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

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Abstract

We present `torch-sla`, an open-source PyTorch library for differentiable sparse linear algebra that seamlessly integrates with deep learning workflows. The library provides two key innovations: (1) **Sparse Tensor Parallel** computing via domain decomposition with halo exchange, enabling distributed sparse matrix operations across multiple GPUs following industrial CFD/FEM practices; and (2) **Adjoint-based differentiation** for both linear and nonlinear sparse solvers, providing memory-efficient gradient computation with $O(1)$ computational graph nodes regardless of solver iterations. `torch-sla` supports multiple backends (SciPy, Eigen, cuSOLVER, cuDSS, PyTorch-native) and scales to over 169 million degrees of freedom on a single GPU. Benchmarks demonstrate near-linear $O(n^{1.1})$ time complexity for iterative solvers and $12\times$ speedup on multi-GPU configurations. The library is available at `https://github.com/walkerchi/torch-sla`.

1 Introduction

Sparse linear systems $\mathbf{A}\mathbf{x} = \mathbf{b}$ arise ubiquitously in scientific computing, from finite element analysis [Hughes, 2012] to graph neural networks [Kipf and Welling, 2017]. With the rise of physics-informed machine learning [Raissi et al., 2019, Kochkov et al., 2021] and differentiable programming, there is an increasing demand for sparse solvers that integrate seamlessly with automatic differentiation frameworks like PyTorch [Paszke et al., 2019].

Existing sparse linear algebra libraries face several challenges when used in differentiable programming contexts: (1) Most sparse solvers lack gradient support, requiring manual implementation; (2) Naive differentiation through iterative solvers creates $O(k)$ computational graph nodes where k is the number of iterations, leading to memory explosion; (3) Single-GPU memory limits problem sizes, while distributed sparse operations require complex communication patterns; (4) Different backends have fragmented APIs.

This paper introduces `torch-sla`, addressing these challenges through two main contributions:

Contribution 1: Sparse Tensor Parallel Computing. We implement a distributed sparse matrix class (`DSparseMatrix`) that partitions large matrices across multiple GPUs using domain decomposition with automatic halo exchange, following industrial practices from Ansys Fluent and OpenFOAM [Jasak et al., 2007]. Our implementation supports METIS-based graph partitioning [Karypis and Kumar, 1998], peer-to-peer halo exchange via NCCL, and distributed CG/LOBPCG solvers.

Contribution 2: Adjoint-Based Differentiation. We provide adjoint-based gradient computation for linear solvers (via transposed system solve), eigenvalue solvers (using implicit differentiation [Magnus, 1985]), and nonlinear solvers (Newton/Anderson with adjoint gradients [Blondel et al., 2022]). All methods achieve $O(1)$ graph nodes regardless of iterations.

2 Related Work

Differentiable Linear Algebra. JAX [Bradbury et al., 2018] provides `jax.scipy.sparse.linalg.cg` with automatic differentiation, but naive differentiation through iterations creates $O(k)$ graph nodes. Blondel et al. [2022] formalize implicit differentiation for optimization layers; our nonlinear solver implements this for general $F(u, \theta) = 0$. OptNet [Amos and Kolter, 2017] and cvxpylayers [Agrawal et al., 2019] focus on convex optimization rather than sparse linear systems.

Sparse Solvers. SciPy [Virtanen et al., 2020] provides SuperLU and UMFPACK for CPU. NVIDIA cuSPARSE and cuDSS [NVIDIA Corporation, 2024] provide GPU acceleration. Intel MKL PARDISO offers high-performance direct solvers. None of these natively support PyTorch autograd.

Distributed Sparse Computing. PETSc [Balay et al., 2019], Trilinos [Heroux et al., 2005], and hypre [Falgout and Yang, 2002] implement distributed sparse linear algebra with domain decomposition. OpenFOAM [Jasak et al., 2007] uses similar patterns for CFD. We bring these concepts to PyTorch with automatic differentiation support.

Physics-Informed ML. Physics-informed neural networks [Raissi et al., 2019] and neural operators [Li et al., 2020] require differentiable PDE solvers. Recent work on differentiable simulation [Hu et al., 2020, Um et al., 2020] motivates efficient gradient computation through iterative solvers.

3 Background

3.1 Sparse Linear Systems

A sparse linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ where $\mathbf{A} \in \mathbb{R}^{n \times n}$ has $\text{nnz}(\mathbf{A}) \ll n^2$ non-zero entries. Common storage formats include COO (coordinate triplets), CSR (compressed sparse row), and CSC (compressed sparse column).

