AN ALE METHOD INCORPORATING MONITOR FUNCTIONS

Mike Baines

University of Reading, UK

Ken Blake
Matthew Hubbard
Ben Wells

SUMMARY

The Geometric Conservation Law has a differential form in terms of a Jacobian which can be used as a monitor.

Generates an ALE velocity when a pseudo-vorticity is prescribed.

Illustrated on a Nonlinear Diffusion Equation.

Remarks on choice of Monitor.

OUTLINE

ALE viewpoint, Geometric Conservation Laws

Monitor Functions, Vorticity, ALE Velocity, Normalization

Discretizations, FV, FE

Scalar PDEs, Nonlinear Diffusion

Effect of Monitors, 1-D examples

Conclusions

FLUID DYNAMICS

Lagrangian Mass Conservation:

$$\int_{\Omega(\mathbf{v})} \rho(\mathbf{x}(t), t) d\mathbf{x}$$

is constant in time, where ρ is the density, $\Omega(\mathbf{v})$ moves with the velocity field $\mathbf{v}$.

Mass Conservation Equations

$$\frac{d}{dt} \int_{\Omega(\mathbf{v})} \rho(\mathbf{x}(t), t) d\mathbf{x} = 0 \quad \text{(Lagrange)}$$

$$\frac{d}{dt} \int_{\Omega_0} \rho(\mathbf{x}, t) d\mathbf{x}_0 = - \oint_{\partial\Omega} \rho \mathbf{v} . d\mathbf{S} \quad \text{(Euler)}$$

where Ω_0 is fixed.

ALE FORM

If $\Omega(\dot{\mathbf{x}})$ is a test volume moving with velocity $\dot{\mathbf{x}}$ the ALE Mass Conservation Equation is

$$\frac{d}{dt}\int_{\Omega(\dot{\mathbf{x}})}\rho d\mathbf{x} = -\oint_{\partial\Omega(\dot{\mathbf{x}})}\rho(\mathbf{v}-\dot{\mathbf{x}}).d\mathbf{S}$$

$$= -\int_{\Omega(\dot{\mathbf{x}})}\nabla\cdot\left(\rho(\mathbf{v}-\dot{\mathbf{x}})\right)d\mathbf{x}$$

using the divergence theorem.

- $\dot{\mathbf{x}}=\mathbf{0}$ corresponds to Eulerian mass conservation

- $\dot{\mathbf{x}}=\mathbf{v}$ corresponds to Lagrangian mass conservation

GENERAL CONSERVATION LAWS

In general, for conserved variables $\vec{w}$ with a flux function $\vec{\mathbf{F}}(\vec{w})$, the ALE equation is

$$\frac{d}{dt}\int_{\Omega(\dot{\mathrm{x}})} \vec{w} d\mathbf{x} = -\oint_{\partial\Omega(\dot{\mathrm{x}})} \left(\vec{\mathbf{F}}(\vec{w}) - \vec{w}\dot{\mathbf{x}}\right) \cdot d\mathbf{S}$$

$$= -\int_{\Omega(\dot{\mathrm{x}})} \nabla \cdot \left(\vec{\mathbf{F}}(\vec{w}) - \vec{w}\dot{\mathbf{x}}\right) d\mathbf{x}$$

using the divergence theorem.

$\dot{\mathbf{x}}$ is the ALE velocity.

THE GEOMETRIC CONSERVATION LAW

(Thomas and Lombard)

For constant $\vec{w}$ the ALE equation reduces to

$$\frac{d}{dt}\int_{\Omega(\dot{\mathbf{x}})} d\mathbf{x} = \int_{\Omega(\dot{\mathbf{x}})} \nabla \cdot \dot{\mathbf{x}} d\mathbf{x}$$

or in flux form

$$\frac{d}{dt}\int_{\Omega(\dot{\mathbf{x}})} d\mathbf{x} = \oint_{\partial\Omega(\dot{\mathbf{x}})} \dot{\mathbf{x}} \cdot d\mathbf{S}$$

which is the Geometric Conservation Law (GCL) (spatial distortions should not affect a constant state).

A compatibility condition.

A DIFFERENTIAL FORM OF THE GCL

Transforming to a fixed frame by the mapping $(\mathbf{x}, t) \to (\xi, \tau)$ with $t = \tau$ and Jacobian $\mathcal{J}$, the GCL leads to the pointwise Eulerian form

$$\frac{\partial \mathcal{J}^{-1}}{\partial \tau} + \nabla \cdot \left(\mathcal{J}^{-1} \dot{\mathbf{x}} \right) = 0$$

where $\mathcal{J} = |\partial \mathbf{x} / \partial \xi|$ and $\dot{\mathbf{x}} = \partial \mathbf{x} / \partial \tau$

It follows that the integral over $\Omega(\dot{\mathbf{x}})$

$$\int_{\Omega(\dot{\mathbf{x}})} \mathcal{J}^{-1} d\mathbf{x}$$

is conserved in time under the velocity $\dot{\mathbf{x}}$.

