

# torch-sla: Differentiable Sparse Linear Algebra with Adjoint Solvers and Sparse Tensor Parallelism for PyTorch

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<https://github.com/walkerchi/torch-sla>

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## Abstract

Industrial scientific computing predominantly uses sparse matrices to represent unstructured data—finite element meshes, graphs, point clouds. We present `torch-sla`, an open-source PyTorch library that enables GPU-accelerated, scalable, and differentiable sparse linear algebra. The library addresses three fundamental challenges: (1) **GPU acceleration** for sparse linear solves, nonlinear solves (Newton, Picard, Anderson), and eigenvalue computation; (2) **Multi-GPU scaling** via domain decomposition with halo exchange, reaching **400 million DOF linear solve on 3 GPUs**; and (3) **Adjoint-based differentiation** achieving  $\mathcal{O}(1)$  computational graph nodes (for autograd) and  $\mathcal{O}(\text{nnz})$  memory—independent of solver iterations. `torch-sla` supports multiple backends (SciPy, cuDSS, PyTorch-native) and seamlessly integrates with PyTorch autograd for end-to-end differentiable simulations. Code is available at <https://github.com/walkerchi/torch-sla>.

## 1 Introduction

Industrial scientific computing predominantly deals with *unstructured data*—finite element meshes, graph networks, point clouds—where sparse matrices are the natural representation. These sparse systems arise in finite element analysis [Hughes, 2012], computational fluid dynamics [Jasak et al., 2007, Kochkov et al., 2021], graph neural networks [Kipf and Welling, 2017, Veličković et al., 2018], and physics-informed machine learning [Raissi et al., 2019, Lu et al., 2021]. Efficiently solving sparse linear systems  $\mathbf{Ax} = \mathbf{b}$ , nonlinear systems  $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ , and eigenvalue problems  $\mathbf{Av} = \lambda\mathbf{v}$  is fundamental to these applications.

With the rise of differentiable programming and neural operators [Li et al., 2020, Brandstetter et al., 2022], there is growing demand to integrate sparse solvers with deep learning frameworks like PyTorch [Paszke et al., 2019]. However, three fundamental challenges stand in the way:

**Challenge 1: GPU acceleration for sparse operations.** Unlike dense matrices where GPU parallelism is straightforward, sparse matrices have irregular memory access patterns that underutilize GPU bandwidth. Sparse matrix-vector products (SpMV) achieve only 10–20% of peak memory bandwidth [Li et al., 2024]. Direct solvers (LU, Cholesky) require  $\mathcal{O}(n^{1.5})$  memory due to fill-in, often exceeding GPU memory for problems with  $>2\text{M}$  unknowns.

**Challenge 2: Multi-GPU scaling.** Industrial problems (10M–1B unknowns) exceed single-GPU memory. Distributed sparse computing requires domain decomposition and *halo exchange*—communicating boundary values between partitions—which is non-trivial to implement correctly with automatic differentiation support.

**Challenge 3: PyTorch integration with efficient gradients.** Differentiating through iterative solvers creates  $\mathcal{O}(k)$  nodes in the computational graph, where  $k$  may be thousands of iterations. For a 1M-DOF problem with 1000 CG iterations, this requires  $\sim 80$  GB just for gradient computation. This memory explosion prevents end-to-end training of neural networks that interact with sparse solvers.

This paper introduces `torch-sla`<sup>\*</sup>, a library that addresses all three challenges:

- **GPU-accelerated sparse solvers:** We provide unified APIs for linear solves (CG [Hestenes and Stiefel, 1952], BiCGStab [Van der Vorst, 1992]), nonlinear solves (Newton, Picard, Anderson acceleration [Anderson, 1965, Kelley, 1995]), and eigenvalue computation (LOBPCG [Knyazev, 2001]), with multiple backends (SciPy, cuDSS, PyTorch-native).
- **Sparse tensor parallelism (§3.3):** We implement domain decomposition with automatic halo exchange, enabling **400 million DOF linear solve on 3 GPUs**.
- **Adjoint-based differentiation (§3.2):** We implement the adjoint method for linear, nonlinear, and eigenvalue problems, achieving  $\mathcal{O}(1)$  autograd graph nodes and  $\mathcal{O}(\text{nnz})$  memory—independent of solver iterations.