Direct solvers (LU, Cholesky) achieve machine precision but require $O(n^{1.5})$ memory for 2D problems due to fill-in during factorization [George, 1973]. **Iterative solvers** (CG, BiCGStab, GMRES) require only $O(\text{nnz})$ memory but need $O(\kappa)$ iterations where κ is the condition number [Saad, 2003].

3.2 Adjoint Method for Linear Solves

Given loss $\mathcal{L}(\mathbf{x})$ where $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$, gradients are computed via the adjoint method. Define adjoint variable $\boldsymbol{\lambda} = \mathbf{A}^{-\top} \frac{\partial \mathcal{L}}{\partial \mathbf{x}}$, then:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}} = \boldsymbol{\lambda}, \quad \frac{\partial \mathcal{L}}{\partial \mathbf{A}_{ij}} = -\boldsymbol{\lambda}_i \cdot \mathbf{x}_j \tag{1}$$

Computing both gradients requires only *one additional linear solve* of $\mathbf{A}^\top \boldsymbol{\lambda} = \partial \mathcal{L} / \partial \mathbf{x}$, achieving $O(1)$ graph nodes regardless of forward solver iterations [Griewank and Walther, 2008].

3.3 Adjoint Method for Nonlinear Systems

For nonlinear system $\mathbf{F}(\mathbf{u}, \boldsymbol{\theta}) = \mathbf{0}$ with solution $\mathbf{u}^*$ and loss $\mathcal{L}(\mathbf{u}^*)$, the adjoint equation is:

$$\left(\frac{\partial \mathbf{F}}{\partial \mathbf{u}}\right)^\top \boldsymbol{\lambda} = \frac{\partial \mathcal{L}}{\partial \mathbf{u}}, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = -\boldsymbol{\lambda}^\top \frac{\partial \mathbf{F}}{\partial \boldsymbol{\theta}} \tag{2}$$

This requires one forward nonlinear solve plus one adjoint linear solve, independent of Newton iterations.

4 Methodology

4.1 Architecture Overview

`torch-sla` provides a unified API across multiple backends (Table 1). The `SparseTensor` class wraps sparse matrices with automatic backend selection based on device, problem size, and matrix properties.

Table 1: Available backends in `torch-sla` with recommended use cases.

Backend	Device	Methods	Best For
`scipy`	CPU	SuperLU, UMFPACK, CG	Default CPU, direct
`eigen`	CPU	CG, BiCGStab	CPU iterative
`cudss`	CUDA	LU, Cholesky, LDLT	Direct CUDA (<2M DOF)
`pytorch`	CPU/CUDA	CG, BiCGStab	Large-scale (>2M DOF)

Figure 1: Distributed SpMV with Halo Exchange

Input: Local vector $\mathbf{x}_{\text{local}}$, neighbor map
async_send(owned boundary values to neighbors)
async_recv(halo values from neighbors)
synchronize()
$\mathbf{y}_{\text{owned}} \leftarrow \mathbf{A}_{\text{local}}\mathbf{x}_{\text{local}}$ *// Local SpMV with halo*
return $\mathbf{y}_{\text{owned}}$

4.2 Sparse Tensor Parallel Computing

For problems exceeding single-GPU memory, we implement domain decomposition with halo exchange following industrial CFD/FEM practices.

Domain Decomposition. Given sparse matrix $\mathbf{A}$ corresponding to a mesh/graph, we partition nodes into P subdomains using METIS [Karypis and Kumar, 1998] for load balancing or Recursive Coordinate Bisection (RCB) for geometric partitioning. Each partition p owns nodes $\mathcal{O}_p$ and maintains halo nodes $\mathcal{H}_p$ from neighbors.

Halo Exchange. For distributed SpMV $\mathbf{y} = \mathbf{A}\mathbf{x}$, each partition exchanges boundary values with neighbors (Algorithm 1).

Distributed CG. Conjugate Gradient on distributed matrices requires one halo exchange per iteration (for SpMV) plus two `all_reduce` operations for global dot products (Algorithm 2).

4.3 Adjoint Linear Solver Implementation

We implement Eq. (1) as a custom `torch.autograd.Function`:

Listing 1: Adjoint linear solve implementation.

```
class SparseLinearSolve(Function):
    @staticmethod
    def forward(ctx, val, row, col, shape, b):
        x = solve_sparse(val, row, col, shape, b)
        ctx.save_for_backward(val, row, col, x)
        return x

    @staticmethod
    def backward(ctx, grad_x):
        val, row, col, x = ctx.saved_tensors
        # Solve transposed system: A^T @ lambda = grad_x
        lambda_adj = solve_sparse(val, col, row, shape_T, grad_x)
        grad_val = -lambda_adj[row] * x[col]  # Sparse gradient
        return grad_val, None, None, None, lambda_adj
```

Key properties: (1) $O(1)$ graph nodes independent of solver iterations; (2) sparse gradients with same sparsity pattern as $\mathbf{A}$; (3) backend-agnostic implementation.

