A flux-corrected transport algorithm for handling the close-packing limit in dense suspensions

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Abstract

Convection of a scalar quantity by a compressible velocity field may give rise to unbounded solutions or nonphysical overshoots at the continuous and discrete level. In this paper, we are concerned with solving continuity equations that govern the evolution of volume fractions in Eulerian models of disperse two-phase flows. An implicit Galerkin finite element approximation is equipped with a flux limiter for the convective terms. The fully multidimensional limiting strategy is based on a flux-corrected transport (FCT) algorithm. This nonlinear high-resolution scheme satisfies a discrete maximum principle for divergence-free velocities and ensures positivity preservation for arbitrary velocity fields. To enforce an upper bound that corresponds to the maximum-packing limit, an FCT-like overshoot limiter is applied to the converged convective fluxes at the end of each time step. This postprocessing step imposes an additional physical constraint on the numerical solution to the unconstrained mathematical model. Numerical results for 2D implosion problems illustrate the performance of the proposed limiting procedure.

Keywords: convection, compressibility, finite elements, flux correction

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1. Introduction

Many modern high-resolution schemes for the equations of fluid dynamics trace their origins to the flux-corrected transport (FCT) algorithm [3, 18]

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which is readily applicable to finite element approximations on unstructured meshes [6, 8, 11, 13]. FCT belongs to the family of *algebraic flux correction* schemes backed by the theory of discrete maximum principles [9, 10, 11]. This theory makes it possible to preserve important properties of the exact solution (nonnegativity, monotonicity, nonincreasing total variation in 1D). However, compressibility effects may trigger an uncontrolled growth of a conserved quantity. In particular, concentrations or volume fractions may exceed 1 and eventually blow up. A consistent numerical scheme does not suppress overshoots that are present in the exact solution. Hence, only solutions to incompressible flow problems are guaranteed to be bounded, whereas there is no upper bound in the case of a compressible velocity field [9].

In the context of Eulerian and Lagrangian two-phase flow models, it is essential to ensure that the volume fraction of the disperse phase is bounded above. A typical model for dense suspensions incorporates an interparticle stress term designed to keep the particle volume fraction below the close-packing value [1, 5, 14]. An interesting alternative to this approach was introduced by Leiderman and Fogelson [12] who multiplied the convective flux by a monotonically decreasing function of the volume fraction to impair the ability of platelets to move into regions packed with other platelets.

The method proposed in this paper combines the idea of Leiderman and Fogelson [12] with algebraic flux correction. Instead of modifying the convective flux at the continuous level, we decompose the discretized convective term into numerical fluxes and limit the magnitude of these fluxes so as to get rid of undesired maxima. The advantages of constraining the discrete solution in this way are twofold. First, there is no need for tuning any free parameters or choosing the 'right' damping function for the convective flux. Second, the FCT-like limiting strategy does not prevent the particles from leaving the regions of high concentration. In this paper, we apply the new limiter to 2D implosion problems discretized with bilinear finite elements.

2. Continuous problem

The evolution of densities and volume fractions in (laminar) multiphase flow models is governed by continuity equations of the form

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v} u) = 0 \qquad \text{in } \Omega, \tag{1}$$

where u is the conserved quantity, $\mathbf{v}$ is a given velocity field and Ω is a bounded domain. Since equation (1) is of hyperbolic type, we prescribe a

Dirichlet boundary condition on the inflow part of the boundary Γ

$$u = u_D \quad \text{on } \Gamma_D := \{\mathbf{x} \in \Gamma \,|\, \mathbf{v} \cdot \mathbf{n} < 0\}, \tag{2}$$

where $\mathbf{n}$ is the unit outward normal to Γ. The initial condition is given by

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega. \tag{3}$$

In the case of an incompressible velocity field ($\nabla \cdot \mathbf{v} = 0$) the solution to problem (1)–(2) is known to satisfy the following maximum principle

$$\min\{u_0, u_D\} \le u \le \max\{u_0, u_D\}. \tag{4}$$

In particular, this useful a priori estimate implies positivity preservation

$$u_0 \ge 0, \quad u_D \ge 0 \quad \Rightarrow \quad u \ge 0. \tag{5}$$

The solution to (1) with $\nabla \cdot \mathbf{v} \neq 0$ satisfies (5) but may violate (4) since

$$\nabla \cdot (\mathbf{v}u) = \mathbf{v} \cdot \nabla u + (\nabla \cdot \mathbf{v})u \tag{6}$$

contains a nonvanishing zero-order term $(\nabla \cdot \mathbf{v})u$. This 'reactive' term acts as a source or a sink, depending on the sign of $\nabla \cdot \mathbf{v}$. It can increase the magnitude of u but cannot change its sign (see [9] and references therein).

