ADJOINT METHODS ARE PARTICLE METHODS: IMPLICATIONS FOR EULERIAN-LAGRANGIAN MODELING OF MULTIPHASE MULTICOMPONENT TRANSPORT

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- Eulerian-Lagrangian methods (ELM) for linear convection-diffusion
- Adjoint ELM formulation (ELLAM)
- Scalar nonlinear hyperbolic adjoint (dual) formulation
- Primal: wave; **dual: particle**
- Illustrative examples
- Numerical results
- Extension to multiphase multicomponent (compositional) flow

SCALAR DUAL FORMULATION

Scalar nonlinear hyperbolic equation (assume $\vec{V}$ known)

$$\mathcal{A}u \equiv \frac{\partial}{\partial t}(g(u)) + \nabla \cdot \left(\vec{V} f(u)\right) = 0, \qquad \vec{x} \in \Omega, \quad t \in J = [t^0, t^1]$$

Weak form: $\langle \mathcal{A}u, w \rangle = 0$ for test function $w(\vec{x}, t)$, thus

$$\begin{aligned} &\int_\Omega (g(u)w)^1 d\vec{x} + \int_{t^0}^{t^1} \int_{\partial\Omega} \vec{V} \cdot \vec{n}\, f(u)\, w\, ds\, dt \\ &= \int_\Omega (g(u)w)^0 d\vec{x} + \int_{t^0}^{t^1} \int_\Omega (g(u)w_t + \vec{V} f(u) \cdot \nabla w)\, d\vec{x}\, dt. \end{aligned}$$

The test function asks of primal functions like u questions such as: How much mass is in a given subdomain? Thus it is really a linear *functional* belonging to the *dual space*. The formal *adjoint* of $\mathcal{A}$ is the operator

$$\mathcal{A}_u^* w \equiv g(u) w_t + \vec{V} f(u) \cdot \nabla w$$

If test function(al) w satisfies $\mathcal{A}_u^* w = 0$, then the primal unknown $u(\vec{x}, t)$ is the solution of the weak form:

$$\int_\Omega (g(u)w)^1 d\vec{x} + \int_{t^0}^{t^1} \int_{\partial\Omega} \vec{V} \cdot \vec{n}\, f(u)\, w\, ds\, dt = \int_\Omega (g(u)w)^0 d\vec{x}$$

t^0 mass on RHS advects to t^1 mass on LHS.

The test function(al) satisfies the *(linear) adjoint equation*

$$w_t + \left(\vec{V}(\vec{x}, t) \frac{f(u)}{g(u)}\right) \cdot \nabla w = 0$$

(*particle velocity* $\vec{v}(\vec{x}, t, u) = \vec{V} f/g$ in parentheses)

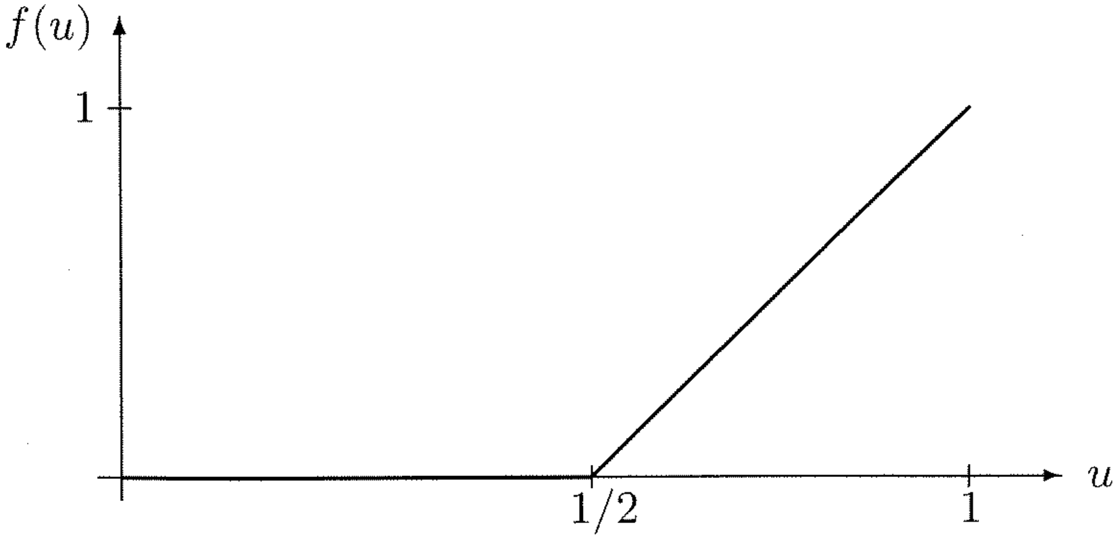
WHY A PARTICLE VELOCITY APPEARS

Test function(al) $w(\vec{x}, t)$: suppose that at ending time t^1, $w^1(\vec{x}, t) = w(\vec{x}, t^1)$ is the indicator function of (evaluates the mass in) a subdomain Ω^1. Since t^0 mass on RHS of weak form advects to t^1 mass on LHS, w^0 at t^0 is the indicator function of the subdomain Ω^0 that advected mass to Ω^1.

Shrink Ω^1 to a point $\vec{x}^1$; then Ω^0 shrinks to the point $\vec{x}^0$ that advects mass to $\vec{x}^1$. Physically, this moves at the particle velocity.

