

Brief communication

On improving mass conservation of level set by reducing spatial discretization errors

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1. Introduction

The impact of the Level Set (LS) method on numerical capturing of interfaces (Osher and Fedkiw, 2003; Sethian, 1999) is well known. Widely-reaching applications include fluid mechanics, combustion, computer vision, and material science. As a way of describing immiscible multi-phase flows, the LS was shown to provide a worthy alternative (Sussman et al., 1994) to the already in existence volume-tracking (VT) (Noh and Woodward, 1976; Hirt and Nichols, 1981; Youngs, 1982) and front-tracking (FT) (Chern et al., 1985; Unverdi and Tryggvason, 1992) methods. A comparative evaluation, made by means of a set of test problems which represent flows with significant deformation, stretching, and tearing, was presented by Rider and Kothe (1995). In this study, the LS method was shown to lead to loss (or gain) of mass when fluid filaments become comparable to grid size, while the VT methods were found prone to producing “blobby” structures. In other words, both methods exhibited low accuracy in under-resolved flows, while particle-based, front-tracking methods were shown to perform better in conserving filamentary structures.

In attempts to improve the mass conservation properties of the LS method a number of modifications have been introduced, including a variety of re-initialization (Sussman et al., 1994; Sussman and Fatemi, 1999) and velocity extension (Adalsteinsson and Sethian, 1999) techniques. While these advancements have been found to be helpful in maintaining the level set as a signed distance function (which is especially important for accurate computation of interface curvature in flows with surface tension), they did not meet the objective for such as the above-mentioned, under-resolved (thin-filament) flows. Recognizing that, several “hybrid” methods have been developed, combining the level set with volume-tracking (Sussman and Puckett, 2000; Sussman, 2003) or front-tracking (Enright et al., 2002, 2005). The method developed by Enright et al. (2002) is particularly interesting. Combining a level set function with Lagrangian marker particles, their Particle Level Set (PLS) method was shown to considerably improve mass conservation in under-resolved flows, while maintaining a smooth geometrical description of the interface. Unfortunately, “hybrid” LS + VT and LS + FT methods become significantly more complicated and computationally expensive, especially in parallel 3D implementations.

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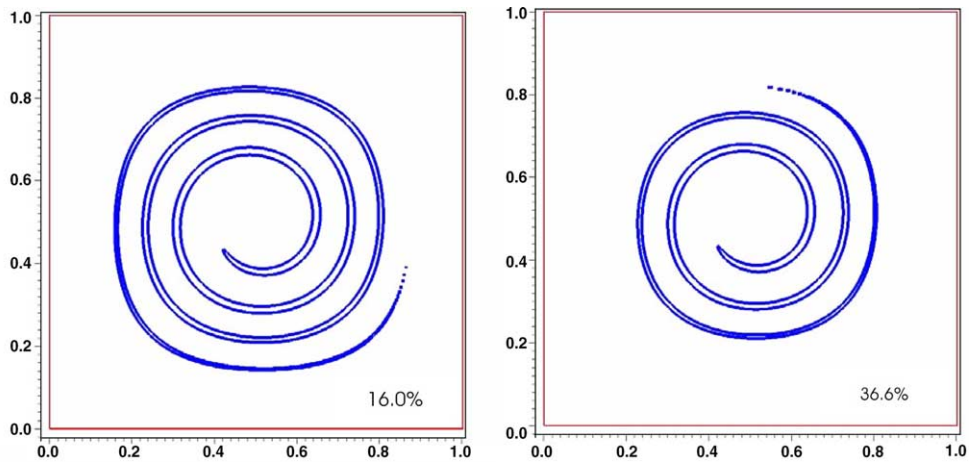


Fig. 1. Effect of non-linear weights of WENO schemes on mass conservation on a “single vortex” numerical test (Rider and Kothe, 1998). Linear (LWENO₅-RK₃, left) vs. non-linear (WENO₅-RK₃, right) schemes. Interface position for $t = 5$. Uniform 256^2 grid. Mass conservation errors are shown in the right lower corners.

