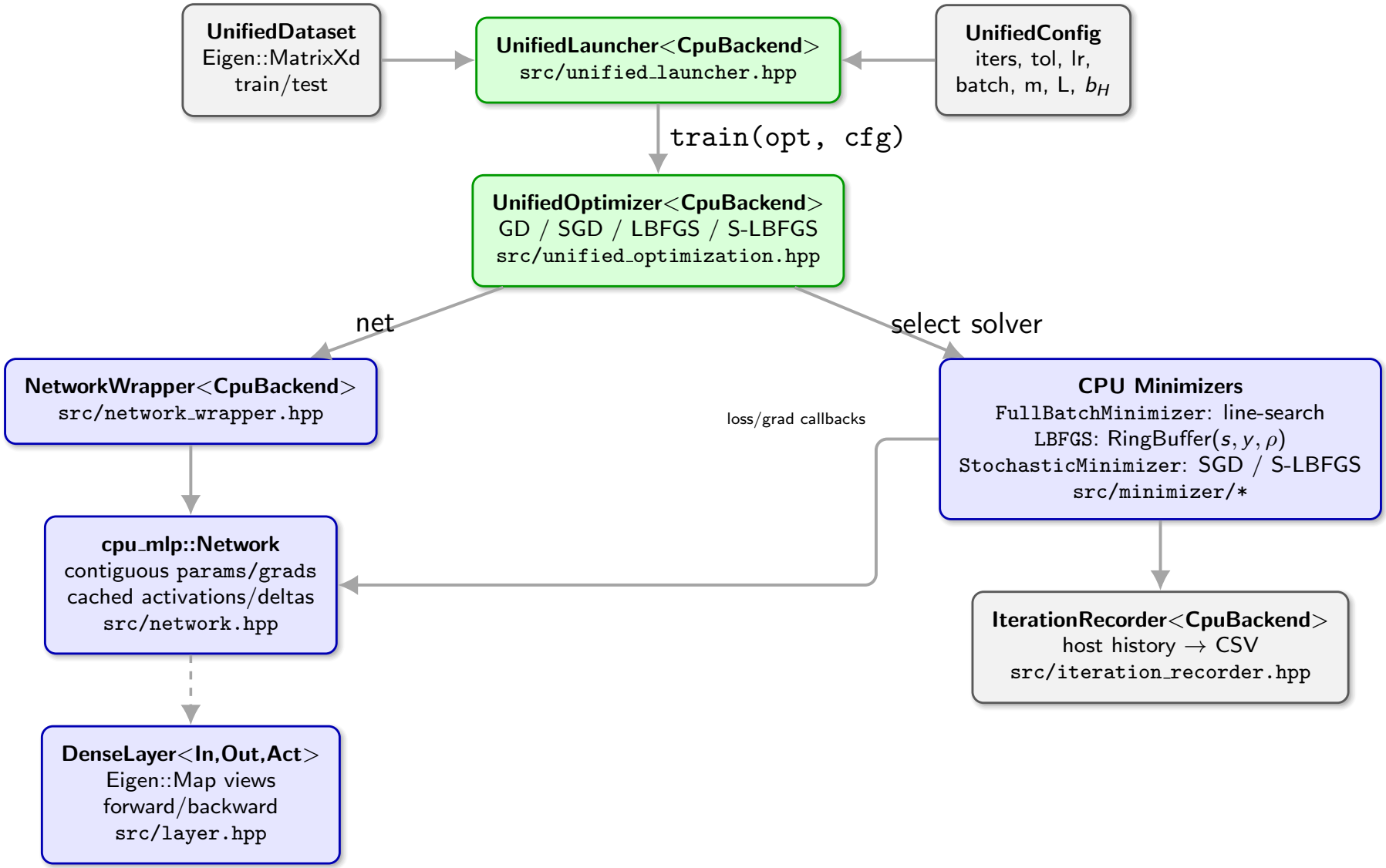
CPU Backend

- **Eigen** for batched linear algebra.
- Optional **OpenMP** to enable Eigen threading.

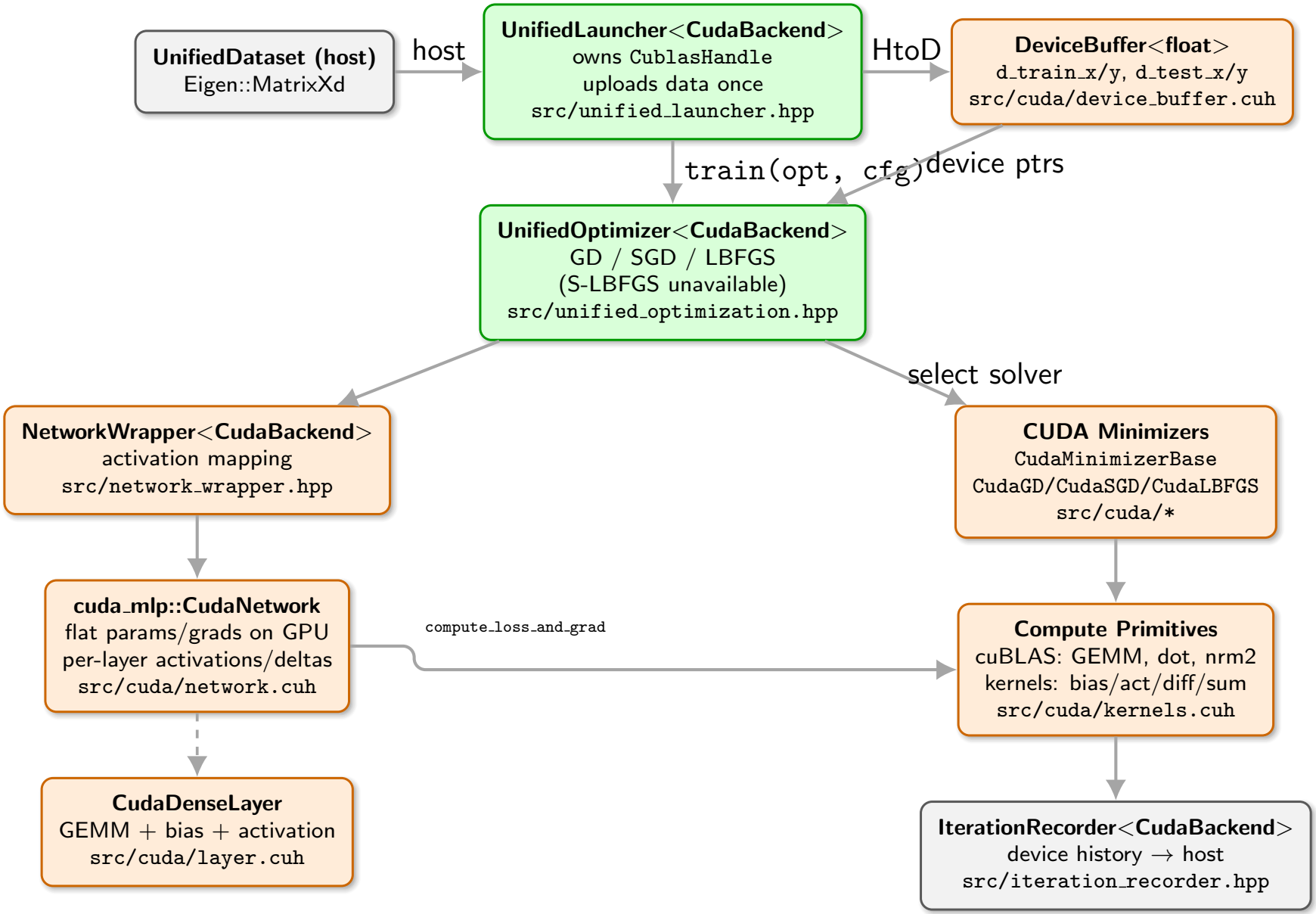
CUDA Backend

- **cuBLAS** for GEMMs + custom CUDA kernels.
- RAII GPU resources: `DeviceBuffer`, `CublasHandle`.