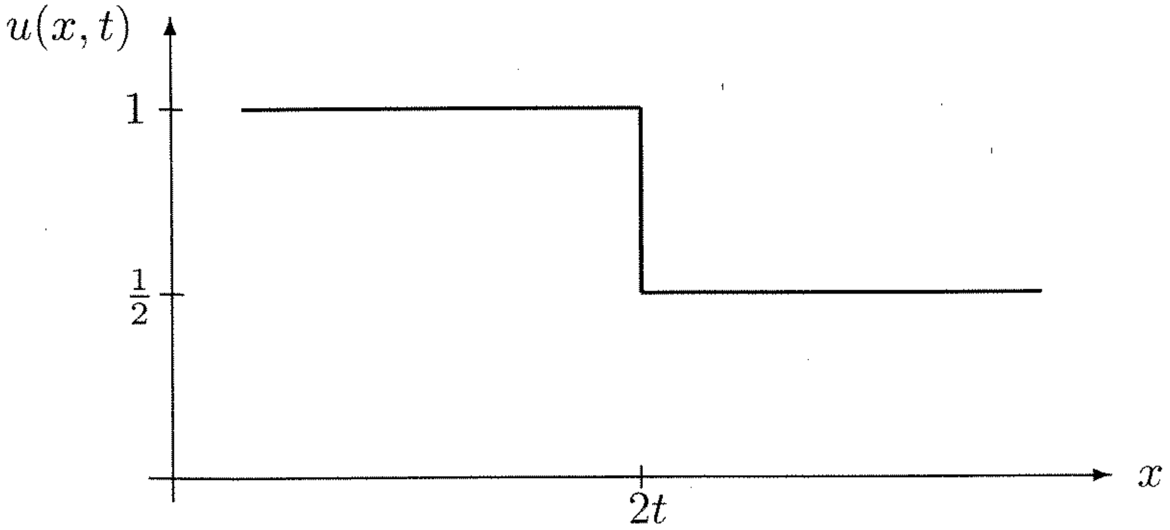
Remark: Since the adjoint equation is linear with respect to the test function(al), its classical (generalized) solution exists — no crossing of characteristics, no formation of shocks. This matches the physical interpretation of particle propagation — trailing particles do not overtake leading ones, particles do not disappear (e.g., into a shock).

Remark: The dual space is the natural framework for a particle equation that propagates sets to sets (masses to masses) and always makes physical sense. Adjoint methods (e.g., ELLAM) operate in this framework. Primal methods (e.g., MMOC, well-known hyperbolic schemes) do not — they see wave velocities (at which solution values propagate) instead of particle velocities.

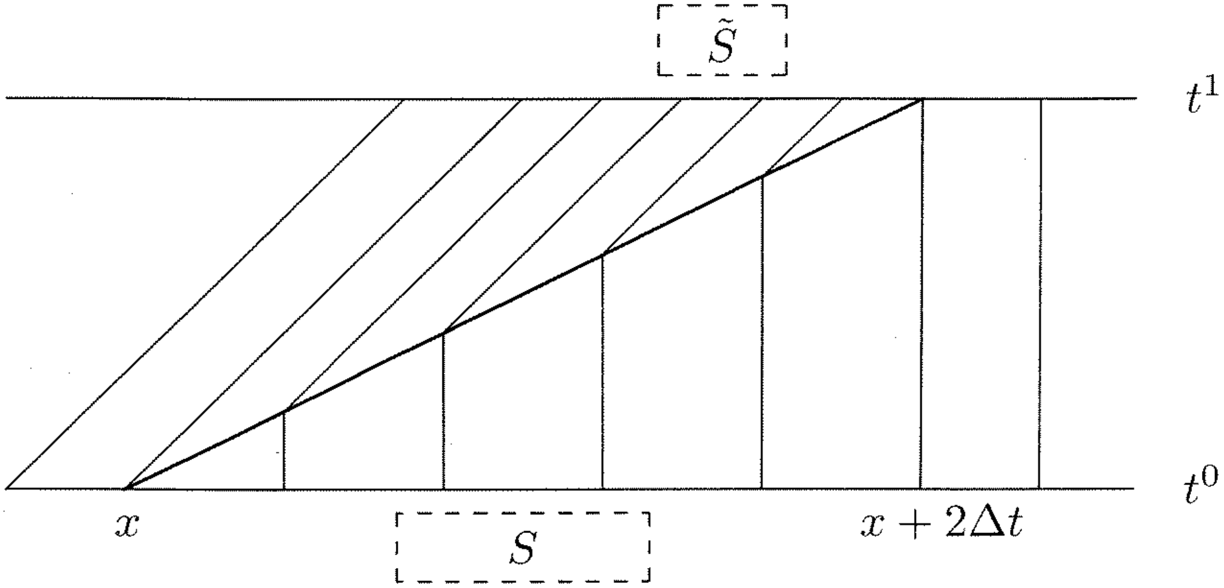


Simple S-shaped flux-function:

$$f(u) = \begin{cases} 0, & 0 \le u \le 1/2, \\ 2u - 1, & 1/2 \le u \le 1, \end{cases}$$



Initial condition for the S-shaped flux.

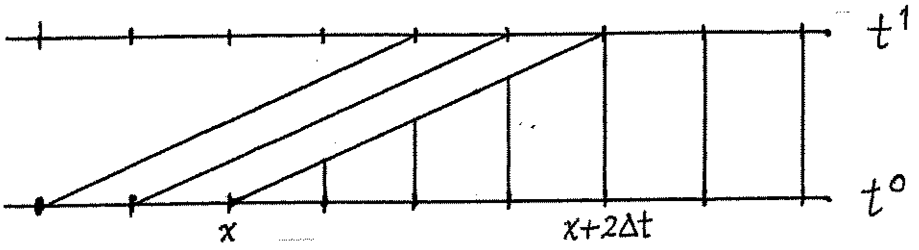


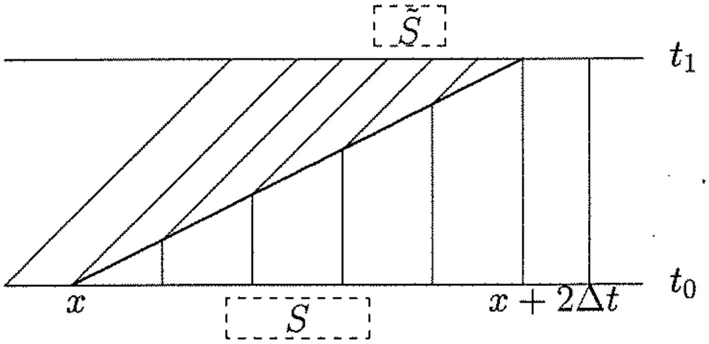
Adjoint characteristics of the S-shaped flux.

