Parallel Adaptive Discontinuous Galerkin Method for Chemical Transport Equations

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• Objective
  • Construct a **3D Parallel Adaptive computer code** to solve a set of chemical transport equations
    • Using **Discontinuous Galerkin Method (DG-FEM)**
• Objective
• Background
• Current Progress
• Acknowledgements
Discontinuous Galerkin Method (DG-FEM)

- Discontinuous Galerkin Method (DG-FEM)
  - A class of Finite Element Method (FEM)
  - Finding approximate solutions to boundary value problems
  - Solving differential equations
Example: Solving Heat Equation (1D)

- **1D** Poisson’s Equation on domain $I = [a, b]$

\[
\begin{align*}
-u'' &= f \\
u(a) &= u(b) = 0
\end{align*}
\]
Example: Solving Heat Equation (1D)

- Multiply by an arbitrary function \( v \)
  (satisfying \( v(a) = v(b) = 0 \))
  \[-u'' v - fv = 0\]

- Integration (Strong-form)
  \[-\int u'' v - \int fv = 0\]
Example: Solving Heat Equation (1D)

- Suppose \( v \) is continuous over \( I \), integration by parts
  \[
  \int u' v' + [u' v]_{I} - \int f v = 0
  \]

- Obtain **Weak-form** of *Finite Element Method*
  \[
  \int u' v' - \int f v = 0
  \]
Example: Solving Heat Equation (1D)

• Choice of \( v \): also serve as basis functions

\[ u \downarrow i = \sum_j u \downarrow j \ n \downarrow j : \text{linear combination of } n \downarrow j \]

\[
\begin{bmatrix}
\int_{f \downarrow 0 \uparrow} \n \downarrow 0
\int_{f \downarrow 1 \uparrow} \n \downarrow 1
\int_{f \downarrow 2 \uparrow} \n \downarrow 2
\end{bmatrix} - \begin{bmatrix}
\int_{f \downarrow 0 \uparrow}
\int_{f \downarrow 1 \uparrow}
\int_{f \downarrow 2 \uparrow}
\end{bmatrix}
\]
Example: Solving Heat Equation (1D)

- Suppose $v$ is discontinuous on $x↓j$

- Integration by parts on each interval

\[-\int u'' \, v = -\sum_j \int_{x↓j}^{x↓j+1} u'' \, v \uparrow = \sum_j \int_{x↓j}^{x↓j+1} (u'' \, v' \uparrow - [u \, v]_{x↓j}^{x↓j+1})\]
Example: Solving Heat Equation (1D)

\[ [u' \uparrow v] \downarrow x \downarrow j \uparrow x \downarrow j + 1 \downarrow \uparrow = \sum_{j=0}^{n} u' (x \downarrow j \uparrow) v(x \downarrow j \uparrow) - u' (x \downarrow j + 1 \uparrow) \]

\[ = u' (x \downarrow 0 \uparrow) v(x \downarrow 0 \uparrow) - u' (x \downarrow 1 \uparrow) v(x \downarrow 1 \uparrow) + u' (x \downarrow 1 \uparrow) + v(x \downarrow 1 \uparrow) - u' (x \downarrow 2 \uparrow) v(x \downarrow 2 \uparrow) + v(x \downarrow 2 \uparrow) - u' (x \downarrow 3 \uparrow) v(x \downarrow 3 \uparrow) \]

\[ = u' (x \downarrow 0 \uparrow) v(x \downarrow 0 \uparrow) + \sum_{\text{interior}} (u' (x \downarrow j \uparrow) v(x \downarrow j \uparrow) - u' (x \downarrow j \uparrow) v(x \downarrow j \uparrow) -) \downarrow - u' (x \downarrow 3 \uparrow) v(x \downarrow 3 \uparrow) \]
Example: Solving Heat Equation (1D)

- Non-zero jumps at interior nodes
- Transfer intervals information between intervals
- Discontinuous Galerkin Methods
Example: Solving Heat Equation (1D)

• Approximate \( u \downarrow h \uparrow (I \downarrow h) \)

\[ v \downarrow k \uparrow (I \downarrow h) \]

• Matrix formulation
  – In terms of blocks

\[
\begin{bmatrix}
  v \downarrow 0 \uparrow (I \downarrow 0) & v \downarrow 0 \uparrow (I \downarrow 1) & v \downarrow 0 \uparrow (I \downarrow 2) \\
  v \downarrow 1 \uparrow (I \downarrow 0) & v \downarrow 1 \uparrow (I \downarrow 1) & v \downarrow 1 \uparrow (I \downarrow 2) \\
  v \downarrow 0 \uparrow (I \downarrow 1) & v \downarrow 1 \uparrow (I \downarrow 1) & v \downarrow 0 \uparrow (I \downarrow 2) \\
  v \downarrow 0 \uparrow (I \downarrow 2) & v \downarrow 1 \uparrow (I \downarrow 2) & v \downarrow 0 \uparrow (I \downarrow 0) \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  u \downarrow 0 \uparrow (I \downarrow 0) \\
  u \downarrow 1 \uparrow (I \downarrow 0) \\
  u \downarrow 0 \uparrow (I \downarrow 1) \\
  u \downarrow 1 \uparrow (I \downarrow 1) \\
  u \downarrow 0 \uparrow (I \downarrow 2) \\
  u \downarrow 1 \uparrow (I \downarrow 2) \\
\end{bmatrix}
\]
Example: Solving Heat Equation (1D)

- 2D Poisson’s Equation on domain $\Omega$

\[
\begin{align*}
-\Delta u \uparrow &= f \\
u &= g\downarrow \Gamma \downarrow D \\
\partial u/\partial n &= g\downarrow N \text{ on } \Gamma \downarrow N
\end{align*}
\]
Example: Solving Heat Equation (1D)

- **2D** Poisson’s Equation on domain $\Omega$
- Partition the domain into triangles
- DG-FEM: Jumps across edges
Why DG-FEM over FEM

• Cons:
  – Large number of degrees of freedom

• Pros:
  – Increase of accuracy
  – Sparse matrix
  – Facilitation of parallelization
    • Information within or across local matrix blocks
• Objective
• Background
• Current Progress
• Acknowledgements
• Understand 1D DG serial code
  • Example: $f = \pi^2 \sin(\pi x)$, $u(0) = u(1) = 0$
  • Basis functions $v_0 = 1 - x$, $v_1 = x$
  • Number of intervals = 20
• Understand 1D DG serial code
  • Example: \( f = \pi^2 \sin(\pi x) \), \( u(0) = u(1) = 0 \)
  • Basis functions \( v_0 = 1 - x \), \( v_1 = x \)
  • Number of intervals = 20
    – Norm behaviors
      • \( \left( \sum I \int I \left( u - u_h \right)^2 \, dx \right)^{1/2} \)
Current Progress

• Understand 1D DG serial code
• **Extend the 1D serial code to parallel code**
• Understand 2D DG serial code
• **Extend the 2D DG serial code to parallel code**
• Extend the 2D DG parallel code to cover chemical transport equations (?)
• Expand to 3D parallel code (?)
• Expand the code to be adaptive (?)
• Objective
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