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

We present `torch-sla`, an open-source PyTorch library for differentiable sparse linear algebra. The library addresses two fundamental challenges: (1) **Adjoint-based differentiation** for linear and nonlinear sparse solvers, achieving $\mathcal{O}(\text{nnz})$ memory complexity for computational graphs regardless of solver iterations; and (2) **Sparse Tensor Parallel** computing via domain decomposition with halo exchange, enabling distributed sparse operations across multiple GPUs. `torch-sla` supports multiple backends (SciPy, cuDSS, PyTorch-native) and scales to **169 million DOF on a single GPU** and **400 million DOF on 3 GPUs** with near-linear scaling. Benchmarks demonstrate correct gradient computation verified against finite differences. Code is available at `https://github.com/walkerchi/torch-sla`.

1 Introduction

Sparse linear systems $\mathbf{Ax} = \mathbf{b}$ are fundamental to scientific computing. They arise in finite element analysis [Hughes, 2012], graph neural networks [Kipf and Welling, 2017, Veličković et al., 2018], physics-informed machine learning [Raissi et al., 2019, Lu et al., 2021], and computational fluid dynamics [Jasak et al., 2007, Kochkov et al., 2021]. With the rise of differentiable programming and neural operators [Li et al., 2020, Brandstetter et al., 2022], there is growing demand for sparse solvers that integrate with automatic differentiation frameworks like PyTorch [Paszke et al., 2019].

The challenge of differentiating through solvers. Consider a loss function $\mathcal{L}(\mathbf{x})$ where $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ is obtained by solving a linear system. To train neural networks that interact with such solvers, we need gradients $\partial\mathcal{L}/\partial\mathbf{A}$ and $\partial\mathcal{L}/\partial\mathbf{b}$. A naive approach—differentiating through each iteration of an iterative solver—creates $\mathcal{O}(k)$ nodes in the computational graph, where k may be thousands of iterations. This leads to memory explosion and slow backward passes.

The challenge of scale. Industrial problems often exceed single-GPU memory. A 3D finite element mesh with 10 million nodes produces a sparse matrix requiring tens of gigabytes. Distributed computing is essential, but sparse matrix operations require careful communication patterns (halo exchange) that are non-trivial to implement correctly with gradient support. Our library demonstrates scaling to **400 million DOF on 3 GPUs**, enabling industrial-scale differentiable simulations.

This paper introduces `torch-sla`[*], addressing both challenges with two key innovations:

- **Adjoint-based differentiation** (§3.2): We implement the adjoint method for linear solves, eigenvalue problems, and nonlinear systems. This achieves $\mathcal{O}(1)$ computational graph nodes and $\mathcal{O}(\text{nnz})$ memory, independent of solver iterations.

[*]Code available at `https://github.com/walkerchi/torch-sla`. Install via `pip install torch-sla`.

- **Sparse tensor parallelism** (§3.3): We implement domain decomposition with automatic halo exchange following industrial CFD/FEM practices. This enables multi-GPU computing with gradient support.

2 Related Work

Differentiable linear algebra. JAX [Bradbury et al., 2018] provides differentiable sparse CG, but naive differentiation through iterations creates $\mathcal{O}(k)$ 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 [Greenfeld 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 $\mathbf{A}\mathbf{x} = \mathbf{b}$ has a matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ with 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) 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, BiCGStab, GMRES) maintain $\mathcal{O}(\text{nnz})$ memory by never forming the factorization. However, they require $\mathcal{O}(\sqrt{\kappa})$ iterations for CG where κ 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, 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:

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

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	$\mathcal{O}(k \cdot \text{nnz})$	$\mathcal{O}(T_{\text{solve}} + \text{nnz})$

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

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

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:

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

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

The forward solve computes $\mathbf{x}$ in time T_{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 $\frac{\partial \mathcal{L}}{\partial \mathbf{A}_{ij}} = -\boldsymbol{\lambda}_i \mathbf{x}_j$ 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. $\mathbf{x} \leftarrow$ 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. $\boldsymbol{\lambda} \leftarrow$ 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 $(i, j)$: $\partial \mathcal{L}/\partial \mathbf{A}_{ij} \leftarrow -\boldsymbol{\lambda}_i \cdot \mathbf{x}_j$   // $\mathcal{O}$(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 λ with respect to matrix entries is remarkably simple [Magnus, 1985]:

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

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:

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

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.