NONLINEAR FLUX, SHOCKS, SYSTEMS

Primal direct equation	**Dual adjoint equation**
Solution u: element of primal space	Test fct w: linear fnal in dual space e.g., evaluate mass in a subdomain
$Au \equiv u_t + (f(u))_x = 0$	$A_u^* w \equiv u w_t + f(u) w_x = 0$
Weak form $\langle Au, w\rangle \equiv \int_t \int_x Au\, w = 0$	$\langle Au, w\rangle = \int_t \int_x A_u^* w +$ boundary terms
Wave velocity $c = f'(u)$ propagates solution values	Particle velocity $v = f(u)/u$ propagates mass
Shocks (waves break)	No shocks (particles don't disappear)
Nonlinear	Linear
Wave methods (Riemann, etc.)	Mass-carrying particle methods

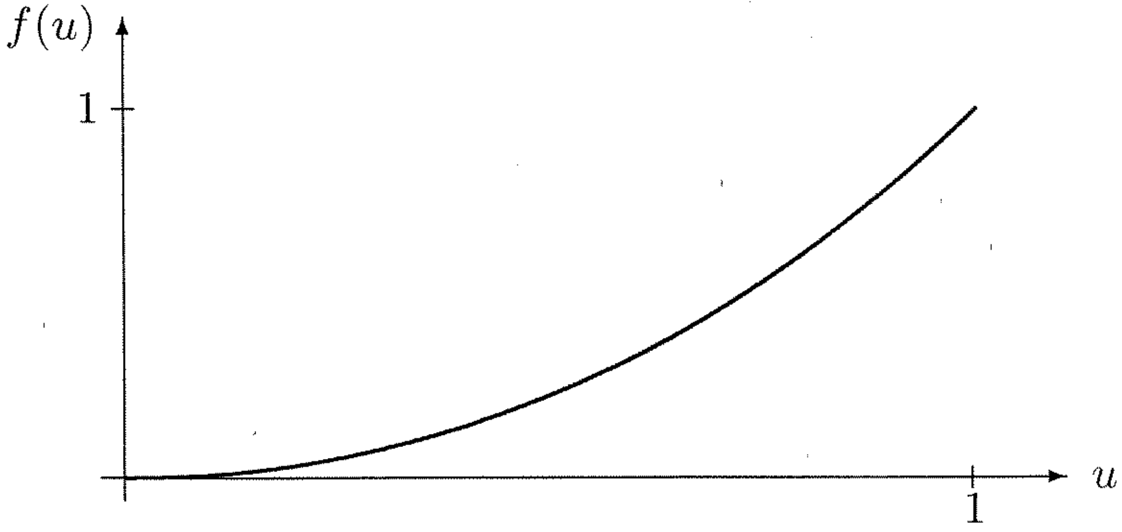
w sat. adjoint eq. $\Rightarrow$ u sat. $\int_x u(t_1) w(t_1) = \int_x u(t_0) w(t_0)$ (advection)





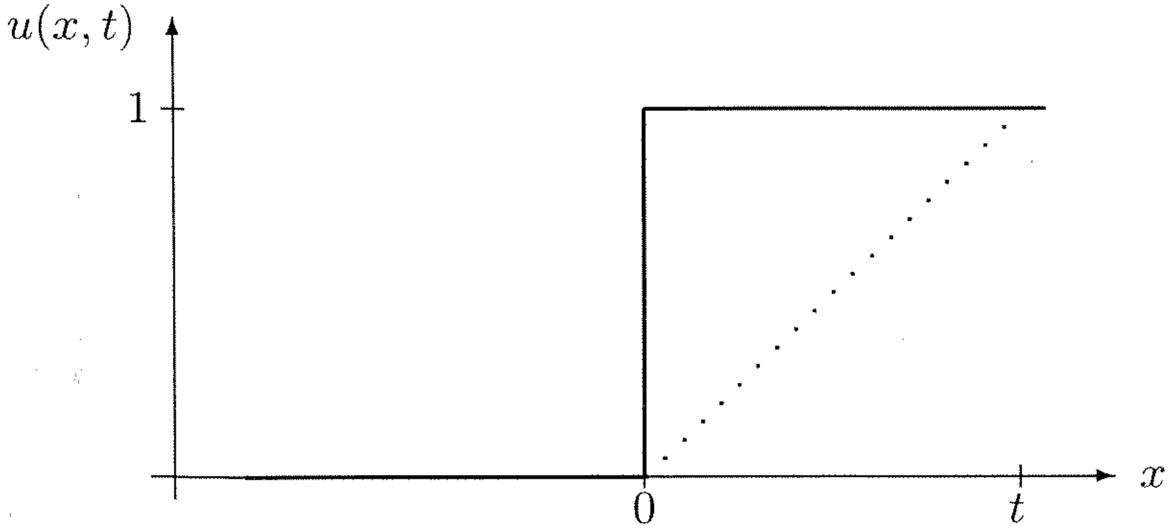
Multiphase multicomponent flow: system of nonlinear PDEs

- Mass particles move in phases
- Test functions w_α, one for each phase
- Conservation eq. for each component, summed over its phases

