Modelling multi-dimensional chemical transport with a parallel Spectral Element Method

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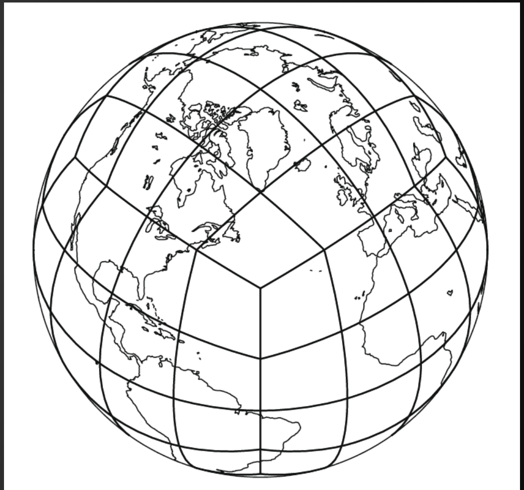
General overview

- Until relatively recently, the finite-element method (FEM) was believed to not be locally conserved
- Chemical transport models are therefore written using the finite *volume* method (FVM), which is explicitly conservative.
- CESM and the HOMME equations, however, are formulated through the FEM because of its use on unstructured grids. This is convenient when solving the equations on a globe.
- The difference in methods used creates difficulty in merging models.
- 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.
- 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.



1D continuous time-dependent case

Chemical equation: $Cl_2 \rightleftharpoons Cl + Cl$

Math Model on population of $[Cl_2]$ and $[Cl]$:

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

1D time-dependent differential equation:

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

➔ ***Goal***: Construct a serial code to solve 1D time-dependent differential equation.

➔ ***Mathematical Scheme***:

1) Galerkin Method
2) Spectral Element Method
3) Gauss-Lobatto Quadrature

$$\frac{\partial U_\alpha}{\partial t} = -[A]U_a + R_\alpha(\vec{U})$$

4) Euler Backward Method (implicit)
(t : time step size)

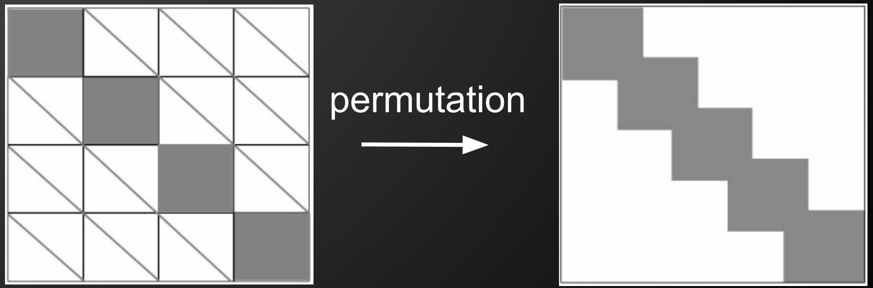
$$U_a^{(n+1)} = U_a^{(n)} - t([A]U_a^{(n+1)} + R_\alpha(\vec{U}^{(n+1)}))$$

5) Newton Method

$$F_\alpha(\vec{x}) = x_\alpha - U_\alpha + t([A]x_\alpha - R_\alpha(\vec{x})) = 0$$

$$J(\Delta\vec{x}) = -F(\vec{x}^*)$$

$$J = \frac{\partial \vec{F}}{\partial \vec{x}} = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} & \cdots & \frac{\partial F_1}{\partial x_{SPI}} \\ \frac{\partial F_2}{\partial x_1} & \frac{\partial F_2}{\partial x_2} & \cdots & \frac{\partial F_2}{\partial x_{SPI}} \\ \cdots & \cdots & \cdots & \\ \frac{\partial F_{SPI}}{\partial x_1} & \frac{\partial F_{SPI}}{\partial x_2} & \cdots & \frac{\partial F_{SPI}}{\partial x_{SPI}} \end{pmatrix}$$



code (language:c)

those can be changed:

- number of species
- diffusion coefficient
- production rate R(u)

input by user:

- *number of elements* (domain:[0,M])
- *tolerance* (for Newton Method)
- *number of time step N* (for Euler Method)
- *time T which you want to solve* (then time step size t = T/N)
- *initial value of u(x) at the nodal points*

output:

- the value of u(x) at time T

compared with FVM :

- SEM can output a smooth function, while FVM can only output a set of points.
- accuracy and running time : need to be tested.

Homer-Hesiod

A pair of Fortran modules intended for use on general SEM problems; intended to eventually model full 3D chemical transport.

CODE STRUCTURE

Data storage

- mesh
  - parameters
  - structure
  - local element matrices
- fields
  - base mesh
  - values by nodes
  - values by element
- fn_ptr
- equation
  - operators
  - splitting?
  - implicit? (θ=?)

Time integration

- Split data by element; divide elements among processors
- Integrate one time step
  - Strang splitting
  - Implicit Euler evolution; solve using Newton-Raphson methods
- Share data on element boundaries with master processor; average out disagreeing values
- Repeat process until integration is complete

Path

1. Write HESIOD, a Fortran module which stores the data types *mesh, fields, fn_ptr,* and *equation*
2. Write HOMER, a module which stores subroutines to time-integrate the problem. Only write explicit Euler method, and then test with a 1D problem with two chemicals:

$$A \rightleftharpoons B$$

$$\frac{d[A]}{dt} = D\frac{d^2[A]}{dx^2} - k_1[A] + k_2[B]$$

$$\frac{d[B]}{dt} = D\frac{d^2[B]}{dx^2} + k_1[A] - k_2[B]$$

3. Add to HOMER subroutines to perform Strang splitting. Test.
4. Add to HOMER subroutines to perform implicit Euler evolution and Newton's method, for small problems. Test.
5. Interface HOMER with Trilinos to allow for larger problems; test on more chemicals, more complex interactions, and higher dimensions.
6. Add to HESIOD more math structures to allow use of layering as seen in CESM.

References

[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.