

Chemical Transport Modelling with Spectral Element Method

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Overview

• Background

• Spectral Element Method

- Basis Function
- Weak Form
- Quadrature
- Global v.s Local Formulation
- Euler and Newton Methods
- Continuous Galerkin v.s Discontinuous Galerkin

• Coding

- Serial Code
- Parallel Code

Background

• CESM (Community Earth System Model) :

Aimed at understanding and predicting the climate system.

• Climate and chemical transport models:

Require the use of unstructured grids and conservation of mass and energy. Therefore, the model is written using the FVM*(Finite Volume Method),* which is explicitly conservative.

• CESM and the HOMME equations:

Formulated through the FEM(*Finite Element Method*) because of its use on unstructured grids. This is convenient when solving the equations on a globe.

• Spectral Element Method:

Mark Taylor [1] has shown that the Spectral Element Method, a type of FEM, is explicitly locally conservative, as well as having other ideal properties, such as a diagonal mass matrix.

• Object:

We want to show that chemical transport problems can be accurately modeled with the SEM, so that they may be integrated with the HOMME equations.



Basis Functions

- A type of continuous-Galerkin Finite Element Method with explicit local and global conservation, and a diagonal mass matrix
- A typical continuous-Galerkin formulation of a problem starts by replacing the fields *u* with a piecewise polynomial function.
- Because of this, *u* can be approximately represented as a sum of basis functions:

 $u(\vec{x}) \approx \sum_{\vec{\iota}} u(\vec{\xi}_{\vec{\iota}}) \phi_{\vec{\iota}}(\vec{x})$

• Because of this, we can also write the first derivatives of *u* as

$$\vec{\nabla} u(\vec{x}) \approx \sum_{\vec{\iota}} u(\vec{\xi}_{\vec{\iota}}) \vec{\nabla} \phi_{\vec{\iota}}(\vec{x})$$



Weak Form

- As a result of the polynomial approximation, *u* is not second-differentiable.
- However, differential equation with a second derivative can be transformed into a differentialintegral equation through integration by parts.
- Integrate the equation with a test function *v*. e.g.:

$$\frac{\partial u}{\partial t} = \nabla^2 u \quad \longrightarrow \quad \int_{\Omega} v \frac{\partial u}{\partial t} dx = \int_{\Omega} v \nabla^2 u dx \quad \longrightarrow \quad \int_{\Omega} v \frac{\partial u}{\partial t} dx = \int_{\partial \Omega} v \nabla u \cdot d\Omega - \int_{\Omega} \nabla v \cdot \nabla u dx$$

• By inserting the polynomial approximation, turn the integro-differential problem into a linear algebra problem:

$$\int_{\Omega} \phi_{\vec{l}} \frac{\partial u}{\partial t} dx = B.C. - \int_{\Omega} \vec{\nabla} \phi_{\vec{l}} \cdot \vec{\nabla} u dx \longrightarrow \sum_{\vec{j}} \frac{\partial u(\vec{\xi}_{\vec{j}})}{\partial t} \int_{\Omega} \phi_{\vec{l}} \phi_{\vec{j}} dx = B.C. - \sum_{\vec{j}} u(\vec{\xi}_{\vec{j}}) \int_{\Omega} \vec{\nabla} \phi_{\vec{l}} \cdot \vec{\nabla} \phi_{\vec{j}} u dx$$

• The integrals are calculated using a Gaussian quadrature.