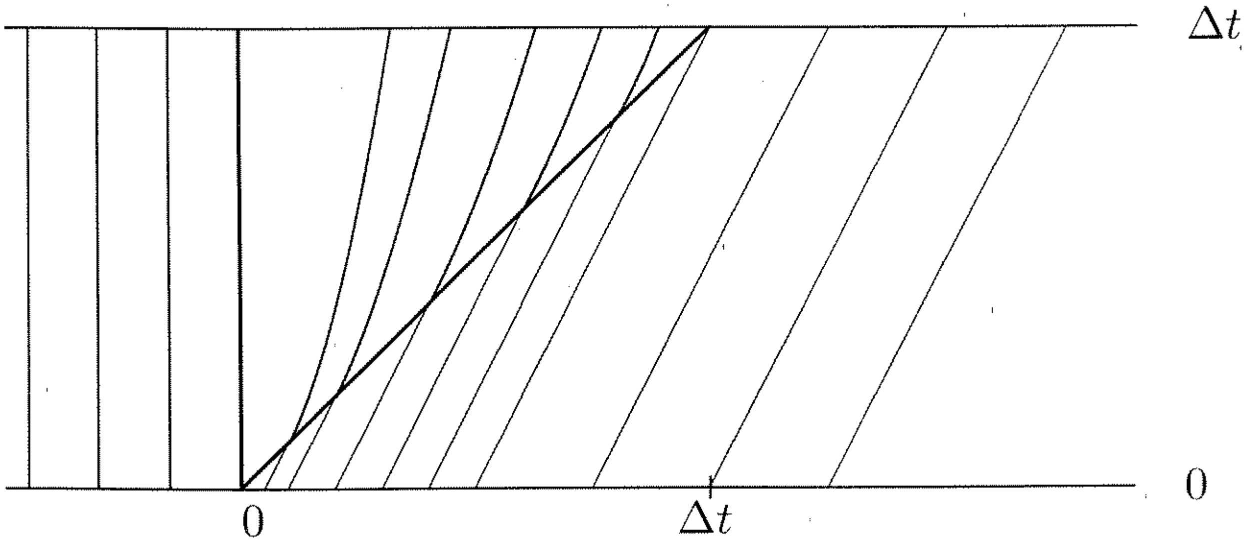


The Burgers flux function:

$$f(u) = \frac{u^2}{2}.$$



Rarefaction wave. Solid is the initial condition, dotted is the analytical solution at time t.



Adjoint characteristics of the S-shaped flux. In the rarefaction region they are parabolas

$$x(t) = C\sqrt{t},$$

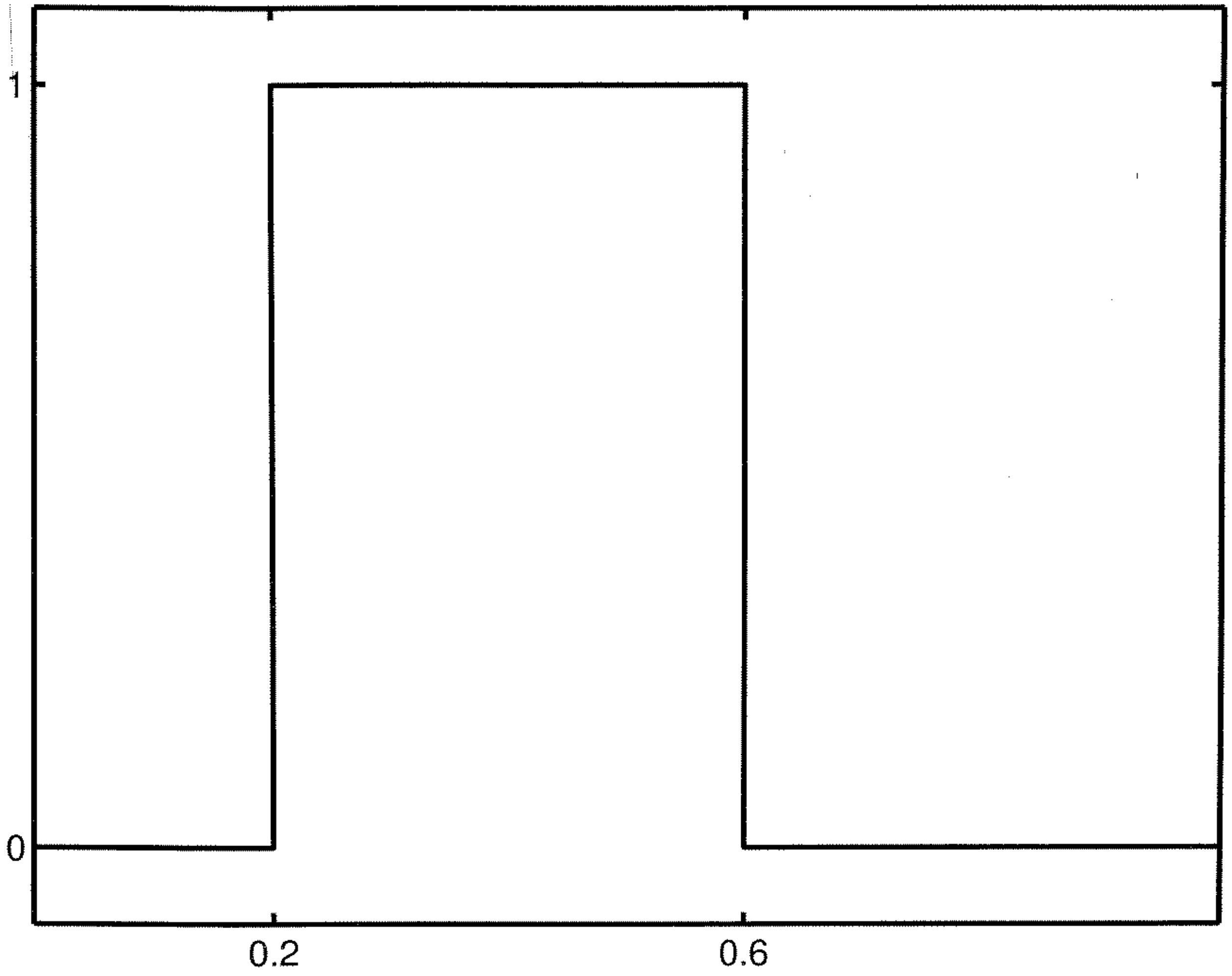
where C is the initial particle position.