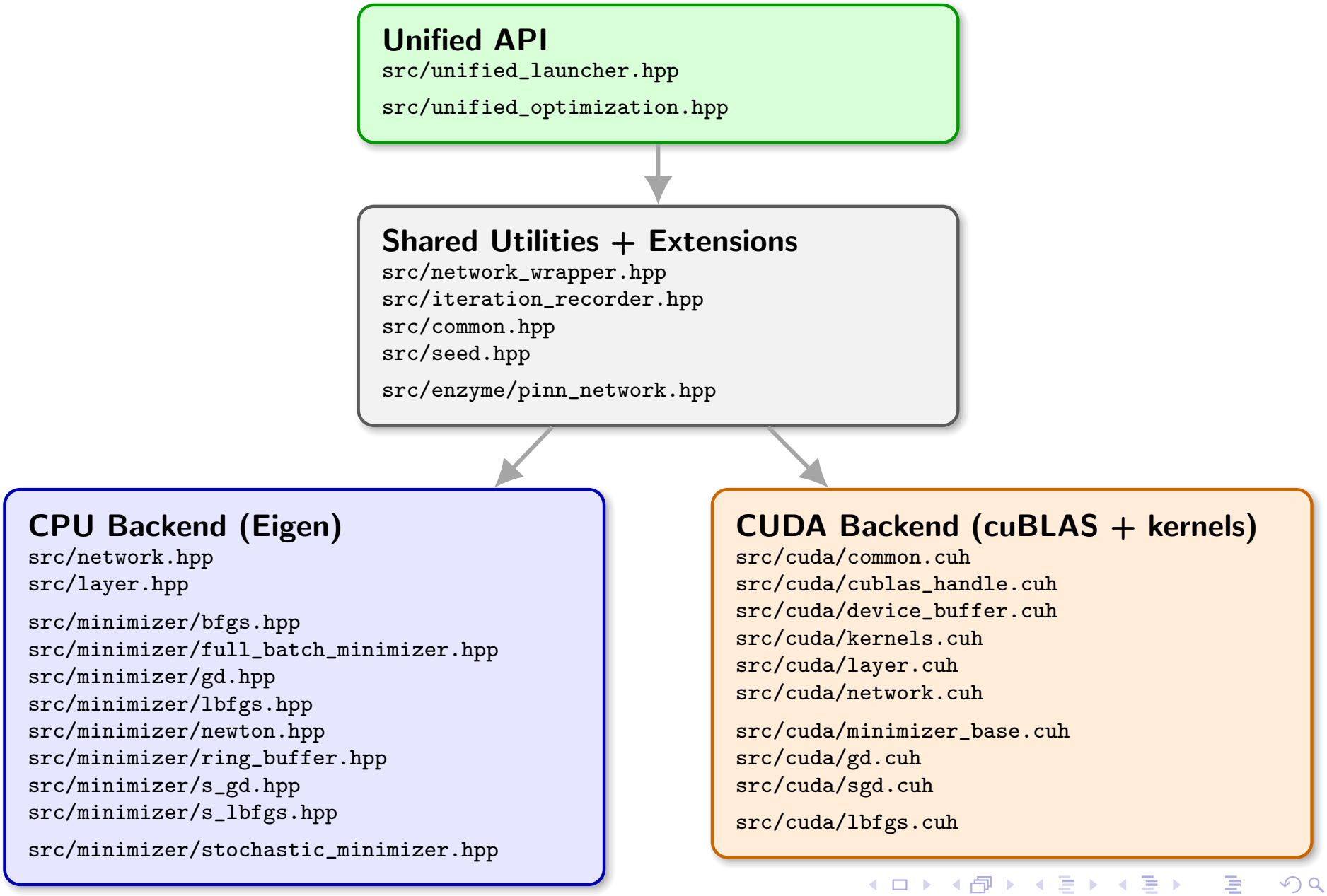
CPU Backend: Modules and Data Flow



CUDA Backend: Modules and Data Flow



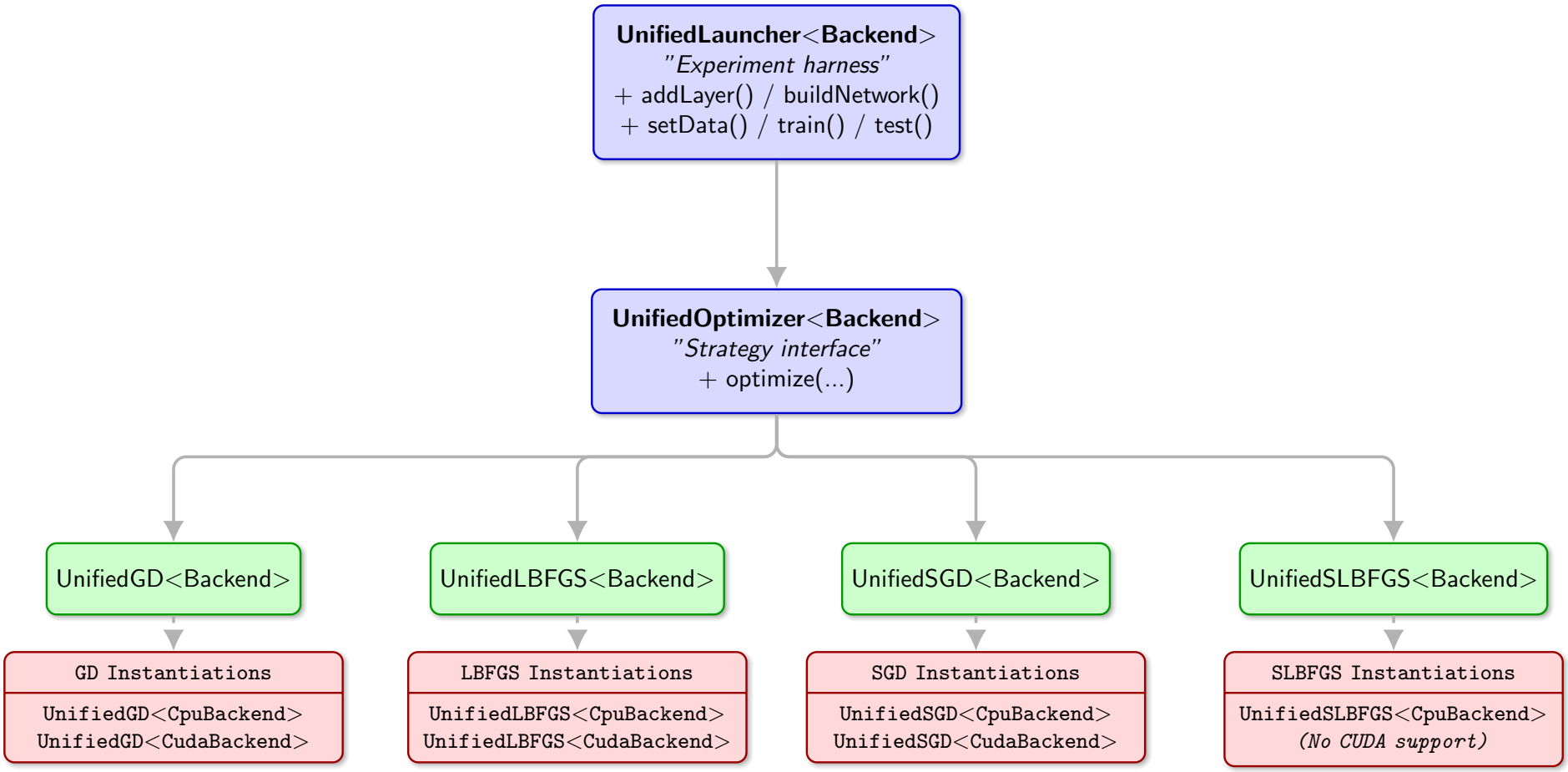
Project File Map (Source Tree)



Test Pattern

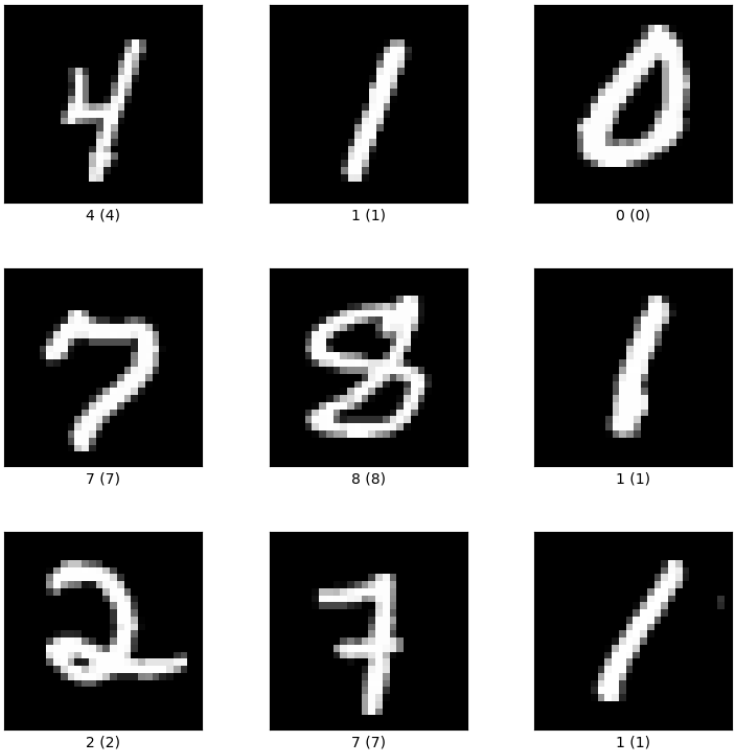
```
// 1) Setup
using Backend = CpuBackend;
UnifiedLauncher<Backend> launcher;

// 2) Build network
launcher.addLayer<in, hidden, Activation>();
launcher.addLayer<hidden, out, Linear>();
...
launcher.buildNetwork();

// 3) Load dataset + bind
UnifiedDataset data;
data.train_x = Loader::loadImages();
...
launcher.setData(data);

// 4) Train and Test
for each experiment e:
  cfg <- makeConfig(e)
  opt <- LBFGS<Backend>
  launcher.train(opt, cfg)
  launcher.test()
```