Gaussian Quadrature

• To approximate an integral by quadrature, we write it as a weighted sum over discrete points:

$$\int_{\Omega_m} f(\vec{x}) dx \approx \sum_{\vec{k}} f(\vec{x}_{\vec{k}}) J_m(x_{\vec{k}}) w_{\vec{k}}$$

• In the Spectral Element Method, we set the nodal points used for polynomial interpolation equal to the quadrature points. This means the mass matrix can be simplified as:

$$\int_{\Omega_m} \phi_{\vec{\iota}} \phi_{\vec{J}} dx \approx \sum_{\vec{k}} \phi_{\vec{\iota}}(\vec{\xi}_{\vec{k}}) \phi_{\vec{J}}(\vec{\xi}_{\vec{k}}) J_m(\vec{\xi}_{\vec{k}}) w_{\vec{k}} = J_m(\vec{\xi}_{\vec{\iota}}) w_{\vec{\iota}} \delta_{\vec{\iota}}$$

- This greatly simplifies the linear algebra involved.
- The Gauss-Lobatto quadrature (which SEM uses) is exact for polynomials of degree *d* <= 2*n*-1, where *n* is the number of quadrature points. This means many vector-calculus identities are preserved in this formulation, which leads to local and global conservation.

Global vs. Local Formulation

- Due to the piecewise approximation, elements are mostly independent of each other.
- The only interdependence between elements occurs at the boundaries, where elements share nodal points.
- When integrating, one can solve the matrices globally, or one can distribute local element data to different processors and integrate each element in parallel.
- This gives the exact same result as the global method for interior points, but points on elemental boundaries may disagree between elements. This discontinuity is resolved by a weighted average.
- After the parallel integration + weighted sum, the local method and global method are mathematically equivalent.





Euler and Newton methods

• Once the time derivative is known, we can calculate the next time step through the Forward Euler Method:

$$\frac{du_i}{dt} = F_i(u) \qquad \qquad u_i(t + \Delta t) = u_i + \Delta u_i$$
$$\Delta u_i = F_i(u)\Delta t$$

- This method can have instabilities, however, which requires a CFL factor to control it (typically has the form $\Delta t = c \Delta x^n$ for some *c* and *n*.
- One way to remove these instabilities is to use an implicit Euler method:

$$u_i(t + \Delta t) = u_i + \Delta u_i$$
$$\Delta u_i = (1 - \theta)F_i(u(t)) + \theta F_i(u(t + \Delta t))$$

• This is typically a nonlinear equation that must be solved via iterative Newton methods and the Jacobian matrix J:

$$\Delta u_i^{(n+1)} = \Delta u_i^{(n)} + \sum_j \frac{1}{\Delta t(1-\theta)} \mathbf{J}(u(t) + \Delta u^{(n)})_{ij}^{-1} \Delta u_j^{(n)} \qquad \mathbf{J}(u)_{ij} = \frac{\partial F_i}{\partial u_j}(u)$$

Euler and Newton methods (cont.)

• The Jacobian matrix will have dimensions $(N_F \times (d + 1)^{dim})^2$, where N_F = number of fields, dim = dimension, and d = interpolation degree.

- For a problem with 10 fields, polynomial degree 4 and 3 dimensions, this is approximately $(10 \times 5^3)^2 \approx 1.5 \times 10^6$ components. If each number is stored in 16 bytes (double precision) this comes to approximately 25 MB.
- Each compute node in BEACON has 256 GB of memory and 16 cores, which comes to 16 GB per core. Problems with a large number of fields or high interpolation degree can strain this memory restriction.
 - Most problems only have a few chemical interactions, which gives the Jacobian a sparse or banded structure that can be split among processors using TRILINOS.



Finite Element Method

Continuous vs. Discontinuous Galerkin Method



Coding

• Serial Code (C):

$$\frac{\partial u_{(\alpha)}}{\partial t} = d_{(\alpha)} \frac{\partial^2 u_{(\alpha)}}{\partial x^2} + R_{(\alpha)} \left(u \right)$$

- 1-dimensional multiple-species diffusion equation with source term
- \circ Method :

Parallel

- Spectral Element Method
- Guassian-Lobatto Quadrature
- Euler Backward Method and Newton Method