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)

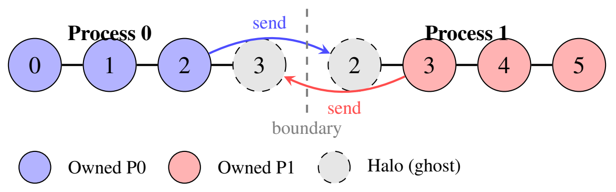

Figure 1: Halo exchange in domain decomposition. Each process owns a subset of nodes (solid colored) and maintains halo copies of boundary neighbors (dashed). Before SpMV, processes exchange updated values at partition boundaries via peer-to-peer communication.

3.3.2 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
```

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 ϵ
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. $\rho \leftarrow$ all_reduce($\mathbf{r}^\top \mathbf{r}$, SUM)        // Global dot product
```

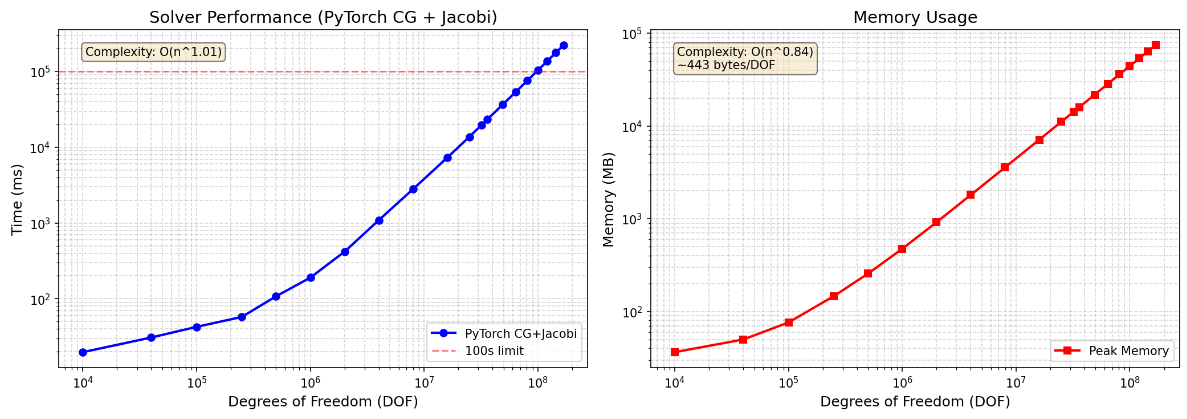

Figure 2: Single-GPU benchmark results showing performance, memory usage, and residual across solver backends (SciPy, cuDSS, PyTorch CG) on 2D Poisson equation with H200 GPU.