Unified Architecture for Testing

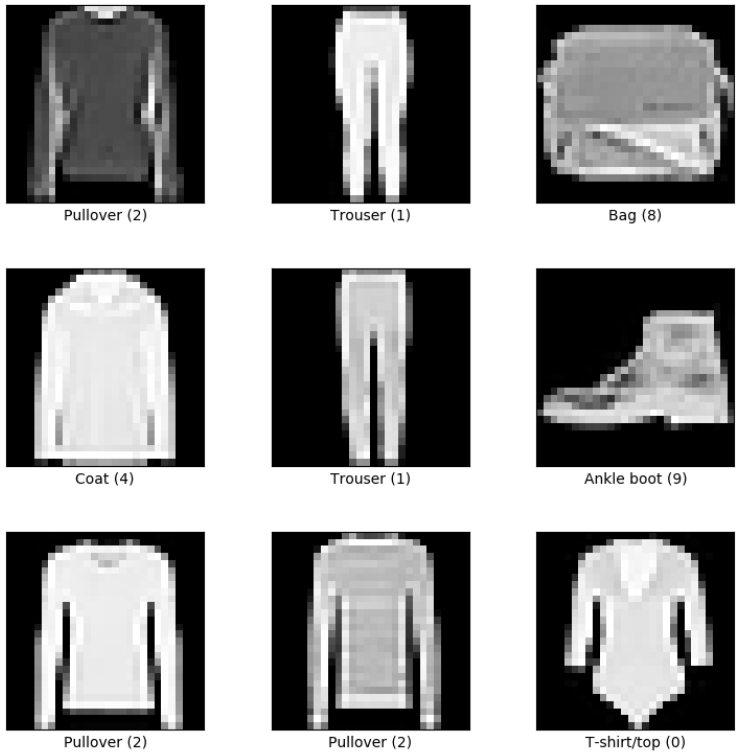


Training set

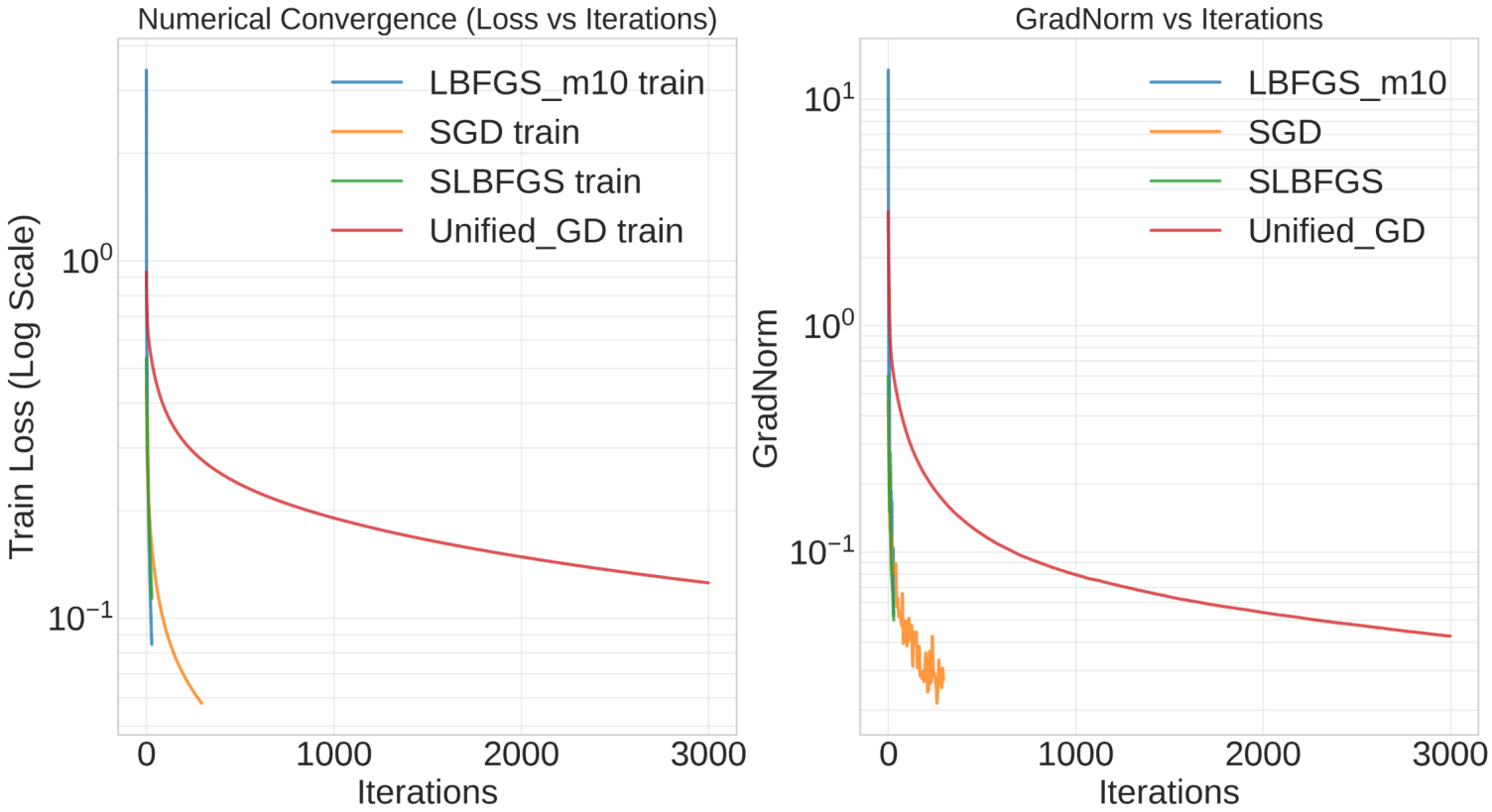
MNIST



Fashion - MNIST



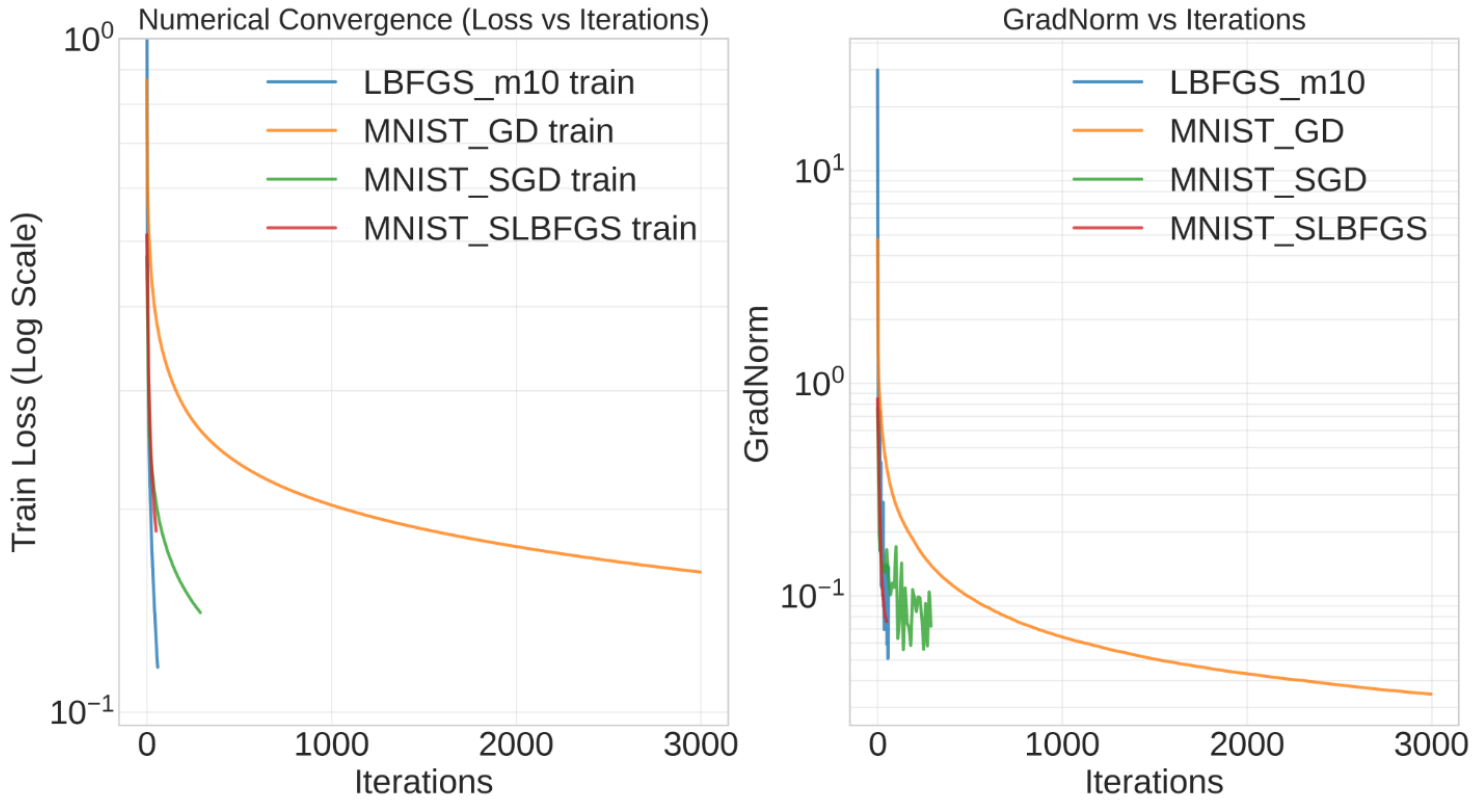
Results: MNIST (CPU)



Setup: $784 \to 128 \to 10$, $N = 5{,}000$ (CPU)