General parameters:

$$\begin{aligned} \Omega &= [0,1], \\ \Delta x &= \frac{1}{100}, \end{aligned}$$

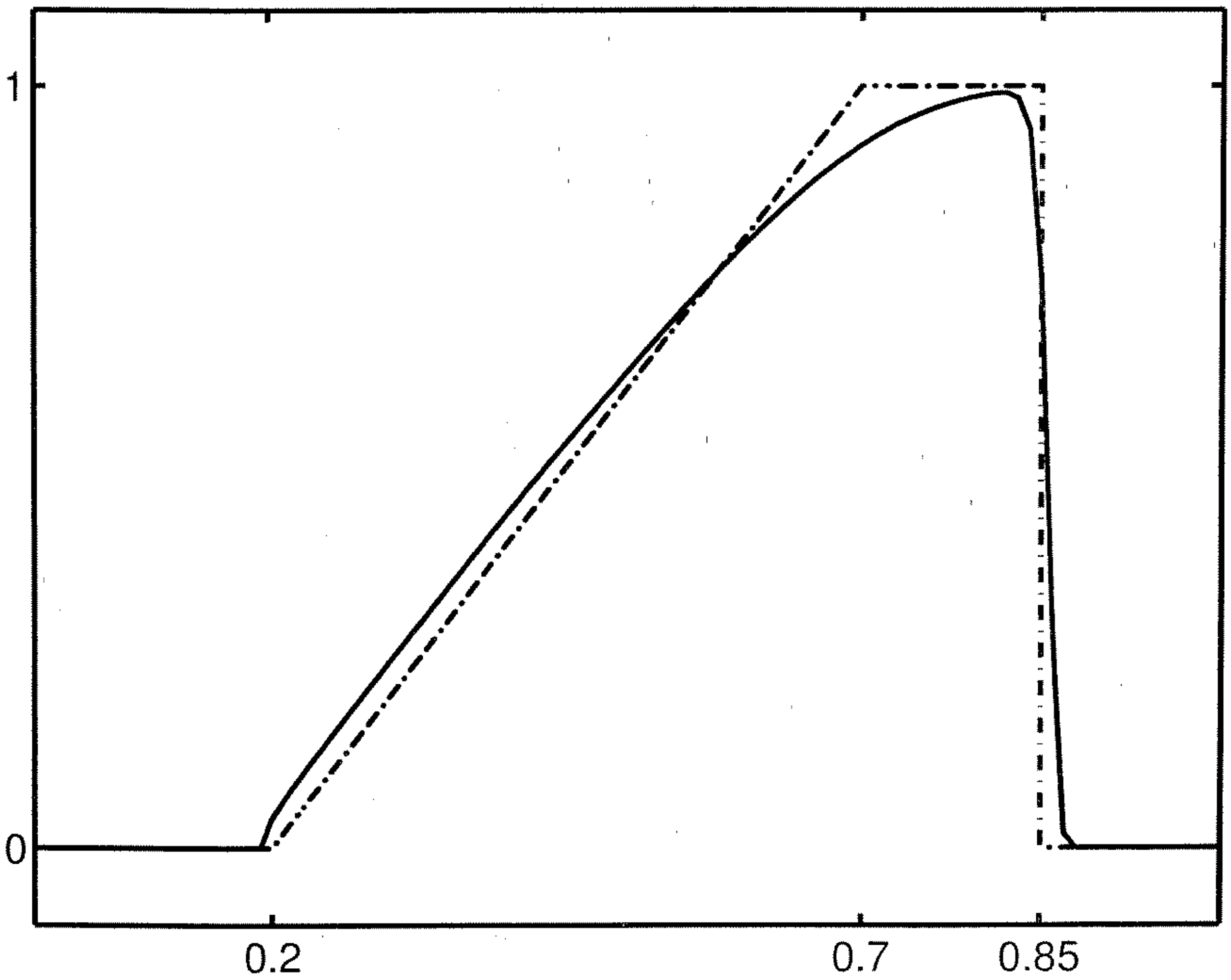
and the timestep is

$$\Delta t = \begin{cases} \frac{\Delta x}{10}, & \text{(upwinding)}, \\ 5\Delta x, & \text{(ELLAM)}. \end{cases}$$

