Project Chemical Species Transport

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Chair for System Simulation

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Outline

Discretization of the concentration convection-diffusion equation

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Fundamental equation I

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \lambda \Delta c + Q(t, x, y, \vec{u}, c) \tag{1}$$

- λ diffusion coefficient
- Q source term (location, time, velocity, concentration), multi-species-systems are modeled here
- the chemical processes under consideration have no effect on the density and hence produce no buoyancy forces $\Rightarrow$ no coupling with the momentum equations
- convective transport: $\vec{u} \cdot \nabla c$
- diffusive spreading: $\lambda \Delta c$

Fundamental equation II

- time step control necessary
- for very stiff equations, implicit procedures might be necessary, we do an explicit time stepping

Boundary conditions

- Dirichlet BC when injecting concentration
- Neumann BC for impermeable walls

Discretization I

$$\left[\frac{\partial c}{\partial t}\right]_{ij}^{n+1} + \left[\frac{\partial uc}{\partial x}\right]_{ij} + \left[\frac{\partial vc}{\partial y}\right]_{ij} = \lambda \left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right]_{ij} + Q_{ij} \tag{2}$$

$$\left[\frac{\partial c}{\partial t}\right]_{ij}^{n+1} = \frac{1}{dt}\left(c_{ij}^{n+1} - c_{ij}^{n}\right) \tag{3}$$

$$\begin{aligned}\left[\frac{\partial uc}{\partial x}\right]_{ij} = \frac{1}{dx}\left(u_{ij}\frac{c_{ij}+c_{i+1,j}}{2} - u_{i-1,j}\frac{c_{i-1,j}+c_{ij}}{2}\right) + \\ \frac{\gamma}{dx}\left(|u_{ij}|\frac{c_{ij}-c_{i+1,j}}{2} - |u_{i-1,j}|\frac{c_{i-1,j}-c_{ij}}{2}\right)\end{aligned} \tag{4}$$

Discretization II

$$\left[\frac{\partial vc}{\partial y}\right]_{ij} = \frac{1}{dy}\left(v_{ij}\frac{c_{ij}+c_{i,j+1}}{2} - v_{i,j-1}\frac{c_{i,j-1}+c_{ij}}{2}\right) + \frac{\gamma}{dy}\left(|v_{ij}|\frac{c_{ij}-c_{i,j+1}}{2} - |v_{i,j-1}|\frac{c_{i,j-1}-c_{ij}}{2}\right) \tag{5}$$

$$\left[\frac{\partial^2 c}{\partial x^2}\right]_{ij} = \frac{c_{i+1,j} - 2c_{ij} + c_{i-1,j}}{(dx)^2} \tag{6}$$

$$\left[\frac{\partial^2 c}{\partial y^2}\right]_{ij} = \frac{c_{i,j+1} - 2c_{ij} + c_{i,j-1}}{(dy)^2} \tag{7}$$

- concentration c lies on the center of the staggered grid cell
- standard central differences of the Laplacian
- add timestep control

Timestep Control

$$dt < \frac{1}{2\lambda_i}\left(\frac{1}{(dx)^2} + \frac{1}{(dy)^2}\right)^{-1} \tag{8}$$

- has to be added for every new species
- depends on the diffusion constant

Implementation

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Implementation I

- array of Arrays for multiple concentrations
- array of reals for the lambdas
- the reaction term Q is also stored in Arrays
- extended parameter reader
- extended initialization

Implementation II

Main loop:

- determineNextDT: added support for the concentration convection diffusion equation
- refreshBoundaries: Dirichlet and Neumann BC according to input for every species (e.g. iterate over all Arrays)
- computeFG: no change
- composeRHS: no change
- calculateConcentrations: explicit concentration update
- updateVelocities: no change
- vtk: support for multiple concentrations

Results

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Results I

- two species come together at an obstacle and create a new one
- one species is coming from west and east
- the other from the south

Results II