Serial

• Parallel Code (Fortran):

$$\frac{\partial u_{\alpha}}{\partial t} = D_{\alpha} \nabla^2 u_{\alpha} - \vec{v} \cdot \vec{\nabla} u_{\alpha} + R_{\alpha}(u)$$

- Fortran modules designed to solve multidimensional PDEs with Spectral Element Method
- module HESIOD:
 - Stores data about mesh, fields and equation
- module HOMER:
 - Performs time-integration on each element separately (parallel)
 - Resolves boundary discontinuities via weighted sum (serial)
- Currently tested on:
 - 1- and 2-dimensional multiple-species diffusion equations with convection and source terms
 - Forward Euler Method, no splitting

Coding

- Testing Example:

 chemical equation:
 Cl₂ ⇒ Cl + Cl
 2-species math model:
 - $\frac{\partial [Cl_2]}{\partial t} = d_1 \frac{\partial^2 [Cl_2]}{\partial x^2} 0.001 [Cl_2] + 0.05 [Cl]^2$ $\frac{\partial [Cl]}{\partial t} = d_2 \frac{\partial^2 [Cl]}{\partial x^2} + 0.002 [Cl_2] 0.1 [Cl]^2$





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.316583e-01 4.464022e-01 1.909972e-03 .618090e-01 4.857160e-01 2.064609e-03 .919598e-01 5.247058e-01 2.214643e-03 .221106e-01 5.633487e-01 2.359897e-03 .522613e-01 6.016203e-01 2.635200e-03 .824121e-01 6.394989e-01 2.635200e-03 .824121e-01 6.79638e-01 2.765040e-03 .125628e-01 7.139945e-01 2.889560e-03 .427136e-01 7.866706e-01 3.122324e-03 .030151e-01 7.866706e-01 3.230610e-03 .6331668e-01 8.222800e-01 3.230610e-03 .6331668e-01 8.573787e-01 3.611300e-03 .633166e-01 9.59667e-01 3.611300e-03 .537688e-01 9.594670e-01 3.611300e-03 .639196e-01 9.259667e-01 3.611300e-03 .839196e-01 9.259667e-01 3.611300e-03 .839196e-01 9.25967e-01 3.611300e-03 .442211e-01 1.056451e+00 3.981612e-03 .743719e-01 1.087590e+00 3.915736e-03 .648241e-01 1.177322e+00 4.103102e-03 <	.015075e-01	4.067898e-01	1.751034e-03
6.618090e-01 4.857160e-01 2.064609e-03 9.919598e-01 5.247058e-01 2.214643e-03 221106e-01 5.633487e-01 2.359897e-03 522613e-01 6.016203e-01 2.500125e-03 824121e-01 6.394989e-01 2.635200e-03 12562e-01 6.769638e-01 2.765040e-03 12562e-01 7.13945e-01 2.889560e-03 227136e-01 7.866706e-01 3.122324e-03 331658e-01 8.222800e-01 3.230610e-03 331658e-01 8.222800e-01 3.230610e-03 331658e-01 8.573787e-01 3.33507e-03 33166e-01 8.573787e-01 3.641300e-03 33166e-01 9.594670e-01 3.611300e-03 339196e-01 9.594670e-01 3.61300e-03 442211e-01 1.024711e+00 3.772236e-03 442211e-01 1.056451e+00 3.846043e-03 743719e-01 1.087590e+00 3.915736e-03 442211e-01 1.07322e+00 4.159311e-03 5442211e-01 1.177322e+00 4.103102e-03 .0346734e-01 1.17732e+00 4.159311e-	.316583e-01	4.464022e-01	1.909972e-03
919598e-01 5.247058e-01 2.214643e-03 .221106e-01 5.633487e-01 2.359897e-03 .522613e-01 6.016203e-01 2.500125e-03 .824121e-01 6.394989e-01 2.635200e-03 .125628e-01 6.769638e-01 2.765040e-03 .125628e-01 7.139945e-01 2.889560e-03 .427136e-01 7.139945e-01 3.008677e-03 .728643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.122324e-03 .6331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.33507e-03 .537686e-01 9.925967e-01 3.611300e-03 .537686e-01 9.594670e-01 3.614075e-03 .546704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.981612e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.177322e+00 4.103102e-03 .949749e-01 1.261383e+00 4.264317e-03	.618090e-01	4.857160e-01	2.064609e-03
