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A Semi-Discrete Lagrangian-Eulerian Formulation for Three-dimensional Hyperbolic Systems and Applications

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Abstract. In this work, we develop a three-dimensional Semi-Discrete formulation for hyperbolic systems of conservation laws in three-space dimensions on structured cubical and tetrahedral meshes, thereby extending the results presented in [2], which is based on the concept of no-flow curves introduced in [7]. A first numerical validation study of the scheme is presented and discussed, addressing several preliminary 3D numerical solutions for systems, namely: (1) compressible Euler flows with positivity of the density, (2) the nontrivial Orszag-Tang problem in magnetohydrodynamics, which is well-known to satisfy the notable involution-constrained partial differential equation, $\nabla \cdot B = 0$ (this condition is verified numerically by the proposed approach, i.e., without any imposition of an additional constraint in the formulation), and (3) a nonstrictly hyperbolic three-phase flow system in porous media with a resonance point (coincidence of eigenvalues). Due to the no-flow framework, there is no need to employ/compute the eigenvalues (exact or approximate values) - in fact there is no need to construct the relevant Jacobian of the hyperbolic flux functions, and thus giving rise to an effective weak CFL-stability condition, which is feasible in the computing practice. Overall, the method is based on locally well-balanced properties, it is Riemann-solver-free and, hence, time-consuming field-by-field type decompositions are avoided in the case of multidimensional systems.

Keywords. 3D Hyperbolic Conservation Laws, Lagrangian-Eulerian Framework, 3D No-flow Curves

1 Introduction

The objective of this work is to formally design and implement a Semi-Discrete Lagrangian-Eulerian scheme for numerically solving three-dimensional systems of hyperbolic conservation laws in tetrahedral grids. A three-dimensional system of hyperbolic conservation laws is a system of partial differential equations in the form

$$\begin{cases} (u_i(\mathbf{x},t))_t + \nabla \cdot \mathbf{f}_i(u(\mathbf{x},t)) &= 0, & \mathbf{x} \in \Omega \subset \mathbb{R}^3,\ t \in (0,T],\ i = 1, \cdots, m, \\ u(\mathbf{x},0) &= u_0(\mathbf{x}), & \mathbf{x} \in \Omega \subset \mathbb{R}^3, \end{cases} \tag{1}$$

with $T > 0$, $u = u(\mathbf{x},t) = (u_1, \cdots, u_m)^T : \Omega \times (0,T] \to \mathbb{R}^m$, $\mathbf{f} = (\mathbf{f}_1, \cdots, \mathbf{f}_m)$, for which each $\mathbf{f}_i$, for $i = 1, \cdots, m$, satisfies $\mathbf{f}_i : \mathbb{R}^m \to \Omega$. Note that if $i = 1$ we have the scalar conservation law. Here, u is called the *conserved quantity* and f is the *flux function*. The condition for system (1) to be considered *hyperbolic* can be found in [5]. Generally speaking, the conservation law expresses that the variation in time of the quantity in a certain domain is equal to the loss (or gain) at its boundaries. In classical continuum physics, such systems express the conservation laws for continuous media where diffusion induced by other phenomena is absent or negligible.

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Systems of multi-dimensional hyperbolic conservation laws presents serious challenges. For example, **there are no global existence results** for solutions of any class of multi-dimensional systems of conservation laws with generic initial data. While entropy solutions are commonly accepted as a suitable solution framework for systems of conservation laws in several space dimensions [5], recent results, like the ones presented in [4, 12], have demonstrated that entropy solutions may not be unique.

Some authors [8] support the concept of entropy measure-valued solutions, first proposed in [6] as the appropriate solution paradigm for systems of conservation laws. But the uniqueness of measure-valued solutions are still an open problem.