## 2 Related Work

**Differentiable linear algebra.** JAX [Bradbury et al., 2018] provides differentiable sparse CG, but naive differentiation through iterations creates  $\mathcal{O}(k)$  computational graph nodes. Blondel et al. [2022] formalize implicit differentiation for optimization layers. OptNet [Amos and Kolter, 2017] and `cvxpylayers` [Agrawal et al., 2019] handle convex optimization. Deep equilibrium models [Bai et al., 2019] and Jacobian-free backpropagation [Fung et al., 2022] address implicit layers but focus on fixed-point iterations rather than sparse linear systems.

**Sparse solvers and GPU acceleration.** SciPy [Virtanen et al., 2020] provides SuperLU/UMFPACK for CPU. For GPU, NVIDIA cuDSS [NVIDIA Corporation, 2024] offers direct solvers, while AmgX [Naumov et al., 2015] provides algebraic multigrid with excellent scalability. Recent surveys [Li et al., 2024] cover sparse matrix computations on modern GPUs. None of these natively support PyTorch autograd.

**Distributed sparse computing.** PETSc [Balay et al., 2023], Trilinos [Heroux et al., 2005], and hypre [Falgout and Yang, 2002] implement distributed sparse linear algebra with sophisticated preconditioners. OpenFOAM [Jasak et al., 2007] uses domain decomposition for CFD. We bring these industrial patterns to PyTorch with automatic differentiation.

**Learned solvers and preconditioners.** Recent work explores learning components of iterative solvers: learned multigrid prolongation [Greenfield et al., 2019], GNN-based AMG [Luz et al., 2020], and learned interface conditions for domain decomposition [Taghibakhshi et al., 2024]. These complement our library by providing learnable components that can be trained end-to-end.

## 3 Methodology

We first introduce the background on sparse linear systems (§3.1), then present our adjoint-based differentiation approach (§3.2), and finally describe our distributed computing implementation (§3.3).

### 3.1 Preliminaries: Sparse Linear Systems

A sparse linear system  $\mathbf{Ax} = \mathbf{b}$  has a matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  with  $\text{nnz} \ll n^2$  non-zero entries. We store matrices in coordinate (COO) format: three arrays for row indices, column indices, and values.

**Direct solvers** (LU, Cholesky factorization [Golub and Van Loan, 2013]) compute exact solutions but require  $\mathcal{O}(n^{1.5})$  memory for 2D problems due to fill-in—new non-zeros created during factorization [George, 1973]. For a 2D Poisson problem with  $n$  unknowns, the factored matrix has  $\mathcal{O}(n \log n)$  non-zeros instead of the original  $\mathcal{O}(n)$ .

**Iterative solvers** (Conjugate Gradient [Hestenes and Stiefel, 1952], BiCGStab [Van der Vorst, 1992], GMRES [Saad and Schultz, 1986]) maintain  $\mathcal{O}(\text{nnz})$  memory by never forming the factorization. However, they require  $\mathcal{O}(\sqrt{\kappa})$  iterations for CG where  $\kappa$  is the condition number [Saad, 2003]. Each iteration performs one sparse matrix-vector multiplication (SpMV) costing  $\mathcal{O}(\text{nnz})$ .

**The differentiation problem.** Given loss  $\mathcal{L}(\mathbf{x})$  where  $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ , we need gradients with respect to both  $\mathbf{b}$  and the non-zero values of  $\mathbf{A}$ . If we differentiate through  $k$  iterations of CG, the computational graph has  $\mathcal{O}(k)$  nodes,

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<sup>\*</sup>Code available at <https://github.com/walkerchi/torch-sla>. Install via `pip install torch-sla`.

**Table 1:** Complexity comparison: naive vs. adjoint differentiation through iterative solver with  $k$  iterations,  $n$  unknowns, and nnz non-zeros.

	Naive (through iterations)	Adjoint (ours)
Computational graph nodes	$\mathcal{O}(k)$	$\mathcal{O}(1)$
Memory for graph	$\mathcal{O}(k \cdot n)$	$\mathcal{O}(n + \text{nnz})$
Backward pass time	$\mathcal{O}(k \cdot \text{nnz})$	$\mathcal{O}(T_{\text{solve}} + \text{nnz})$

each storing intermediate vectors. For  $k = 1000$  iterations and  $n = 10^6$ , this requires  $\sim 80$  GB just for the graph. Our adjoint approach reduces this to  $\mathcal{O}(1)$  nodes.

