A combined GDM–ELLAM–MMOC (GEM) scheme with local volume conservation for advection dominated PDEs

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Australian Government

Australian Research Council

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1 Introduction

- **2** Characteristic-Based Schemes for Advection-reaction PDEs
 - ELLAM
 - MMOC
 - ELLAM-MMOC
- **3** Application: The miscible flow model
- GEM scheme
- 5 Numerical tests

$$\begin{cases} \phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) &= f(c) \text{ on } Q_T := \Omega \times (0, T) \\ c(\cdot, 0) &= c_{\text{ini}} & \text{ on } \Omega \end{cases}$$

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Assumptions on the Data

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$$c_{\text{ini}} \in L^{\infty}(\Omega)$$

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- $\mathbf{u} \in L^{\infty}(0, T; L^2(\Omega)^d)$ and $\nabla \cdot \mathbf{u} \in L^{\infty}(Q_T)$
- $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial \Omega$

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- $\mathbf{u} \in L^{\infty}(0, T; L^{2}(\Omega)^{d})$ and $\nabla \cdot \mathbf{u} \in L^{\infty}(Q_{T})$
- $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial \Omega$
- $f(c) = f(c, \mathbf{x}, t) : \mathbb{R} \times Q_T \to \mathbb{R}$ is Lipschitz continuous w.r.t. its first variable and $f(0, \cdot, \cdot) \in L^{\infty}(Q_T)$.

Gradient discretisation

Gradient discretisation: $\mathcal{D} = (X_{\mathcal{D}}, \Pi_{\mathcal{D}}, \nabla_{\mathcal{D}})$ with

- $X_{\mathcal{D}}$ finite dimensional space (encodes the unknowns).
- $\Pi_{\mathcal{D}}: X_{\mathcal{D}} \to L^{\infty}(\Omega)$ (reconstructs a function).
- $\nabla_{\mathcal{D}}: X_{\mathcal{D}} \to L^{\infty}(\Omega)^d$ (reconstructs a gradient).

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Weak formulation between two time steps $t^{(n)}$ and $t^{(n+1)}$: for $\varphi \in C^{\infty}(\overline{\Omega} \times [t^{(n)}, t^{(n+1)}])$:

$$\begin{vmatrix} -\int_{t^{(n)}}^{t^{(n+1)}} \int_{\Omega} c(\phi \partial_t \varphi + \mathbf{u} \cdot \nabla \varphi) \\ + \int_{\Omega} \phi c(t^{(n+1)}) \varphi(t^{(n+1)}) - \int_{\Omega} \phi c(t^{(n)}) \varphi(t^{(n)}) \\ = \int_{t^{(n)}}^{t^{(n+1)}} \int_{\Omega} f(c, \mathbf{x}, t) d\mathbf{x} dt. \end{cases}$$

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Choice of test function: φ that satisfy $\phi \partial_t \varphi + \mathbf{u} \cdot \nabla \varphi = 0...$

Weak formulation between two time steps $t^{(n)}$ and $t^{(n+1)}$: for $\varphi \in C^{\infty}(\overline{\Omega} \times [t^{(n)}, t^{(n+1)}])$:

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Choice of test function: φ that satisfy $\phi \partial_t \varphi + \mathbf{u} \cdot \nabla \varphi = 0...$ **>** With $\frac{dF_t}{dt} = \frac{\mathbf{u}^{(n+1)}(F_t)}{\phi(F_t)}$, $F_0(\mathbf{x}) = \mathbf{x}$, we have $\varphi(\mathbf{x}, t) = \varphi(F_{t^{(n+1)}-t}(\mathbf{x}), t^{(n+1)}).$