3. Space discretization

The variational form of the above initial-boundary value problem reads

$$\int_\Omega w \left(\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) \right) \mathrm{d}\mathbf{x} = 0 \tag{7}$$

for all admissible test functions w vanishing at the inlet Γ_D. For notational simplicity, we refrain from a formal definition of the functional spaces.

In this paper, we discretize (7) in space using the Galerkin finite element method. Let $\{\varphi_j\}$ denote a finite set of continuous piecewise-linear or multilinear basis functions. The numerical solution u_h is defined as

$$u_h = \sum_j u_j \varphi_j. \tag{8}$$

The unknowns of the semi-discrete problem are the coefficients u_j which represent the time-dependent values of u_h at the vertices of the mesh.

The Galerkin discretization of the convective term can be defined by differentiating $\mathbf{v}u_h$. For our purposes, it is more convenient to work with Fletcher's [4] *group finite element* interpolant of the convective flux

$$(\mathbf{v}u)_h = \sum_j (\mathbf{v}_j u_j)\varphi_j. \tag{9}$$

This formula implies the following discretization of the divergence operator

$$\nabla \cdot (\mathbf{v}u)_h = \sum_j u_j(\mathbf{v}_j \cdot \nabla\varphi_j). \tag{10}$$

Using approximations (8) and (10) in the Galerkin weak form (7) with the test function $w_h = \varphi_i$, we obtain the following semi-discrete equation

$$\sum_j \left(\int_\Omega \varphi_i\varphi_j \,\mathrm{d}\mathbf{x} \right) \frac{\mathrm{d}u_j}{\mathrm{d}t} = -\sum_j \mathbf{v}_j \cdot \left(\int_\Omega \varphi_i \nabla\varphi_j \,\mathrm{d}\mathbf{x} \right) u_j. \tag{11}$$

The system of equations for all unknowns can be written in the generic form

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} = Ku, \tag{12}$$

where u is the vector of unknowns, $M_C = \{m_{ij}\}$ is the consistent mass matrix, and $K = \{k_{ij}\}$ is the discrete transport operator. We have

$$m_{ij} = \int_\Omega \varphi_i\varphi_j \,\mathrm{d}\mathbf{x} \tag{13}$$

and $k_{ij} = -\mathbf{v}_j \cdot \mathbf{c}_{ij}$, where $\mathbf{c}_{ij}$ is the vector of discretized space derivatives

$$\mathbf{c}_{ij} = \int_\Omega \varphi_i \nabla\varphi_j \,\mathrm{d}\mathbf{x}. \tag{14}$$

In the case of an unsteady velocity field, the discrete transport operator must be updated at each time step. If the mesh is fixed, then the coefficients $\mathbf{c}_{ij}$ do not change and need to be evaluated just once. Hence, the group finite element formulation makes it possible to update K in a very efficient way.

4. Algebraic flux correction

A semi-discrete scheme of the form (12) proves *local extremum diminishing* for $\nabla \cdot \mathbf{v} = 0$ and/or positivity-preserving for any $\mathbf{v}$ if [9, 10, 11]

$$m_{ii} > 0, \quad m_{ij} = 0, \quad k_{ij} \geq 0, \quad \forall j \neq i. \tag{15}$$

The standard Galerkin discretization fails to satisfy these sufficient conditions, so it tends to produce nonphysical oscillations (also known as 'wiggles') in a neighborhood of discontinuities and steep fronts. This is unacceptable when it comes to solving continuity equations in multiphase flow models. Therefore, we will use algebraic flux correction [10] to constrain the contribution of matrix entries that have a wrong sign ($m_{ij} > 0$ and $k_{ij} < 0$).