In this regard, recently, in [8] the authors showed that a Monte-Carlo algorithm, based on underlying entropy stable finite volume schemes, converges to an entropy measure-valued solution of multi-dimensional systems of conservation laws on mesh refinement. This provided the first rigorous convergence result (existence) for numerical approximations of generic multi-dimensional systems of conservation laws, but based on the construction of a novel solution concept termed as statistical solutions. However, note that only evidence of uniqueness is presented, as a rigorous proof is still in development.

In this context we present this work, advancing the results presented in [2, 9], analyzing the use of the weak positive Lagrangian-Eulerian methods free of explicit computation of the eigenstructure, based on the concept of no-flow curves, recently developed and analyzed in [1]. These methods respect a weak positivity principle, generalizing results of P. Lax and X.-D. Liu [11] and are able to obtain the same stable numerical results as in the papers [8], but avoiding the computationally expensive Monte Carlo Algorithm.

2 3D Semi-Discrete Lagrangian-Eulerian Scheme

Let $\mathcal{T}$ be a family of tetrahedrons of $\mathbb{R}^3$ such that the common face $(K|L)$ between cells K and L of $\mathcal{T}$ is included in a plane on $\mathbb{R}^3$. For any control volume (K), we denote its 3D measure (volume) by $|K|$, and the set of its neighbors by $N(K)$. If $L \in N(K)$, then $|K|L|$ is the 2D measure (superficial area) of $K|L$.
In [2] the following Fully-Discrete scheme was presented

$$u_K^{n+1} = u_K^n - \frac{\Delta t}{|K|} \sum_{L \in N(K)} F(u_K^n, u_L^n, n_{K|L}) |K|L|, \tag{2}$$

$$F(u_K^n, u_L^n, n_{KL}) = \frac{1}{2}\Big(\mathbf{f}(u_K^n) + \mathbf{f}(u_L^n)\Big) \cdot \mathbf{n}_{KL} + \sup_{u,K,L} \left| \frac{\mathbf{f}(u)}{u} \cdot \mathbf{n}_{KL} \right| (u_K^n - u_L^n). \tag{3}$$

While the scheme (2)–(3) have the desired properties for solving scalar hyperbolic laws (as the Total Variation Non Increasing (TVNI) property and convergence to entropy solution [9]), these properties are not valid for any multi-D system of hyperbolic laws, as they may not be bounded [5] or may have infinite entropic solutions [4] For such systems, the current paradigm is to guarantee the "positivity principle" as proposed in [11]. For this end, from the fully-discrete scheme (2)–(3), a new semi-discrete 3D Lagrangian-Eulerian scheme on tetrahedral grids can be constructed as follows: thanks to the no-flow stability coefficient, $sup_{u,\mathbf{n}} |(\mathbf{f}(u)/u) \cdot \mathbf{n}|$, it can be seen that the Lagrangian-Eulerian numerical flux function (3) do not depend on $\mathcal{O}(1/\Delta t)$ and do not have a blow-up singularity as $\Delta t \to 0^+$. Therefore, taking the limit as $\Delta t \to 0^+$ in equation (2), we get

$$\begin{cases} u_K^0 = \dfrac{1}{m(K)} \displaystyle\int_K u(\mathbf{x}, 0) d\mathbf{x}, \\ \dfrac{d}{dt} u_K(t) = -\dfrac{1}{|K|} \displaystyle\sum_{L \in N(K)} \mathcal{F}(u_K(t), u_L(t); \mathbf{n}_{KL}) := \mathcal{L}(u_K(t), u_L(t)). \end{cases} \tag{4}$$

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Equations (3)–(4) constitute the **3D Semi-Discrete Lagrangian-Eulerian (SDLE3D)** scheme on tetrahedral grids. The semi-discrete scheme (3)–(4) satisfies the positivity principle presented in [11] (the 2D case is presented in [1] and the 3D case will be presented in [9]). Also, note that the positivity principle is strongly dependent of the eigen-structure of the system. Since our scheme **does not use any eigenvalue or eigenvector**, it is also proposed that the scheme satisfies a weak formulation of the positivity principle, as seen in [1].