ELLAM scheme

 \blacktriangleright Given C gradient discretisation,

Find
$$c^{(n+1)} \in X_{\mathcal{C}}$$
 such that for all $z \in X_{\mathcal{C}}$,

$$\int_{\Omega} \phi \Pi_{\mathcal{C}} c^{(n+1)} \Pi_{\mathcal{C}} z - \int_{\Omega} \phi \Pi_{\mathcal{C}} c^{(n)} v_z(t^{(n)})$$

$$= w \delta t^{(n+\frac{1}{2})} \int_{\Omega} f_n v_z(t^{(n)}) + (1-w) \delta t^{(n+\frac{1}{2})} \int_{\Omega} f_{n+1} \Pi_{\mathcal{C}} z,$$

where $w \in [0,1]$, $f_k := f(\Pi_\mathcal{C} c^{(k)},\cdot,t^{(k)})$

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where $w \in [0, 1]$, $f_k := f(\Pi_{\mathcal{C}} c^{(k)}, \cdot, t^{(k)})$ and
 $v_z : \Omega \times (t^{(n)}, t^{(n+1)}] \to \mathbb{R}$ solves
 $\phi \partial_t v_z + \mathbf{u}^{(n+1)} \cdot \nabla v_z = 0$ on $(t^{(n)}, t^{(n+1)}), \quad v_z(\cdot, t^{(n+1)}) = \Pi_{\mathcal{C}} z,$
with $\mathbf{u}^{(n+1)} \in L^2(\Omega)^d$ and $\nabla \cdot \mathbf{u}^{(n+1)} \in L^\infty(\Omega).$

ELLAM scheme - condensed

•
$$f^{(n,w)}(\mathbf{x}) := \left(wf(\mathbf{x}, t^{(n)}), (1-w)f(\mathbf{x}, t^{(n+1)}) \right)$$

• $g_F(\mathbf{x}) := \left(g(F_{\delta t^{(n+\frac{1}{2})}}(\mathbf{x})), g(\mathbf{x}) \right)$

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Find $c^{(n+1)} \in X_{\mathcal{C}}$ such that for all $z \in X_{\mathcal{C}}$,

$$\int_{\Omega} \phi \Pi_{\mathcal{C}} c^{(n+1)} \Pi_{\mathcal{C}} z - \int_{\Omega} \phi \Pi_{\mathcal{C}} c^{(n)} v_z(t^{(n)}) = \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot (\Pi_{\mathcal{C}} z)_F.$$

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Find $c^{(n+1)} \in X_{\mathcal{C}}$ such that

$$\int_{\mathcal{K}} \phi c_{\mathcal{K}}^{(n+1)} d\mathbf{x} = \int_{\Omega} \phi \sum_{M \in \mathcal{M}} c_{M}^{(n)} \mathbb{1}_{M}(\mathbf{x}) \mathbb{1}_{\mathcal{K}}(F_{\delta t^{(n+\frac{1}{2})}}(\mathbf{x})) d\mathbf{x}$$
$$+ \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot (\mathbb{1}_{\mathcal{K}})_{F} d\mathbf{x},$$

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write $\Pi_{\mathcal{C}} c^{(k)} = \sum_{K \in \mathcal{M}} c_{K}^{(k)} \mathbb{1}_{K}$
 $|K|_{\phi} c_{K}^{(n+1)} = \sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} c_{M}^{(n)}$
 $+ \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot (\mathbb{1}_{K})_{F} d\mathbf{x},$

$$egin{aligned} &\sum_{K\in\mathcal{M}}|K|_{\phi}c_{K}^{(n+1)}=\sum_{M\in\mathcal{M}}|M|_{\phi}c_{M}^{(n)}\ &+\sum_{K\in\mathcal{M}}\delta t^{(n+rac{1}{2})}\int_{\Omega}f^{(n,w)}\cdot\mathbf{e}dm{x}, \end{aligned}$$
 where $\mathbf{e}:=(1,1).$

$$\sum_{K \in \mathcal{M}} |K|_{\phi} c_{K}^{(n+1)} = \sum_{M \in \mathcal{M}} |M|_{\phi} c_{M}^{(n)}$$