This form of the GCL shows the connection between the Jacobian $\mathcal{J}$ and the ALE velocity $\dot{\mathbf{x}}$.

A RELATED FORM OF GCL

In an Eulerian frame

$$\int_{\Omega_0} d\xi = \text{fixed area}$$

constant in time. Transforming to a frame moving with velocity $\dot{\mathbf{x}}$ by the mapping $(\xi, \tau) \rightarrow (\mathbf{x}, t)$ with $\tau = t$, it follows that the integral

$$\int_{\Omega(\dot{\mathbf{x}})} J d\mathbf{x}$$

is constant in time, where $\dot{\mathbf{x}} = \partial \mathbf{x} / \partial t$ and the Jacobian $J = |\partial \mathbf{x}_0 / \partial \mathbf{x}|$.

This is another form of GCL connecting the Jacobian J and $\dot{\mathbf{x}}$.

MONITOR FUNCTIONS (Cao,Huang)

We shall use J as a monitor function to generate the ALE velocity $\dot{\mathbf{x}}$.

Let J be a monitor function $\mathcal{M}(\vec{w})$ satisfying the monitor equation

$$\int_{\Omega(\dot{\mathrm{x}})} \mathcal{M}(\vec{w})d\mathbf{x} = \text{constant in time} \qquad (1)$$

$\mathcal{M}$ can be thought of as the density of a pseudo fluid moving with pseudo velocity $\dot{\mathbf{x}}$.

THE VELOCITY OF THE PSEUDO FLUID

Differentiating (1) wrt t we have

$$\int_{\Omega(\dot{\mathrm{x}})} \nabla \cdot (\mathcal{M}\dot{\mathbf{x}})\, d\mathbf{x} = -\int_{\Omega(\dot{\mathrm{x}})} \frac{\partial \mathcal{M}}{\partial t} d\mathbf{x}$$

or in differential form

$$\nabla \cdot (\mathcal{M}\dot{\mathbf{x}}) = -\frac{\partial \mathcal{M}}{\partial t} \qquad (2)$$

(equations for the ALE velocity $\dot{\mathbf{x}}$).

The right hand sides are driven by the pointwise form of the conservation law giving

$$\frac{\partial \mathcal{M}}{\partial t} = \frac{\partial \mathcal{M}}{\partial \vec{w}}\frac{\partial \vec{w}}{\partial t} = -\frac{\partial \mathcal{M}}{\partial \vec{w}} \nabla \cdot \vec{\mathbf{F}}(\vec{w})$$

THE ALE VELOCITY POTENTIAL (1)

The ALE velocity $\dot{\mathbf{x}}$ is not uniquely determined by (2) but the addition of a curl condition and a consistent boundary condition is sufficient.

So prescribe the vorticity $curl\dot{\mathbf{x}} = curl\mathbf{u}$ and pose a suitable condition at the boundary.

We may then write

$$\dot{\mathbf{x}} - \mathbf{u} = \nabla\boldsymbol{\Psi} \tag{3}$$

where Ψ is the ALE velocity potential. Either Ψ or $\frac{\partial\Psi}{\partial n}$ is to be prescribed at the boundary.

THE ALE VELOCITY POTENTIAL (2)

We then have the following elliptic problem for the ALE velocity potential Ψ:

$$\left.\begin{array}{ll} \nabla \cdot (\mathcal{M}\nabla\Psi) = -\frac{\partial \mathcal{M}}{\partial t} - \nabla \cdot (\mathcal{M}\mathbf{u}) & \text{in } \Omega \\ \Psi \text{ or } \frac{\partial \Psi}{\partial n} \text{ given} & \text{on } \partial\Omega \end{array}\right\} \tag{4}$$

Having found Ψ, the ALE velocity $\dot{\mathbf{x}}$ can be obtained from (3) and used in the ALE equation.

The character of the ALE velocity $\dot{\mathbf{x}}$ is controlled by the monitor function $\mathcal{M}$ and the prescribed vorticity $curl \mathbf{u}$.

EXAMPLES OF MONITORS

(with conserved quantities)

- $\mathcal{M} = \text{const}, \quad \nabla \cdot \dot{\mathbf{x}} = 0$ (volume)
- $\mathcal{M} = \rho, \quad \nabla \cdot (\rho \dot{\mathbf{x}}) = \frac{\partial \rho}{\partial t}$ (mass)
- $\mathcal{M} = \nabla \cdot \mathbf{Q}$ (flux of $\mathbf{Q}$)
- $\mathcal{M} =$error density (error)

VORTICITY can be taken for example to be a convenient fraction of the fluid vorticity.

