Parallel Discontinuous Galerkin Method

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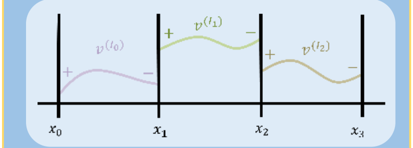
Overview

Discontinuous Galerkin Method (DG-FEM) is a class of Finite Element Method (FEM) for finding approximation solutions to systems of differential equations that can be used to simulate chemical transport phenomena.

The goal of my project is to implement parallelization on DG-FEM codes that can be scaled on existing supercomputers.

DG-FEM

In standard Finite Element Method, test functions are chosen for the weak formulation of the differential equation. DG-FEM chooses test functions that are discontinuous across adjacent elements, resulting jump conditions on the shared boundaries.



v+, v- : test function values on element boundaries

Mathematics behind

1D Poisson's Equation on domain $I = [a,b]$

$$\begin{cases} -u'' = f \\ u(a) = u(b) = 0 \end{cases}$$

Weak formulation using test function *v*

$$-\int u''v = -\sum_{j=0}^{j=N}\int_{x_j}^{x_{j+1}} u''v$$
$$= \sum_{j=0}^{j=N}\left(\int_{x_j}^{x_{j+1}} u'v' + u'(x_j^+)\,v(x_j^+) - u'(x_{j+1}^-)\,v(x_{j+1}^-)\right)$$
$$= \sum_{j=0}^{j=N}\int_{x_j}^{x_{j+1}} u'v' + u'(x_0^+)\,v(x_0^+) + \Bigg(\Big(-u'(x_1^-)\,v(x_1^-) + u'(x_1^+)\,v(x_1^+)\Big) + \dots$$
$$+ \Big(-u'(x_N^-)\,v(x_N^-) + u'(x_N^+)\,v(x_N^+)\Big)\Bigg) - u'(x_{N+1}^-)\,v(x_{N+1}^-)$$
$$= \sum_{j=0}^{j=N}\int_{x_j}^{x_{j+1}} u'v' + u'(x_0^+)\,v(x_0^+) + \sum_{j=1}^{j=N}[\mathbf{u'v}]_{\mathbf{x_j}} - u'(x_{N+1}^-)\,v(x_{N+1}^-)$$

Jump conditions: $[u'v]_{x_j} = \{u'\}_j[v]_j + [u']_j\{v\}_j$

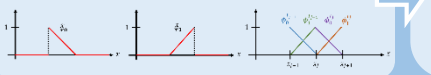
$$= \{\tfrac{1}{2}\left(u'(x_j^+) + u'(x_j^-)\right)\}\,[v(x_j^+) - v(x_j^-)] + [u'(x_j^+) - u'(x_j^-)]\,\{\tfrac{1}{2}\left(v(x_j^+) + v(x_j^-)\right)\}$$

1D Linear System Construction

Bilinear Function for Stiffness Matrix:

$$a(u,v) \equiv \sum_{j=0}^{j=N}\int_{x_j}^{x_{j+1}} u'v' + \sum_{j=0}^{j=N+1}\Big(\{u'\}_j[v]_j + \underbrace{\{v'\}_j[u]_j}_{\text{symmetric term}}\Big) + \gamma\underbrace{\sum_{j=0}^{N+1}\frac{1}{|I_j|}[u]_j[v]_j}_{\text{penalty term}}$$

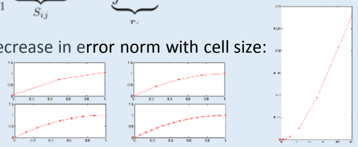
Basis Functions for *u*, *v*:



Solving Linear System:

$$\sum_{j=1}^{j=M}\underbrace{a(\phi_j,\phi_i)}_{S_{ij}}\alpha_j = \underbrace{\int f\,\phi_i}_{F_i} + \text{symmetric term} + \text{penalty term}$$

Decrease in error norm with cell size:



Parallel Computing over Serial Computing

LAPACK / ScaLAPACK
- Dense matrix solver only

DG-FEM Stiffness Matrix
- Positive Definite - Sparse

Less time
Less storage
Larger problem

Trilinos
- Compressed row storage
- Also sparse matrix solver

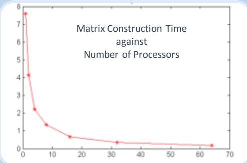
1D Parallelization

Matrix Construction → Solving Linear System

Serial: Global Matrix — Serial: *LAPACK*; Parallel: *ScaLAPACK*

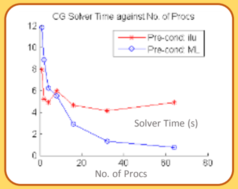
Parallel: Local Matrices — Serial: *LAPACK* on *MPI*; Parallel: *Trilinos*

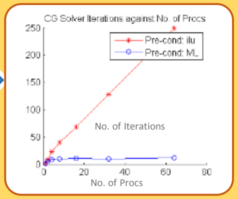
Parallel: *Trilinos* — Solver: Iterative; Preconditioner: ML Library



AztecOO on Trilinos

No. of Cells = 5,000,000
No. of Procs = 1,2,4,8,16,32,64

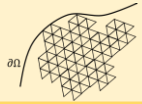


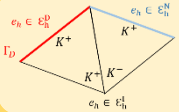


CG Iterative Solver + ML Preconditioner = LESS solver time + STABLE no. of iter.

From 1D to 2D

Partition of Domain:
Intervals (1-D)
=> Triangles (2-D)




$e_h \in \mathcal{E}_h^D$
Γ_D
K^+
K^+
K^-
K^-
$e_h \in \mathcal{E}_h^N$
Γ_N
$e_h \in \mathcal{E}_h^I$

Jump conditions
Over nodes (1-D)
=> Over edges (2-D)

2D DG-FEM: more complex code structure

Why DG-FEM matters

Discontinuity between element boundaries provides local support and leads to :

✓ Local refinement ✓ Complex geometries
✓ Parallelization ✓ Higher-order accuracy

My Work

✓ Construct a 1-D DG-FEM serial code

✓ Construct a 1-D DG-FEM partial parallel code (*LAPACK* on *MPI)*

✓ Construct a 1-Dimension DG-FEM fully parallel code (*Trilinos*)

✓ Analyze parallelization performances

Future

-- Extend the code to 2-D and 3-D DG-FEM fully parallel code

-- Expand the code to be adaptive for local refinement, and cover chemical transport equations

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