 $+ \sum_{K \in \mathcal{M}} \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot \mathbf{e} d\mathbf{x},$
where $\mathbf{e} := (1, 1).$

discrete mass balance error

$$egin{aligned} & e_{ ext{mass}} := igg| \sum_{K \in \mathcal{M}} |K|_{\phi} c_K^{(n+1)} - \sum_{M \in \mathcal{M}} |M|_{\phi} c_M^{(n)} \ & - \sum_{K \in \mathcal{M}} \delta t^{(n+rac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot \mathbf{e} doldsymbol{x} igg|. \end{aligned}$$

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For each $K \in \mathcal{M}$, $|K|_{\phi}c_{K}^{(n+1)} = \sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi}c_{M}^{(n)}$ $+ \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot (\mathbb{1}_{K})_{F} d\mathbf{x}.$

Sum over $K \in \mathcal{M}$.

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 \triangleright $e_{\text{mass}} = 0.$

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ELLAM scheme (piecewise constant approximations)

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$$|\mathcal{K}|_{\phi}c_{\mathcal{K}}^{(n+1)} = \sum_{M\in\mathcal{M}} |M\cap \mathcal{F}_{-\delta t^{(n+rac{1}{2})}}(\mathcal{K})|_{\phi}c_{M}^{(n)}$$

Figure: Interpretation: Piecewise constant approximations



$$|\mathcal{K}|_{\phi}c_{\mathcal{K}}^{(n+1)} = \sum_{M\in\mathcal{M}} |M\cap \mathcal{F}_{-\delta t^{(n+rac{1}{2})}}(\mathcal{K})|_{\phi}c_{M}^{(n)}$$

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Figure: Numerical implementation: Piecewise constant approximations



Local volume conservation

$$\blacktriangleright |\widetilde{K}| \neq |F_{-\delta t^{(n+\frac{1}{2})}}(K)|$$

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Figure: Trace back regions \widetilde{K}_i (left: initial; right: illustration of possible perturbed cells after local volume adjustments).
Local volume conservation

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Figure: Trace back regions \widetilde{K}_i (left: initial; right: illustration of possible perturbed cells after local volume adjustments).

▶ Note: Dotted figures are not explicitly computed

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- iii) Obtain local volume conservation for K_1 by

$$|\widetilde{K}_1 \cap M_i| \rightsquigarrow |\widetilde{K}_1 \cap M_i| + \frac{|\mathbf{u}_{1,i}|}{\sum_{j=2}^4 |\mathbf{u}_{1,j}|} e_{K_1}.$$

- i) Measure the defect in local volume conservation $e_{\mathcal{K}_1} := |\mathcal{F}_{-\delta t^{(n+\frac{1}{2})}}(\mathcal{K}_1)| - |\widetilde{\mathcal{K}}_1|.$
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iv) Adjust volumes of cells adjacent to \widetilde{K}_1 .

•

$$|\widetilde{K}_2 \cap M_2| \rightsquigarrow |\widetilde{K}_2 \cap M_2| - \frac{|\mathbf{u}_{1,2}|}{\sum_{j=2}^4 |\mathbf{u}_{1,j}|} e_{K_1}$$

Figure: Mesh cells K

Figure: Back-tracked regions $F_{-\delta t^{(n+\frac{1}{2})}}(K)$



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MMOC



characteristics-based scheme

MMOC

characteristics-based scheme

 characteristic derivative is approximated in a different manner compared to ELLAM

► MMOC

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$$\begin{split} |\mathcal{K}|_{\phi} c_{\mathcal{K}}^{(n+1)} &= \sum_{M \in \mathcal{M}} |\mathcal{F}_{\delta t^{(n+\frac{1}{2})}}(M) \cap \mathcal{K}|_{\phi} c_{M}^{(n)} \\ &+ \delta t^{(n+\frac{1}{2})} \int_{\mathcal{K}} f^{(n,w)} \cdot \mathbf{e} d\mathbf{x} \\ &- \delta t^{(n+\frac{1}{2})} \int_{\mathcal{K}} \left[(c_{\mathcal{K}})^{(n,w)} \nabla \cdot \mathbf{u}^{(n+1)} \right] \cdot \mathbf{e} d\mathbf{x}. \end{split}$$