Solver	**Train Acc. (%)**	**Test Acc. (%)**
GD	91.98	89.50
SGD	97.64	93.15
S-LBFGS	93.42	90.94
L-BFGS ($m = 10$)	94.30	92.11

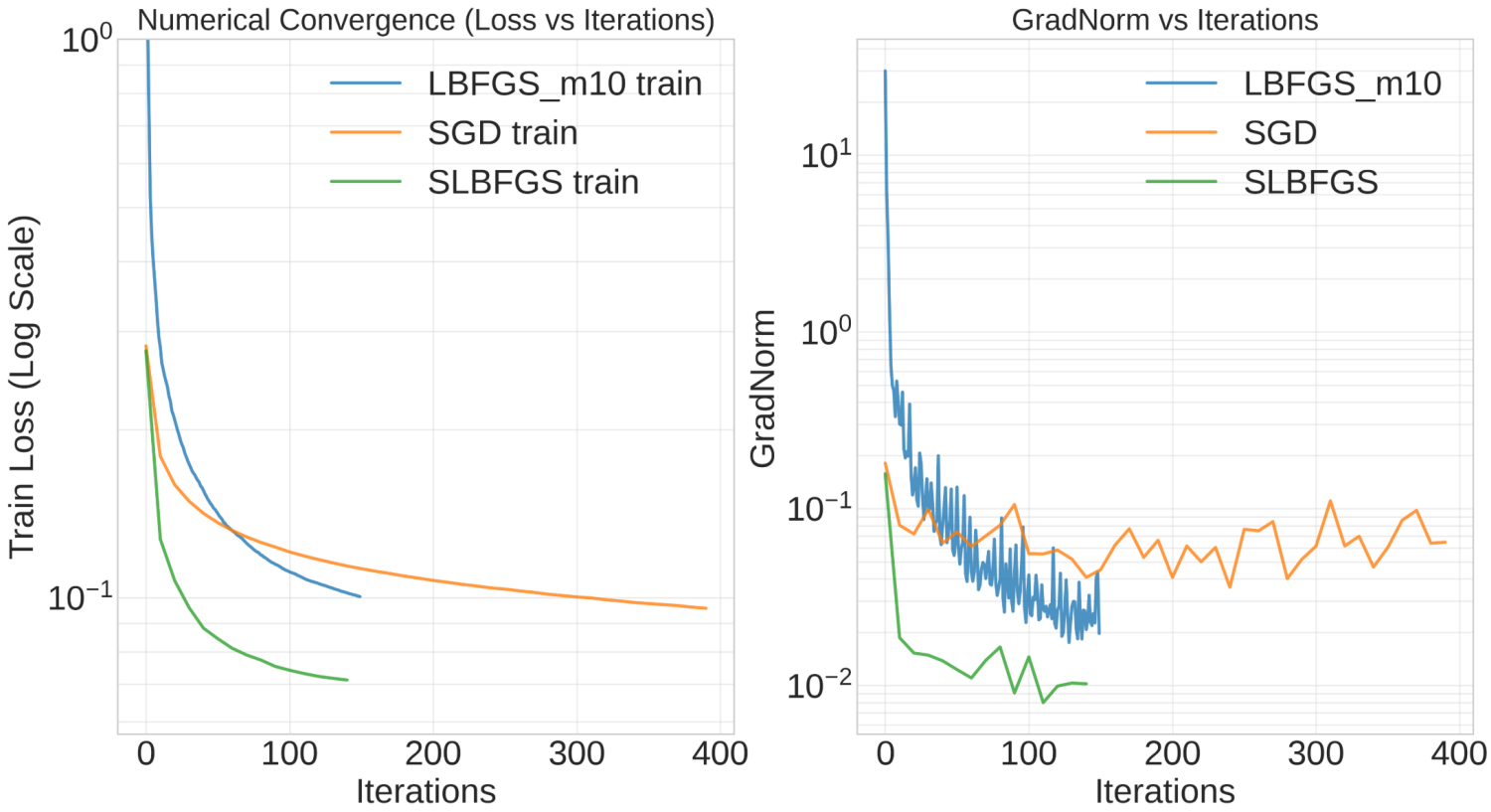
Results: Fashion-MNIST (CPU)



Setup: $784 \to 128 \to 10$, $N = 5{,}000$ (CPU)

Solver	**Train Acc. (%)**	**Test Acc. (%)**
GD	84.40	79.58
SGD	86.40	81.42
S-LBFGS	83.84	79.72
L-BFGS ($m = 10$)	88.10	82.38

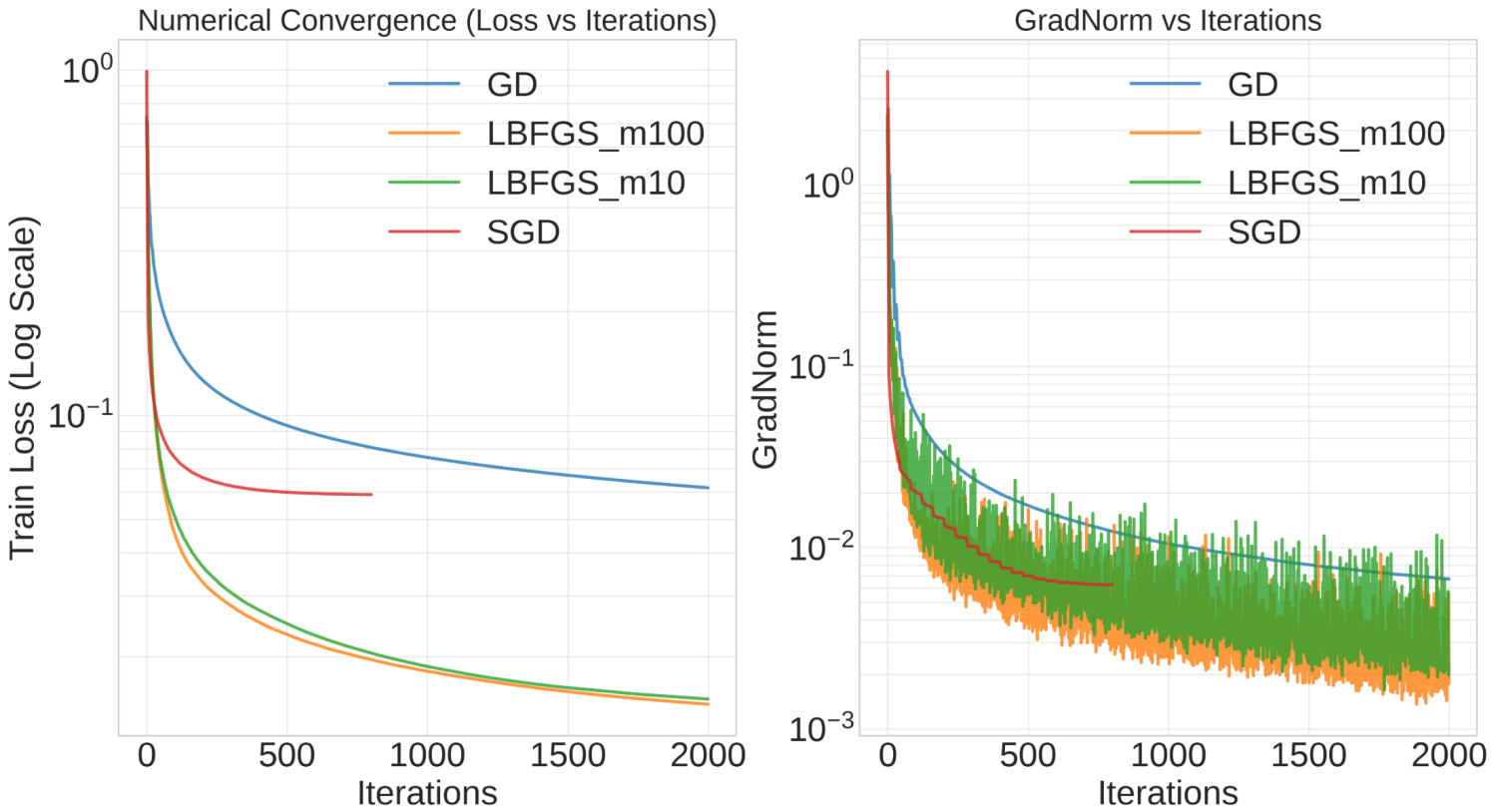
Results: Fashion-MNIST (CPU, Full Dataset)



Setup: $784 \to 128 \to 10$, $N = 60{,}000$ (CPU)