SPACE DISCRETIZATION

Let Ω be partitioned into elements $\Omega_i(\dot{\mathbf{x}})$ and let the monitor equation (1) on element $\Omega_i(\dot{\mathbf{x}})$ be written

$$\int_{\Omega_i(\dot{\mathbf{x}})} \mathcal{M}(\vec{w})d\mathbf{x} = f_i\Theta \tag{5}$$

where Θ is a fixed quantity and f_i are fixed fractions such that

$$\Theta = \int_{\Omega(\dot{\mathbf{x}})} \mathcal{M}(\vec{w})d\mathbf{x}, \qquad \sum_i f_i = 1$$

(similar to 1-D equidistribution)

FINITE VOLUME DISCRETIZATION

In integral form the ALE velocity potential equation from (4) becomes $\forall i$

$$\int_{\Omega_i(\dot{\mathbf{x}})} \nabla \cdot (\mathcal{M} \nabla \Psi)\, d\mathbf{x} =$$

$$\int_{\Omega_i(\dot{\mathbf{x}})} \nabla \cdot (\mathcal{M} \mathbf{u})\, d\mathbf{x} - \int_{\Omega_i(\dot{\mathbf{x}})} \frac{\partial \mathcal{M}}{\partial t} d\mathbf{x} \qquad (6)$$

We solve for Ψ from (6), obtain $\dot{\mathbf{x}}$ from (3) and use it in the ALE equation.

NORMALIZATION (1)

If constancy in time of the monitor integral (5) is inconsistent with the problem at hand we can choose J to be the *normalized* monitor function

$$\overline{\mathcal{M}}(\vec{w}) = \frac{\mathcal{M}(\vec{w})}{\Theta(t)}$$

where $\Theta(t)$ is the global unknown

$$\Theta(t) = \int_{\Omega(\dot{\mathrm{x}})} \mathcal{M}(\vec{w}) d\mathbf{x}$$

This monitor automatically satisfies

$$\int_{\Omega(\dot{\mathrm{x}})} \overline{\mathcal{M}}(\vec{w}) d\mathbf{x} = \frac{1}{\Theta(t)} \int_{\Omega(\dot{\mathrm{x}})} \mathcal{M}(\vec{w}) d\mathbf{x} = 1 \tag{7}$$

constant in time.

In order to determine $\Theta(t)$ an additional global property of the problem is required.

FINITE ELEMENT DISCRETIZATION (1)

Define a distributed monitor equation

$$\int_{\Omega_i(\dot{\mathrm{x}})} \mathcal{M}(\vec{w}) \phi_{ik} d\mathbf{x} = f_{ik}\Theta \qquad (8)$$

$ik = 1, 2, 3$, where the $\phi_{ik}(\mathbf{x})$'s are a partition of the unit function.

Again Θ and f_{ik} are constants such that

$$\Theta = \int_{\Omega(\dot{\mathrm{x}})} \mathcal{M}(\vec{w}) d\mathbf{x}, \qquad \sum_i \sum_{ik} f_{ik} = 1$$

FINITE ELEMENT DISCRETIZATION (2)

Differentiating (8) wrt t gives

$$\int_{\Omega_i(\dot{\mathbf{x}})} \nabla \cdot (\phi_{ik}\mathcal{M}\dot{\mathbf{x}})\, d\mathbf{x} + \int_{\Omega_i(\dot{\mathbf{x}})} \mathcal{M}\frac{\partial \phi_{ik}}{\partial t} d\mathbf{x}$$

$$= - \int_{\Omega_i(\dot{\mathbf{x}})} \phi_{ik}\frac{\partial \mathcal{M}}{\partial t} d\mathbf{x}$$

For Lagrangian basis functions ϕ_{ik},

$$\frac{\partial \phi_{ik}}{\partial t} = \sum_l \left(\nabla_{\mathbf{x}_l}\phi_l\right) \cdot \dot{\mathbf{x}}_{ik}$$

$$= - \sum_l \phi_l \left(\nabla_{\mathbf{x}}\phi_{ik}\right) \cdot \dot{\mathbf{x}}_l = -\nabla\phi_{ik} \cdot \dot{\mathbf{x}}$$

which leads to the ALE velocity equation

$$\int_{\Omega_i(\dot{\mathbf{x}})} \phi_{ik}\nabla \cdot (\mathcal{M}\dot{\mathbf{x}})\, d\mathbf{x} = - \int_{\Omega_i(\dot{\mathbf{x}})} \phi_{ik}\frac{\partial \mathcal{M}}{\partial t} d\mathbf{x} \tag{9}$$

FINITE ELEMENT DISCRETIZATION (3)

To ensure a unique $\dot{\mathbf{x}}$ at each node we assemble the contributions from a patch Π_i of elements surrounding node i to obtain

$$\int_{\Pi_i(\dot{\mathbf{x}})} \phi_i \nabla \cdot (\mathcal{M}\dot{\mathbf{x}})\, d\mathbf{x} = -\int_{\Pi_i(\dot{\mathbf{x}})} \phi_i \frac{\partial \mathcal{M}}{\partial t} d\mathbf{x}$$

where ϕ_i is now a standard FE basis function.