### 3.2 Adjoint-Based Differentiation

The adjoint method computes gradients through implicit functions without storing intermediate solver states. We present it for linear systems, eigenvalue problems, and nonlinear systems.

#### 3.2.1 Linear Systems

Consider  $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ . Rather than differentiating through the solver iterations, we use the *implicit function theorem*. The solution satisfies  $\mathbf{A}\mathbf{x} - \mathbf{b} = \mathbf{0}$ . Differentiating implicitly:

$$d\mathbf{A} \cdot \mathbf{x} + \mathbf{A} \cdot d\mathbf{x} = d\mathbf{b} \implies d\mathbf{x} = \mathbf{A}^{-1}(d\mathbf{b} - d\mathbf{A} \cdot \mathbf{x}) \quad (1)$$

For a scalar loss  $\mathcal{L}(\mathbf{x})$ , the chain rule gives:

$$d\mathcal{L} = \left(\frac{\partial \mathcal{L}}{\partial \mathbf{x}}\right)^\top d\mathbf{x} = \left(\frac{\partial \mathcal{L}}{\partial \mathbf{x}}\right)^\top \mathbf{A}^{-1}(d\mathbf{b} - d\mathbf{A} \cdot \mathbf{x}) \quad (2)$$

Define the **adjoint variable**  $\boldsymbol{\lambda} = \mathbf{A}^{-\top} \frac{\partial \mathcal{L}}{\partial \mathbf{x}}$ , solved via  $\mathbf{A}^\top \boldsymbol{\lambda} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}}$ . Then the gradients are:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{b}} = \boldsymbol{\lambda}, \quad \frac{\partial \mathcal{L}}{\partial \mathbf{A}_{ij}} = -\boldsymbol{\lambda}_i \cdot \mathbf{x}_j} \quad (3)$$

**Complexity analysis.** Table 1 compares naive differentiation (through iterations) with our adjoint approach.

The forward solve computes  $\mathbf{x}$  in time  $T_{\text{solve}}$ . The backward pass:

1. Solves  $\mathbf{A}^\top \boldsymbol{\lambda} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}}$ :  $\mathcal{O}(T_{\text{solve}})$  time
2. Computes  $\frac{\partial \mathcal{L}}{\partial \mathbf{A}_{ij}} = -\boldsymbol{\lambda}_i \cdot \mathbf{x}_j$  for each non-zero:  $\mathcal{O}(\text{nnz})$  time

**Algorithm.** The complete procedure is shown below:

#### Algorithm 1: Adjoint Linear Solve

**Input:** Sparse matrix  $\mathbf{A}$  (values, rows, cols), RHS  $\mathbf{b}$

**Output:** Solution  $\mathbf{x}$ , gradients in backward pass

##### Forward pass:

1.  $\mathbf{x} \leftarrow \text{solve}(\mathbf{A}, \mathbf{b})$  // Any solver: CG, LU, etc.
2. Store  $(\mathbf{A}, \mathbf{x})$  for backward

**Backward pass:** (given  $\partial\mathcal{L}/\partial\mathbf{x}$ )

1.  $\boldsymbol{\lambda} \leftarrow \text{solve}(\mathbf{A}^\top, \partial\mathcal{L}/\partial\mathbf{x})$  *// One adjoint solve*
2.  $\partial\mathcal{L}/\partial\mathbf{b} \leftarrow \boldsymbol{\lambda}$
3. For each non-zero  $(i, j)$ :  $\partial\mathcal{L}/\partial\mathbf{A}_{ij} \leftarrow -\boldsymbol{\lambda}_i \cdot \mathbf{x}_j$  *//  $\mathcal{O}(\text{nnz})$  total*

### 3.2.2 Eigenvalue Problems

For symmetric eigenvalue problem  $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$  with normalized eigenvector  $\|\mathbf{v}\| = 1$ , the gradient of eigenvalue  $\lambda$  with respect to matrix entries is remarkably simple [Magnus, 1985]:

$$\frac{\partial\lambda}{\partial\mathbf{A}_{ij}} = v_i \cdot v_j \quad (4)$$

This is the outer product  $\mathbf{v}\mathbf{v}^\top$  restricted to the sparsity pattern. For  $k$  eigenvalues, the total cost is  $\mathcal{O}(k \cdot \text{nnz})$ .