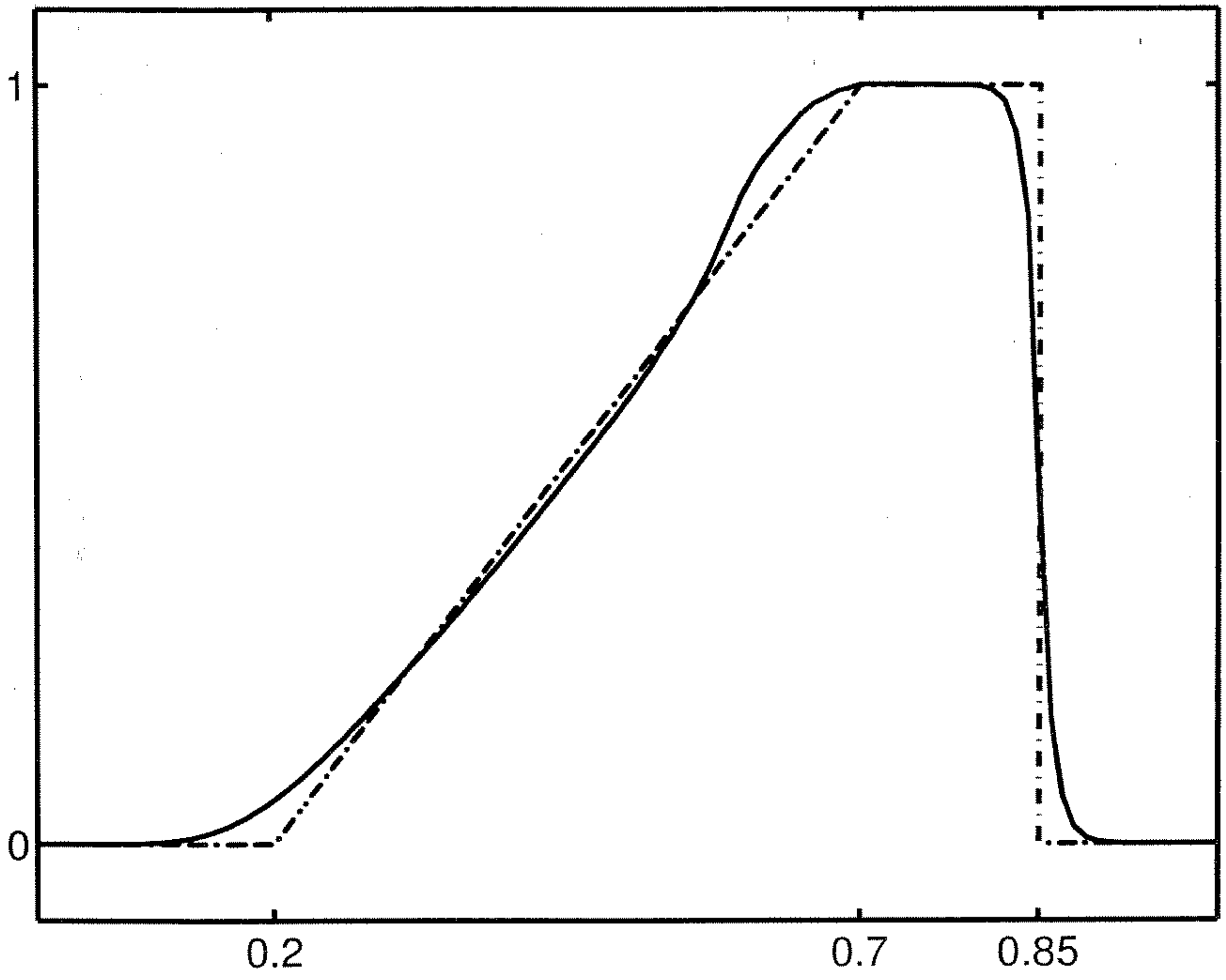


Burgers equation with periodic boundary conditions:

$$u_t + \left(\frac{u^2}{2}\right)_x = 0.$$



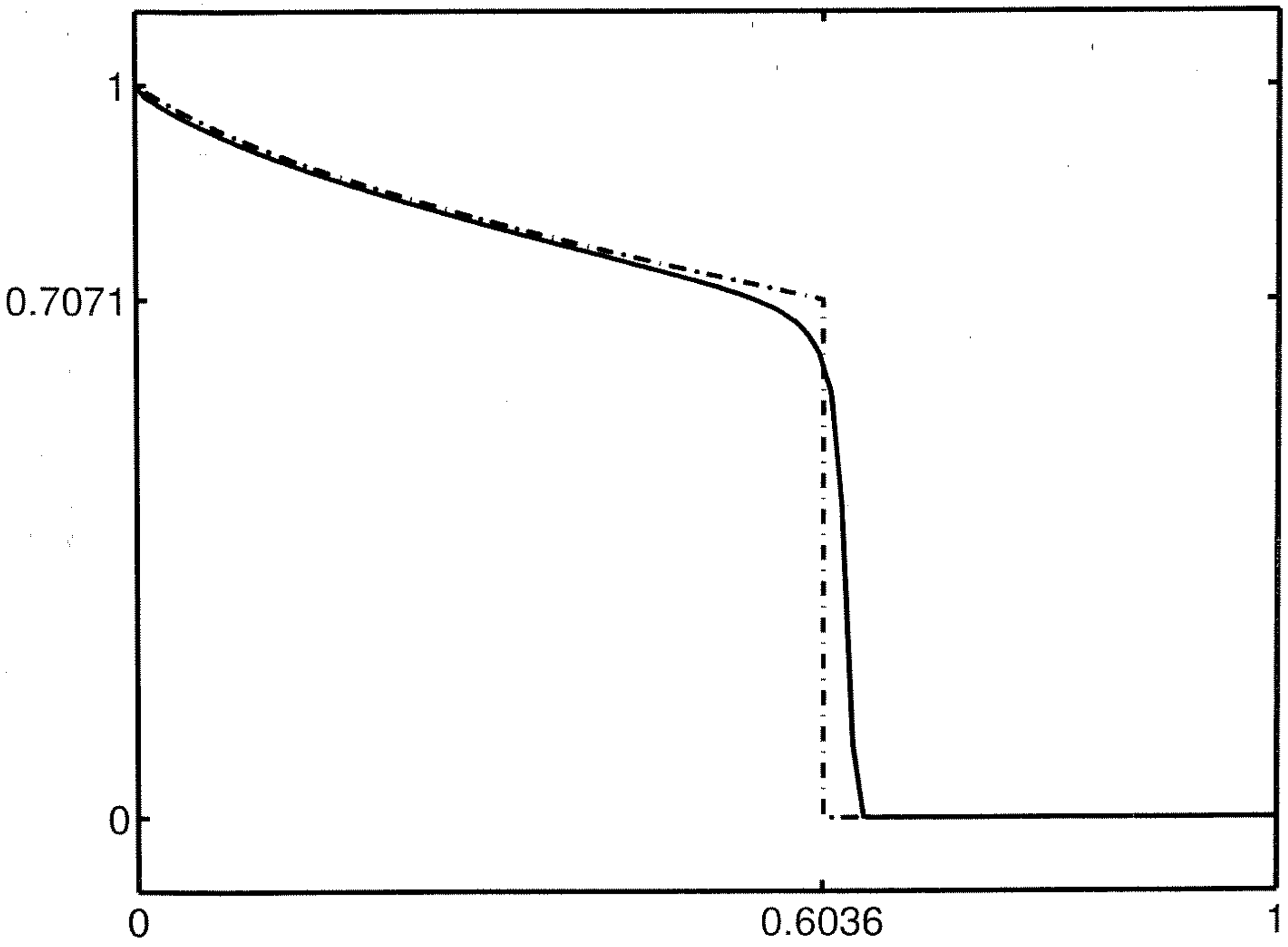
Solution of the Burgers equation with a simple upwinding scheme. The dashed line is the analytical solution and the solid line is the computed, both displayed at $t = 1/2$.