3 Numerical Results

All models are numerically solved using the 3D Semi-Discrete Lagrangian-Eulerian scheme (scheme (4) with flux (3)), solving the time derivative using Forward-Euler (results labeled as "Fully-Discrete") or using the Runge-Kutta scheme presented in [11] (results labeled as "Semi-Discrete"). Also, all models are solved using a tetrahedral mesh. Results were obtained using the Santos Dumont supercomputer.

The numerical mesh are composed of tetrahedral elements. They are created using a regular mesh of cubic elements and splitting each cube is into six tetrahedron. On the following results, we present the Relative Error considering the numerical result in the finer possible mesh (with 512 subdivisions per axis, and each cubic element split into six tetrahedrons, which we will note as $(512 \times 512 \times 512) \times 6)$ as a "reference solution", dubbed $(e_i^*)_1$, and the Relative Error between two consecutive meshes, marked as $(e_i)_1$, both computed using the norm l_1. Since the theory in multi-D systems of hyperbolic conservation laws is still mostly open [12], there is still no widely accepted numerical scheme to use as basis of comparison. Therefore, our results will be presented in terms of the behavior of the scheme under mesh refinement and comparison with well accepted results.

3.1 Euler Equations

While Euler Equations are common in fluid dynamics, here we present them in the context of gas dynamics. As in [1], the Euler Equations can be written as

$$\begin{cases} \rho_t + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ (\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + pI) &= 0, \\ e_t + \nabla \cdot (\mathbf{v}(e+p)) &= 0, \\ p &= (\gamma - 1)(e - (1/2)\rho \mathbf{v}^2). \end{cases} \tag{5}$$

Here we consider a problem with Slip Line Initial Data on unit cube $\Omega = [0,1]^3$ as the domain, with two planes, $x = 0.5$ and $z = 0.5$ subdividing the domain in four subdomains. Each subdomain receive a distinct constant initial condition, starting with discontinuities. A initial condition constant in the $y-$axis will be used, where any slice in the xz-plane can be compared to a 2D case. All boundaries uses the homogeneous Neumann condition. The $y-$axis constant initial condition is the same as [1, 10]

$$IC : \begin{cases} \rho = 1, & \mathbf{v} = [-0.75, 0, -0.5]^T, & p = 1, & \text{if } x > 0.5 \text{ and } z > 0.5, \\ \rho = 3, & \mathbf{v} = [0.75, 0, -0.5]^T, & p = 1, & \text{if } x > 0.5 \text{ and } z < 0.5, \\ \rho = 2, & \mathbf{v} = [-0.75, 0, 0.5]^T, & p = 1, & \text{if } x < 0.5 \text{ and } z > 0.5, \\ \rho = 1, & \mathbf{v} = [0.75, 0, 0.5]^T, & p = 1, & \text{if } x < 0.5 \text{ and } z < 0.5. \end{cases} \tag{6}$$

In Table 1 we can observe a steady decrease in the the relative error for both the fully- and semi-discrete schemes. Note that the error is calculated using the values of the density ρ. While the

gains per mesh refinement seems small, we remember that for hyperbolic conservation laws, which presents discontinuous weak solutions, the convergence is expected to be slow. For the 2D case, for example, a convergence of order 0.5 is expected for the smooth cases [1] The solution profile shown in Figure 1 (left) can be compared with the results shown in [1] and references therein.

Table 1: Relative Error for the Euler Equations on tetrahedral mesh with initial datum (6). CFL=0.04 and $t = 0.23$.