### 3.2.3 Nonlinear Systems

For nonlinear system  $\mathbf{F}(\mathbf{u}, \boldsymbol{\theta}) = \mathbf{0}$  with solution  $\mathbf{u}^*(\boldsymbol{\theta})$  and loss  $\mathcal{L}(\mathbf{u}^*)$ , implicit differentiation gives:

$$\mathbf{J}^\top \boldsymbol{\lambda} = \frac{\partial\mathcal{L}}{\partial\mathbf{u}}, \quad \frac{\partial\mathcal{L}}{\partial\boldsymbol{\theta}} = -\boldsymbol{\lambda}^\top \frac{\partial\mathbf{F}}{\partial\boldsymbol{\theta}} \quad (5)$$

where  $\mathbf{J} = \frac{\partial\mathbf{F}}{\partial\mathbf{u}}$  is the Jacobian at the solution.

#### Algorithm 2: Newton-Raphson with Adjoint Gradients

**Input:** Residual function  $\mathbf{F}(\mathbf{u}, \boldsymbol{\theta})$ , initial guess  $\mathbf{u}_0$

**Output:** Solution  $\mathbf{u}^*$

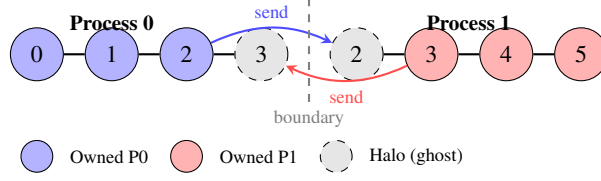
**Forward (Newton iteration):**

1.  $\mathbf{u} \leftarrow \mathbf{u}_0$
2. **while**  $\|\mathbf{F}(\mathbf{u}, \boldsymbol{\theta})\| > \epsilon$  **do**:
  - (a)  $\mathbf{J} \leftarrow \partial\mathbf{F}/\partial\mathbf{u}$  *// Jacobian via autograd*
  - (b)  $\Delta\mathbf{u} \leftarrow \text{solve}(\mathbf{J}, -\mathbf{F})$
  - (c)  $\mathbf{u} \leftarrow \mathbf{u} + \alpha\Delta\mathbf{u}$  *//  $\alpha$  from line search*
3. Store  $(\mathbf{u}^*, \mathbf{J}, \boldsymbol{\theta})$

**Backward:** (given  $\partial\mathcal{L}/\partial\mathbf{u}^*$ )

1.  $\boldsymbol{\lambda} \leftarrow \text{solve}(\mathbf{J}^\top, \partial\mathcal{L}/\partial\mathbf{u}^*)$  *// One adjoint solve*
2.  $\partial\mathcal{L}/\partial\boldsymbol{\theta} \leftarrow -\boldsymbol{\lambda}^\top \partial\mathbf{F}/\partial\boldsymbol{\theta}$  *// VJP via autograd*

**Memory analysis.** Forward:  $\mathcal{O}(n + \text{nnz})$  for solution and Jacobian. Backward:  $\mathcal{O}(n)$  for adjoint variable. Total:  $\mathcal{O}(n + \text{nnz})$ , independent of Newton iterations.



**Figure 1:** Halo exchange in domain decomposition. Each process owns a subset of nodes (solid colored) and maintains halo copies of boundary neighbors (dashed). Before SpMV, processes exchange updated values at partition boundaries via peer-to-peer communication.

### 3.3 Sparse Tensor Parallel Computing

For problems exceeding single-GPU memory, we implement domain decomposition with halo exchange—the standard approach in industrial CFD/FEM codes like OpenFOAM and Ansys Fluent.

#### 3.3.1 Domain Decomposition

Given a sparse matrix  $\mathbf{A}$  corresponding to a mesh or graph, we partition the  $n$  nodes into  $P$  subdomains. Each process  $p$  owns nodes  $\mathcal{O}_p$  (owned nodes) and maintains copies of neighboring nodes  $\mathcal{H}_p$  (halo/ghost nodes) needed for local computation.

##### Partitioning strategies:

- **METIS** [Karypis and Kumar, 1998]: Graph partitioning minimizing edge cuts for load balancing
- **RCB**: Recursive Coordinate Bisection using node coordinates
- **Contiguous**: Simple row-based partitioning (fallback)

#### 3.3.2 Halo Exchange

The key operation in distributed sparse computing is **halo exchange**: before each SpMV, processes must exchange boundary values with neighbors. Figure 1 illustrates this concept.