To begin with, we replace the matrix M_C with its lumped counterpart

$$M_L := \mathrm{diag}\{m_i\}, \qquad m_i = \sum_j m_{ij}. \tag{16}$$

Next, we fix K by adding a discrete diffusion operator $D = \{d_{ij}\}$ with [10, 11]

$$d_{ij} = \max\{-k_{ij}, 0, -k_{ji}\} = d_{ji}, \qquad \forall j \neq i \tag{17}$$

so that $K + D$ has no negative off-diagonal coefficients. The diagonal entries of D are defined so that this symmetric matrix has zero row sums

$$d_{ii} := -\sum_{j \neq i} d_{ij}. \tag{18}$$

Due to symmetry, the column sums are also equal to zero. In the 1D case, the lumped-mass Galerkin approximation on a uniform mesh of linear finite elements is equivalent to the central difference scheme, while the modified operator $K + D$ corresponds to the first-order upwind difference [11].

In summary, the semi-discrete Galerkin scheme (12) can be split as follows

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = (K + D)u + f(u), \tag{19}$$

where $f(u)$ is the sum of antidiffusive terms that may destroy positivity

$$f(u) = (M_L - M_C)\frac{\mathrm{d}u}{\mathrm{d}t} - Du. \tag{20}$$

Since $M_L - M_C$ and D are symmetric with zero row sums, we have

$$(M_L u - M_C u)_i = m_i u_i - \sum_j m_{ij} u_j = \sum_{j \neq i} m_{ij}(u_i - u_j), \tag{21}$$

$$(Du)_i = \sum_j d_{ij} u_j = d_{ii} u_i + \sum_{j \neq i} d_{ij} u_j = \sum_{j \neq i} d_{ij}(u_j - u_i). \tag{22}$$

Thus, each component of (20) admits a flux decomposition of the from

$$f_i = \sum_{j \neq i} f_{ij}, \qquad f_{ji} = -f_{ij}. \tag{23}$$

The formula for the *raw antidiffusive fluxes* f_{ij} follows from (21)–(22)

$$f_{ij} = \left(m_{ij} \frac{\mathrm{d}}{\mathrm{d}t} + d_{ij} \right) (u_i - u_j), \qquad \forall j \neq i. \tag{24}$$

Some fluxes are harmless but others may create an undershoot or overshoot. The contribution of these "bad" fluxes must be limited so as to make the antidiffusive term local extremum diminishing for a given solution. The flux-corrected counterpart of (12) is a semi-discrete problem of the form

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = (K + D)u + \bar{f}(u), \tag{25}$$

where $\bar{f}(u)$ stands for the sum of limited antidiffusive fluxes

$$\bar{f}_i = \sum_{j \neq i} \bar{f}_{ij}, \qquad \bar{f}_{ji} = -\bar{f}_{ij}. \tag{26}$$

A well-designed flux limiter produces $\bar{f}_{ij} \approx f_{ij}$ in smooth regions and $\bar{f}_{ij} = 0$ elsewhere. The unconstrained Galerkin scheme (12) and its nonoscillatory "good" part correspond to $\bar{f} = f$ and $\bar{f} = 0$, respectively.

In general, the best definition of $\bar{f}_{ij}$ is given by the solution of a constrained optimization problem [2]. A nonoptimal but cost-effective alternative is the multiplication by a solution-dependent correction factor

$$\bar{f}_{ij} := \alpha_{ij} f_{ij}, \qquad 0 \leq \alpha_{ij} \leq 1. \tag{27}$$

This kind of flux correction traces its origins to the FCT algorithm and forms the basis for the construction of our algebraic flux correction schemes.

5. Time discretization

Let $0 = t_0 < t^1 < t^2 < \ldots < t^M = T$ be the sequence of time levels for the fully discrete problem. For simplicity, we assume that the time step $\Delta t := t^{n+1} - t^n$ is constant, whence $t^n = n\Delta t$. The two-level θ-scheme with $\theta = \frac{1}{2}$ or $\theta = 1$ yields a nonlinear algebraic system of the form

$$Au^{n+1} = Bu^n + \bar{f}, \tag{28}$$

where $\bar{f} = \bar{f}(u^{n+1}, u^n)$ is the limited antidiffusive term and

$$A = \frac{1}{\Delta t} M_L - \theta(K + D), \tag{29}$$

$$B = \frac{1}{\Delta t} M_L + (1 - \theta)(K + D). \tag{30}$$

In this paper, we solve the nonlinear system (28) in an iterative way. Let $\{u^{(m)}\}$ be a sequence of successive approximations to u^{n+1}. A reasonable initial guess is $u^{(0)} = u^n$ or $u^{(0)} = 2u^n - u^{n-1}$. These settings correspond to the constant and linear extrapolation in time, respectively. Given the current iterate $u^{(m)}$ and the vector of approximate time derivatives

