Unique Linear Solver Needs of the Los Alamos Radiation Transport Team

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DANTE

Problem Characteristics

- Radiation Transport (S_N, SP_N, P_N)
- 1–D, 2–D, 3–D Cartesian
- Arbitrary Finite Element (Hexahedra, Tetrahedra, etc.)
- Unstructured Mesh — Node-Based
- Variables: Intensity for every point, angle and energy group (energy groups always decouple)

DANTE

Matrix Characteristics

- Size (rows): S_N & SP_N: n_{nodes};
  P_N: $n_{nodes} \times F\left(n_{angles}\right)$

- Absolute size (rows): 10,000 – 1,000,000

- Sparse ($\approx$ 10 non-zeroes per row)

- Actual number of non-zeroes per row unknown

- Symmetric Positive Definite

- P_N: full block matrix, each block has same non-zero pattern

- S_N & SP_N: block diagonal matrix (angles uncouple)

DANTE

System Storage

- Multi-D Vectors: `v(npoints, nangles)`
- Matrix: complicated, never assembled
- Reverse communication necessary
- Some treatment of dot products necessary

DANTE

Current Solution

- Conjugate Gradient with Jacobi preconditioning
  (developed in-house)

- Algebraic Unstructured Multigrid
  (Mantueffel et al., experimental)

- Would like to be able to use standard preconditioners with
  reverse communication

Augustus / Spartan
Problem Characteristics

- Radiation Transport (SPARTAN: SP_N, AUGUSTUS: P_1)

- AUGUSTUS: 1–D (Cartesian, Cylindrical & Spherical), 2–D (Cartesian & Cylindrical), 3–D (Cartesian)

- SPARTAN: 2–D (Cartesian & Cylindrical)

- SPARTAN uses AUGUSTUS as its solver, so multi–D version of SPARTAN is on the way

- 3–D: Hexahedra & Degenerates,
  2–D: Quadrilaterals & Degenerates,
  1–D: Line Segments

- Unstructured Mesh

- SPARTAN Variables: Intensity for every point, angle and energy group (energy groups and angles always decouple)

Augustus / Spartan
Matrix Characteristics

Main Matrix System:

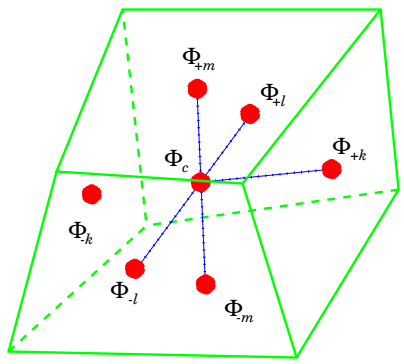
- Size (rows): $4\ n_{cells} + n_{bf}/2$
- Absolute size (rows): 10,000 – 100,000
- Sparse (7 or 11 non-zeroes per row)
- Unsymmetric
- ELL Storage

Preconditioner Matrix System:

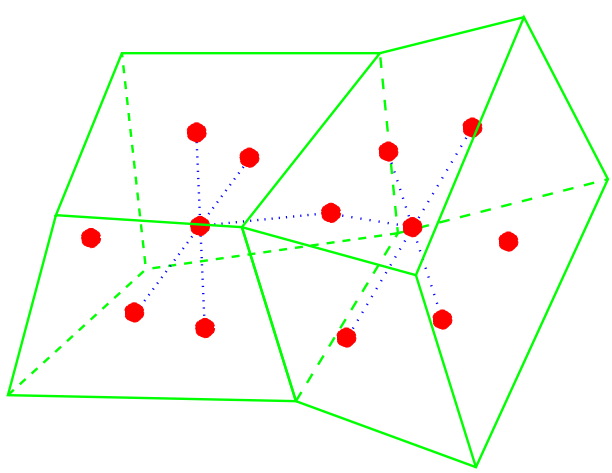
- Size (rows): n_{cells}
- Sparse (7 non-zeroes per row)
- Symmetric
- ELL Storage

Augustus / Spartan Discretization

Main system involves cell-equations ($+\boldsymbol{k}$ flux shown, all points would be involved in cell-equation):



and cell-face equations:



Preconditioner eliminates minor directions in flux terms to yield a system involving only cell-centers.

Augustus / Spartan
Current Solution

Main system:

- Krylov space solvers (GMRES, BCGS, etc.) in JTPACK by John Turner, LANL
- UMFPACK: incomplete direct method (the unstructured multi-frontal method) by Tim Davis, U of FL

Preconditioner:

- Jacobi, SSOR, ILU from JTPACK
- Specialized Low-Order Preconditioner, solved with Conjugate Gradient with SSOR preconditioning using JTPACK
- UMFPACK: none

Overall Needs of Radiation Transport

- JTpack, UMFPACK serving most needs
- Would like to be able to use standard preconditioners with reverse communication
- Reverse communication for matrix multiplication and system solution (possibly for dot products)
- Support for 2–D vectors
- Arithmetic Unstructured Multigrid Package with Documentation

Implementation:
The Augustus Code Package

Author:	Michael L. Hall (1/94 - present)
Architectures:	Sun (SunOS and Solaris), SGI (IRIX), HP (HP-UX), IBM (AIX)
Language:	Fortran-77, plans for Fortran-90
Solver Packages:	JTPACK (by John Turner, LANL) for Krylov Space methods, UMFPACK (by Tim Davis, U of FL) for sparse direct methods
Installations:	SNLA ALEGRA hydrodynamics code, LANL TELLURIDE low-speed flow code, Solver for the SPARTAN SP_N radiation transport code.
Status:	Completed, active development of new features
Availability:	Email `hall@lanl.gov` and we'll talk