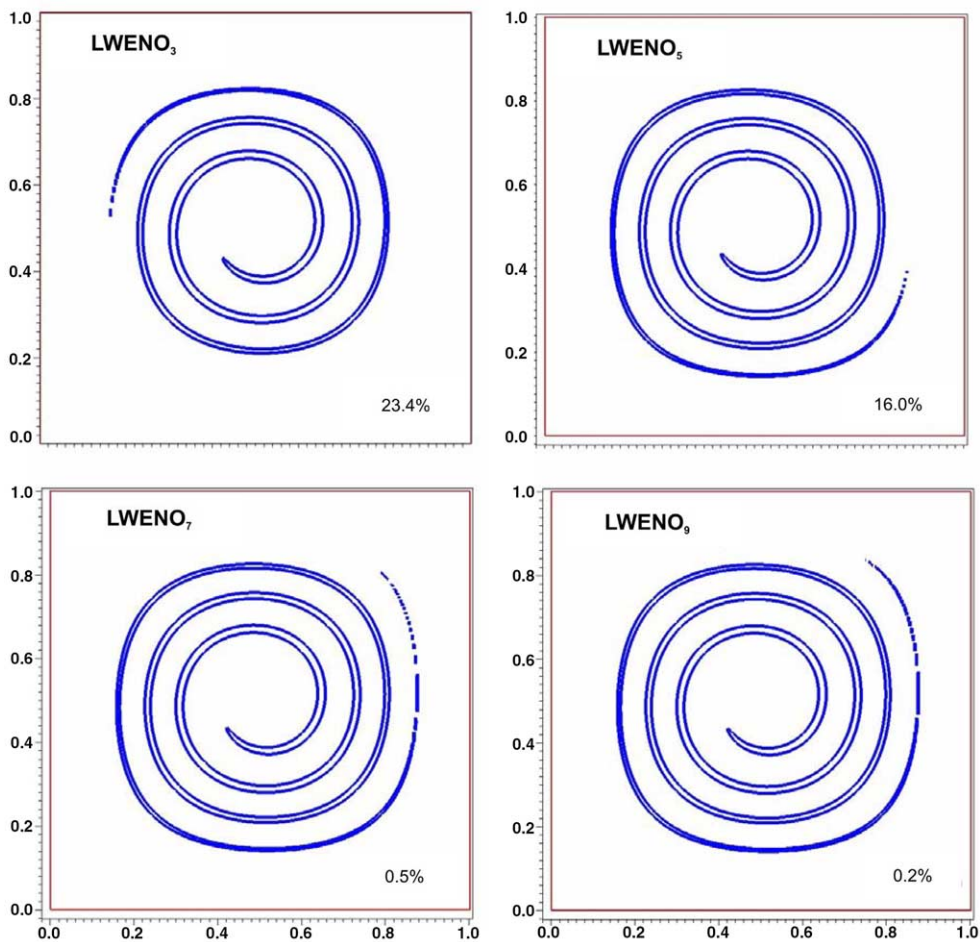


Fig. 2. Effect of accuracy of discretization scheme on mass conservation on a “single vortex” numerical test (Rider and Kothe, 1998). Interface position for $t = 5$. Uniform 256^2 grid. Mass conservation errors are shown in the right lower corners.

The purpose of this note is to suggest that mass conservation of the level set method can be significantly improved by reducing spatial discretization errors, and that this can be accomplished without significant complications in coding, or computational burden. Our approach consists of two synergistic elements: (i) increasing space discretization accuracy by using Linear WENO (LWENO) schemes; and (ii) increasing local resolution by Structured Adaptive Mesh Refinement (SAMR). While the use of AMR for better resolution of interface structures has been attempted previously (e.g., Sussman et al., 1999; Strain, 1999; Sussman, 2003), only Enright et al. (2005) made an effort to demonstrate explicitly improvements in mass conservation. Moreover all these works employed either non-linear third- or non-linear fifth-order schemes (limited MUSCL₃, ENO₃ or WENO₅), which leaves open the potential impact of even higher-order discretization on mass conservation, a rather non-obvious effect, especially in regards to using limiters for a generally smooth level set function. Here, we will demonstrate that with the combination of the LWENO_{7,9} and SAMR, the level set method becomes essentially free of mass conservation errors, while it is still highly efficient, and readily amenable to 3D parallel implementations. The basic ideas and illustrative computational results are described below.