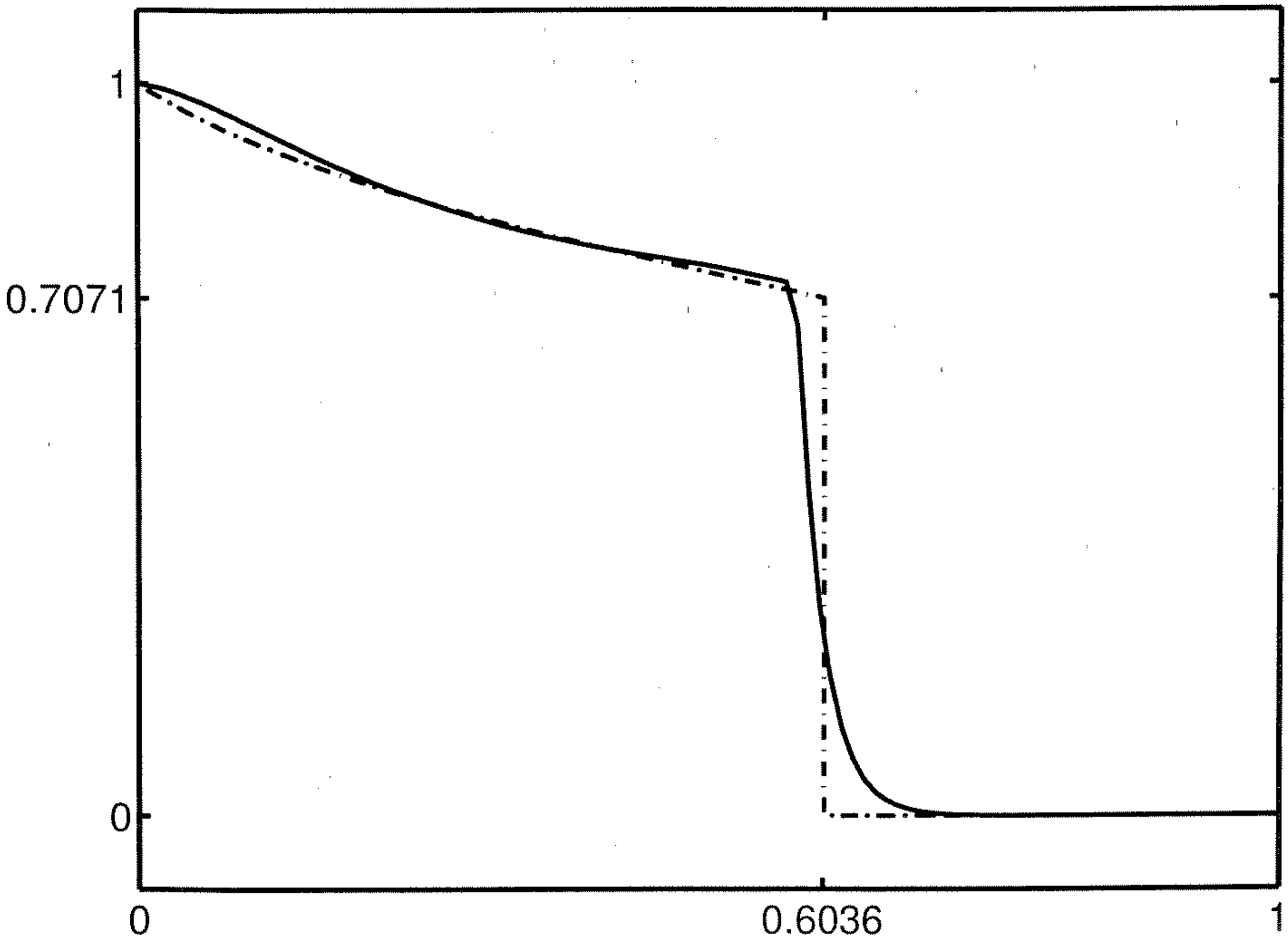
ELLAM solution with a frontal Riemann solver. Artificial diffusion of $2 \cdot 10^{-2}$ added.

The Buckley-Leverett equation

$$\begin{aligned} u_t + \left(\frac{u^2}{u^2+(1-u)^2}\right)_x &= 0, \\ u(0,t) &= 1, \\ u(x,0) &= 0, \quad x \in (0,1], \\ f(u(1,t)) \cdot n &= 0, \quad t \geq 0. \end{aligned}$$



Solution of Buckley-Leverett with an upwinding scheme, shown at $t = 1/2$.



Non-linear ELLAM solver for the Buckley-Leverett problem with diffusion of 10^{-2}.

The 2D rotational Buckley-Leverett equation

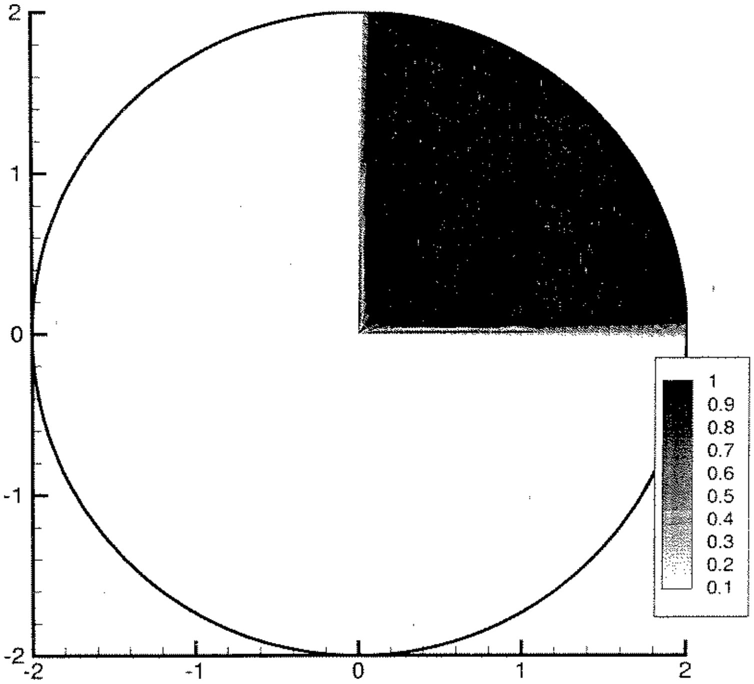
$$u_t + \nabla \cdot \left(\vec{V} \frac{u^2}{u^2 + (1-u)^2} \right) = 0,$$