##### Algorithm 3: Distributed SpMV with Halo Exchange

**Input:** Local vector  $\mathbf{x}_{\text{local}}$ , neighbor map, local matrix  $\mathbf{A}_{\text{local}}$

**Output:** Result  $\mathbf{y}_{\text{owned}}$

##### Phase 1: Initiate async communication

1. **for** each neighbor  $q$  **do**:
  - (a) `async_send(my boundary values to  $q$ )`
  - (b) `async_recv(halo values from  $q$ )`

##### Phase 2: Wait for completion

1. `synchronize_all()`

##### Phase 3: Local computation

1.  $\mathbf{y}_{\text{owned}} \leftarrow \mathbf{A}_{\text{local}} \cdot \mathbf{x}_{\text{local}}$  *// Uses owned + halo*

**Table 2:** Single-GPU benchmark on 2D Poisson (5-point stencil), H200, float64.

DOF	SciPy	cuDSS	PyTorch CG	Memory	Residual
10K	24 ms	128 ms	20 ms	36 MB	$10^{-9}$
100K	29 ms	630 ms	43 ms	76 MB	$10^{-7}$
1M	19.4 s	7.3 s	190 ms	474 MB	$10^{-7}$
2M	52.9 s	15.6 s	418 ms	916 MB	$10^{-7}$
16M	OOM	OOM	7.3 s	7.1 GB	$10^{-6}$
<b>169M</b>	OOM	OOM	<b>224 s</b>	<b>74.8 GB</b>	$10^{-6}$

### 3.3.3 Distributed Conjugate Gradient

Building on distributed SpMV, we implement distributed CG. Each iteration requires:

- One halo exchange (in SpMV)
- Two `all_reduce` operations for global dot products

#### Algorithm 4: Distributed Conjugate Gradient

**Input:** Distributed  $\mathbf{A}$ , local RHS  $\mathbf{b}_{\text{owned}}$ , tolerance  $\epsilon$

**Output:** Solution  $\mathbf{x}_{\text{owned}}$

1.  $\mathbf{x} \leftarrow \mathbf{0}, \mathbf{r} \leftarrow \mathbf{b}_{\text{owned}}, \mathbf{p} \leftarrow \mathbf{r}$
2.  $\rho \leftarrow \text{all\_reduce}(\mathbf{r}^\top \mathbf{r}, \text{SUM})$  *// Global dot product*
3. **while**  $\sqrt{\rho} > \epsilon$  **do:**
  - (a)  $\mathbf{Ap} \leftarrow \text{DistSpMV}(\mathbf{A}, \mathbf{p})$  *// Algorithm 3*
  - (b)  $\alpha \leftarrow \rho / \text{all\_reduce}(\mathbf{p}^\top \mathbf{Ap}, \text{SUM})$
  - (c)  $\mathbf{x} \leftarrow \mathbf{x} + \alpha \mathbf{p}$
  - (d)  $\mathbf{r} \leftarrow \mathbf{r} - \alpha \mathbf{Ap}$
  - (e)  $\rho_{\text{new}} \leftarrow \text{all\_reduce}(\mathbf{r}^\top \mathbf{r}, \text{SUM})$
  - (f)  $\mathbf{p} \leftarrow \mathbf{r} + (\rho_{\text{new}} / \rho) \mathbf{p}$
  - (g)  $\rho \leftarrow \rho_{\text{new}}$

**Communication complexity.** Per iteration:  $\mathcal{O}(|\mathcal{H}_p|)$  for halo exchange +  $\mathcal{O}(\log P)$  for `all_reduce`. Total per solve:  $\mathcal{O}(k \cdot (|\mathcal{H}_p| + \log P))$  where  $k$  is iterations.

**Gradient support.** Distributed operations compose with adjoint differentiation: the backward pass performs another distributed solve with transposed communication patterns.