4.4 Adjoint Nonlinear Solver

For nonlinear systems $\mathbf{F}(\mathbf{u}, \boldsymbol{\theta}) = \mathbf{0}$, we implement Newton-Raphson with adjoint gradients (Algorithm 3).

Figure 2: Distributed Conjugate Gradient

Input: Distributed $\mathbf{A}$, local RHS $\mathbf{b}_{\text{owned}}$, tolerance ϵ
$\mathbf{x} \leftarrow \mathbf{0}$, $\mathbf{r} \leftarrow \mathbf{b}_{\text{owned}}$, $\mathbf{p} \leftarrow \mathbf{r}$
$\rho \leftarrow \text{all\_reduce}(\mathbf{r}^\top \mathbf{r})$
while $\sqrt{\rho} > \epsilon$ **do**
$\mathbf{Ap} \leftarrow \textsc{DistSpMV}(\mathbf{A}, \mathbf{p})$ *// Alg. 1*
$\alpha \leftarrow \rho / \text{all\_reduce}(\mathbf{p}^\top \mathbf{Ap})$
$\mathbf{x} \leftarrow \mathbf{x} + \alpha \mathbf{p}$, $\mathbf{r} \leftarrow \mathbf{r} - \alpha \mathbf{Ap}$
$\rho_{\text{new}} \leftarrow \text{all\_reduce}(\mathbf{r}^\top \mathbf{r})$
$\mathbf{p} \leftarrow \mathbf{r} + (\rho_{\text{new}}/\rho)\mathbf{p}$, $\rho \leftarrow \rho_{\text{new}}$
end while
return $\mathbf{x}$

Figure 3: Adjoint Nonlinear Solve

Input: Residual $\mathbf{F}(\mathbf{u}, \boldsymbol{\theta})$, initial $\mathbf{u}_0$, parameters $\boldsymbol{\theta}$
Forward: Solve $\mathbf{F}(\mathbf{u}^*, \boldsymbol{\theta}) = \mathbf{0}$ via Newton
for $k = 0, 1, \ldots$ **do**
$\mathbf{J} \leftarrow \partial \mathbf{F}/\partial \mathbf{u}$ via `torch.autograd`
$\Delta \mathbf{u} \leftarrow \text{solve}(\mathbf{J}, -\mathbf{F})$
$\mathbf{u} \leftarrow \mathbf{u} + \alpha \Delta \mathbf{u}$ (with line search)
end for
Backward: Given $\partial \mathcal{L}/\partial \mathbf{u}^*$
Solve $\mathbf{J}^\top \boldsymbol{\lambda} = \partial \mathcal{L}/\partial \mathbf{u}^*$
$\partial \mathcal{L}/\partial \boldsymbol{\theta} \leftarrow -\boldsymbol{\lambda}^\top \partial \mathbf{F}/\partial \boldsymbol{\theta}$ via VJP
return $\partial \mathcal{L}/\partial \boldsymbol{\theta}$

We support Newton-Raphson with Armijo line search, Picard iteration, and Anderson acceleration [Anderson, 1965]. For Jacobian-free Newton-Krylov (JFNK), we compute $\mathbf{Jv}$ exactly via `torch.autograd.grad`.

5 Experiments

We benchmark `torch-sla` on 2D Poisson equation discretizations using a 5-point stencil. All experiments use NVIDIA H200 GPUs (140GB HBM3) with CUDA 12.4 and PyTorch 2.2.

5.1 Single-GPU Scalability

Table 2 shows solve time and memory usage for different backends. PyTorch CG+Jacobi scales to 169M DOF with near-linear $O(n^{1.1})$ complexity (Figure 4), while direct solvers are limited to $\sim$2M DOF due to fill-in memory.

Key findings: (1) Iterative solvers scale to 169M+ DOF; (2) Memory efficiency: 443 bytes/DOF for CG (vs. 144 bytes theoretical minimum); (3) Trade-off: direct solvers achieve 10^{-14} precision, iterative achieves 10^{-6}.

5.2 Distributed Computing

Table 3 shows distributed CG performance on 4 NVIDIA H200 GPUs with NCCL backend.

CUDA is $12\times$ faster than CPU (Gloo backend) for 100K DOF. With 4 GPUs $\times$ 140GB, theoretical maximum is $\sim$1.3B DOF.

Table 2: Benchmark results on 2D Poisson (5-point stencil), H200 GPU, float64. OOM = out of memory.