This gives the velocity potential equation

$$\int_{\Pi_i(\dot{\mathbf{x}})} \phi_i \nabla \cdot (\mathcal{M}\nabla\Psi)\, d\mathbf{x}$$

$$= -\int_{\Pi_i(\dot{\mathbf{x}})} \phi_i \nabla \cdot (\mathcal{M}\mathbf{u})\, d\mathbf{x} - \int_{\Pi_i(\dot{\mathbf{x}})} \phi_i \frac{\partial \mathcal{M}}{\partial t} d\mathbf{x} \tag{10}$$

ALGORITHM

- Solve (6) or (10) for Ψ
- Evaluate $\dot{\mathbf{x}}$ from (4)
- Use in the ALE Conservation Laws

SCALAR PDEs

Consider the scalar PDE

$$\frac{\partial u}{\partial t} = \mathcal{N}(u)$$

where $\mathcal{N}$ is a nonlinear operator.

In scalar PDEs the final step in the algorithm can be modified to

- Integrate $\dot{\mathbf{x}}$ in time to obtain $\mathbf{x}(t)$
- Reconstruct u from the monitor equation (5)

i.e there is no need to solve the differential equation for u after the ALE velocity has been found.

EXAMPLE:

A NONLINEAR DIFFUSION EQUATION

Consider the Nonlinear Diffusion Equation

$$\frac{\partial T}{\partial t} = \nabla \cdot (T^4 \nabla T)$$

for temperature T with boundary condition

$$T = 0 \text{ at } \mathbf{x} = \mathbf{X}(t) \quad \text{(a moving boundary).}$$

This equation has self-similar solutions which can be used to test the numerical method.

A SELF-SIMILAR SOLUTION

For the 2-D radial problem

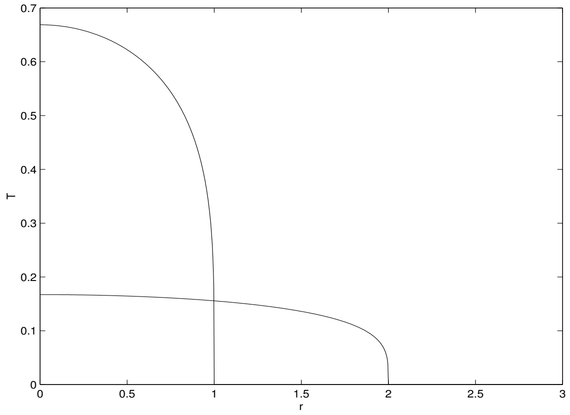
$$u(r,t) = \begin{cases} \left\{\frac{r(t)}{r_0}\right\}^2 \left[1 - \left\{\frac{r}{r(t)}\right\}^2\right]^{1/m} & |r| \leq r(t) \\ 0 & |r| > r(t) \end{cases}$$

where

$$r(t) = r_0 \, (t/t_0)^{1/(2+2m)}$$

is the position of the moving front and

$$r_0^2 = \frac{Q}{\pi}\left(1 + \frac{1}{m}\right) \qquad t_0 = \frac{r_0^2 m}{4(m+1)}$$



Evolution of the 2-D Radially Symmetric Self-Similar Solution.

SCALE INVARIANCE

Physically based PDEs have invariance properties which can be used to inform the choice of monitor functions. Since it is readily shown that the total "mass" (heat)

$$\int_{\Omega} T dx = \Theta$$

is constant in time we can use the monitor function $\mathcal{M} = T$, giving the monitor equation

$$\int_{\Omega_i(x)} T dx = f_i \Theta \text{ (constant in time)}$$

VELOCITY POTENTIAL EQUATIONS

Taking the vorticity to be zero so that $\dot{\mathrm{x}} = \nabla\Psi$, we solve