		Fully-Discrete		Semi-Discrete	
Mesh	Elements	$(e_i^*)_1$	$(e_i)_1$	$(e_i^*)_1$	$(e_i)_1$
$(32 \times 32 \times 32) \times 6$	196608	7.980e-02	3.209e-02	8.016e-02	3.220e-02
$(64 \times 64 \times 64) \times 6$	1572864	5.222e-02	2.299e-02	5.249e-02	2.309e-02
$(128 \times 128 \times 128) \times 6$	12582912	3.076e-02	1.761e-02	3.096e-02	1.772e-02
$(256 \times 256 \times 256) \times 6$	100663296	1.352e-02	1.352e-02	1.362e-02	1.362e-02

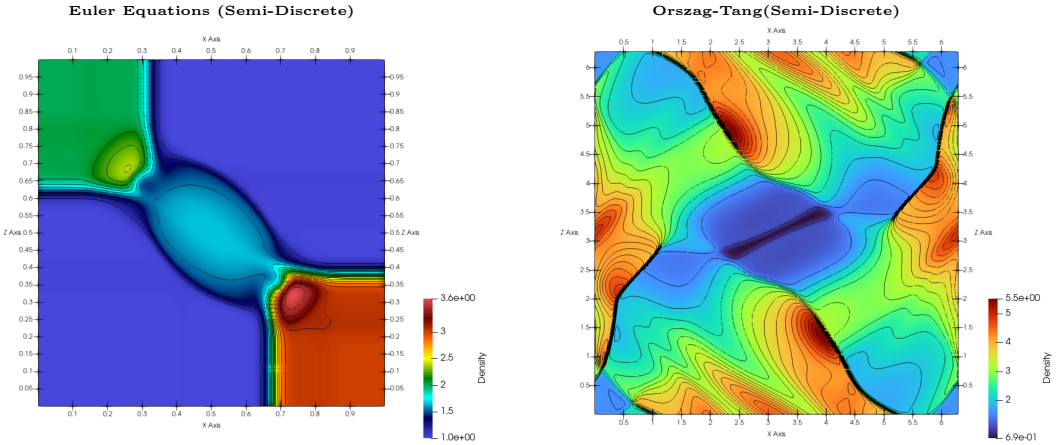

Figure 1: 2D Slice of the numerical solution for the Euler Equations (left) and Orszag-Tang Vortex System (right) on tetrahedral mesh using the Semi-Discrete scheme. The Fully-Discrete generates similar results.

3.2 Orszag-Tang Vortex System

The Orszag-Tang Vortex System is a well-known problem in magneto-hydrodynamics. From [1], in the conservative form, the Orszag-Tang Vortex System is given by

$$\begin{cases} \rho_t + \nabla \cdot (\rho \mathbf{v}) = 0, \\ (\rho \mathbf{v})_t + \nabla \cdot \left[\rho \mathbf{v} \otimes \mathbf{v} + \left(p + \frac{1}{2}\mathbf{B}^2\right) I - \mathbf{B} \otimes \mathbf{B}\right] = 0, \\ \mathbf{B}_t - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0, \\ e_t + \nabla \cdot \left[\left(\frac{\gamma}{\gamma - 1} p + \frac{1}{2}\rho \mathbf{v}^2\right)\mathbf{v} - (\mathbf{v} \times \mathbf{B}) \times \mathbf{v}\right] = 0, \\ p = (\gamma - 1)(e - (1/2)\rho \mathbf{v}^2 - (1/2)\mathbf{B}^2). \end{cases} \tag{7}$$

Note that system (7) is subject to the divergence-free constraint, that is,$\nabla \cdot \mathbf{B} = 0$, by Gauss's laws for magnetism. Failure in keeping this constraint leads to nonphysical behavior of the system.

As in [3], we will measure the global divergence error of the numerical magnetic field at each time step to validate the results.