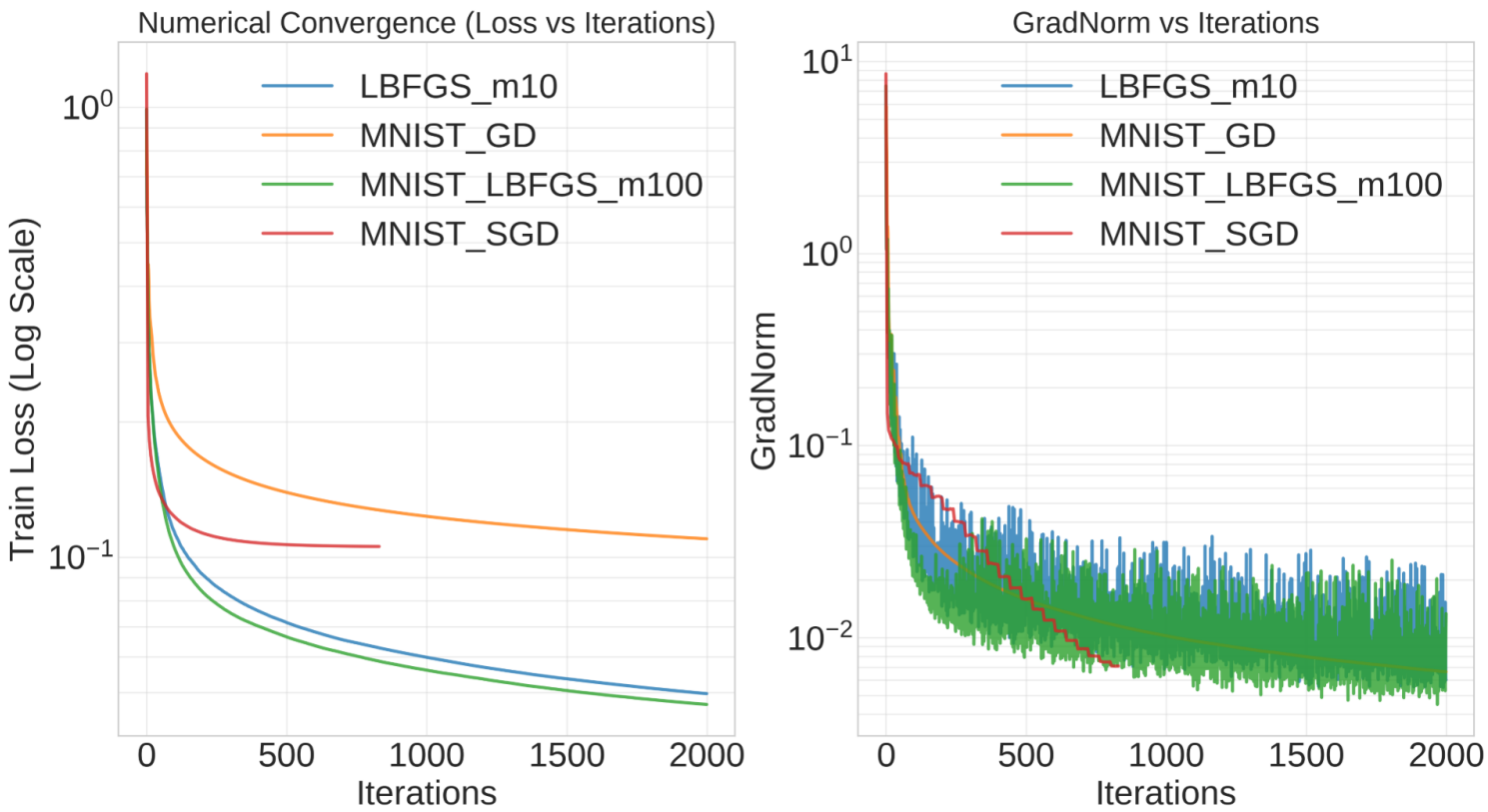
Solver	**Train Acc. (%)**	**Test Acc. (%)**
SGD	89.43	86.98
L-BFGS ($m = 10$)	88.59	86.62
S-LBFGS	**93.46**	**87.98**

Results: MNIST (GPU)



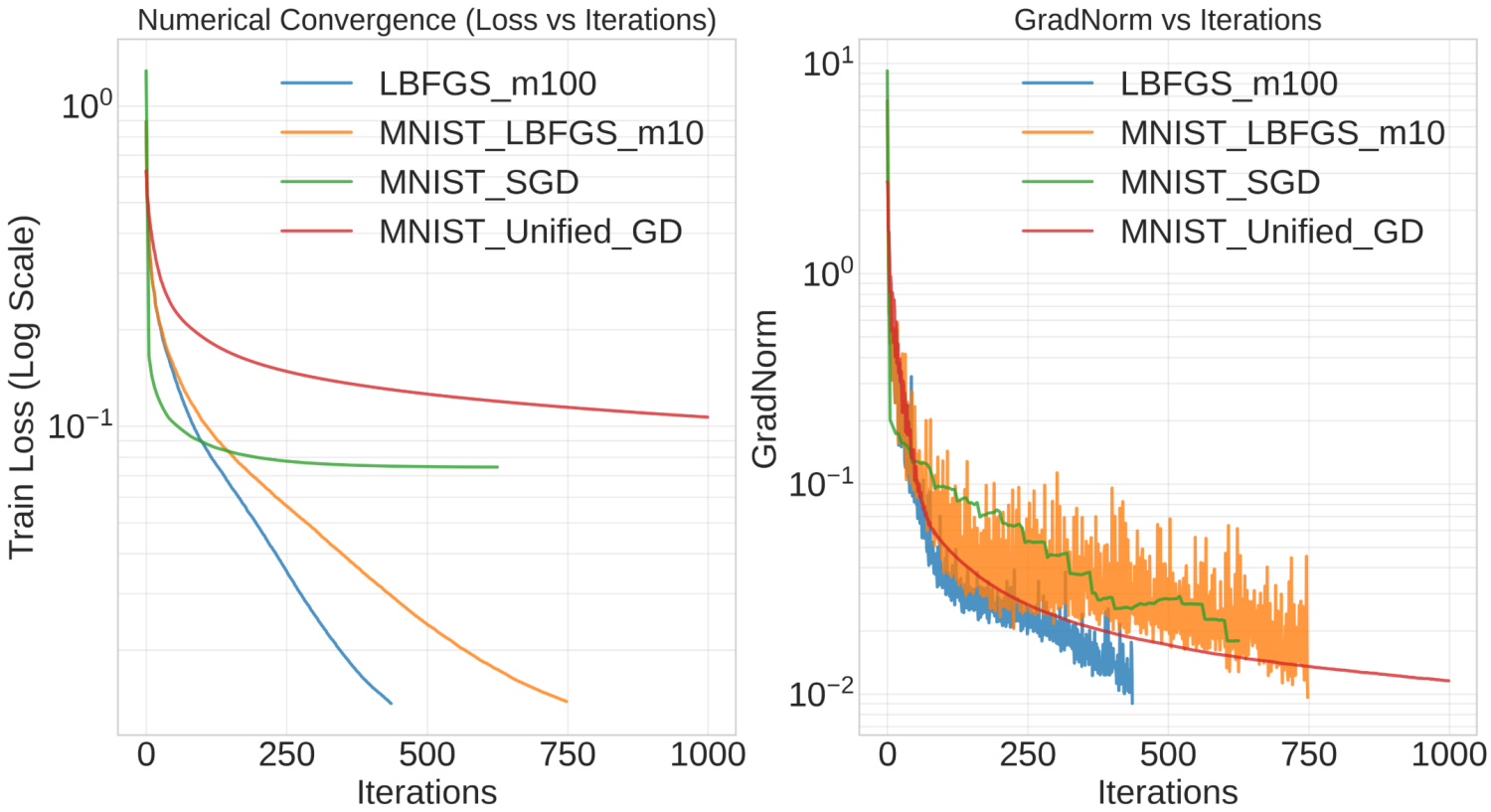
Setup: $784 \to 128 \to 10$, $N = 60{,}000$ (GPU)

Results: Fashion-MNIST (GPU)



Setup: $784 \to 128 \to 10$, $N = 60{,}000$ (GPU)

Results: Fashion-MNIST (GPU, Deep Network)



Setup: $784 \to 256 \to 128 \to 64 \to 10$

Solver	**Train Acc. (%)**	**Test Acc. (%)**
GD	87.55	85.37
SGD	91.37	88.16
L-BFGS ($m = 10$)	98.32	88.75
L-BFGS ($m = 100$)	98.40	88.30

