Research Directions in Scalable Algorithms

Robert D. Falgout
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

Panel Discussion
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The scalable solution of linear systems is crucial in large-scale simulations

- **Multigrid** linear solvers are optimal ($O(N)$ operations), and hence have good scaling potential.

The Multigrid V-cycle

The near null space (kernel) is important!

MG uses a sequence of coarse-grid problems to accelerate the solution of the original problem.
Error left by relaxation can be geometrically oscillatory

- 7 GS sweeps on
  \[-a u_{xx} - b u_{yy} = f\]
  \[a = b \quad a \gg b\]

- AMG automatically coarsens grids — can “follow physics”
- This example still targets geometric smoothness and pointwise smoothers
- Not sufficient for some problems!
Electromagnetic problems have huge near null spaces that are geometrically oscillatory

- Three classes of PDEs:
  \[
  \nabla \times \alpha \nabla \times E + \beta E = f \quad \text{– Definite Maxwell (}\alpha, \beta > 0) \n  \nabla \times \alpha \nabla \times E - k^2 E = f \quad \text{– Indefinite Maxwell (}\alpha > 0) \n  -\nabla^2 u - k^2 u = f \quad \text{– Helmholtz} \n  \]

- Requires specialized smoothers and coarse grids

  - Local: specialized relaxation (Definite Maxwell, Indefinite Maxwell)
  - Global: specialized coarse grids (Helmholtz, Indefinite Maxwell)

- Good recent progress for Definite Maxwell!
Adaptive AMG employs the idea of: using the method to improve the method

- Requires no a-priori knowledge of near null-space
- **Idea:** uncover slowly-converging error components by applying the “current method” to the system $Ax = 0$, then use these to adapt (improve) the method

- **PCG can be viewed as an adaptive method**
  - Not optimal because it uses a global view
  - The key is to view slow-to-converge components as “representatives” of locally smooth error

- **Two methods:** $\alpha$AMG and $\alpha$SA (SISC pubs)
- **Prolongation in $\alpha$SA formed by**
  - “chopping up” the representatives, then
  - smoothing to lower the overall energy
We are applying our adaptive AMG methods to QCD

- Quantum Chromodynamics (QCD) is the theory of strong forces in Standard Model of particle physics
- Challenges:
  - The system is complex and indefinite
  - The system can be extremely ill-conditioned
  - Near null space is unknown and oscillatory!

- Uniform convergence of $\alpha_{SA}$ in 2D (first such result)
- Extending to 4D
Scalable, robust simulation of transport is a major issue in many codes

- Transport plays a crucial role in many applications
  - Stockpile stewardship, astrophysics, ICF
- High dimensionality makes it a challenging problem
  - 6D phase space (space, angle, energy) + time
- **Mono-energetic Boltzmann equation** is a key kernel in radiative transfer and neutron transport

\[
\frac{1}{\nu} \frac{\partial \psi}{\partial t} + \vec{\Omega} \cdot \nabla \psi + \sigma(r) \psi = \sigma_s(r) \int_{S^2} \psi(r, \Omega', t) d\Omega' + q
\]

Stream: Streaming, Absorption, (In)Scattering
Underlying nature of transport equation changes in different parameter regimes

- Discretization in angle ($S_N$ discrete ordinates) and space (Petrov-Galerkin, corner balance) leads to

\[
\begin{pmatrix}
H_1 & \cdots & H_n \\
-\Sigma_1 & \ddots & -\Sigma_n \\
-\Sigma_1 & \cdots & -\Sigma_n
\end{pmatrix}
\begin{pmatrix}
\psi_1 \\
\vdots \\
\psi_n \\
\Phi
\end{pmatrix}
=
\begin{pmatrix}
Q_1 \\
\vdots \\
Q_n \\
0
\end{pmatrix}
\]

- Traditional source iteration (SI) = block Gauss-Seidel

- Thin limit (little scattering): nearly block lower triangular and SI converges rapidly

- Thick limit (high scattering): the system for the scalar flux $\Phi$ behaves like diffusion
  - SI converges slowly
  - DSA / TSA used to accelerate convergence
Very little work has been done on MG for the Boltzmann transport equations

- MG developed mainly for 2\textsuperscript{nd} order elliptic problems
- **Challenges:** not elliptic, not symmetric, involves 1\textsuperscript{st} order terms & integral terms
- Many methods require so-called **sweeps** to invert the triangular streaming operators $H_i$

\[
H_i = \begin{bmatrix}
\end{bmatrix}
\]

- **Current parallelization techniques** may be sufficient even for BG/L $\Rightarrow O(dP^{1/d} + M)$
  - Sweeping many directions $M$ delays effect of $P$ term
- Parallel MG alternative to sweeps an open problem
True scalability will require parallel multilevel methods in time

- As we refine the mesh, we also refine the time step
- To date, have relied on increases in processor speed
- **This “solution” probably won’t work indefinitely**

- Doing concurrent work in time is not a natural concept (we live our lives sequentially in time)
- It is possible, however, though not trivial

- Related to the sweep problem in transport
- Some work has been done on this already (e.g., Stefan Vandewalle at Leuven, Belgium)
- **Still a very open (and interesting) problem!**
New assumed partition (AP) algorithm enables scaling to 100K+ processors

- Answering global data distribution queries previously required $O(P)$ storage and computations
- On BG/L, storing $O(P)$ data is not always practical or possible — e.g., no MPI_AllGather()
- New algorithm employs an assumed partition to answer queries through a kind of rendezvous algorithm
- Reduces storage to $O(I)$ and computations to $O(\log P)$!
- Now available in hypre
- AP idea has general applicability beyond hypre
AMG is 16x faster and uses less memory with new AP and coarsening algorithms on BG/L

<table>
<thead>
<tr>
<th># of procs</th>
<th>global partition (old)</th>
<th>assumed partition (new)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C-old</td>
<td>C-new</td>
</tr>
<tr>
<td>4,096</td>
<td>12.42</td>
<td>3.06</td>
</tr>
<tr>
<td>64,000</td>
<td>67.19</td>
<td>10.45</td>
</tr>
</tbody>
</table>

7pt 3D Laplacian; 30x30x30 unknowns per processor; co-processor mode;
BoomerAMG-CG; total times in seconds; coarsening algorithms C-old & C-new

- 15x overall speedup on 64K procs!
- 2 billions unknowns on 125K procs!
Guest Editors-in-Chief:
Chris Johnson
David Keyes
Ulrich Ruede

Call for papers:
- Modeling techniques
- Simulation techniques
- Analysis techniques
- Tools for realistic problems

Deadline for submissions:
April 30, 2007
Thank You!

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