$$\dot{u}^{(m)} := \frac{u^{(m)} - u^n}{\Delta t}, \tag{31}$$

we recalculate the implicit part of the raw antidiffusive fluxes given by

$$\begin{aligned} f_{ij}^{(m)} &= m_{ij}(\dot{u}_j^{(m)} - \dot{u}_i^{(m)}) + \theta d_{ij}(u_j^{(m)} - u_i^{(m)}) \\ &+ (1 - \theta) d_{ij}(u_j^n - u_i^n), \qquad j \neq i. \end{aligned} \tag{32}$$

Then we apply the FCT limiter (to be presented in the next section), assemble the limited antidiffusive term $\bar{f}^{(m)}$, and solve the linear system

$$Au^{(m+1)} = Bu^n + \bar{f}^{(m)}. \tag{33}$$

The solution, the raw antidiffusive fluxes, and the corresponding correction factors are updated in this way until the residuals or relative changes become smaller than a prescribed tolerance. It can be shown that each solution update is positivity-preserving under the CFL-like condition [10, 11]

$$\Delta t \leq \frac{1}{\theta - 1} \frac{m_i}{k_{ii} + d_{ii}}, \qquad \forall i. \tag{34}$$

Note that there is no time step restriction in the fully implicit case ($\theta = 1$).

6. Zalesak's FCT limiter

In this section, we present Zalesak's limiter [18] that we use to calculate the correction factors α_{ij}. Consider an explicit update of the form

$$m_i u_i = m_i \tilde{u}_i + \Delta t \sum_{j \neq i} \alpha_{ij} f_{ij}, \tag{35}$$

where $\tilde{u} := M_L^{-1} B u^n$ is an explicit low-order approximation to $u^{n+1-\theta}$. Let $S_i = \{j \neq i \,|\, m_{ij} \neq 0\}$ be the set of nearest neighbors of node i. Define

$$u_i^{\max} := \max\{\tilde{u}_i, \max_{j \in S_i} \tilde{u}_j\}, \tag{36}$$

$$u_i^{\min} := \min\{\tilde{u}_i, \min_{j \in S_i} \tilde{u}_j\}. \tag{37}$$

In accordance with the FCT philosophy, the flux limiting procedure must render the antidiffusive term local extremum diminishing. That is, the solution to (35) must satisfy the local discrete maximum principle

$$u_i^{\min} \leq u_i \leq u_i^{\max}. \tag{38}$$

The process of flux correction begins with the optional 'prelimiting' step

$$f_{ij} := 0 \quad \text{if} \quad f_{ij}(\tilde{u}_j - \tilde{u}_i) > 0. \tag{39}$$

This adjustment was found to eliminate spurious ripples created by fluxes that flatten the solution profiles instead of steepening them [10, 18].

The right choice of the correction factors α_{ij} for $\bar{f}_{ij} = \alpha_{ij} f_{ij}$ ensures that positive antidiffusive fluxes cannot create an overshoot, while negative ones cannot create an undershoot. Assuming the worst-case scenario, we enforce condition (38) using Zalesak's multidimensional FCT algorithm [18]:

1. Compute the sums of positive/negative antidiffusive fluxes

$$P_i^+ = \sum_{j \neq i} \max\{0, f_{ij}\}, \qquad P_i^- = \sum_{j \neq i} \min\{0, f_{ij}\}. \tag{40}$$

2. Define the upper/lower bounds for admissible increments

$$Q_i^+ = \frac{m_i}{\Delta t}(u_i^{\max} - \tilde{u}_i), \qquad Q_i^- = \frac{m_i}{\Delta t}(u_i^{\min} - \tilde{u}_i). \tag{41}$$

3. Compute the nodal correction factors for the components of $P_i^{\pm}$

$$R_i^+ = \min\left\{1, \frac{Q_i^+}{P_i^+}\right\}, \qquad R_i^- = \min\left\{1, \frac{Q_i^-}{P_i^-}\right\}. \tag{42}$$

4. Check the sign of the unconstrained flux and multiply f_{ij} by

$$\alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\} & \text{if } f_{ij} > 0, \\ \min\{R_i^-, R_j^+\} & \text{if } f_{ij} < 0. \end{cases} \tag{43}$$

This definition of α_{ij} guarantees that the corrected nodal value u_i satisfies (38). As shown in [10, 11], this implies positivity preservation for (33).