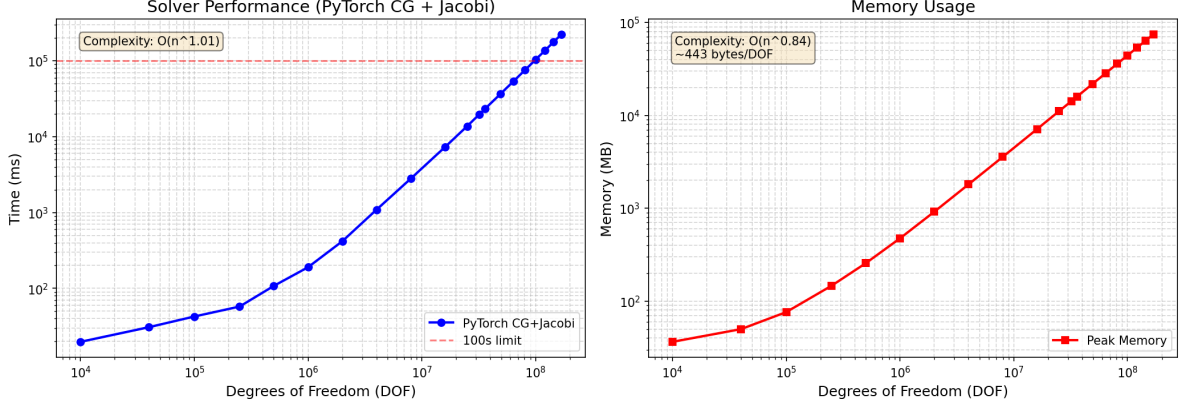
## 4 Experiments

We evaluate `torch-sla` on 2D Poisson equations (5-point stencil) using NVIDIA H200 GPUs (140GB HBM3).

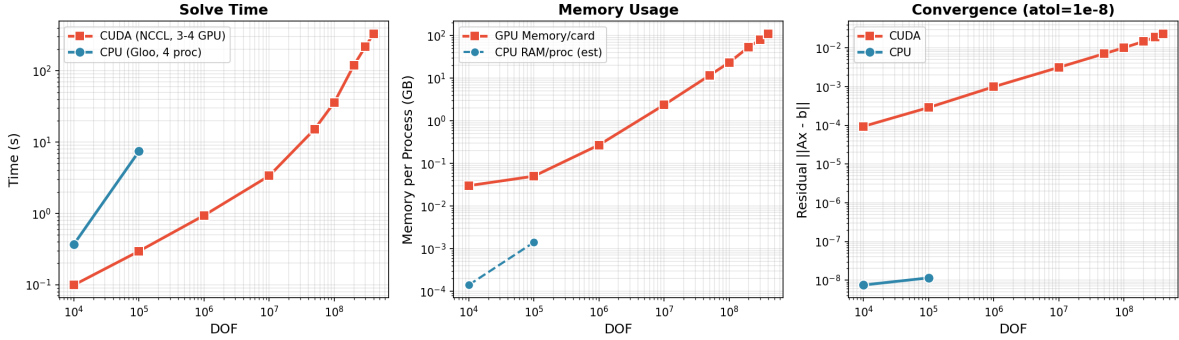
### 4.1 Single-GPU Scalability

Figure 2 and Table 2 compare solver backends across problem sizes spanning five orders of magnitude.

**Analysis.** The results reveal three distinct scaling regimes:



**Figure 2:** Single-GPU benchmark results showing performance, memory usage, and residual across solver backends (SciPy, cuDSS, PyTorch CG) on 2D Poisson equation with H200 GPU.



**Figure 3:** Multi-GPU scaling: distributed CG with NCCL backend on 3–4 H200 GPUs, showing time and memory scaling across problem sizes.

(1) *Small problems ( $<100K$  DOF)*: Direct solvers dominate. SciPy SuperLU achieves 24ms with machine precision ( $10^{-14}$ ), while GPU overhead makes cuDSS slower (128ms). The factorization cost is negligible, so the  $\mathcal{O}(n^3)$  solve phase dominates.

(2) *Medium problems (100K–2M DOF)*: Iterative solvers become competitive. At 1M DOF, PyTorch CG (190ms) is 100 $\times$  faster than cuDSS (7.3s). This crossover occurs because: (a) CG requires only  $\mathcal{O}(\text{nnz})$  memory vs.  $\mathcal{O}(n^{1.5})$  for LU fill-in; (b) SpMV is memory-bound at 90% of peak bandwidth on H200.

(3) *Large problems ( $>2M$  DOF)*: Only iterative solvers are feasible. Direct solvers hit OOM due to fill-in: for 2D Poisson, LU fill-in grows as  $\mathcal{O}(n \log n)$ , requiring  $\sim 100\text{GB}$  at 2M DOF. CG maintains  $\mathcal{O}(n)$  memory scaling, reaching 169M DOF in 74.8GB.