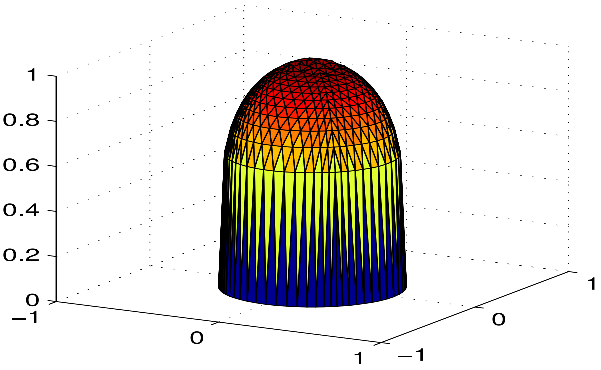
$$\int_{\Omega_i(\dot{\mathrm{x}})} \nabla \cdot (T\nabla\Psi)\, d\mathrm{x} = -\int_{\Omega_i(\dot{\mathrm{x}})} \frac{\partial T}{\partial t} d\mathrm{x}$$

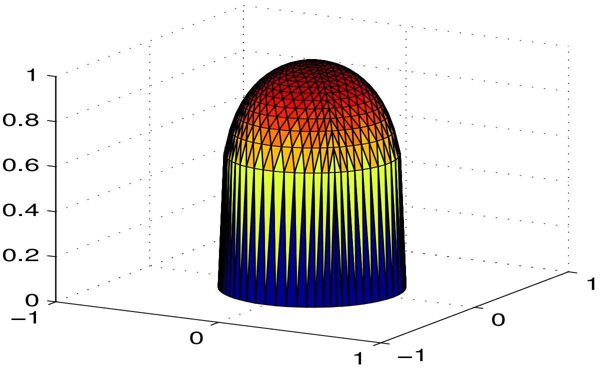
in the finite volume case and

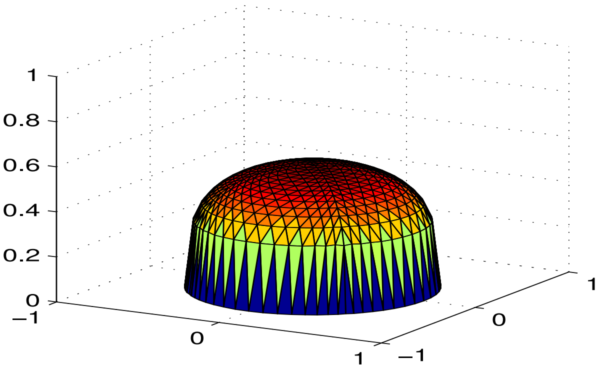
$$\int_{\Pi_i(\dot{\mathrm{x}})} \phi_i \nabla \cdot (T\nabla\Psi)\, d\mathrm{x} = -\int_{\Pi_i(\dot{\mathrm{x}})} \phi_i \frac{\partial T}{\partial t} d\mathrm{x}$$

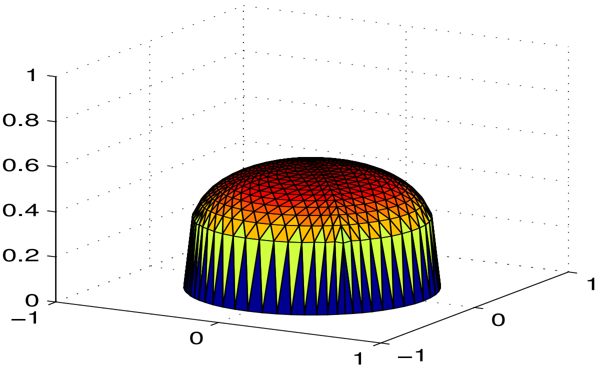
in the finite element case.

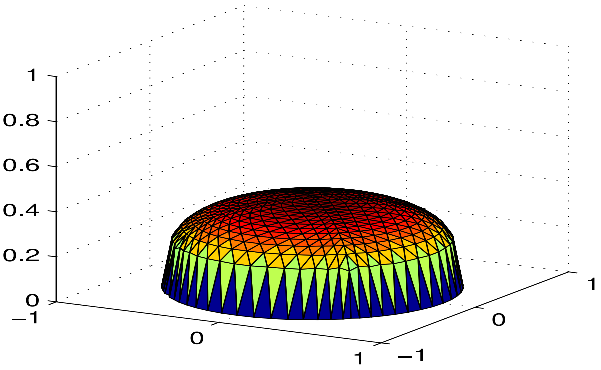
The PDE is used in calculating the right hand sides and we take $\Psi = 0$ at the boundary.