► MMOC

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► ELLAM

$$\begin{split} |\mathcal{K}|_{\phi} c_{\mathcal{K}}^{(n+1)} &= \sum_{M \in \mathcal{M}} |M \cap \mathcal{F}_{-\delta t^{(n+\frac{1}{2})}}(\mathcal{K})|_{\phi} c_{M}^{(n)} \\ &+ \delta t^{(n+\frac{1}{2})} \int_{\Omega} f^{(n,w)} \cdot (\mathbb{1}_{\mathcal{K}})_{\mathcal{F}} d\mathbf{x}, \end{split}$$

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$$\triangleright \delta t^{(n+\frac{1}{2})} \rightarrow 0$$

►
$$\delta t^{(n+\frac{1}{2})} \rightarrow 0$$

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$$\triangleright \delta t^{(n+\frac{1}{2})} \rightarrow 0$$

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▶ c is almost constant in the non-divergence free regions

Interpretation

$$|\mathcal{K}|_{\phi} c_{\mathcal{K}}^{(n+1)} = \sum_{M \in \mathcal{M}} |\mathcal{F}_{\delta t^{(n+rac{1}{2})}}(M) \cap \mathcal{K}|_{\phi} c_{M}^{(n)}$$

Figure: Interpretation: Piecewise constant approximations



Forward-tracked regions





Figure: Forward-tracked regions $F_{\delta t^{(n+\frac{1}{2})}}(K)$



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advection-reaction equation

$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = f(c).$$

advection-reaction equation

$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = f(c).$$

$$\triangleright c = \alpha c + (1 - \alpha)c$$

advection-reaction equation

$$\phi \frac{\partial(\alpha c)}{\partial t} + \nabla \cdot ((\alpha c)\mathbf{u}) + \phi \frac{\partial((1-\alpha)c)}{\partial t} + \nabla \cdot (((1-\alpha)c)\mathbf{u}) = \alpha f + (1-\alpha)f.$$

▶ For each cell $K \in \mathcal{M}$, take $\Pi_{\mathcal{C}} z_K = \mathbb{1}_K$.

► For each cell
$$K \in \mathcal{M}$$
, take $\prod_{\mathcal{C}} z_K = \mathbb{1}_K$.
► Write $\prod_{\mathcal{C}} c^{(k)} = \sum_{K \in \mathcal{M}} c_K^{(k)} \mathbb{1}_K$.

For each cell
$$K \in \mathcal{M}$$
, take $\prod_{\mathcal{C}ZK} = \mathbb{1}_{K}$.
Write $\prod_{\mathcal{C}C} c^{(k)} = \sum_{K \in \mathcal{M}} c_{K}^{(k)} \mathbb{1}_{K}$.
Choose α piecewise constant, 1 for ELLAM, 0 for MMOC.
 $c_{K}^{(n+1)} |K|_{\phi} - \sum_{M \in \mathcal{M}_{ELLAM}} c_{M}^{(n)} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi}$
 $- \sum_{M \in \mathcal{M}_{MMOC}} c_{M}^{(n)} |F_{\delta t^{(n+\frac{1}{2})}}(M) \cap K|_{\phi}$
 $= \delta t^{(n+\frac{1}{2})} \int_{\Omega} \alpha f^{(n,w)} \cdot (\mathbb{1}_{K})_{F}$
 $+ \delta t^{(n+\frac{1}{2})} \int_{\Omega} [(1-\alpha)f^{(n,w)} \cdot \mathbf{e}] \mathbb{1}_{K}$
 $- \delta t^{(n+\frac{1}{2})} \int_{\Omega} [(1-\alpha)\nabla \cdot \mathbf{u}^{(n+1)}(\Pi_{\mathcal{C}}c)^{(n,w)} \cdot \mathbf{e}] \mathbb{1}_{K}$