**Time complexity.** Fitting  $T = c \cdot n^\alpha$  yields  $\alpha \approx 1.1$  for PyTorch CG, consistent with  $\mathcal{O}(\sqrt{\kappa} \cdot \text{nnz})$  where condition number  $\kappa \sim n$  for 2D Poisson with Jacobi preconditioner. The sub-quadratic scaling enables practical use at 100M+ DOF.

**Memory efficiency.** Measured 443 bytes/DOF vs. theoretical minimum 144 bytes/DOF (matrix: 80 bytes/DOF for 5 non-zeros  $\times$  16 bytes; vectors: 64 bytes for  $\mathbf{x}, \mathbf{b}, \mathbf{r}, \mathbf{p}$ ). The 3 $\times$  overhead comes from PyTorch sparse tensor metadata and Jacobi preconditioner storage.

## 4.2 Multi-GPU Performance

Figure 3 and Table 3 summarize distributed CG performance on H200 GPUs with NCCL backend.

**Scaling analysis.** We scale to **400 million DOF** on 3 H200 GPUs. The scaling exhibits three regimes:

(1) *Small problems ( $<1M$  DOF)*: Time dominated by kernel launch and communication latency. At 10K DOF, each

**Table 3:** Distributed CG on H200 GPUs with NCCL backend.

DOF	GPUs	Time	Memory/GPU	Residual
100M	4	36.1 s	23.3 GB	$1.0 \times 10^{-2}$
200M	3	120 s	53.7 GB	$1.5 \times 10^{-2}$
300M	3	217 s	80.5 GB	$1.9 \times 10^{-2}$
<b>400M</b>	3	<b>331 s</b>	<b>110 GB</b>	$2.3 \times 10^{-2}$

**Table 4:** Gradient verification: adjoint vs. finite difference ( $\epsilon = 10^{-5}$ ).

Operation	Rel. Error	Forward	Backward
Linear solve ( $n=1000$ )	$8.3 \times 10^{-7}$	1 solve	1 solve
Eigenvalue ( $k=6$ )	$2.1 \times 10^{-6}$	LOBPCG	1 outer product
Nonlinear (5 Newton)	$4.7 \times 10^{-7}$	5 solves	1 solve

CG iteration takes  $\sim 0.1$ ms, with 50% spent on `all_reduce` synchronization.

(2) *Medium problems (1M–100M DOF)*: Near-linear scaling with  $T \propto n^{1.05}$ . At 100M DOF, we achieve 2.8M DOF/s throughput, close to the memory bandwidth limit of H200 ( $3.9 \text{ TB/s} \times 4 \text{ GPUs}$ ).

(3) *Large problems ( $>100$ M DOF)*: Memory capacity becomes the bottleneck. At 200M+ DOF, we reduce to 3 GPUs to fit within 140GB/GPU limit. The time scaling remains efficient: 400M DOF in 331s corresponds to 1.2M DOF/s.

**Memory efficiency.** Measured 275 bytes/DOF at 400M DOF (110GB / 400M), consistent with sparse matrix storage (80 bytes/DOF) plus solver vectors and halo buffers. The per-GPU memory scales as  $\mathcal{O}(n/P + |\mathcal{H}_p|)$  where halo size  $|\mathcal{H}_p| \sim \mathcal{O}(\sqrt{n/P})$  for 2D grids.

**Convergence.** Residual increases from  $10^{-4}$  at 10K DOF to  $10^{-2}$  at 400M DOF. This is expected: fixed iteration count (1000) with Jacobi preconditioner, where condition number  $\kappa \sim n$  for 2D Poisson. For tighter tolerance, multigrid preconditioning would reduce iterations by  $10\times$ .

### 4.3 Gradient Verification

We verify gradient correctness by comparing adjoint gradients against finite differences:

$$\frac{\partial \mathcal{L}}{\partial \theta} \approx \frac{\mathcal{L}(\theta + \epsilon) - \mathcal{L}(\theta - \epsilon)}{2\epsilon} \quad (6)$$

**Analysis.** Relative errors  $< 10^{-5}$  confirm correct implementation. Notably, the nonlinear solver’s backward pass requires only 1 adjoint solve regardless of Newton iterations (5 in this case), validating the  $\mathcal{O}(1)$  graph complexity claim. The eigenvalue gradient uses Eq. (4), requiring no additional solves—just  $\mathcal{O}(k \cdot \text{nnz})$  outer product computations.