.221106e-01 5.633487e-01 2.359897e-03 .522613e-01 6.016203e-01 2.500125e-03 .824121e-01 6.394989e-01 2.635200e-03 .125628e-01 6.769638e-01 2.765040e-03 .427136e-01 7.139945e-01 2.889560e-03 .728643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.122324e-03 .0331658e-01 8.222800e-01 3.233610e-03 .331658e-01 8.573787e-01 3.333507e-03 .3331658e-01 9.259867e-01 3.523709e-03 .236181e-01 9.259867e-01 3.611300e-03 .389196e-01 9.923791e-01 3.694075e-03 .442211e-01 1.056451e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.126333e+00 4.26317e-03 .025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.261360e-03 .055276e+00 1.261383e+00 4.361660e-03	.919598e-01	5.247058e-01	2.214643e-0
.522613e-01 6.016203e-01 2.500125e-03 .824121e-01 6.394989e-01 2.635200e-03 .125628e-01 6.769638e-01 2.765040e-03 .427136e-01 7.139945e-01 2.889560e-03 .728643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.122324e-03 .331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.33507e-03 .331658e-01 9.259867e-01 3.523709e-03 .236181e-01 9.259867e-01 3.61300e-03 .839196e-01 9.923791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.177322e+00 4.03969e-03 .045226e-01 1.261383e+00 4.264317e-03 .055276e+00 1.261382e+00 4.31788e-03 .055276e+00 1.38638e+00 4.264317e-03 .055276e+00 1.386438e+00 4.408278e-03 <th>.221106e-01</th> <th>5.633487e-01</th> <th>2.359897e-03</th>	.221106e-01	5.633487e-01	2.359897e-03
.824121e-01 6.394989e-01 2.635200e-03 .125628e-01 6.769638e-01 2.765040e-03 .427136e-01 7.139945e-01 2.889560e-03 .728643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.122324e-03 .331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.33507e-03 .633166e-01 8.573787e-01 3.523709e-03 .236181e-01 9.259867e-01 3.61300e-03 .537688e-01 9.594670e-01 3.611300e-03 .5331656e-01 9.259867e-01 3.694075e-03 .100704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.1205979e+00 4.103102e-03 .045276e+00 1.2261383e+00 4.264317e-03 .055276e+00 1.288122e+00 4.313783e-03 .055276e+00 1.314218e+00 4.361660e-03	.522613e-01	6.016203e-01	2.500125e-03
.125628e-01 6.769638e-01 2.765040e-03 .427136e-01 7.139945e-01 2.889560e-03 .728643e-01 7.505702e-01 3.008677e-03 .30151e-01 7.866706e-01 3.122324e-03 .331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.33507e-03 .934673e-01 8.919524e-01 3.431159e-03 .934673e-01 9.259867e-01 3.523709e-03 .236181e-01 9.259867e-01 3.611300e-03 .236181e-01 9.259867e-01 3.614300e-03 .537688e-01 9.594670e-01 3.614300e-03 .633194e-01 1.024711e+00 3.772236e-03 .140704e-01 1.024711e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .045226e-01 1.118120e+00 3.981612e-03 .045226e-01 1.1205979e+00 4.103102e-03 .055276e+00 1.261383e+00 4.24317e-03 .055276e+00 1.288122e+00 4.313783e-03 .115578e+00 1.314218e+00 4.361660e-03 .15578e+00 1.39670e+00 4.408278e-03 <th>.824121e-01</th> <th>6.394989e-01</th> <th>2.635200e-0</th>	.824121e-01	6.394989e-01	2.635200e-0