2. Linear Weighted, Essentially Non-Oscillatory (LWENO) schemes

Traditionally, the level set equation is solved using Essentially Non-Oscillatory based (ENO₃ or WENO₅) schemes for polynomial reconstruction in space (Jiang and Shu, 1996; Fedkiw et al., 1999; Sethian, 1999; Osher and Fedkiw, 2003), together with different approximate Riemann solvers for computation of the Hamiltonian. The *N*th-order-accurate WENO_{*N*} reconstruction scheme is a combination of $n = \frac{N+1}{2}$, *n*th-order-accurate polynomials:

$$P_{\text{WENO}_N}(x) = \sum_k^n w_k P_k^{(n)}(x) \tag{1}$$

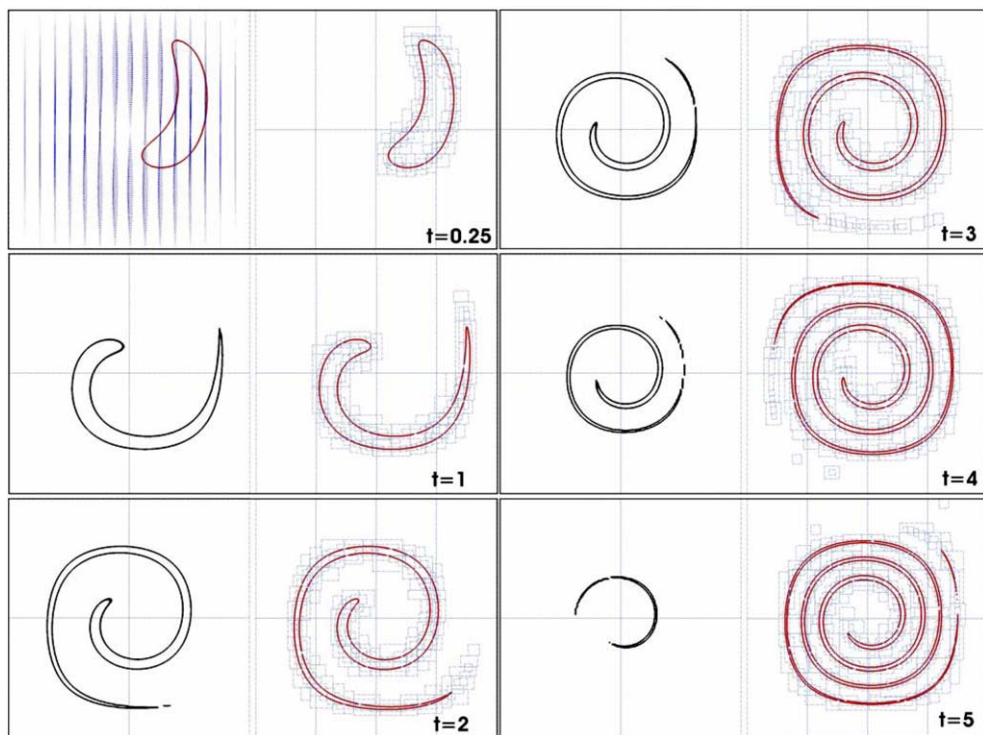


Fig. 3. Dynamics of interface on a “single vortex” numerical test (Rider and Kothe, 1998). Uniform 128² grid (left) vs. SAMR_{512²}^{2/3} (right), both using WENO₅-RK₃.

where w_k are non-linear weights, designed to “catch” discontinuities and eliminate oscillations associated with them. Computation of non-linear weights is the most expensive part, taking roughly half of total time for WENO-based reconstructions. In addition, these weights introduce extra numerical diffusion—so that in practice the accuracy of these schemes is always between n th and N th order. Since the level set is a smooth function, computation of non-linear weights is not needed, and instead we can use “optimal”, constant weights. Hereafter, we will denote these schemes as Linear WENO (LWENO). Optimal weights for N ranging from 5th to 11th-order have been obtained by Balsara and Shu (2000).

The effects of high-order-accurate discretization of the level set equation are demonstrated by sample results shown in Figs. 1 and 2 for a single-vortex flow (Rider and Kothe, 1998). Importantly, no re-initialization techniques are employed here. The use of optimal instead of non-linear weights, both in the 5th-order scheme, allows to reduce mass losses in this example from 37% to 16%. Further reductions of error are possible by increasing the order of the discretization scheme, until, at the 9th order, errors in this example are virtually eliminated. Such mass conservation errors of the LWENO₉ for rotating, stretching, and tearing flows are comparable to those of the PLS method (Enright et al., 2002, 2005).