7. Overshoot limiter

In this section, we present a new limiter for overshoots created by the discrete counterpart of $(\nabla \cdot \mathbf{v})u$. Given a global bound $u^{\max}$, such as the close-packing value of a particle volume fraction, we eliminate nonphysical maxima using the following representation of the discrete problem

$$m_i u_i^{n+1} = m_i u_i^n + \Delta t \sum_{j \neq i} g_{ij}, \tag{44}$$

where u^{n+1} is the converged solution to (28) and g_{ij} denotes the corrected convective flux from node j into node i. It can be shown that [9, 10]

$$(Ku)_i = \sum_{j \neq i} (\mathbf{c}_{ji} \cdot \mathbf{v}_j u_j - \mathbf{c}_{ij} \cdot \mathbf{v}_i u_i) \tag{45}$$

for each internal node. If i is a node on the boundary, then a surface integral is added. The vector-valued coefficients $\mathbf{c}_{ij}$ are given by (14). A very similar flux decomposition was presented by Selmin and Formaggia [15, 16].

By virtue of (45), the semi-discrete form of the convective flux g_{ij} reads

$$\begin{aligned} g_{ij} : \;&=\; \mathbf{c}_{ji} \cdot \mathbf{v}_j u_j - \mathbf{c}_{ij} \cdot \mathbf{v}_i u_i \\ &+\; d_{ij}(u_j - u_i) + \bar{f}_{ij}. \end{aligned} \tag{46}$$

Since the solution updates (35) and (44) have the same structure, we use a one-sided version of Zalesak's limiter to enforce the upper bound

$$u_i^{n+1} \leq u^{\max}.$$

As in the case of algebraic flux correction for the antidiffusive part, each convective flux g_{ij} is multiplied by a solution-dependent correction factor $\beta_{ij} \in [0,1]$. Since there are no undershoots, only positive fluxes require limiting. The algorithm for the practical computation of β_{ij} becomes:

1. Compute the sums of positive convective fluxes into node i
$$P_i^+ = \sum_{j \neq i} \max\{0, g_{ij}\}. \tag{47}$$
2. Define the upper bounds for admissible increments
$$Q_i^+ = \frac{m_i}{\Delta t}(u^{\max} - u_i^n). \tag{48}$$
3. Compute the nodal correction factors for the components of P_i^+
$$R_i^+ = \min\left\{1, \frac{Q_i^+}{P_i^+}\right\}. \tag{49}$$
4. Check the sign of the unconstrained flux and multiply g_{ij} by
$$\beta_{ij} = \begin{cases} R_i^+ & \text{if } g_{ij} > 0, \\ R_j^+ & \text{if } g_{ij} < 0. \end{cases} \tag{50}$$

This FCT-like limiter makes it possible to fix u^{n+1} with a single postprocessing step. However, the formula for β_{ij} is based on the worst-case scenario. Since positive fluxes are limited without knowing the magnitude of negative ones, unnecessary flux correction is performed if there is no overshoot at node i but the removal of negative fluxes would create an overshoot. This may lead to some erosion in regions where $u^{n+1} \approx u^{\max}$. A possible remedy is iterative flux limiting. The contribution of negative fluxes can be taken into account using β_{ij} from the previous iteration to sharpen the bounds thus:

$$Q_i^+ = \frac{m_i}{\Delta t}(u^{\max} - u_i^n) + \sum_{j \neq i} \beta_{ij} \min\{0, g_{ij}\}. \tag{51}$$

At the first iteration, we use $\beta_{ij} = 1$ so that the solution remains unchanged if the constraint $u_i^{n+1} \leq u^{\max}$ is satisfied from the outset for all nodes.

8. Numerical examples

To test the new overshoot limiter, we apply it to 2D model problems with highly compressible velocity fields. Computations are performed in the square domain $\Omega := (0, 1)^2$ on a uniform mesh of 128×128 bilinear elements using the Crank-Nicolson time-stepping ($\theta = \frac{1}{2}$) with $\Delta t = 10^{-3}$. The presented solutions were calculated with the iterative overshoot limiter. The single-step version produces almost identical results for both examples.