## 5 Conclusion

We presented `torch-sla`, a differentiable sparse linear algebra library with two innovations: (1) adjoint-based differentiation achieving  $\mathcal{O}(\text{nnz})$  graph complexity, and (2) distributed sparse computing with halo exchange. The library scales to **169M DOF on a single GPU** and **400M DOF on 3 GPUs**, demonstrating industrial-scale capability with full gradient support.

### 5.1 Future Work

- **Roofline-guided tuning for distributed solvers:** Current distributed CG achieves  $\sim 50\%$  parallel efficiency at billion-scale DOF due to communication bottlenecks. We plan to develop roofline-based auto-tuning that: (a) overlaps halo exchange with local SpMV computation; (b) dynamically adjusts partition granularity based



on compute/communication ratio; (c) implements communication-avoiding CG variants [Hoemmen, 2010] to reduce `all_reduce` frequency.

- **Learned preconditioners:** GNN-based multigrid [Luz et al., 2020] and meta-learned preconditioner selection [Chen et al., 2022] could adaptively choose optimal preconditioners based on matrix structure, potentially improving convergence rates.
- **Mixed precision:** Following FlashAttention [Dao et al., 2022], we plan FP16/BF16 SpMV with FP64 accumulation, potentially doubling throughput while maintaining convergence for well-conditioned problems.
- **Neural operator hybrid:** Combining with FNO [Li et al., 2020], DeepONet [Lu et al., 2021], and mesh-based GNNs [Pfaff et al., 2021] enables hybrid neural-classical solvers where neural networks provide coarse corrections and classical solvers refine to high precision.
- **Differentiable simulation integration:** Seamless integration with  $\Phi$ Flow [Holl et al., 2024] and DiffTaichi [Hu et al., 2020] for end-to-end differentiable physics pipelines, enabling gradient-based optimization of simulation parameters.

**Availability.** MIT license: <https://github.com/walkerchi/torch-sla>

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## A Implementation Details

### A.1 Backend Selection

`torch-sla` automatically selects backends based on device and problem size:

- CPU, any size: `scipy` with SuperLU
- CUDA,  $<2M$  DOF: `cudss` with Cholesky (if SPD) or LU
- CUDA,  $>2M$  DOF: `pytorch` with CG+Jacobi preconditioner

### A.2 API Examples

**Listing 1:** Basic usage with gradient support.

```
1 import torch
2 from torch_sla import SparseTensor
3
4 # Create sparse matrix (COO format)
5 A = SparseTensor(val, row, col, shape)
6 b = torch.randn(n, requires_grad=True)
7
8 # Solve with automatic differentiation
9 x = A.solve(b) # Forward: any backend
10 loss = x.sum()
11 loss.backward() # Backward: adjoint method
12 print(b.grad) # Gradient w.r.t. RHS
```

**Listing 2:** Distributed multi-GPU solve.

```
1 import torch.distributed as dist
2 from torch_sla import DSparseMatrix
3
4 dist.init_process_group(backend='nccl')
5 rank = dist.get_rank()
6
7 # Each process loads its partition
8 A = DSparseMatrix.from_global(
9     val, row, col, shape,
10     num_partitions=4, my_partition=rank
11 )
12
13 # Distributed CG with halo exchange
14 x = A.solve(b_local, atol=1e-10)
```

## B Complexity Proofs

**Theorem 1** (Adjoint memory complexity). *The adjoint method for linear solve requires  $\mathcal{O}(n + \text{nnz})$  memory, independent of solver iterations.*

*Proof.* Forward pass stores: solution  $\mathbf{x} \in \mathbb{R}^n$ , matrix indices ( $\mathcal{O}(\text{nnz})$ ), matrix values ( $\mathcal{O}(\text{nnz})$ ). Backward pass computes adjoint  $\boldsymbol{\lambda} \in \mathbb{R}^n$  and gradients  $\partial\mathcal{L}/\partial\mathbf{A} \in \mathbb{R}^{\text{nnz}}$ . No intermediate solver states are stored. Total:  $\mathcal{O}(n + \text{nnz})$ .  $\square$