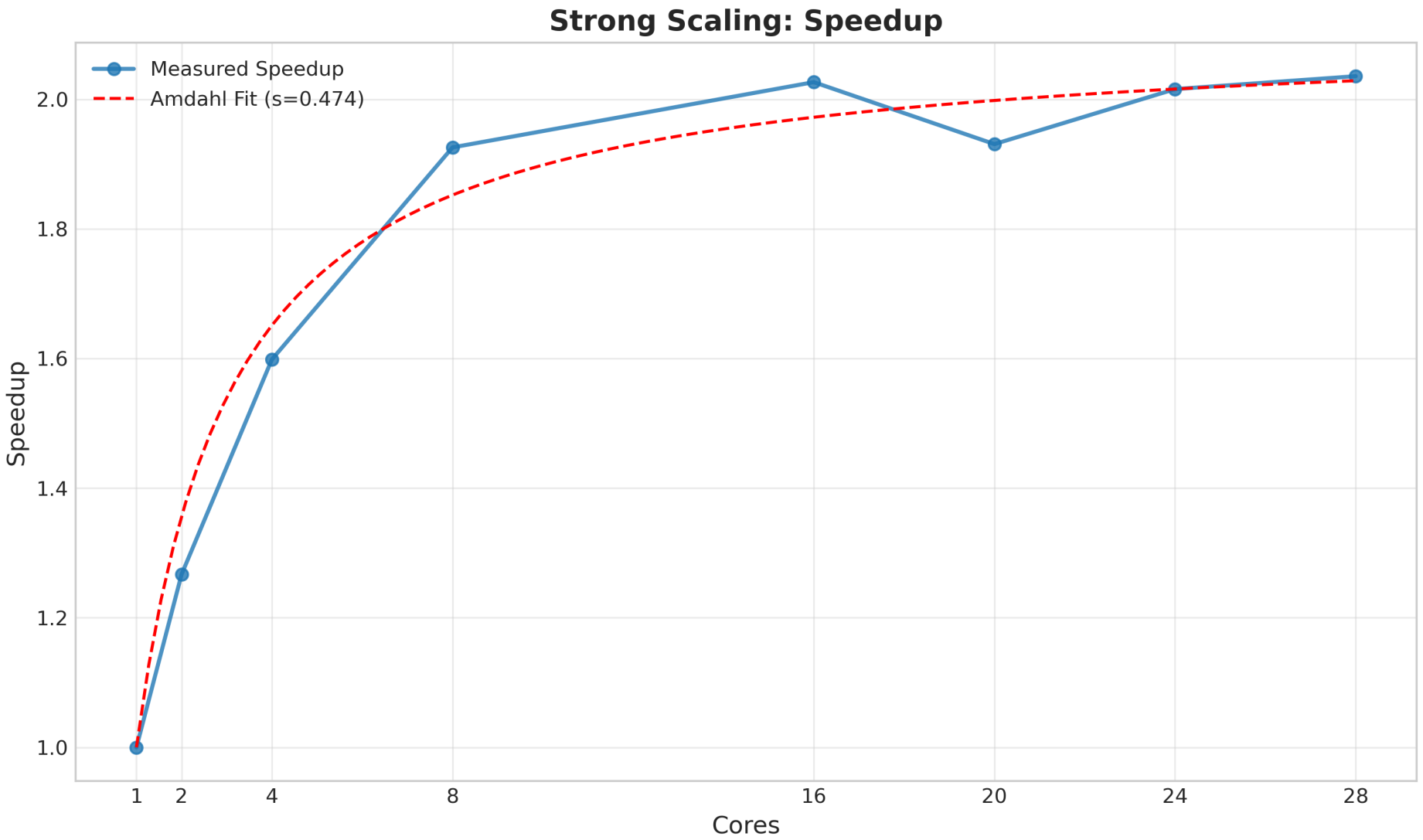
Scalability on Multi-Core CPU

Speedup analysis of S-LBFGS on a 28-core cluster node.

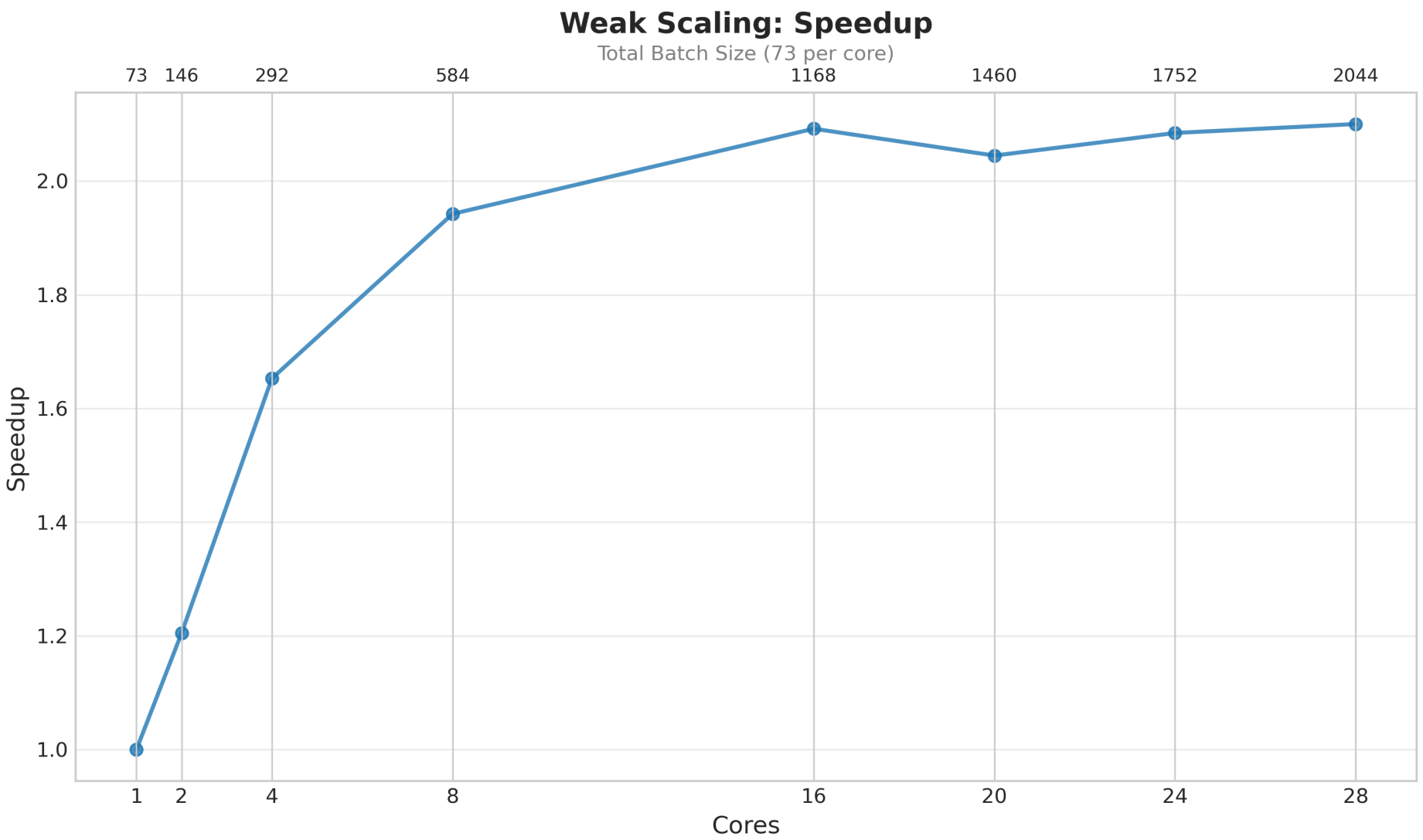
- **Memory-Bound Behavior:**
- Speedup saturates at approximately **2.1x** (Amdahl's Law).
- About 47% of time is dominated by serial components or memory access.

Hardware Conclusion:
For small/medium networks the CPU is competitive, but memory bandwidth quickly becomes the bottleneck for parallel stochastic algorithms.

Scalability CPU: Strong Scaling of S-LBFGS



Scalability CPU: Weak Scaling of S-LBFGS



Beyond Classification: PINNs

Application to Burgers' Equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \qquad x \in [-1, 1], t \in [0, 1]$$

$$u_0(x) = sin(\pi x) \qquad \forall x \in [-1, 1]$$

$$u(-1, t) = u(1, t) = 0 \qquad \forall t \in [0, 1]$$

$$F_{\text{PDE}} = \frac{1}{N_{\text{PDE}}} \sum_{i=1}^{N_{\text{PDE}}} \left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2}\right)^2$$

Loss Function

$$F(\omega) = w_{\text{IC}}\, F_{\text{IC}} + w_{\text{BC}}\, F_{\text{BC}} + w_{\text{PDE}}\, F_{\text{PDE}}$$

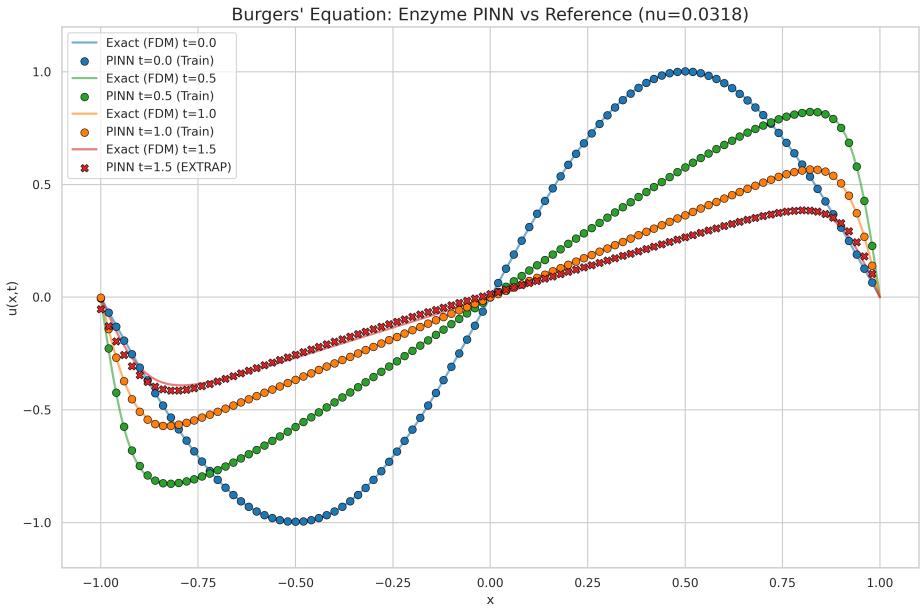
$$F_{\text{PDE}} = \frac{1}{N_{\text{PDE}}} \sum_{i=1}^{N_{\text{PDE}}} \left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2}\right)^2$$