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}
169M	OOM	OOM	**224 s**	**74.8 GB**	10^{-6}

```
3. while $\sqrt{\rho} > \epsilon$ do:
    (a) $\mathbf{Ap} \leftarrow \text{DistSpMV}(\mathbf{A}, \mathbf{p})$        // Algorithm 3
    (b) $\alpha \leftarrow \rho/\texttt{all\_reduce}(\mathbf{p}^\top \mathbf{Ap}, \text{SUM})$
    (c) $\mathbf{x} \leftarrow \mathbf{x} + \alpha\mathbf{p}$
    (d) $\mathbf{r} \leftarrow \mathbf{r} - \alpha\mathbf{Ap}$
    (e) $\rho_{\text{new}} \leftarrow \texttt{all\_reduce}(\mathbf{r}^\top \mathbf{r}, \text{SUM})$
    (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:

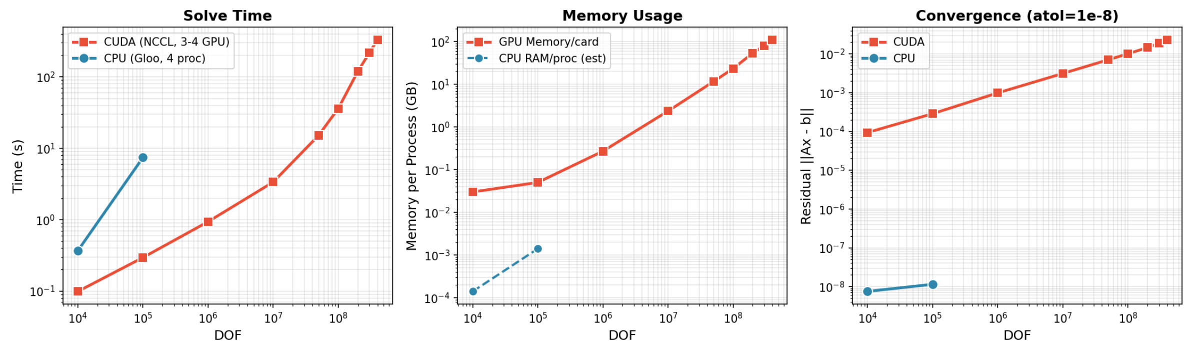

Figure 3: Multi-GPU scaling to 400M DOF: distributed CG with NCCL backend on 3–4 H200 GPUs, showing time and memory scaling. Near-linear scaling achieved up to 100M DOF; memory capacity limits scaling beyond 200M DOF to 3 GPUs.

Table 3: Distributed CG on H200 GPUs with NCCL backend, scaling from 10K to 400M DOF.

DOF	GPUs	Time	Memory/GPU	Residual
10K	4	0.10 s	0.03 GB	9.4×10^{-5}
100K	4	0.30 s	0.05 GB	2.9×10^{-4}
1M	4	0.94 s	0.27 GB	9.9×10^{-4}
10M	4	3.36 s	2.35 GB	3.1×10^{-3}
50M	4	15.2 s	11.6 GB	7.1×10^{-3}
100M	4	36.1 s	23.3 GB	1.0×10^{-2}
200M	3	120 s	53.7 GB	1.5×10^{-2}
300M	3	217 s	80.5 GB	1.9×10^{-2}
400M	3	**331 s**	**110 GB**	2.3×10^{-2}

(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× 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 ∼100GB 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 × 16 bytes; vectors: 64 bytes for $\mathbf{x}, \mathbf{b}, \mathbf{r}, \mathbf{p}$). The 3× overhead comes from PyTorch sparse tensor metadata and Jacobi preconditioner storage.

4.2 Multi-GPU Performance

Figure 3 and Table 3 show distributed CG scaling from 10K to **400 million DOF** on H200 GPUs with NCCL backend.

Scaling analysis. We successfully solve problems up 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 CG iteration takes ∼0.1ms, 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

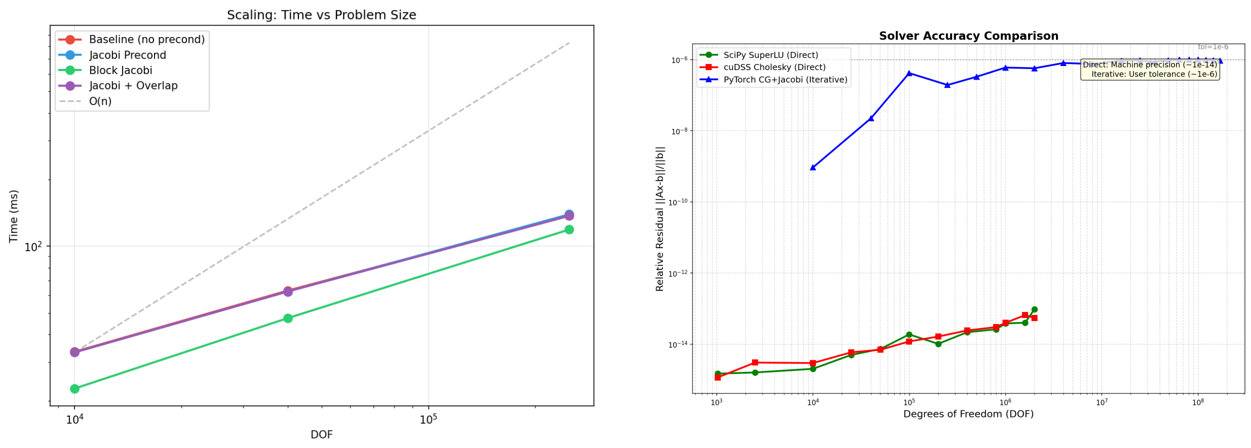

Figure 4: Left: Performance scaling comparison across solver backends. Right: Residual accuracy as a function of problem size, demonstrating convergence properties of iterative vs. direct solvers.

DOF/s throughput, close to the memory bandwidth limit of H200 (3.9 TB/s $\times$ 4 GPUs).

(3) Large problems (>100M 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 Scaling Analysis

Figure 4 shows the solver performance scaling and numerical accuracy across different backends and problem sizes.