8.1. Implosion of a circle

In the first test, we solve equation (1) with the compressible velocity field

$$\mathbf{v}(x, y) := \frac{(0.5 - x, 0.5 - y)}{r + \epsilon},$$

where

$$r := \sqrt{(x - 0.5)^2 + (y - 0.5)^2}$$

is the distance to (0.5,0.5) and $\epsilon = 10^{-12}$ is added to prevent division by zero.

The initial solution u_0 depicted in Fig. 1a is a circle of constant density

$$u_0(x, y) := \begin{cases} 0.5 & \text{if } r \leq 0.4 \\ 0.0 & \text{otherwise.} \end{cases}$$

Homogeneous Dirichlet boundary conditions are prescribed at the inlet Γ.

Since the velocity vector $\mathbf{v}$ points into the center of the domain Ω, the unconstrained solution to (1) exhibits unlimited growth. As time goes on, the entire initial mass is convected towards and concentrated at the point (0.5,0.5). Hence, the final solution is a delta function. The snapshots shown in Fig. 1 b–d were calculated using FEM-FCT with the overshoot limiter that stops the growth of u as soon as the largest admissible value $u^{\max} := 1$ is attained. This prevents the blowup of the solution. The total 'mass', i.e., the integral of u is the same in all diagrams. The final solution is again a circle of constant density ($u = 1$ inside, $u = 0$ outside), see Fig. 1d.

8.2. Implosion of a ring

In the second test, we employ the following definition of the velocity field

$$\mathbf{v}(x, y) := \frac{(1 - 2x, 1 - 2y)}{r} \max\{0, r - 0.1\}.$$

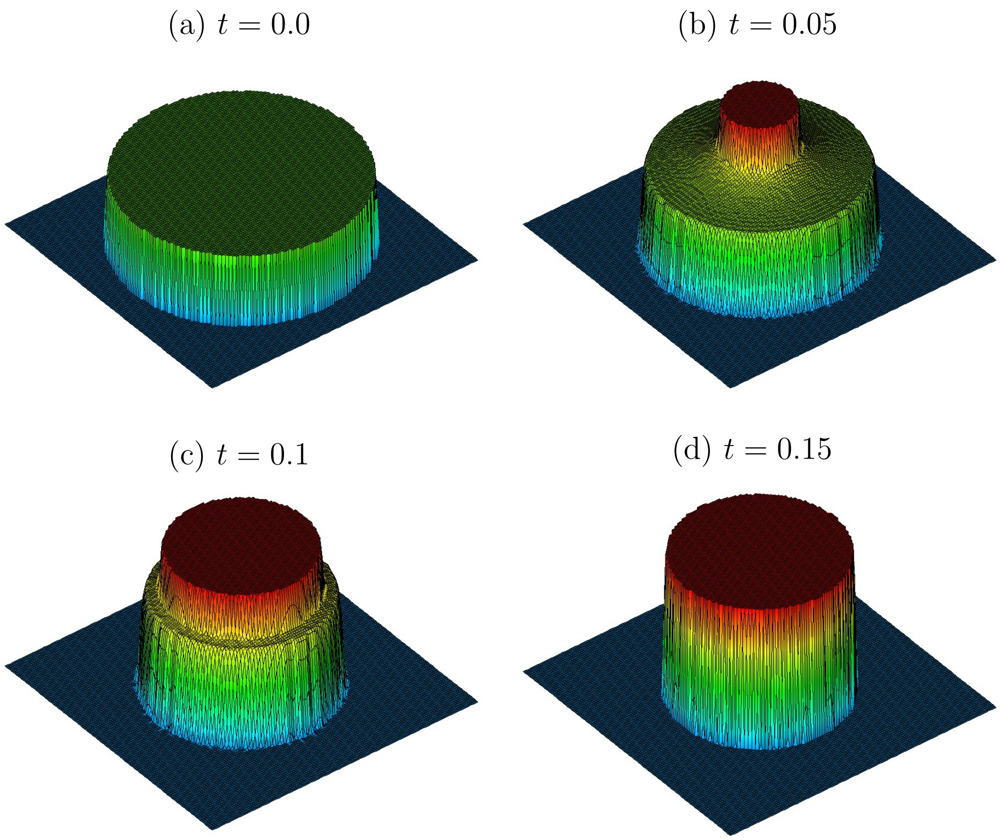

Figure 1: Constrained implosion of a density circle (FEM-FCT simulation).