.427136e-01 7.139945e-01 2.889560e-03 .728643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.12324e-03 .331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.333507e-03 .633166e-01 8.573787e-01 3.33507e-03 .236181e-01 9.259667e-01 3.523709e-03 .236181e-01 9.259667e-01 3.611300e-03 .339196e-01 9.923791e-01 3.694075e-03 .346734e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.846043e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.118120e+00 4.043969e-03 .045226e-01 1.177322e+00 4.103102e-03 .045226e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.288122e+00 4.31783e-03 .055276e+00 1.339670e+00 4.361660e-03 .115578e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 <th>.125628e-01</th> <th>6.769638e-01</th> <th>2.765040e-03</th>	.125628e-01	6.769638e-01	2.765040e-03
7.28643e-01 7.505702e-01 3.008677e-03 .030151e-01 7.866706e-01 3.122324e-03 .030151e-01 8.222800e-01 3.230610e-03 .331658e-01 8.222800e-01 3.230610e-03 .633166e-01 8.573787e-01 3.333507e-03 .934673e-01 8.919524e-01 3.431159e-03 .236181e-01 9.259667e-01 3.523709e-03 .53768e-01 9.594670e-01 3.611300e-03 .53768e-01 9.594670e-01 3.611300e-03 .639196e-01 9.023791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.846043e-03 .045226e-01 1.118120e+00 3.915736e-03 .045226e-01 1.11822e+00 4.103102e-03 .045226e-01 1.177322e+00 4.103102e-03 .045226e+00 1.205979e+00 4.103102e-03 .045226e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.314218e+00 4.361660e-03 .115578e+00 1.314218e+00 4.361660e-03 <th>.427136e-01</th> <th>7.139945e-01</th> <th>2.889560e-0</th>	.427136e-01	7.139945e-01	2.889560e-0
0.030151e-01 7.866706e-01 3.122324e-03 0.331658e-01 8.222800e-01 3.230610e-03 0.633166e-01 8.573787e-01 3.333507e-03 0.934673e-01 8.919524e-01 3.431159e-03 0.236181e-01 9.259867e-01 3.6311300e-03 0.236181e-01 9.594670e-01 3.611300e-03 0.537688e-01 9.594670e-01 3.611300e-03 0.537688e-01 9.594670e-01 3.694075e-03 0.442211e-01 1.024711e+00 3.772236e-03 0.442211e-01 1.056451e+00 3.846043e-03 0.442211e-01 1.087590e+00 3.915736e-03 0.45226e-01 1.118120e+00 3.915736e-03 0.45226e-01 1.11820e+00 4.043969e-03 0.45226e-01 1.205979e+00 4.159311e-03 0.949749e-01 1.205979e+00 4.159311e-03 0.95276e+00 1.288122e+00 4.313783e-03 0.055276e+00 1.288122e+00 4.313783e-03 0.15578e+00 1.314218e+00 4.361660e-03 1.15578e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e	.728643e-01	7.505702e-01	3.008677e-03
331658e-01 8.222800e-01 3.230610e-03 6.33166e-01 8.573787e-01 3.333507e-03 6.33166e-01 8.919524e-01 3.431159e-03 2.236181e-01 9.259867e-01 3.523709e-03 2.336168e-01 9.594670e-01 3.61300e-03 2.336168e-01 9.923791e-01 3.64075e-03 3.839196e-01 9.923791e-01 3.694075e-03 3.140704e-01 1.024711e+00 3.772236e-03 2.442211e-01 1.056451e+00 3.846043e-03 2.442211e-01 1.087590e+00 3.915736e-03 2.442211e-01 1.087590e+00 3.915736e-03 2.442211e-01 1.18120e+00 3.915736e-03 2.442211e-01 1.18120e+00 3.915736e-03 2.442211e-01 1.18120e+00 3.915736e-03 2.442211e-01 1.177322e+00 4.03969e-03 2.442211e-01 1.177322e+00 4.103102e-03 2.4422126e+00 1.2261383e+00 4.24317e-03 2.055276e+00 1.261383e+00 4.264317e-03 .015578e+00 1.314218e+00 4.361660e-0	.030151e-01	7.866706e-01	3.122324e-03
