Structured ILU Preconditioner for Boltzmann Transport

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Overview

- 1D BOLTZTRAN for multi-group Boltzmann and convective hydrodynamics transport.
- Block tridiagonal systems.
- ADI like preconditioner.
- Sparse ILU for diagonal blocks
- Matlab experiments
1D hydrodynamics coupled to multi-group Boltzmann neutrino transport and used in modeling supernova core collapse.

**BOLTZTRAN** uses full Newton iteration with explicit construction of Jacobian. Typically require 6 newton iterations per time step for over 20,000 time steps.

- The sparse Jacobian is block tridiagonal, $[B_i, D_i, C_i]$ where $D_i$ is $M \times M$ and dense but $B_i, C_i$ are exactly diagonal.

- Dense diagonal block arising from discrete ordinates formulation of Boltzmann transport, off-diagonal blocks from 1D spatial discretization in hydrodynamic transport.
Development of 2D and 3D BOLTZTRAN as possible SciDAC application.

The sparse Jacobian has overall size $M \times N$, where $N$ is number of spatial grid points, $M$ is size of dense diagonal block.

In 1D, $M = 2 \times G \times Q + 2$, $M = 2 \times G \times (Q \times Q) + 2$ in 2D and 3D where $G$ is number of energy groups, $Q$ is number of quadrature points.

Astrophysicists consider $G = 12$, $Q = 4$, $N = 128 \times 64$ to be a low resolution ($M = 386$), and $G = 24$, $Q = 8$, $N = 512 \times 512$ a high resolution case ($M = 3074$).

High memory and computational costs associated with large dense diagonal blocks.
Linear solver

- Original code used a block variant of Thomas algorithm for tridiagonal systems. Recently added LAPACK DGBSV band solver.

- Consider iterative solver such as GMRES, BICGSTAB and even fixed point iteration.

- We consider two easily parallelizable preconditioners:
  - DBLOCK: just using the diagonal $D_i$ dense blocks
  - ADI: additional correction using the diagonal part of $D_i$ and off-diagonal blocks, $[B_i, \text{diag}(D_i), C_i]$.

- Preconditioner DBLOCK still requires $O(NM^3)$ work for factoring diagonal dense blocks. Band solver also requires $O((NM)M^2)$ work.
Sparisty Pattern

![Graph showing the sparisty pattern with nz = 6036]
By reordering spatial variables together, the second correction in ADI can be viewed as performing $M$ independent tridiagonal solutions of size $N$.

ADI-like sweep where we alternately sweep along the spatial direction and separately handle the coupling among multi-group variables.

This correction may require costly ‘transpose-like’ communication in a parallel environment.

# Solve $A \times x = b$, $[B_i, D_i, C_i] \times x_i = b_i$

# (1) block diagonal part

B = diag(diag(A,-m),-m);

C = diag(diag(A,m),m);

DBLOCK = A - B - C;

y = DBLOCK \ b;

# (2) ADI correction after DBLOCK

r = -(B + C) * x; # residual $r = b - A \times x$

# compute correction

x = y + ( diag(diag(A,0),0) + B + C ) \ r;

Figure 1: Algorithm for ADI-like preconditioner in MATLAB notation.
Test cases

- Jacobian matrix has 102 blocks, each block is $34 \times 34$ ($34 = 4 \times 4 \times 2 + 2$)

<table>
<thead>
<tr>
<th>case</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>30-1,2,3,4</td>
<td>at core bounce with complex physics</td>
</tr>
<tr>
<td>60-1</td>
<td>well into the post-bounce heating phase, shock still moving out</td>
</tr>
<tr>
<td>90-1</td>
<td>shock has stalled, explosion might occur shortly</td>
</tr>
</tbody>
</table>

Table 1: Brief description of test cases.
Convergence of ADI preconditioner

![Graph showing convergence of ADI preconditioner](image)
Sparse ILU of 60_1

nz = 98

L with 1e−3

nz = 285

U with 1e−3
ILU of diagonal block

- Sparsity in L: \(\text{nz} = 795\)
- Sparsity in U: \(\text{nz} = 5547\)
- Sparser U: \(\text{nz} = 795\)
**Sparse ILU with structure**

- ILU as preconditioner to dense block.
- Exploit internal structure of diagonal block such as tight coupling within energy group, retain high energy interactions.
- Matrix-free method or on-the-fly recomputation to avoid high memory cost.
- Even sparser approximation to operate and store only approximate Jacobian.
- Approximate Jacobian likely lead to more newton iterations but may still have overall savings.
Significant entries in diagonal blocks

M30

\(nz = 232\)

M60

\(nz = 228\)

M90

\(nz = 233\)

M30 + M60 + M90

\(nz = 262\)
High energy coupling in $U$
High energy coupling in L and U

nz = 211
L

nz = 307
U

nz = 484
L*U
Comparison for 30-1

Problem 30−1: relative error, norm(A−LU)/norm(A)

U coupling
L&U coupling

condest before LU

condest after LU

U coupling
L&U coupling
Comparison for 30-1
Comparison for 60-1

Problem 60–1: relative error, \( \frac{\text{norm}(A-LU)}{\text{norm}(A)} \)

- **U coupling**
- **L&U coupling**

![Graphs showing relative error comparison for 60-1 problem](image)
Comparison for 60-1

nse60–1

10^0

10^−7

10^−6

10^−5

10^−4

10^−3

10^−2

10^−1

1
2
3
4
5
6
7
8
9
10

BICGSTAB+ILU
GMRES+ILU
BICGSTAB+LU
GMRES+LU
Comparison for 90-1

Problem 90–1: relative error, \( \text{norm}(A-\text{LU}) / \text{norm}(A) \)

- **U coupling**
- **L&U coupling**

**condest before LU**

**condest after LU**

\( \times \) U coupling

\( \circ \) L&U coupling
Comparison for 90-1

![Comparison graph for 90-1](image)
Larger problem

- 6 quadrature points, 12 energy groups

![Graphs of M140, M160, and M140+M160 showing nz counts of 967, 1051, and 1150 respectively.](image-url)
Comparison for 140-1

Problem nse140: relative error, norm(A−LU)/norm(A)

- L&U coupling
- L2&U2 coupling
- L3&U3 coupling
- L4&U4 coupling

condest before LU

condest after LU
Comparison for 140-1

![Comparison for 140-1](image)
Comparison for 160-1

Problem nse160: relative error, \( \text{norm}(A-LU)/\text{norm}(A) \)

- L&U coupling
- L2&U2 coupling
- L3&U3 coupling
- L4&U4 coupling

condest before LU

condest after LU
Comparison for 160-1
Nonlinear Newton iterations
Nonlinear Newton iterations

- The neutrino luminosities look to be different at only the 1% level.
- The inner iteration count (for the BiCG-STAB) seems essentially unchanged throughout collapse.
- More realistic energy gridding (12 groups instead of 4) is needed.
Summary

- Enhancement to ADI preconditioner to avoid costly LU factorization in diagonal blocks by taking advantage of structure in ILU.

- Structured ILU with predetermined sparsity pattern (within group coupling and highest energy coupling) seems to be an effective preconditioner for the diagonal blocks.

- Explore using sparse diagonal blocks as inexact Jacobian to reduce storage requirements.

- Simulations with more energy groups are needed.