The initial data for this test is a ring of constant density (Fig. 2a)

$$u_0(x, y) := \begin{cases} 0.5 & \text{if } 0.3 \leq r \leq 0.4 \\ 0.0 & \text{otherwise.} \end{cases}$$

Again, the mass is convected towards the point (0.5,0.5) but the magnitude of the velocity vector $\mathbf{v}$ decreases linearly with r and vanishes inside the circle $r = 1$. The resultant compression wave makes the imploding density ring thinner, while the maximum value of u increases as time goes on. The results of the FEM-FCT simulation are shown in Fig. 2b–d. The overshoot limiter is activated when the threshold value $u^{\max} := 1$ is reached. In the steady-state limit, all mass is concentrated in a thin ring of constant height $u = 1$. As in the first example, the radial symmetry is preserved, and the numerical solutions remain free of spurious undershoots/overshoots.

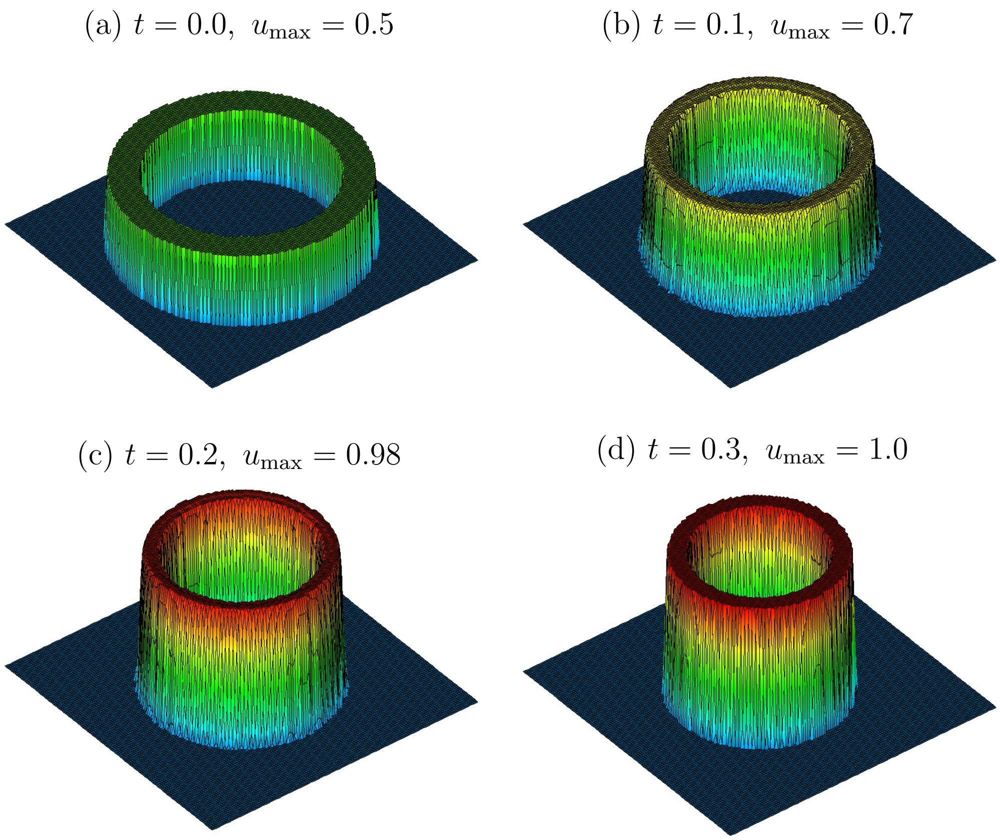

Figure 2: Constrained implosion of a density ring (FEM-FCT simulation).

9. Conclusions

A new approach to enforcing physically-motivated upper bounds for volume/mass fractions was developed on the basis of an implicit FEM-FCT algorithm. The presented scheme is nonlinear even for a linear transport equation. The cost of flux correction can be significantly reduced using a suitable linearization [8] or convergence acceleration techniques [7, 17]. An application of particular importance is the numerical treatment of continuity equations in Eulerian two-phase flow models (granular materials, fluidized beds). This research will be presented in a forthcoming publication.

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