6.633166e-01 8.573787e-01 3.333507e-03 6.934673e-01 8.919524e-01 3.431159e-03 .236181e-01 9.259867e-01 3.523709e-03 .537688e-01 9.594670e-01 3.611300e-03 .537688e-01 9.923791e-01 3.694075e-03 .839196e-01 9.923791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.72236e-03 .442211e-01 1.056451e+00 3.846043e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .045226e-01 1.11820e+00 3.981612e-03 .045226e-01 1.177322e+00 4.103102e-03 .045226e-01 1.261383e+00 4.264317e-03 .025126e+00 1.261382e+00 4.264317e-03 .025276e+00 1.261382e+00 4.316160e-03 .0155276e+00 1.328612e+00 4.361660e-03 .115578e+00 1.339670e+00 4.408278e-03 .145729e+00 1.364477e+00 4.45964e-03 .206030e+00 1.388638e+00 4.499034e-03	.331658e-01	8.222800e-01	3.230610e-03
934673e-01 8.919524e-01 3.431159e-03 .236181e-01 9.259867e-01 3.523709e-03 .537688e-01 9.594670e-01 3.611300e-03 .839196e-01 9.923791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.846043e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .045226e-01 1.148033e+00 4.043969e-03 .045226e-01 1.177322e+00 4.103102e-03 .045226e-01 1.261383e+00 4.264317e-03 .025126e+00 1.261383e+00 4.264317e-03 .025126e+00 1.288122e+00 4.313783e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.349670e+00 4.361660e-03 .115578e+00 1.339670e+00 4.361660e-03 .175879e+00 1.364477e+00 4.493964e-03 .206030e+00 1.388638e+00 4.499034e-03 .206030e+00 1.388638e+00 4.499034e-03	.633166e-01	8.573787e-01	3.333507e-0
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537688e-01 9.594670e-01 3.611300e-03 .839196e-01 9.923791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.915736e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .346734e-01 1.148033e+00 4.043969e-03 .648241e-01 1.177322e+00 4.103102e-03 .949749e-01 1.205979e+00 4.159311e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.288122e+00 4.313783e-03 .115578e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.408278e-03 .206030e+00 1.388638e+00 4.499034e-03 .206030e+00 1.388638e+00 4.499034e-03 .206181e+00 1.412156e+00 4.543781e-03	.236181e-01	9.259867e-01	3.523709e-03
.839196e-01 9.923791e-01 3.694075e-03 .140704e-01 1.024711e+00 3.772236e-03 .442211e-01 1.056451e+00 3.846043e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .346734e-01 1.148033e+00 4.043969e-03 .648241e-01 1.177322e+00 4.103102e-03 .648241e-01 1.205979e+00 4.159311e-03 .025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.314218e+00 4.361660e-03 .115578e+00 1.314218e+00 4.408278e-03 .175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.537688e-01	9.594670e-01	3.611300e-03
1.1024711e+00 3.772236e-03 442211e-01 1.056451e+00 3.846043e-03 743719e-01 1.087590e+00 3.915736e-03 0.045226e-01 1.118120e+00 3.981612e-03 0.346734e-01 1.148033e+00 4.043969e-03 0.648241e-01 1.177322e+00 4.103102e-03 0.648241e-01 1.205379e+00 4.159311e-03 0.055276e+00 1.261383e+00 4.264317e-03 0.055276e+00 1.288122e+00 4.313783e-03 0.055276e+00 1.314218e+00 4.361660e-03 115578e+00 1.314218e+00 4.361660e-03 125739e+00 1.386438e+00 4.49934e-03 206030e+00 1.388638e+00 4.49934e-03 236181e+00 1.412156e+00 4.543781e-03	.839196e-01	9.923791e-01	3.694075e-0
.442211e-01 1.056451e+00 3.846043e-03 .743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .346734e-01 1.148033e+00 4.043969e-03 .648241e-01 1.177322e+00 4.103102e-03 .949749e-01 1.205979e+00 4.159311e-03 .025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .055276e+00 1.314218e+00 4.31678e-03 .115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.386438e+00 4.493964e-03 .206030e+00 1.388638e+00 4.499034e-03 .226181e+00 1.412156e+00 4.543781e-03	.140704e-01	1.024711e+00	3.772236e-03