For this work we will use the same initial data as [1], so any xz-slice of the 3D solution can be compared to the well-known 2D solution. The initial data is

$$\begin{array}{llll} \rho(x,y,z,0)=\gamma^2, & v_x(x,y,z,0)=-sin(z), & v_y(x,y,z,0)=0 & v_z(x,y,z,0)=sin(x), \\ p(x,y,z,0)=\gamma, & B_x(x,y,z,0)=-sin(z), & B_y(x,y,z,0)=0 & B_z(x,y,z,0)=sin(2x). \end{array} \tag{8}$$

In Table 2 we can see that even in coarser meshes, the Global Divergence Error is very small, suggesting the numerical solution preserves the systems physical properties. Also, the Global Divergence Error diminishes under mesh refinement consistently with the relative error, as expected. The solution profile shown in Figure can be compared with the results shown in Figure 1 (right) can be compared with the results shown in [1] and references therein.

Table 2: Relative Error and Maximum Global Divergence Error $\max(\xi_{div})$[3] for the Orszag-Tang Vortex System on tetrahedral mesh with initial datum (8). CFL=0.04 and $t = 2$.

		Fully-Discrete			Semi-Discrete		
Mesh	Elements	$(e_i^*)_1$	$(e_i)_1$	$\max(\xi_{div})$	$(e_i^*)_1$	$(e_i)_1$	$\max(\xi_{div})$
$(32\times32\times32)\times6$	196608	1.431e-01	5.451e-02	3.413e-02	1.435e-01	5.456e-02	3.403e-02
$(64\times64\times64)\times6$	1572864	9.832e-02	4.348e-02	2.030e-02	9.860e-02	4.361e-02	2.026e-02
$(128\times128\times128)\times6$	12582912	6.059e-02	3.412e-02	1.158e-02	6.078e-02	3.423e-02	1.157e-02
$(256\times256\times256)\times6$	100663296	2.798e-02	2.798e-02	6.447e-03	2.807e-02	2.807e-02	6.443e-03

3.3 Three-Phase Flow System

In this section we focus on the Three-Phase Flow System. Multiphase flow systems are very common in petroleum engineering as they model the flow of fluids through porous media, which is the case of hydrocarbon reservoirs. As in [13], the Three-Phase Flow System may be written as

$$\begin{array}{rl} \frac{\partial S_w}{\partial t}+\frac{\partial f_w^1(S_w,S_g)}{\partial x}+\frac{\partial f_w^2(S_w,S_g)}{\partial y}+\frac{\partial f_w^3(S_w,S_g)}{\partial z} & =0; \\ \frac{\partial S_g}{\partial t}+\frac{\partial f_g^1(S_w,S_g)}{\partial x}+\frac{\partial f_g^2(S_w,S_g)}{\partial y}+\frac{\partial f_g^3(S_w,S_g)}{\partial z} & =0; \\ S_w+S_g+S_o & =1. \end{array} \tag{9}$$

In this work we will consider Corey-Pope type permeability models, with $f_w^1=f_w^2=f_w^3=\frac{S_w^2}{S_w^2+(5/3)S_g^2+(1/2)S_o^2}$ and $f_g^1=f_g^2=f_g^3=\frac{S_w^2}{0.6S_w^2+S_g^2+0.3S_o^2}$.

System (9) will be solved in the spatial domain $\Omega=(0,\,512)\times(0,\,128)\times(0,\,128)$. On the boundaries, we will impose the following conditions:

- On $\mathbf{x}=(0,y,z)$ we will have the Water and Gas injection and therefore use a Dirichlet condition prescribed with the initial condition.
- On $\mathbf{x}=(512,y,z)$ a homogeneous Neumann boundary will let the fluids freely flow out of the domain, in direction of the producing well.
- In the remaining boundaries, a barrier is placed, so the outward velocity is zero.

We will consider the following initial data

$$RP:\begin{cases} S_w^L=0.613 & \text{if } \mathbf{x}=(0,y,z) \text{ and } \quad S_w^R=0.05 \quad \text{elsewhere;} \\ S_g^L=0.387 & \text{if } \mathbf{x}=(0,y,z) \text{ and } \quad S_g^R=0.15 \quad \text{elsewhere.} \end{cases} \tag{10}$$

The results are presented in Tables 3 and illustrated in Figure 2. Again, the schemes presents a consistently diminishing relative error under mesh refinement for both formulations. In Figure 2 (left) we show the Oil Saturation profile, which is composed of a combination of the Water and Gas solution and gives a good overall depiction of the results. Also, to facilitate the evaluation of the results, for this problem we display a 1D slice of the three fluids that can easily be compared to the well-known results presented in [13].