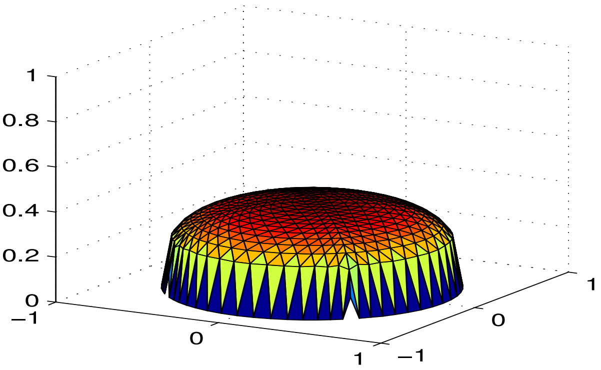

m=4: t=0.05 (t0=0.05) –– approximate


m=4: t=0.05 (t0=0.05) –– exact


m=4: t=1.0 (t0=0.05) –– approximate


m=4: t=1.0 (t0=0.05) –– exact


m=4: t=5.0 (t0=0.05) –– approximate


m=4: t=5.0 (t0=0.05) –– exact

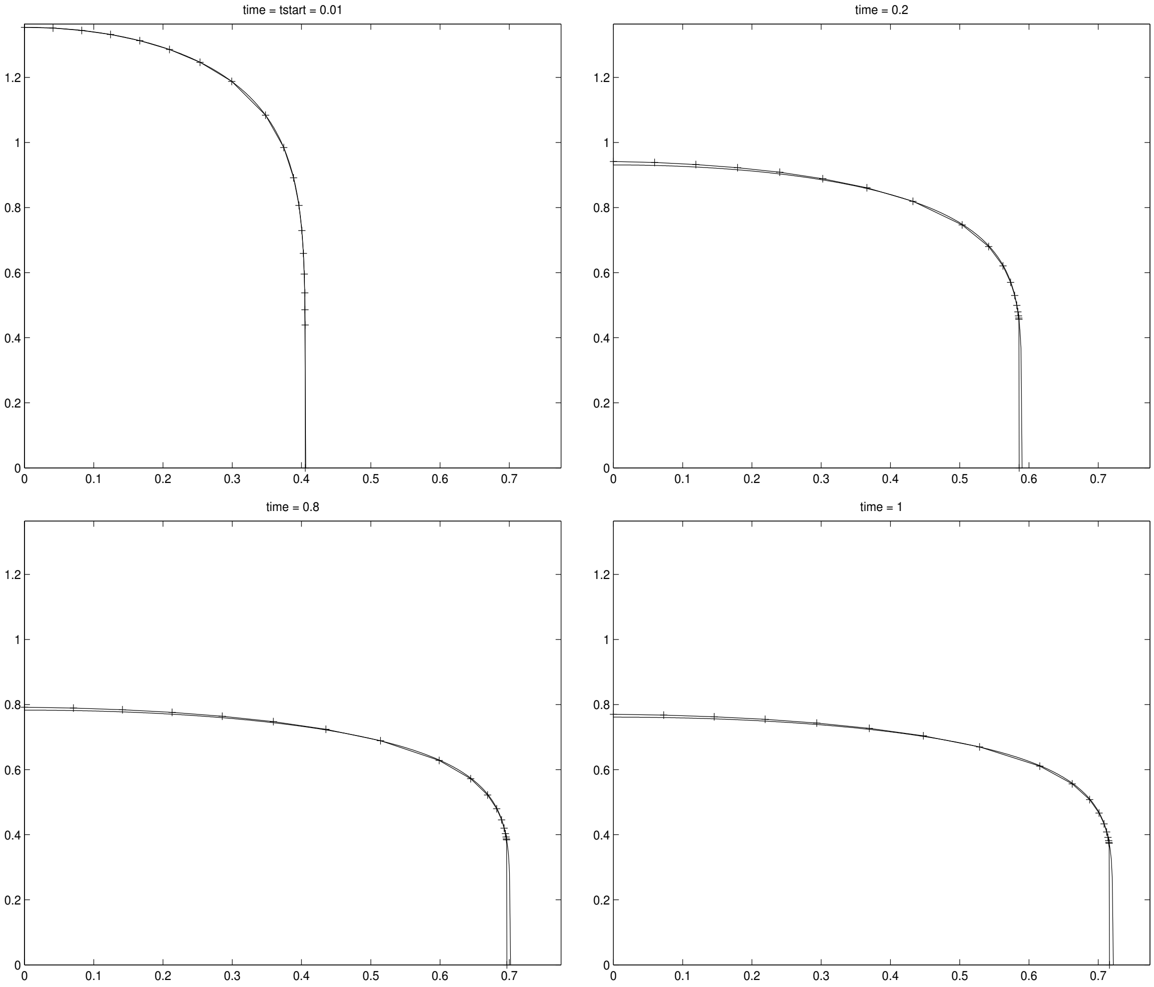
MESH REFINEMENT AT THE FRONT

It is clear that the monitor $M = T$ is poor at resolving the solution near the steep front. We study this in 1-D.

There are two ways forward:

- Refine the mesh near the front
- Change the monitor

The former can be achieved by redistributing the total heat amongst the cells by modifying the f_i values. This may be done by successively subdividing the cell next to the boundary until a tolerance is reached.


time = tstart = 0.01

time = 0.2

time = 0.8

time = 1

Approximate and reference solutions using mesh refinement in the rightmost cell.