3. Structured Adaptive Mesh Refinement (SAMR)

Numerical discretization errors can be further reduced by adaptive mesh refinement. Here, we utilize the structured adaptive mesh refinement technology, developed by Berger and co-authors for hyperbolic conservation laws (Berger, 1986; Berger and Collela, 1989; Berger and Rigoutsos, 1991), and implemented as the SAMRAI library (Hornung and Kohn, 2002; Wissink et al., 2003) at the Lawrence Livermore National

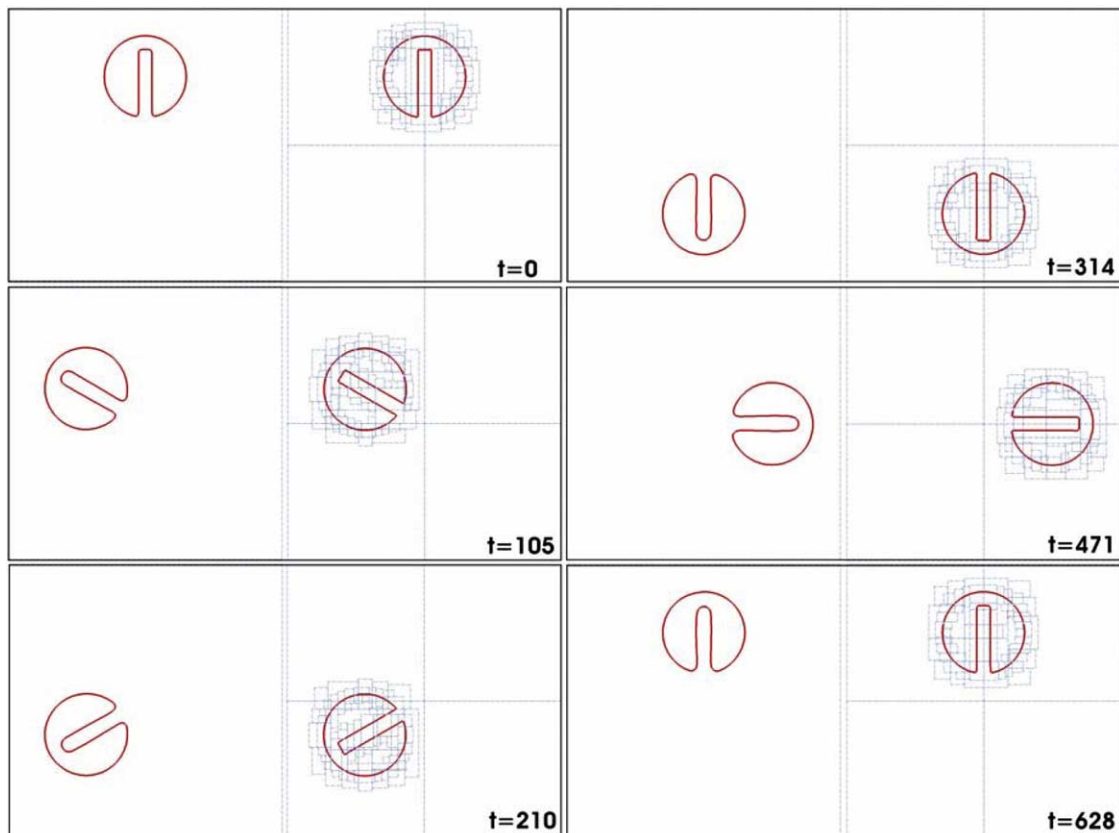


Fig. 4. Dynamics of interface on a “Zalesak’s disk” numerical test (Zalesak, 1979). Uniform 100^2 grid (left) vs. SAMR $_{400^2}^{2/3}$ (right), both using WENO₅-RK₃. Mass conservation errors: 1% (left), 0.1% (right).

Laboratory (LLNL). The SAMR solution techniques share certain characteristics with parallel uniform structured grid methods, such as storage of simulation data by arrays, and representation of the numerical solution on logically rectangular regions. In the present study, we modified this approach to make it suitable for solving the level set (non-conservative Hamilton–Jacobi) equation, it being addressed via Linear Weighted Essentially Non-Oscillatory schemes as described above. In addition, the algorithm was adapted for the multi-level Runge–Kutta, time-discretization scheme (RK₃-TVD) (Shu and Osher, 1989), used in place of the single-level, “corner-transport” scheme originally used in (Berger and Collela, 1989). Hereafter, we denote AMR simulations as SAMR_C^{A/B}, where *A* is the grid refinement ratio between levels of adaptation in a hierarchy of SAMR grids, *B* is the total number of levels in a hierarchy, and *C* is the effective grid resolution if corresponding uniform grids were applied.