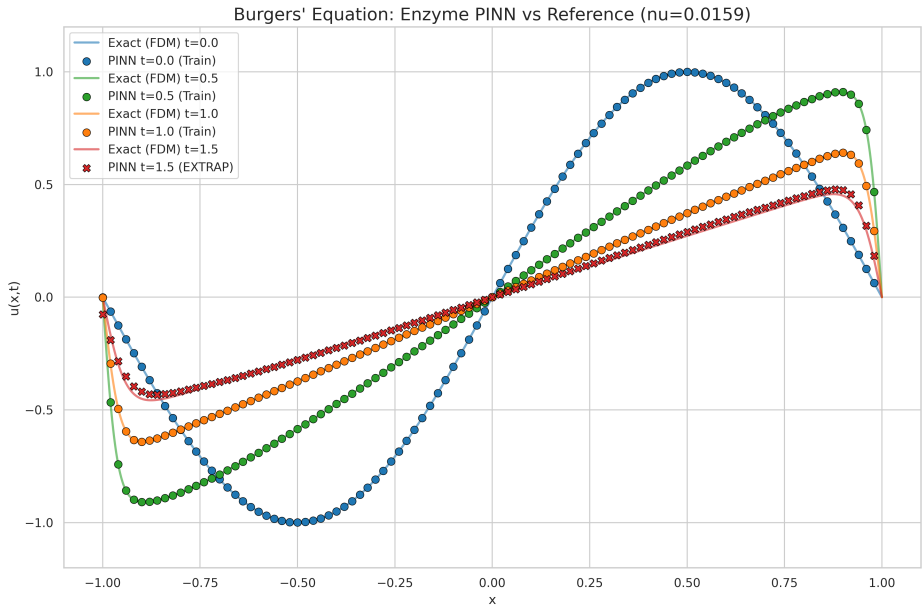
$$F_{\text{BC}} = \frac{1}{N_{\text{BC}}} \sum_{i=1}^{N_{\text{BC}}} \left(u(x_i, t_i) - g(x_i, t_i)\right)^2$$

$$F_{\text{IC}} = \frac{1}{N_{\text{IC}}} \sum_{i=1}^{N_{\text{IC}}} \left(u(x_i, 0) - u_0(x_i)\right)^2$$

PINN Results: Burgers' Equation

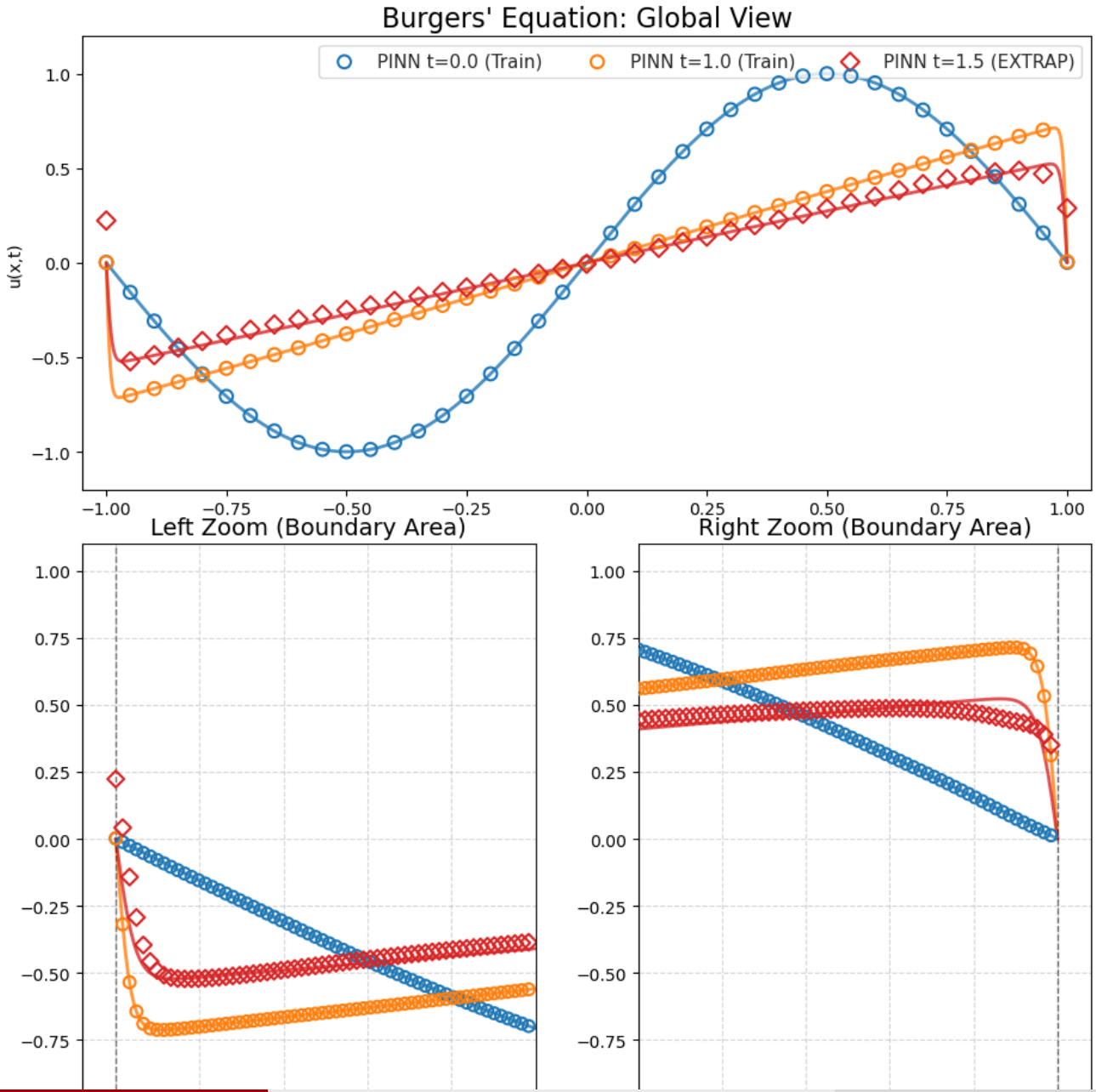
- **Optimizer Strategy:** L-BFGS
  - Good convergence on physics based loss compared to standard GD.
- **Prediction** from the PINN at $t = 1.5s$
- **Outcome:** The model accurately captures the solution dynamics and shock formation across different viscosity regimes (ν).





- Solid Line: Exact analytical solution.
- Dots: Neural Network estimation (PINN output).