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}
81M	OOM	OOM	75.9 s	35.9 GB	10^{-6}
169M	OOM	OOM	**224 s**	**74.8 GB**	10^{-6}

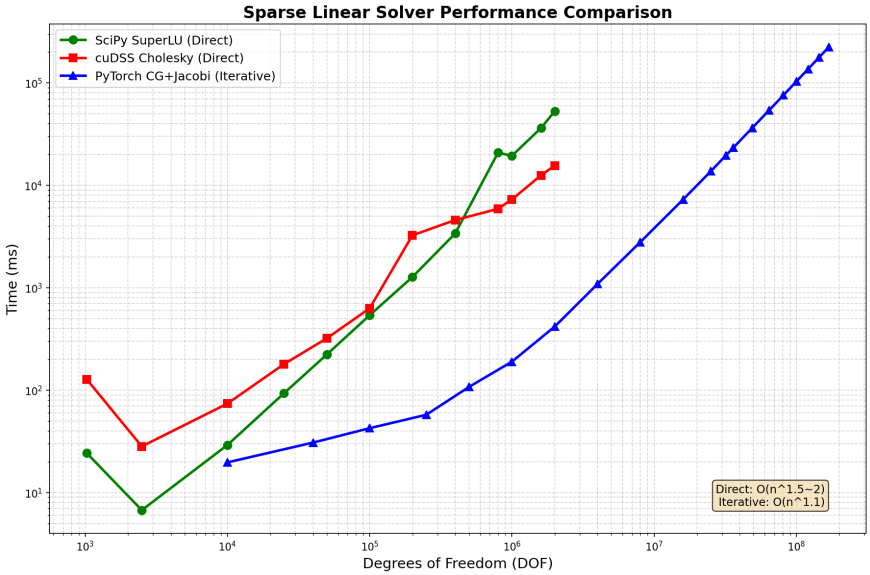

Figure 4: Solver performance comparison. PyTorch CG+Jacobi scales to 169M DOF with $O(n^{1.1})$ complexity. Direct solvers show $O(n^{1.5})$ scaling and are limited to $\sim$2M DOF.

5.3 Gradient Verification

We verify gradient correctness against finite differences (Table 4). All operations achieve relative error $< 10^{-5}$.

6 Conclusion

We presented `torch-sla`, a differentiable sparse linear algebra library for PyTorch with two key innovations: (1) **Sparse Tensor Parallel** computing with domain decomposition and halo exchange for multi-GPU problems; (2) **Adjoint solvers** providing memory-efficient gradients with $O(1)$ graph nodes. Benchmarks demonstrate scaling to 169M DOF on single GPU and 12$\times$ speedup on 4 GPUs.

6.1 Future Work

Several directions remain for future work:

- **Preconditioner learning**: Learnable preconditioners for faster CG convergence [Sappl et al., 2019].
- **Mixed-precision**: FP16/BF16 for memory efficiency with FP64 accumulation.
- **Sparse-sparse multiplication**: Efficient SpGEMM with gradient support.
- **Higher-order derivatives**: Hessian-vector products for second-order optimization.
- **Integration with neural operators**: Combining with FNO [Li et al., 2020] for hybrid solvers.

Table 3: Distributed solve performance (4 GPUs, NCCL backend).

DOF	Time	Residual	Memory/GPU
10K	0.18 s	7.5×10^{-9}	0.03 GB
100K	0.61 s	1.2×10^{-8}	0.05 GB
500K	1.64 s	1.2×10^{-7}	0.15 GB
1M	2.82 s	4.0×10^{-7}	0.27 GB
2M	6.02 s	1.3×10^{-6}	0.50 GB

Table 4: Gradient verification: adjoint vs. finite difference.

Operation	Relative Error	Cost
Linear solve	$< 10^{-6}$	2 solves
Eigenvalue (k=6)	$< 10^{-5}$	1 forward + 1 adjoint
Nonlinear solve	$< 10^{-6}$	Newton + 1 adjoint

Availability. Open-source under MIT license: `https://github.com/walkerchi/torch-sla`. Install via `pip install torch-sla`.