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Table 3: Relative Error for the Three-Phase Flow System on tetrahedral mesh with initial datum (10). CFL=0.04 and $t = 200$.

		Fully-Discrete		Semi-Discrete	
Mesh	Elements	$(e_i^*)_1$	$(e_i)_1$	$(e_i^*)_1$	$(e_i)_1$
$(32 \times 32 \times 32) \times 6$	196608	3.534e-02	1.511e-02	3.530e-02	1.507e-02
$(64 \times 64 \times 64) \times 6$	1572864	2.107e-02	1.031e-02	2.108e-02	1.030e-02
$(128 \times 128 \times 128) \times 6$	12582912	1.099e-02	6.704e-03	1.101e-02	6.712e-03
$(256 \times 256 \times 256) \times 6$	100663296	4.431e-03	4.431e-03	4.325e-03	4.325e-03

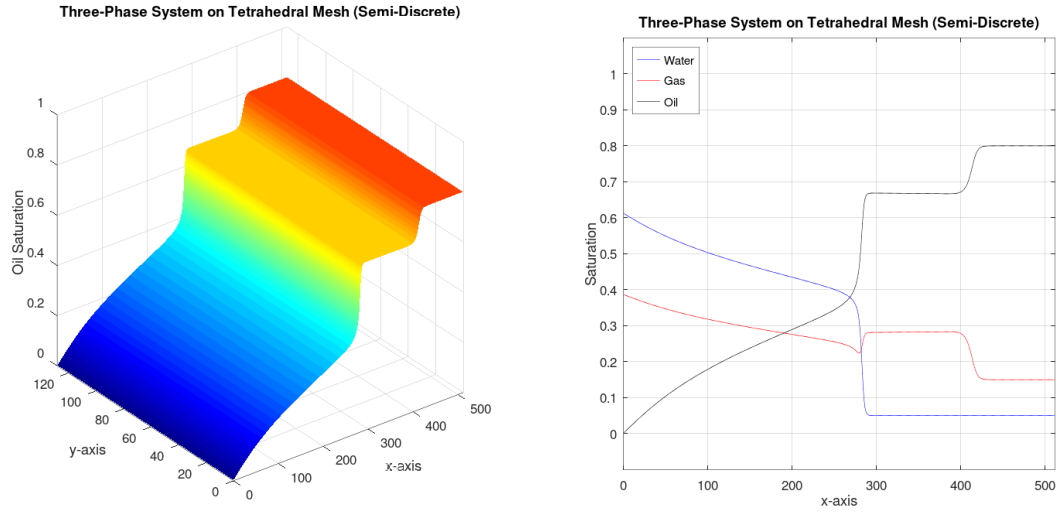

Figure 2: 2D Slice for Oil and 1D Slice of the numerical solution of the Three-Phase Flow System using the Semi-Discrete scheme. The Fully-Discrete generates similar results.

4 Concluding Remarks

In this work, we show an extension of the 3D Lagrangian-Eulerian scheme in a semi-discrete form and apply it to hyperbolic systems from physics and engineering. The 3D Semi-Discrete Lagrangian-Eulerian is independent of the eigen-structure and therefore does not need the use of eigenvalues, calculated or approximated. The proposed systems were numerically solved using the proposed scheme directly in each equation, without any corrective step. The numerical experiments show that the scheme is able to correctly approximate the solution of the problems, with consistent diminishing errors under mesh refinement, giving numerical evidence of the scheme convergence.

These results reinforce the need for a formal mathematical analysis of the scheme properties along with further validating experiments, as are already in work in [9], since the scheme shows promising results for hyperbolic systems.

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