PINN results

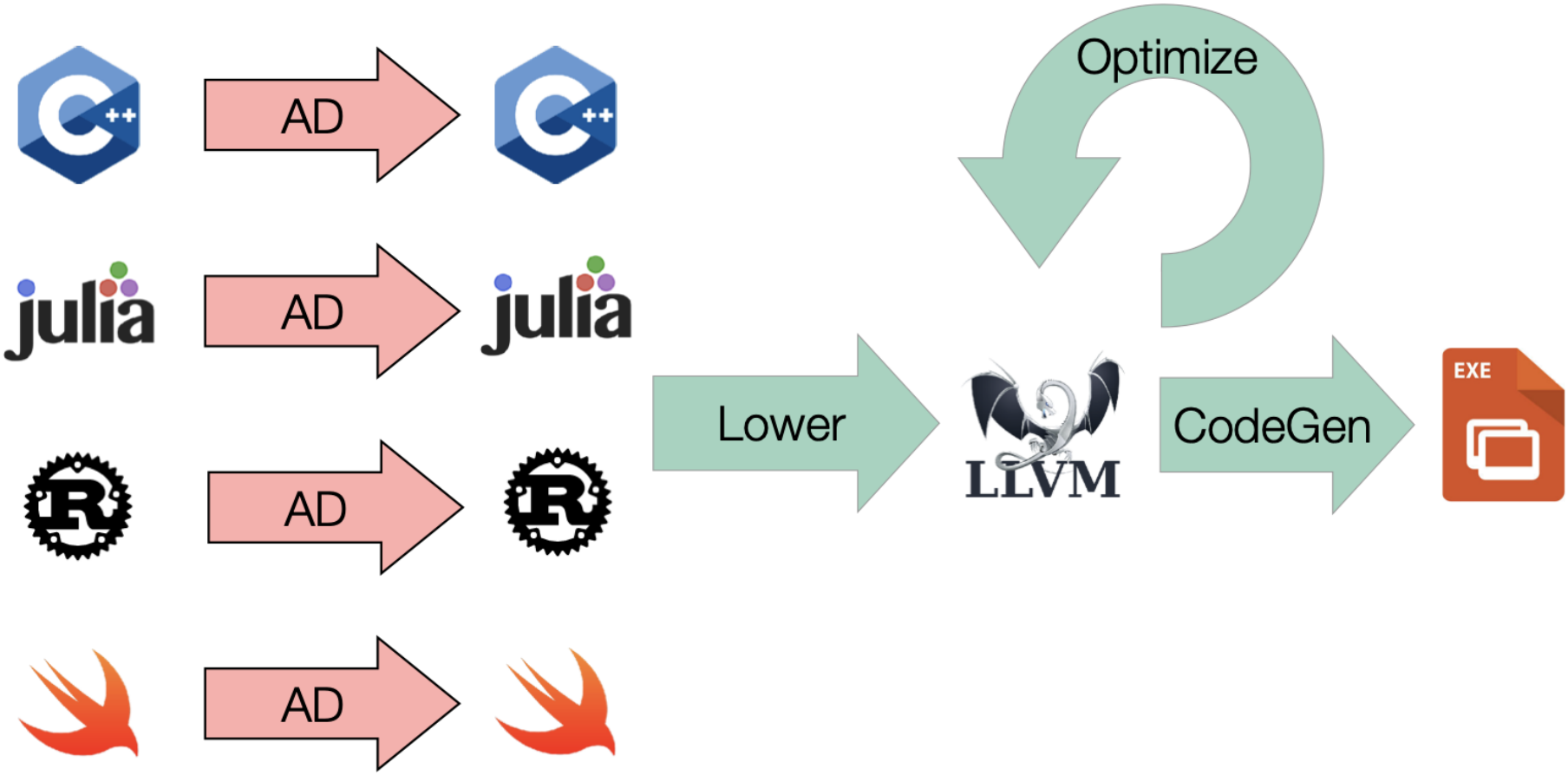


EnzymeAD

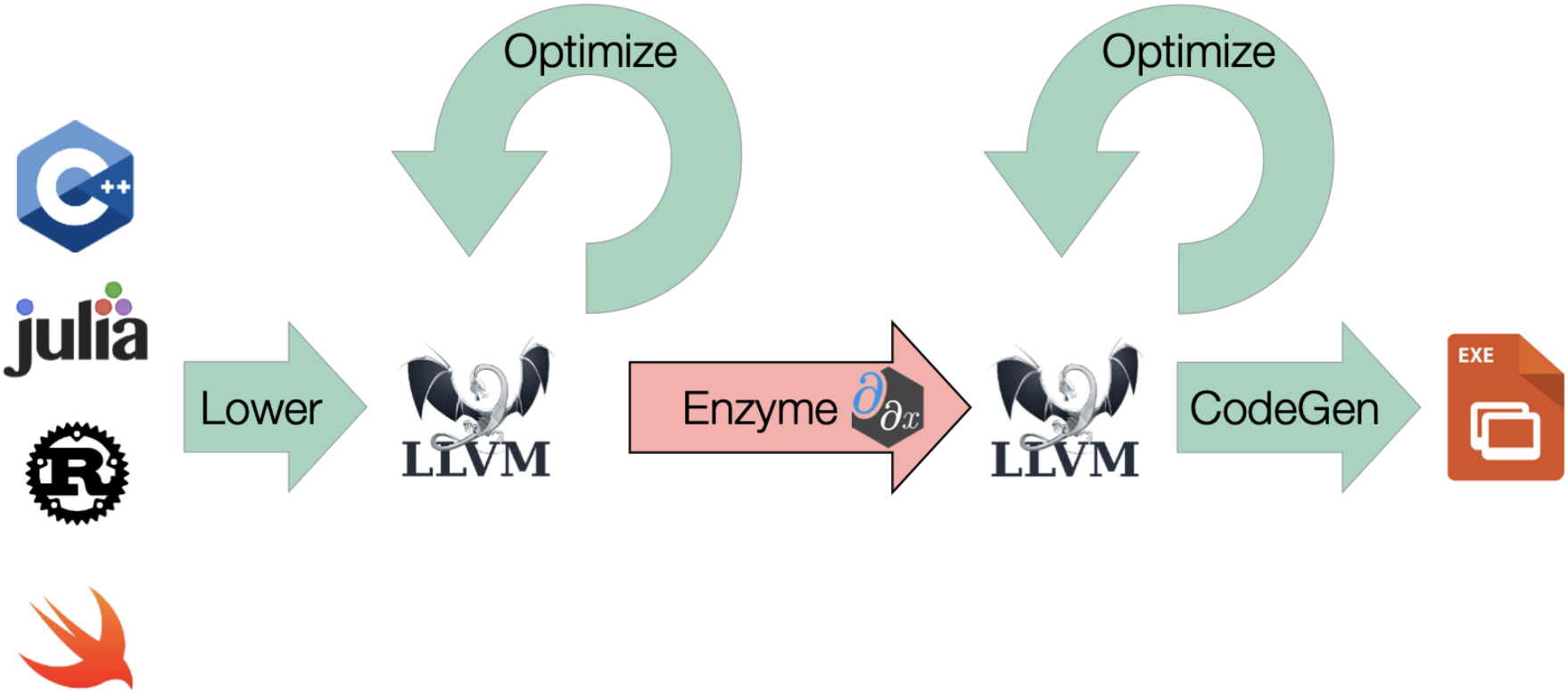
The Differentiation Challenge:

- Standard frameworks (AutoDiff) fail with nested high-order derivatives in the loss function.
- **Solution:** Integration of **EnzymeAD** (LLVM IR level).
- Enables differentiation through the derivative code itself without breaking the computation graph.
- An implementation that would also work on GPU with CUDA

Existing AD Flow

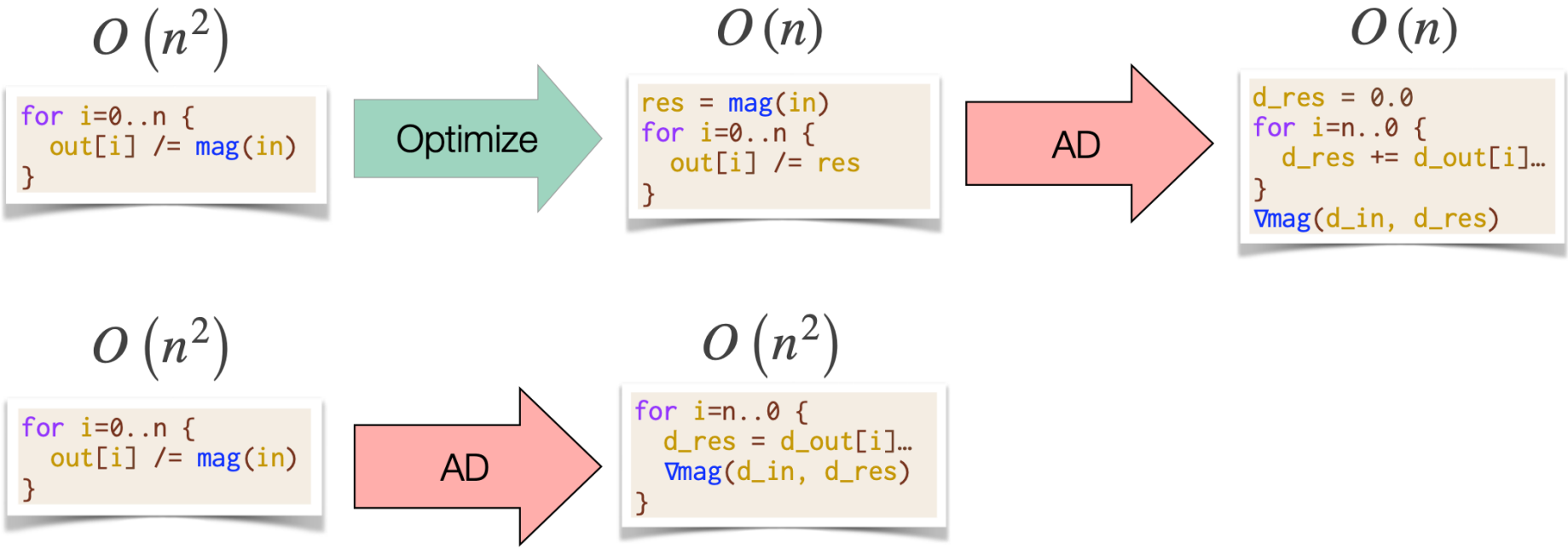


EnzymeAD Flow



EnzymeAD

An example from EnzymeAD docs:



EnzymeAD

While working on the understanding and implementation of PINNs on a CUDA backend using EnzymeAD:

```
/home/gio/amsc_temp/tests/mnist/../../src/cuda/network.cuh:18:68:   required from here
/usr/include/c++/13/bits/stl_construct.h:197:1: internal compiler error: Segmentation fault
  197 |     }
      | ^
0xd32248 crash_signal
        ../../src/gcc/toplev.cc:314
0x70cca744251f ???
        ./signal/../sysdeps/unix/sysv/linux/x86_64/libc_sigaction.c:0
0x1697e1b lookup_page_table_entry
        ../../src/gcc/ggc-page.cc:630
0x1697e1b ggc_set_mark(void const*)
        ../../src/gcc/ggc-page.cc:1550
0x1690eed gt_ggc_mx_lang_tree_node(void*)
        ./gt-cp-tree.h:107
0x16922d5 gt_ggc_mx_lang_tree_node(void*)
        ./gt-cp-tree.h:439
0x16910e1 gt_ggc_mx_lang_tree_node(void*)
        ./gt-cp-tree.h:418
0x16912bd gt_ggc_mx_lang_tree_node(void*)
        ./gt-cp-tree.h:569
0x169a3f0 gt_ggc_mx(tree_node*&)
        /build/gcc-13-IvzKaI/gcc-13-13.1.0/build/gcc/gtype-desc.cc:1806
0x169a3f0 void gt_ggc_mx<tree_node*>(vec<tree_node*, va_gc, vl_embed>*)
```

Thank you!