AN ALTERNATIVE MONITOR

A possible monitor in 1-D is the gradient monitor $\mathcal{M} = T_x$ (assuming a monotonic solution).

This monitor is not consistent with global heat conservation and is therefore normalized via

$$\overline{\mathcal{M}} = \frac{T_x}{\Theta(t)}$$

where

$$\Theta(t) = \int_{x_0}^{x_N} T_x dx = T_N - T_0$$

MONITOR EQUATION

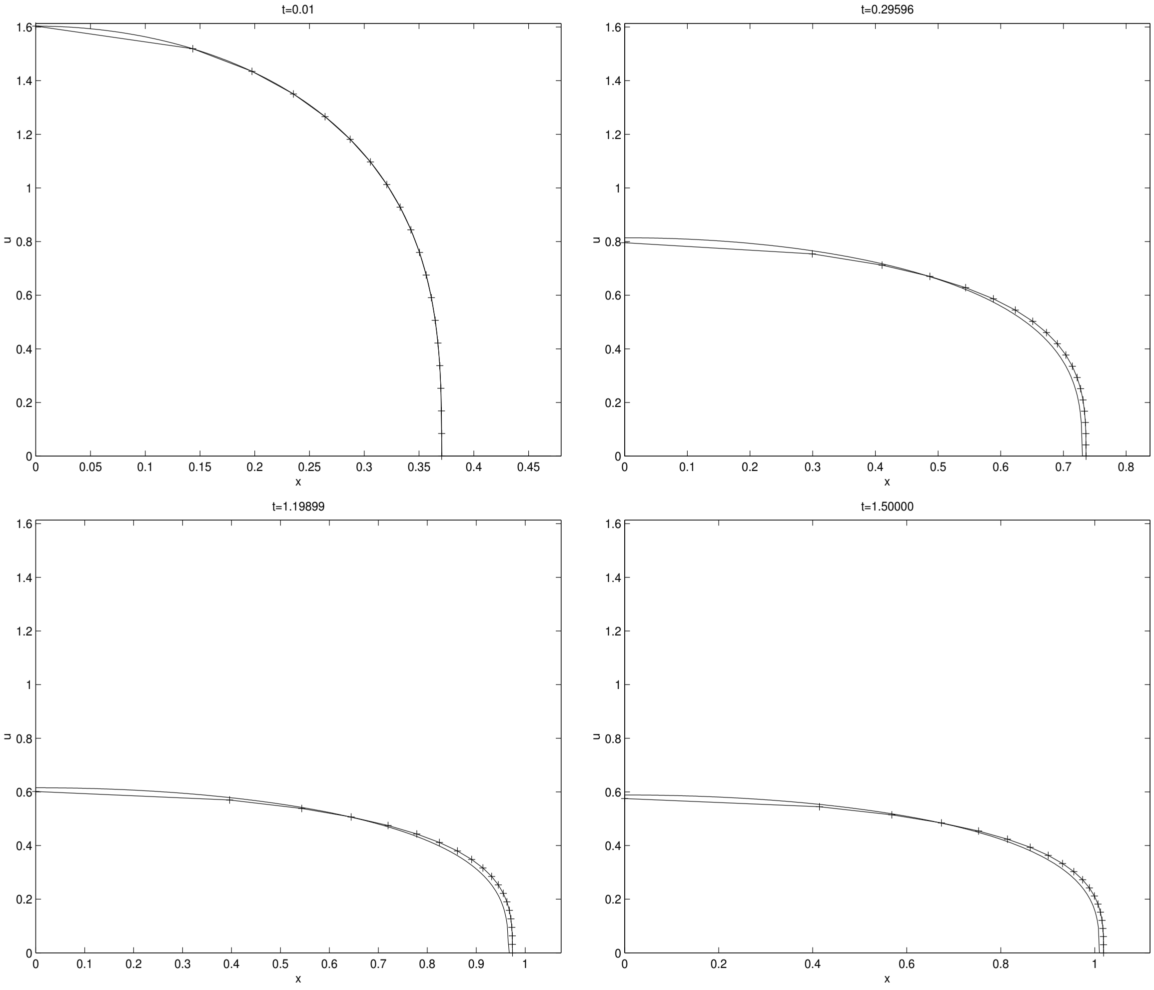
Hence for each interval i

$$\int_{x_{i-1}}^{x_i} T_x dx = \frac{T_i - T_{i-1}}{\Theta(t)} = f_i \qquad (11)$$