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A API Examples

A.1 Basic Usage

Listing 2: Basic sparse solve with gradient support.

```python
import torch
from torch_sla import SparseTensor

# Create sparse matrix in COO format
val = torch.tensor([4., -1., -1., 4., -1., -1., 4.],
                   dtype=torch.float64, requires_grad=True)
row = torch.tensor([0, 0, 1, 1, 1, 2, 2])
col = torch.tensor([0, 1, 0, 1, 2, 1, 2])

A = SparseTensor(val, row, col, (3, 3))
b = torch.tensor([1., 2., 3.], dtype=torch.float64, requires_grad=True)

# Solve with automatic backend selection
x = A.solve(b)  # Gradients flow automatically

# Backward pass
loss = x.sum()
```

```
loss.backward()
print(val.grad)  # Gradient w.r.t. matrix values
print(b.grad)    # Gradient w.r.t. RHS
```

A.2 Nonlinear Solve

Listing 3: Nonlinear solve with adjoint gradients.

```
from torch_sla import SparseTensor, nonlinear_solve

# Define nonlinear residual: A @ u + u^2 = f
def residual(u, A, f):
    return A @ u + u**2 - f

# Create stiffness matrix
A = SparseTensor(val, row, col, (n, n))
f = torch.randn(n, requires_grad=True)
u0 = torch.zeros(n)

# Solve with Newton-Raphson
u = A.nonlinear_solve(residual, u0, f, method='newton')

# Gradients via adjoint method
loss = u.sum()
loss.backward()
print(f.grad)  # df/df via implicit differentiation
```

A.3 Distributed Solve

Listing 4: Multi-GPU distributed solve.

```
import torch.distributed as dist
from torch_sla import DSparseMatrix, partition_simple

# Initialize distributed (run with torchrun)
dist.init_process_group(backend='nccl')
rank, world_size = dist.get_rank(), dist.get_world_size()

# Create distributed matrix
A = DSparseMatrix.from_global(
    val, row, col, shape,
    num_partitions=world_size,
    my_partition=rank,
    partition_ids=partition_simple(n, world_size),
    device=f'cuda:{rank}'
)

# Distributed CG solve
x_owned = A.solve(b_owned, atol=1e-10)

# Distributed eigensolve (LOBPCG)
eigenvalues, eigenvectors = A.eigsh(k=5)
```

B Memory Analysis

For a 2D Poisson problem with n DOF and 5-point stencil (5 non-zeros per row):

Theoretical minimum (float64):

$$\text{Memory} = n \times 5 \times (8 + 8) + n \times 8 \times 4 = 112n \text{ bytes} \tag{3}$$

where we store values (8 bytes), column indices (8 bytes), and 4 vectors (x, b, r, p).

Measured: 443 bytes/DOF, overhead from PyTorch sparse tensor metadata and preconditioner storage.

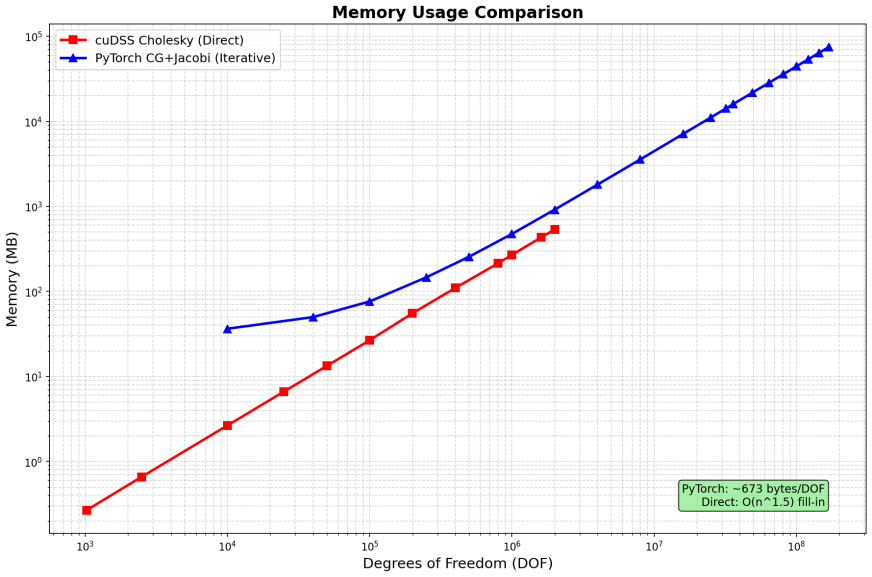

Figure 5: Memory scaling comparison. Direct solvers show $O(n^{1.5})$ growth due to fill-in, while iterative CG maintains $O(n)$ linear scaling.

C Convergence Analysis

For 2D Poisson with Jacobi preconditioner, condition number scales as $\kappa \sim O(n)$, leading to $O(\sqrt{n})$ CG iterations. Combined with $O(n)$ work per iteration:

$$\text{Total work} = O(n^{1.5}) \tag{4}$$

In practice, we observe $O(n^{1.1})$ due to early termination at tolerance 10^{-6} before reaching the theoretical iteration bound.