.743719e-01 1.087590e+00 3.915736e-03 .045226e-01 1.118120e+00 3.981612e-03 .346734e-01 1.148033e+00 4.043969e-03 .648241e-01 1.177322e+00 4.103102e-03 .949749e-01 1.205979e+00 4.159311e-03 .025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .115578e+00 1.314218e+00 4.316786e-03 .145729e+00 1.339670e+00 4.408278e-03 .206030e+00 1.388638e+00 4.499034e-03 .226181e+00 1.412156e+00 4.543781e-03	.442211e-01	1.056451e+00	3.846043e-03
0.045226e-01 1.118120e+00 3.981612e-03 0.346734e-01 1.148033e+00 4.043969e-03 0.648241e-01 1.177322e+00 4.103102e-03 0.949749e-01 1.205979e+00 4.159311e-03 0.025126e+00 1.234001e+00 4.212935e-03 0.055276e+00 1.261383e+00 4.264317e-03 0.055427e+00 1.314218e+00 4.3161660e-03 .115578e+00 1.314218e+00 4.361660e-03 .175879e+00 1.364477e+00 4.45964e-03 .206030e+00 1.388638e+00 4.499034e-03 .226181e+00 1.412156e+00 4.543781e-03	.743719e-01	1.087590e+00	3.915736e-03
3.346734e-01 1.148033e+00 4.043969e-03 0.648241e-01 1.177322e+00 4.103102e-03 0.949749e-01 1.205979e+00 4.159311e-03 0.025126e+00 1.234001e+00 4.222935e-03 0.055276e+00 1.261383e+00 4.264317e-03 0.055427e+00 1.314218e+00 4.361660e-03 .115578e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.045226e-01	1.118120e+00	3.981612e-03
0.648241e-01 1.177322e+00 4.103102e-03 0.949749e-01 1.205979e+00 4.159311e-03 0.025126e+00 1.234001e+00 4.212935e-03 0.055276e+00 1.261383e+00 4.264317e-03 0.055276e+00 1.288122e+00 4.313783e-03 1.15578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.45964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.346734e-01	1.148033e+00	4.043969e-03
.949749e-01 1.205979e+00 4.159311e-03 .025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .085427e+00 1.288122e+00 4.313783e-03 .115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.648241e-01	1.177322e+00	4.103102e-03
.025126e+00 1.234001e+00 4.212935e-03 .055276e+00 1.261383e+00 4.264317e-03 .085427e+00 1.288122e+00 4.313783e-03 .115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.949749e-01	1.205979e+00	4.159311e-03
.055276e+00 1.261383e+00 4.264317e-03 .085427e+00 1.288122e+00 4.313783e-03 .115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.025126e+00	1.234001e+00	4.212935e-03
.085427e+00 1.288122e+00 4.313783e-03 .115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.055276e+00	1.261383e+00	4.264317e-03
.115578e+00 1.314218e+00 4.361660e-03 .145729e+00 1.339670e+00 4.408278e-03 .175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.085427e+00	1.288122e+00	4.313783e-03
145729e+00 1.339670e+00 4.408278e-03 175879e+00 1.364477e+00 4.453964e-03 206030e+00 1.388638e+00 4.499034e-03 236181e+00 1.412156e+00 4.543781e-03	.115578e+00	1.314218e+00	4.361660e-03
.175879e+00 1.364477e+00 4.453964e-03 .206030e+00 1.388638e+00 4.499034e-03 .236181e+00 1.412156e+00 4.543781e-03	.145729e+00	1.339670e+00	4.408278e-03
206030e+00 1.388638e+00 4.499034e-03 236181e+00 1.412156e+00 4.543781e-03	.175879e+00	1.364477e+00	4.453964e-03
.236181e+00 1.412156e+00 4.543781e-03	.206030e+00	1.388638e+00	4.499034e-03
	.236181e+00	1.412156e+00	4.543781e-0



