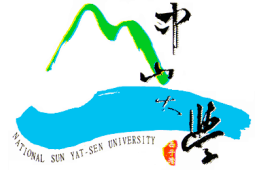




Properties of the Volume Corrected Characteristic Mixed Method

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Goal

Accurate, long-time simulation of transport processes.

Miscible, Incompressible Transport

Conservation of bulk fluid mass

$$\nabla \cdot \mathbf{u} = q$$

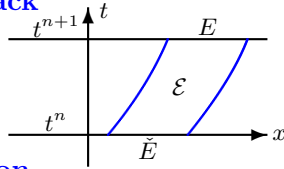
Conservation of component mass (ignore diffusion)

$$\phi c_t + \nabla \cdot (c\mathbf{u}) = q_c(c)$$

\mathbf{u} is bulk fluid velocity q are wells
 c is component concentration ϕ is porosity

Characteristic Trace-back

Fluid particles travel along **characteristics**. Particles in grid element E trace back to \tilde{E} .



Local Mass Conservation

The local mass constraint

$$\int_E \phi c^{n+1} dx = \int_{\tilde{E}} \phi c^n dx + \iint_{\mathcal{E}} q_c dx dt$$

The local volume constraint ($c = 1$ above)

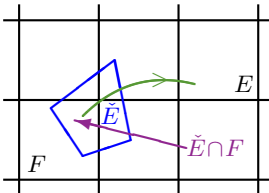
$$\int_E \phi dx = \int_{\tilde{E}} \phi dx + \iint_{\mathcal{E}} q dx dt$$

Volume Corrected Characteristics Mixed Method (VCCMM) in Algebraic Form

Pore volume in set S is $|S|_\phi$. Up to treatment of wells:

- Trace back the corners of each grid element E .
- Adjust traceback points so $|\tilde{E}|_\phi = |E|_\phi$.
- Define the **transport matrix** indexed by the grid elements as

$$\mathbf{A}_{EF} = \frac{|\tilde{E} \cap F|_\phi}{|E|_\phi}$$



- Transport c (\mathbf{b} comes from wells) by

$$\mathbf{c}_E^{n+1} = \sum \mathbf{A}_{EF} \mathbf{c}_F^n + \mathbf{b}_E$$

- (Optional) Postprocess \mathbf{c}_h^{n+1} into a local linear \tilde{c}_h^{n+1} .

Letting \mathbf{c}_h be the vector of element concentrations, this is

$$\mathbf{c}_h^{n+1} = \mathbf{A} \mathbf{c}_h^n + \mathbf{b} \quad (\text{local mass constraint})$$

Algebraic Properties

Ignoring wells:

Nonnegativity $\mathbf{A}_{EF} \geq 0$

Row sum $\sum_F \mathbf{A}_{EF} = 1$ (local volume constraint)

Weighted column sum

$$\sum_E |E|_\phi \mathbf{A}_{EF} = |F|_\phi \quad (\text{tessellation constraint})$$

Monotonicity and Maximum Principles

For two transport problems, if initially one concentration is below the other, then it stays below for all time:

$$c_{1,h}^0 \leq c_{2,h}^0 \implies c_{1,h}^n \leq c_{2,h}^n \quad \text{for all } n \geq 0.$$

There are no overshoots nor undershoots:

$$0 \leq c_h^0 \leq 1 \quad \text{for all } n \geq 0.$$

Stability

VCCMM is stable: if ξ_h^n satisfies the perturbed scheme

$$\xi_h^{n+1} = \mathbf{A} \xi_h^n + \mathbf{b} + \Delta t^n \delta^n$$

where δ^n is a perturbation, then to time T ,

$$\max_{0 \leq n \leq N} |\xi_h^n - c_h^n|_\infty \leq |\xi_h^0 - c_h^0|_\infty + T \max_{0 \leq n \leq N} |\delta^n|_\infty.$$

Convergence

The convergence rate is optimal.

With physical diffusion

$$\max_{0 \leq n \leq N} \| \tilde{c}_h^n - c^n \|_{L^2} \leq C(h^2 + \Delta t),$$

$$\max_{0 \leq n \leq N} \| c_h^n - c^n \|_{L^2} \leq C(h + \Delta t).$$

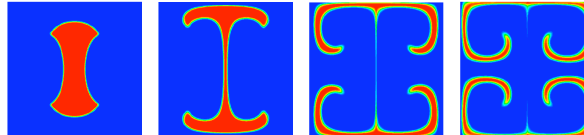
Without physical diffusion

$$\max_{0 \leq n \leq N} \| c_h^n - c^n \|_{L^1} \leq \| c_h^0 - c^0 \|_{L^1} + C \left(\frac{h}{\sqrt{\Delta t}} + h + (\Delta t)^r \right),$$

where r is the accuracy of the traceback tracing. There is no restriction on Δt , and the results improve for large Δt .

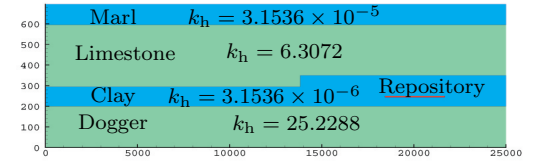
Example: Pure Curl Flow

Evolution of a tracer at steps 10, 30, 60, and 80.

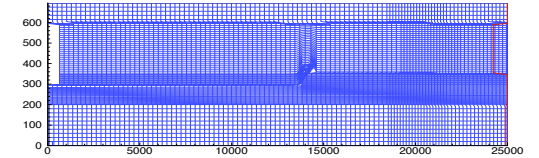


Extremely little numerical diffusion is seen!

Example: A Nuclear Waste Repository

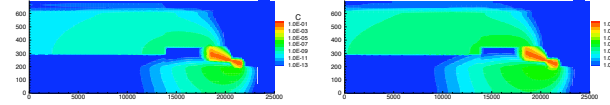


Characteristic trace-back mesh.

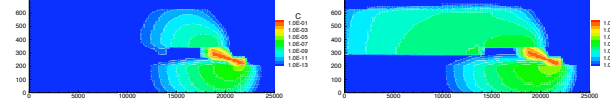


Concentration at 2.5×10^5 and 3×10^5 years.

Godunov's method



VCCMM



Computation time (sec).

| | flow | trace & adjust | transport |
|---------|------|----------------|-----------|
| Godunov | 0.05 | N/A | 66.77 |
| VCCMM | 0.05 | 2.97 | 39.77 |

Conclusions

- VCCMM is stable and accurate, even for large Δt ;
- has no overshoots nor undershoots;
- is locally conservative for component *and* bulk fluid;
- exhibits very little numerical diffusion;
- can be more efficient for long-time simulations.

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