where

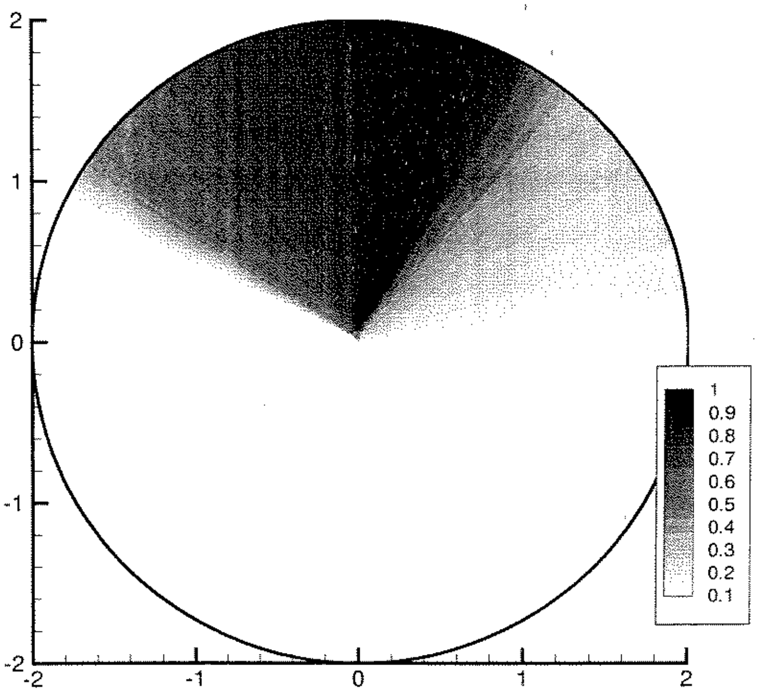
$$\vec{V}\left(\vec{x}\right) = 2\pi\left[y, -x\right],$$

and the domain is $\Omega = \{r, \theta \mid r < 2\}$ with

$$u(r,\theta) = \begin{cases} 1, & \theta \in (0, \pi/2) \\ 0, & \theta \in [\pi/2, 2\pi]. \end{cases}$$



Initial state of the rotational 2D Buckley-Leverett problem.



Solution of the rotational 2D Buckley-Leverett problem with a streamline, non-linear ELLAM, shown at $t = 1$. The motion is clockwise. 30 streamlines were used.

CONCEPTS OF PARTICLE-BASED E.L.M.

- Phase Darcy velocities v_α available from pressure (flow) equation (e.g., IMPES pressure equation, or a total-velocity / fractional-flow formulation)
- In the advection algorithm only: Each phase modeled as a separate overlapping continuum (as in the dual-porosity conceptual model)
- Each continuum has a single-phase flow with ϕs = (phase volume)/(bulk volume) playing the role of porosity
- In each continuum, advect as in forward-tracking single-phase ELLAM (e.g., Wang, Liang, Ewing, Lyons, & Qin, *Comp. Geosci.,* 2002), i.e., compute right-hand-side contributions to destination cells
- Track with phase interstitial velocity $v_\alpha/\phi s_\alpha$
- Iterative loop with pressure eq., this advection algorithm, flash (mass transfer), other processes … *precise form of decoupling ??* Issues should be similar to existing upstream finite-difference codes
- If just one iteration, advected masses summed over phases may not add up to pore volume at given pressure (non-accumulating volume error as in formulation of Watts *et al.*)

MULTIPHASE MULTICOMPONENT FLOW

Assume phase Darcy velocities $\vec{V}_\alpha$ available from flow solver (previous time step or iteration)

Conservation of mass equation for component i:

$$\Big(\sum_\alpha \phi S_\alpha \rho_\alpha c_{i\alpha}\Big)_t + \nabla \cdot \Big(\sum_\alpha \rho_\alpha \vec{V}_\alpha c_{i\alpha}\Big) = R_i, \qquad i = 1, \ldots, n_i,$$

where $\alpha = 1, \ldots, n_\alpha$.

Weak form: Space-time test function $w_\alpha(\vec{x}, t)$ for each phase. Decompose component i conservation equation into n_α sub-equations. Weak form *for component i in phase α* is

$$\begin{aligned} &\int_\Omega (\phi S_\alpha \rho_\alpha c_{i\alpha} w_\alpha)^{n+1} + \int_{t^n}^{t^{n+1}} \int_{\partial\Omega} \rho_\alpha \vec{V}_\alpha \cdot \vec{n} c_{i\alpha} w_\alpha \\ &= \int_{t^n}^{t^{n+1}} \int_{\partial\Omega} R_{i\alpha} w_\alpha + \int_\Omega (\phi S_\alpha \rho_\alpha c_{i\alpha} w_\alpha)^n \end{aligned}$$

subject to the adjoint particle-velocity equation

$$\phi S_\alpha (w_\alpha)_t + \vec{V}_\alpha \cdot \nabla w_\alpha = 0, \qquad \alpha = 1, \ldots, n_\alpha.$$

Reduction from $n_i n_\alpha$ equations to n_i equations in terms of global concentrations c_i or global mole numbers comes from phase equilibria. Advection is done (explicitly, via Lagrangian tracking) for each component in each phase as above. Assuming that phase equilibria can be defined in terms of global concentrations, re-sum the above weak form over the phases after the advection step.

Remark: $\vec{v}_\alpha = \vec{V}_\alpha / \phi S_\alpha$ is the particle velocity (of all components) in phase α.

Remark: This reduces to familiar special cases under simplifying assumptions; e.g., two-component incompressible oil-water with no mass transfer, single-phase multicomponent.

Remark: In $\vec{V}_\alpha$, could encounter discontinuities or rapid changes that propagate at wave speed (not particle speed). In a realistic problem, these are not likely to be as severe as those in the 1D examples.

CONCLUSIONS

- Nonlinear transport equations can be more computationally tractable in an adjoint framework
- Adjoint equations track particles; primal equations track waves
- Adjoint equations are linear, with a nonlinear primal-solution dependence in their coefficients
- The well-known hyperbolic complexities can affect the coefficients, but are not directly seen in the adjoint test function(al)
- The extension of Eulerian-Lagrangian methods to multiphase multicomponent systems in an adjoint framework is *conceptually* straightforward, due to the physical particle interpretation
- The most severe practical drawbacks may appear in idealized 1D examples, which are currently performing reasonably well