Efficient Numerical Simulation of Advection Diffusion Systems

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Seminar Series
• History of machine and algorithmic speedup
• Introduction to Advection-Diffusion Systems
• Choice of Numerical Discretization
• Development of Numerical Solvers
• Results
• Conclusion/Future Directions
Motivation - Efficient Solvers

Faster machines and computational algorithms can dramatically reduce simulation time. (Centuries to milliseconds).
Simulating complex flows doesn’t scale as well.
## Complexity of Modern Linear Solvers

<table>
<thead>
<tr>
<th>Method</th>
<th>Type</th>
<th>Serial</th>
<th>Parallel</th>
</tr>
</thead>
<tbody>
<tr>
<td>FFT</td>
<td>Direct</td>
<td>nlog(n)</td>
<td>log(n)</td>
</tr>
<tr>
<td>Multigrid</td>
<td>Iterative</td>
<td>(n)</td>
<td>(log(n))^2</td>
</tr>
<tr>
<td>GMRES</td>
<td>Iterative</td>
<td>(n)</td>
<td>(n)</td>
</tr>
<tr>
<td>Lower Bound</td>
<td></td>
<td>(n)</td>
<td>log(n)</td>
</tr>
</tbody>
</table>
Model - Steady Advection Diffusion

\[-\epsilon \nabla^2 u + (\vec{w} \cdot \nabla) u = f\]

Inertial and viscous forces occur on disparate scales causing **sharp flow features** which:

- require fine numerical grid resolution
- cause poorly conditioned non-symmetric discrete systems.

These properties make solving the discrete systems **computationally expensive**.
High order methods are accurate & efficient.
Spectral elements provide:
- **flexible geometric boundaries**
- **large volume to surface ratio**
- **low storage requirements**
The discrete system of advection-diffusion equations are of the form:

$$F(\vec{w})u = Mf$$

When $w$ is constant in each direction on each element we can use

• Fast Diagonalization & Domain Decomposition as a solver.

$$\tilde{F} = \hat{M} \otimes \hat{F}(w_x) + \hat{F}(w_y) \otimes \hat{M}$$
Otherwise, we can use this as a **Preconditioner** for an iterative solver such as GMRES

\[ F(\vec{w}) P_F^{-1} P_F u = M f \]
What does $\otimes$ mean?

Suppose $A_{k \times l}$ and $B_{m \times n}$

The Kronecker Tensor Product

$$C_{km \times ln} = A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \ldots & a_{1l}B \\ a_{21}B & a_{22}B & \ldots & a_{2l}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1}B & a_{k2}B & \ldots & a_{kl}B \end{pmatrix}.$$ 

Matrices of this form have properties that make computations very efficient and save lots of memory!
Matrix-vector multiplies \((A \otimes B)\bar{u} = BU A^T\)
done in \(O(n^3)\) flops instead of \(O(n^4)\)

Fast Diagonalization Property
\(C = A \otimes B + B \otimes A\)
\(V^T AV = \Lambda, \quad V^T BV = I\)
\(C = (V \otimes V)(I \otimes \Lambda + \Lambda \otimes I)(V^T \otimes V^T)\)
\(C^{-1} = (V \otimes V)(I \otimes \Lambda + \Lambda \otimes I)^{-1}(V^T \otimes V^T)\)

Only need an inverse of a **diagonal matrix**!
We use Flexible GMRES with a **preconditioner** based on:

- Local constant wind approximations
- Fast Diagonalization
- Domain Decomposition

\[
F(\vec{w})P_F^{-1}P_Fu = Mf
\]

\[
P_F^{-1} = R_0^T \tilde{F}_0^{-1}(\vec{w}_0)R_0 + \sum_{e=1}^{N} R_e^T \tilde{F}_e^{-1}(\vec{w}^e)R_e
\]

\[
\tilde{F}_e^{-1} = (\hat{M}^{-1/2} \otimes \hat{M}^{-1/2})(S \otimes T)(\Lambda \otimes I + I \otimes V)^{-1}(S^{-1} \otimes T^{-1})(\hat{M}^{-1/2} \otimes \hat{M}^{-1/2})
\]
\[ \vec{w} = 200(-\sin\left(\frac{\pi}{6}\right), \cos\left(\frac{\pi}{6}\right)) \]

Solution and contour plots of a steady advection-diffusion flow. Via Domain Decomposition & Fast Diagonalization. Interface solve takes 150 steps to obtain $10^5$-5 accuracy.
Hot plate at wall forms internal boundary layers.

\[ \vec{w} = 200(y(1 - x^2), -x(1 - y^2)) \]

Residual Plot above.

\[ (P + 1) \begin{bmatrix} 1 & 2 & 0 & N & + & (P + 1) \end{bmatrix} \]

additional flops per step
Coupling Fast Diagonalization & Domain Decomposition provides an efficient solver for the advection-diffusion equation.

- Precondition Interface Solve
- Coarse Grid Solve (multilevel DD)
- Multiple wind sweeps
- Time dependent flows
- 2D & 3D Navier-Stokes
- Apply to study of complex flows