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►
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▶ $(1 - \alpha)c$ is almost constant in the non-divergence free regions

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Model for enhanced oil recovery

$$\begin{cases} \nabla \cdot \mathbf{u} = q^{+} - q^{-} := q \\ \mathbf{u} = -\frac{\mathbf{K}}{\mu(c)} \nabla p \end{cases}$$
$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{x}, \mathbf{u}) \nabla c) + q^{-}c = q^{+}$$

Unknowns

- *p*(**x**, *t*) pressure of the mixture
- $\mathbf{u}(\mathbf{x}, t)$ Darcy velocity
- c(x, t) concentration of the injected solvent

Parameters

- K(x) permeability tensor
- $\phi(\mathbf{x})$ porosity

Source Terms

- q^+ injection well
- q⁻ production well

Model for enhanced oil recovery

Diffusion Tensor

$$\mathbf{D}(\mathbf{x}, \mathbf{u}) = \phi(\mathbf{x}) \left[d_m \mathbf{I} + d_l |\mathbf{u}| \mathcal{P}(\mathbf{u}) + d_t |\mathbf{u}| \left(\mathbf{I} - \mathcal{P}(\mathbf{u}) \right) \right]$$

- *d_m* molecular diffusion coefficient
- d₁ longitudinal dispersion coefficient
- *d_t* transverse dispersion coefficient
- $\bullet \ \mathcal{P}(u)$ the projection matrix along the direction of u

Viscosity

$$\mu(c) = \mu(0) \left[(1-c) + M^{1/4} c \right]^{-4}$$

• $M = \mu(0)/\mu(1)$ - mobility ratio of the two fluids
Model for enhanced oil recovery

No-flow Boundary Conditions	
$\mathbf{u}\cdot\mathbf{n}=0,$	on $\partial\Omega imes [0, T]$
$(\mathbf{D} abla c)\cdot\mathbf{n}=0,$	on $\partial\Omega imes [0, T]$

Features

Pressure Equation

$$\begin{cases} \nabla \cdot \mathbf{u} &= q \\ \mathbf{u} &= -\frac{\mathbf{K}}{\mu(c)} \nabla p \end{cases}$$

in
$$Q_T := \Omega \times [0, T]$$
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anisotropic diffusion equation

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Concentration Equation

$$\phi rac{\partial c}{\partial t} +
abla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{x}, \mathbf{u})
abla c) + q^{-}c = q^{+}$$
 in Q_{T} .

- advection-diffusion-reaction equation
- mostly advection dominated

Introduction

- 2 Characteristic-Based Schemes for Advection-reaction PDEs
 - ELLAM
 - MMOC
 - ELLAM-MMOC
- **3** Application: The miscible flow model

GEM scheme

5 Numerical tests

 $0 = t^{(0)} < t^{(1)} < \cdots < t^{(N)} = T$ time steps.

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- (II) Reconstruction of velocity: reconstruct $\mathbf{u}^{(n+1)}$ Darcy velocity in $H_{\text{div}}(\Omega)$ from $p^{(n+1)}$.

(II) Reconstruction of $H_{\rm div}$ Darcy velocity

► $p^{(n+1)} \in X_{\mathcal{P}}$ known, find $\mathbf{u}^{(n+1)} \in H_{\text{div}}(\Omega)$ approximation of $-\frac{\kappa}{\mu(c(t^{(n)}))} \nabla p(t^{(n+1)}).$

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 - ► HMM produces fluxes at the cell faces. These fluxes can be used to re-construct u⁽ⁿ⁺¹⁾ which is RT₀ on a subdivision of each cell.