Initial Condition



Parallel

Serial

Solution run by the serial code **Compare with FVM** \bullet

-Cl





FVM : solution given by Jian Sun(UTK)



Program Solution VS Theoretical Solution

- Differential Equation :
- Initial Condition :

• Theoretical Solution :

$$\frac{\partial u}{\partial t} = 0.1 \frac{\partial^2 u}{\partial x^2} + 0.1 u \qquad u = \sin(\pi x) \text{ at } T = 0 \qquad u = e^{0.1 - 0.1 \pi^2 T} \sin(\pi x)$$





Program Solution VS Theoretical Solution





Convergence of the Solution

Fix the domain to be [0, 20] and Vary the number of elements from 13 to 70



Coding

Convergence testing Equation: $\frac{\partial u}{\partial t} = 0.1 \frac{d^2 u}{dx^2} - 1.0u$

Theoretical Solution:

$$u(x,t) = e^{-1.0t} (1 + e^{-0.1\pi^2 t} \cos(\pi x))$$



elem40



Convergence Test

0.8 0.9



2D test case: $2A \Leftrightarrow A_2$

$$\frac{\partial [A_2]}{\partial t} = 2.0\nabla^2 [A_2] - \vec{v} \cdot \vec{\nabla} [A_2] - 500.0 [A_2] + 80.0 [A]^2$$

$$\frac{\partial [A]}{\partial t} = 2.0\nabla^2 [A] - \vec{v} \cdot \vec{\nabla} [A] + 1000.0 [A_2] + 160.0 [A]^2$$

 $v_x = 50.0$ • Tested on 5 x 5 (=25) elemental grid

$$v_y = 0.0$$
 • dx = 0.2, dt = 0.0001



Serial



$2D \text{ test case: } 2A \Leftrightarrow A_2$ $t = 0 \longrightarrow t = 0.002 \longrightarrow t = 0.004$



Parallel

Coding Scalability

Tested previous example with 32 x 32 (=1024) element grid on 1, 2, 4, 8, ..., 1024 processors.

- Minimum time at 512 processors
- Can be improved by parallelizing
- the weighted average process

Parallel

Computing time may be improved
 by adding operator
 Serial splitting



Next Steps

• Serial Code:

Serial

Parallel

- Finish the current discontinuous Galerkin serial code and test the accuracy of this code
- Write a discontinuous Galerkin code based on Dr.Chung's(CUHK) algorithm
- Combine the code of the discontinuous serial code with the parallel code with Trilinos
- Hopefully, a discontinuous parallel code would be obtained

• Parallel Code:

- Parellelize the averaging process on the boundaries by sending boundary data only to neighbors
- Implement option for operator splitting to improve computational efficiency
- Implement options for Implicit Euler and Newton methods
- Allow user to set more general boundary conditions: Dirichlet, Neumann, Robin and Periodic
- Interface with Trilinos to allow for higher dimensional problems and a large number of fields

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• [1] Mark A. Taylor and Aime Fournier. A compatible and conservative spectral element method on unstructured grids. Journal of Computational Physics, 229(17):5879 – 5895, 2010.