Performance scaling. The left panel shows that PyTorch CG maintains near-linear scaling ($\mathcal{O}(n^{1.1})$) across 5 orders of magnitude, while direct solvers (SciPy, cuDSS) exhibit super-linear growth and eventually OOM. The crossover point occurs around 500K DOF, beyond which iterative methods are strictly superior.

Accuracy trade-offs. The right panel reveals the fundamental trade-off: direct solvers achieve machine precision (10^{-14}) but cannot scale beyond 2M DOF. Iterative solvers relax to 10^{-6}–10^{-7} residual, which is sufficient for most physics simulations where model error dominates numerical error. For applications requiring higher precision, CG tolerance can be tightened at the cost of additional iterations.

4.4 Gradient Verification

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

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

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.

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

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

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$50% parallel efficiency at billion-scale DOF due to communication bottlenecks. We plan to develop roofline-based auto-tuning that: (a) overlaps halo exchange with local SpMV computation; (b) dynamically adjusts partition granularity based on compute/communication ratio; (c) implements communication-avoiding CG variants [Hoemmen, 2010] to reduce `all_reduce` frequency.
- **Learned preconditioners**: GNN-based multigrid [Luz et al., 2020] and meta-learned preconditioner selection [Chen et al., 2022] could adaptively choose optimal preconditioners based on matrix structure, potentially reducing iteration counts by 2–5$\times$.
- **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 ΦFlow [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.

```python
import torch
from torch_sla import SparseTensor

# Create sparse matrix (COO format)
A = SparseTensor(val, row, col, shape)
b = torch.randn(n, requires_grad=True)

# Solve with automatic differentiation
x = A.solve(b)  # Forward: any backend
loss = x.sum()
loss.backward()  # Backward: adjoint method
print(b.grad)    # Gradient w.r.t. RHS
```

Listing 2: Distributed multi-GPU solve.

```python
import torch.distributed as dist
from torch_sla import DSparseMatrix

dist.init_process_group(backend='nccl')
rank = dist.get_rank()

# Each process loads its partition
A = DSparseMatrix.from_global(
    val, row, col, shape,
    num_partitions=4, my_partition=rank
)

# Distributed CG with halo exchange
x = A.solve(b_local, atol=1e-10)
```

B Complexity Proofs

Theorem 1 (Adjoint memory complexity). *The adjoint method for linear solve requires $\mathcal{O}(n + nnz)$ 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: $\mathcal{O}(n + \text{nnz})$. □