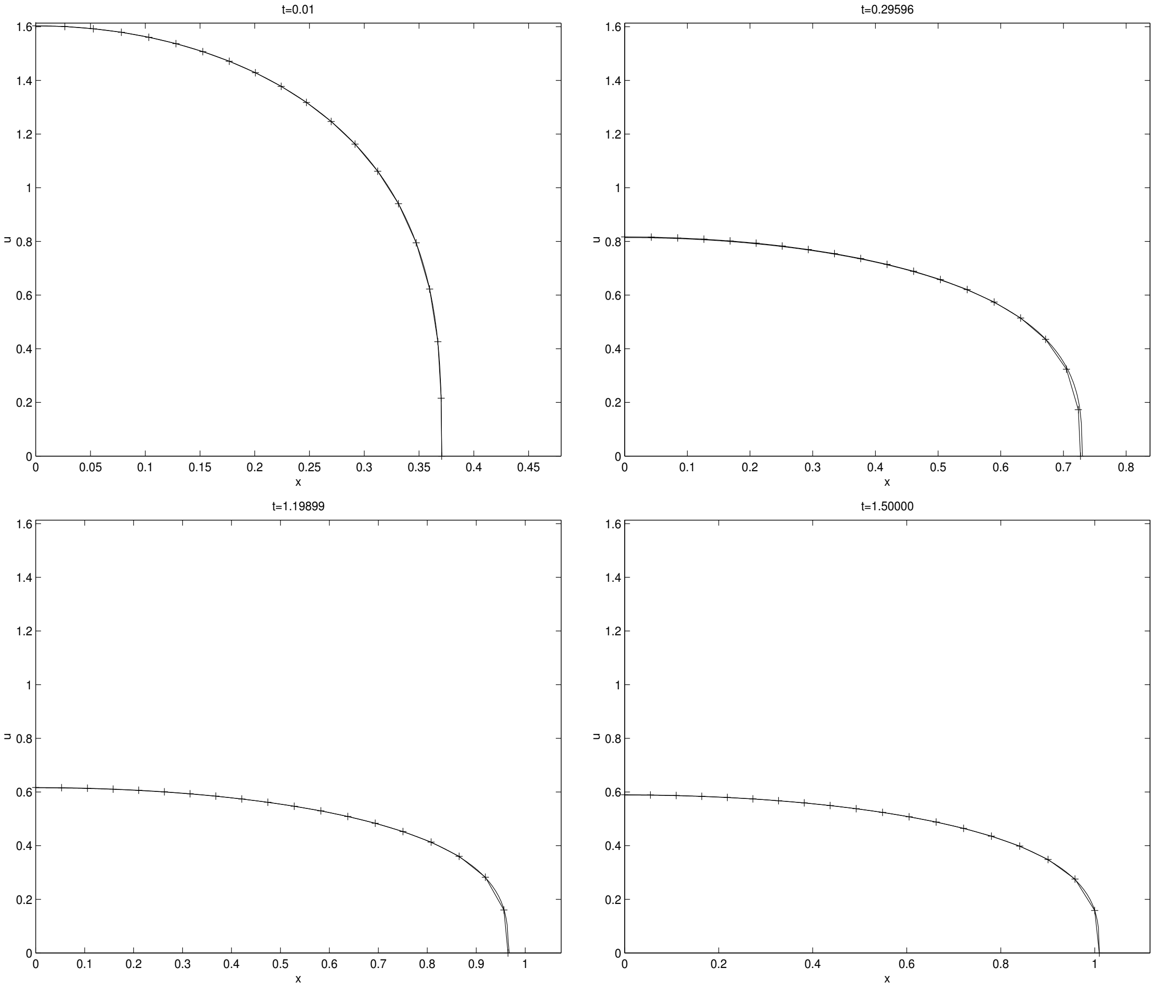
$\Theta(t)$ can be obtained from invariance of the total mass, which, if T is piecewise linear, can be approximated as

$$\int_{x_0}^{x_N} T dx = \sum_{i=1}^{N} \frac{1}{2}(x_i - x_{i-1})(T_{i-1} + T_i) = \text{const}$$

Substituting for T_i from the solution of the system (11) yields an equation for $\Theta(t)$.



Approximate and reference solutions using the gradient monitor.



Approximate and reference solutions using a combination monitor.

CONCLUSIONS (1)

The differential form of the Geometric Conservation Law is a Lagrangian Conservation Law for a Jacobian which can be taken as a monitor function.

The monitor function equation together with the field equations can be used generate a differential equation for the ALE velocity.

Uniqueness of the ALE velocity is provided by prescribing a pseudo vorticity.

FV and FE discretizations can be constructed.

CONCLUSIONS (2)

For scalar PDEs the dependent variable can be reconstructed from the monitor function equation.

The method is illustrated for a nonlinear diffusion equation.

The choice of monitor can be informed by scale invariance, but may fail to deal with problems of resolution.