Figure: Triangulation of a cell



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- (1) Pressure equation: find approximation $p^{(n+1)}$ of p at $t^{(n+1)}$ by using $c^{(n)}$.
- (II) Reconstruction of velocity: reconstruct u⁽ⁿ⁺¹⁾ Darcy velocity in H_{div}(Ω) from p⁽ⁿ⁺¹⁾.
- (III) Concentration equation: find approximation $c^{(n+1)}$ of c at $t^{(n+1)}$ using $p^{(n+1)}$ and $\mathbf{u}^{(n+1)}$ for the characteristics (ELLAM-MMOC).





(αc): ELLAM
 ((1 - α)c): MMOC

► HMM-ELLAM: $\alpha = 1$ on Ω

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Choices for α

- ▶ HMM-ELLAM: $\alpha = 1$ on Ω
- ► HMM–MMOC: $\alpha = 0$ on Ω
- ► HMM–GEM:

$$\alpha(\mathbf{x}) = \begin{cases} 1 & \text{if } |\mathbf{x} - C_+| \ge |\mathbf{x} - C_-| \\ 0 & \text{otherwise.} \end{cases}$$

Choices for α

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Set up



Mesh Types

Figure: Cartesian Mesh

Figure: Hexahedral Mesh



Figure: Kershaw Mesh



Cartesian mesh

Figure: HMM–ELLAM



Figure: HMM–MMOC



Figure: HMM–GEM, 1 point per edge



Figure: HMM–GEM, 3 points per edge



 Table:
 Comparison between HMM–ELLAM, HMM–MMOC and HMM–GEM schemes, Cartesian mesh

	points per edge	overshoot	$e_{\rm mass}^{(N)}$	recovery
HMM-ELLAM	1	1.11%	0.19%	70.09%
HMM-ELLAM	3	0.18%	0.21%	69.76%
HMM-MMOC	1	< 0.01%	5.60%	71.97%
HMM-MMOC	3	< 0.01%	2.80%	69.94%
HMM–GEM	1	< 0.01%	2.35%	68.44%
HMM–GEM	3	< 0.01%	0.85%	69.14%

Hexahedral mesh

Figure: HMM–ELLAM



Figure: HMM–MMOC



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Figure: HMM–ELLAM (with local volume adjustment)



Figure: HMM–GEM



Table: Comparison between HMM–ELLAM, HMM–MMOC and HMM–GEM scheme, hexahedral mesh, $\Delta t = 18$ days

	points per edge	overshoot	$e_{\rm mass}$	recovery
HMM-ELLAM	$\lceil \log_2(m_{Kreg}) \rceil$	3.65%	0.62%	62.50%
(no adjustment)				
HMM-ELLAM	$2\lceil \log_2(m_{Kreg}) \rceil + 1$	4.47%	0.19%	63.41%
(adjusted)	_			
HMM–MMOC	$\lceil \log_2(m_{Kreg}) \rceil$	< 0.01%	1.82%	61.43%
HMM–GEM	$2\lceil \log_2(m_{Kreg}) \rceil + 1$	0.26%	0.70%	64.02%

Forward-tracked regions





Figure: Forward-tracked regions $F_{\delta t^{(n+\frac{1}{2})}}(K)$



Kershaw mesh

Figure: HMM–ELLAM



Figure: HMM–MMOC



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Figure: HMM–GEM



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 Table:
 Comparison between HMM–ELLAM, HMM–MMOC and HMM–GEM scheme, Kershaw mesh

	points per edge	overshoot	$e_{ m mass}$	recovery
HMM–ELLAM	$\lceil \log_2(m_{Kreg}) \rceil$	0.28%	0.38%	72.63%
HMM–MMOC	$\lceil \log_2(m_{Kreg}) \rceil$	0%	4.28%	73.21%
HMM–GEM	$\lceil \log_2(m_{Kreg}) \rceil$	0.32%	0.13%	72.36%

- ▶ Mass balance analysis for characteristics based schemes
 - ELLAM
 - MMOC
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► Gradient Discretisation Method-ELLAM-MMOC (GEM) scheme

- acceptable mass balance
- improvement on HMM-ELLAM

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Conclusion

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Thank you.