Modeling Chemical Transport with Galerkin Methods

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JICS Joint Institute for Computational Sciences — UT ORNL Computational Sciences — A UT/ORNL PARTNERSHIP — NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES — NICS — NSF — UT

Overview

Chemical transports are typically done using the Finite Volume Method (FVM), which is explicitly locally conservative.

However, climate models such as CESM and the HOMME equations use continuous Galerkin methods to simulate meteorological phenomena on the globe. It is desirable to also use the same method for both climate and chemical transport.

Mark Taylor[1] has shown relatively recently that the Spectral Element Method, a type of Galerkin method, is explicitly locally conservative.

Our goal is to test the advantage of using Galerkin methods like the SEM to model chemical transport in the form of the equation:

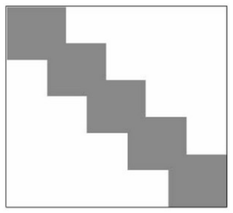
$$\frac{\partial u^\alpha}{\partial t} = D\nabla^2 u^\alpha + R^\alpha(u)$$

Acknowledgements Thanks to our mentors Dr. Drake, Dr. Fu and Dr. Wong for guidance and helpful conversations. Additional thanks to PhD student Jian Sun for providing FVM comparison code.

[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.

Mathematical Scheme

- Approximate function with piecewise polynomial interpolation

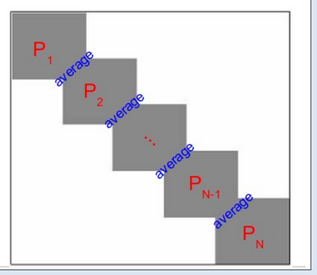


- Calculate matrices and solve for time derivative.

- Integrate PDE using Implicit Euler and Newton's method.

Serial: Integrate on the entire domain.

Parallel: Integrate on individual elements first,



Introduction to the Serial Code

The Serial Code written in C is aim to solve the diffusion equation with source term formed as the following differential equation.

$$\frac{\partial u^\alpha}{\partial t} = D\nabla^2 u^\alpha + R^\alpha(u)$$

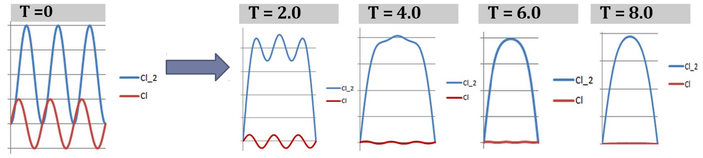
This code is basically Spectral Element Method, Gaussian-Lobatto Quadrature, Euler Backward Method as well as Newton Method.

Example of Running the Serial Code to Solve the Diffusion Equation with source term

Based on the chemical equation $Cl_2 \rightleftharpoons Cl + Cl$, we construct a model on the quantity of these 2 species:

$$\frac{\partial [Cl_2]}{\partial t} = d_1 \frac{\partial^2 [Cl_2]}{\partial x^2} - 0.001[Cl_2] + 0.05[Cl]^2$$
$$\frac{\partial [Cl]}{\partial t} = d_2 \frac{\partial^2 [Cl]}{\partial x^2} + 0.002[Cl_2] - 0.1[Cl]^2$$

Given the initial value at time T=0, the serial code can provide us the distribution of these two species in the future.



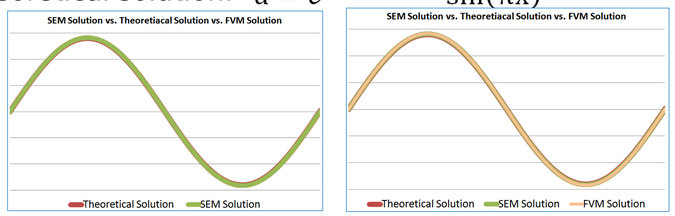
Accuracy of the Serial Code SEM Solution vs. Theoretical Solution vs. FVM Solution

To test whether the serial code (based on Spectral Element Method) can give us a basically correct result, a good way is to compare the result withthe analytical result.

Equation: $\frac{\partial u}{\partial t} = 0.1\frac{\partial^2 u}{\partial x^2} + 0.1u$

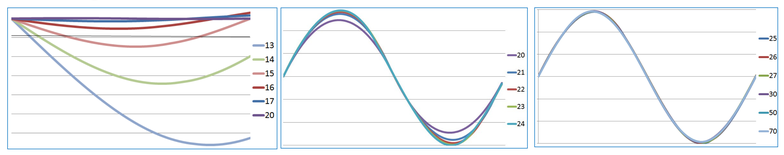
Initial condition: $u = \sin(\pi x)$ at T=0

Theoretical solution: $u = e^{0.1-0.1\pi^2 T}\sin(\pi x)$



Convergence

By varying the number of elements from 13 to 70, the convergence of the result is shown as follows.

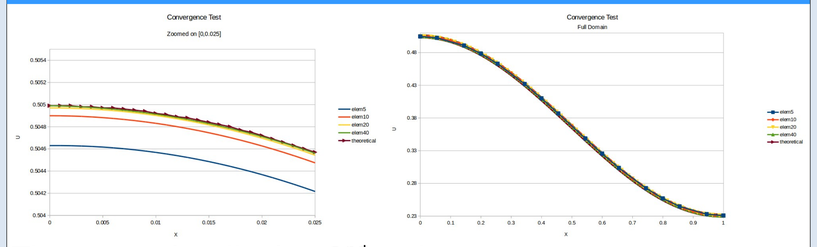


Parallel Code Overview

The parallel code is a pair of Fortran modules designed to solve a general multi-dimensional Spectral Element problem. It was tested on chemical diffusion-convection models in both 1 and 2 dimensions. Currently the code uses Forward Euler method for the time integration.

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

Parallel Code Convergence Results

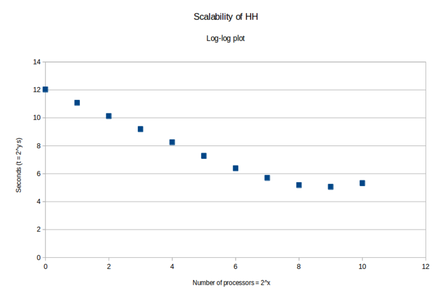


These results display 2nd-order convergence. This can be improved with higher-order interpolation and operator splitting.

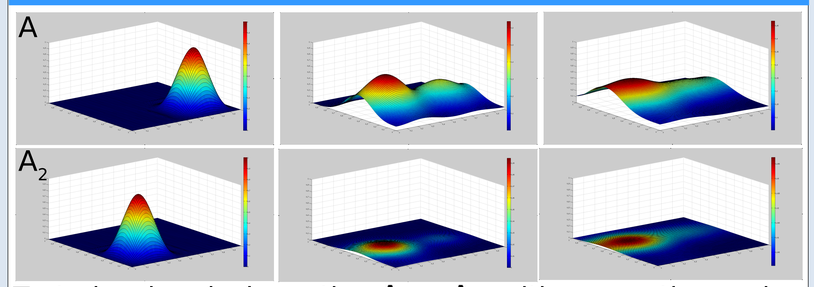
Parallel Code Scalability Results

The code proves to be highly scalable when processors < elements.

Results can be improved by paralellizing boundary calculations and adding operator splitting.



Parallel Code 2D Results



Tested a chemical reaction $A \leftrightharpoons A_2$ with convection and diffusion.