Considering first the single-vortex problem, Fig. 3 shows that with AMR we can negate the deficiency of non-linear WENO relative to LWENO (shown in Fig. 2). For the “Zalesak disk” problem, Fig. 4 shows that in single rotation the non-linear WENO is not as detrimental, while the AMR still is of benefit in maintaining the sharpness in corners. In the “rigid-body rotation of a 3D slotted cube” and the “time reversed single vortex” problems, Figs. 5 and 6 demonstrate the combined benefit of LWENO on AMR grids.

As a concluding note, we would like to mention that in some types of flows, such as time-reversed 2D and 3D deformation tests (Rider and Kothe, 1995, 1998; Enright et al., 2002, 2005), performance of high-order-

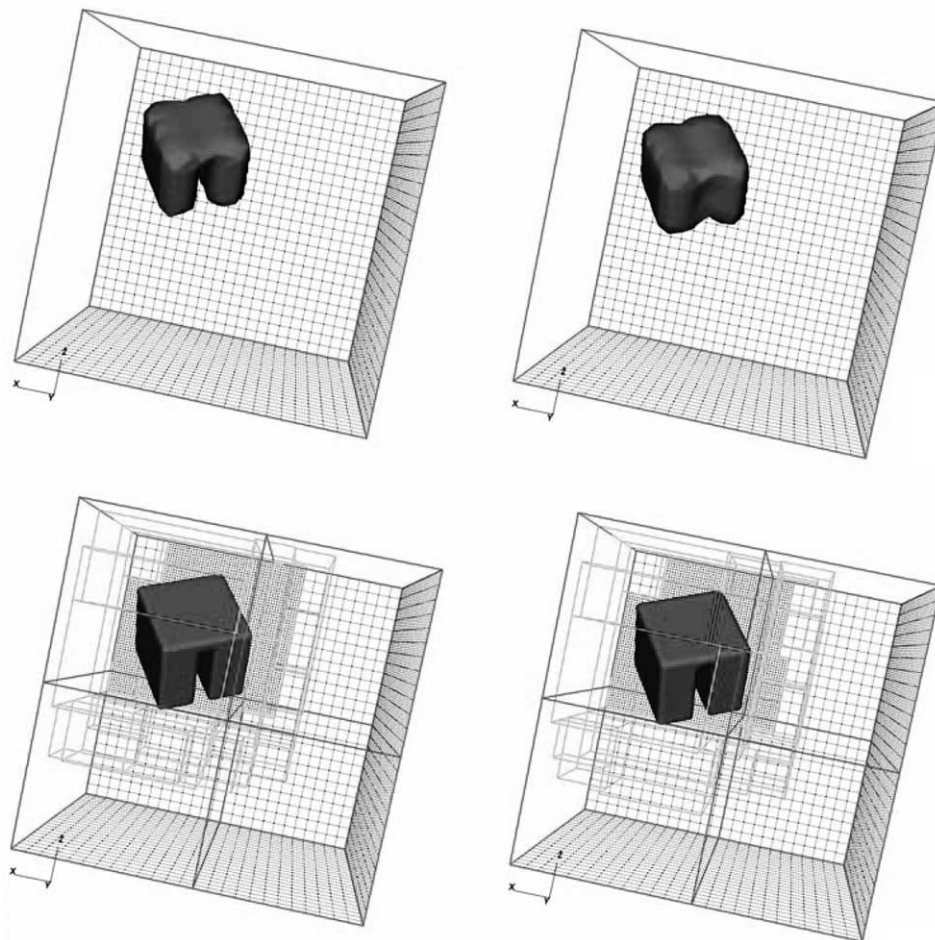


Fig. 5. Interface position on a “rigid-body rotation of 3D slotted cube” numerical test, at the beginning (left) and after one revolution (right). Uniform 25^3 grid (top) vs. SAMR_{100²}^{4/2} (bottom), both using LWENO₇-RK₃. AMR patches are shown in red and green (for color version of this figure, the reader is referred to the web version of this article). Mass conservation errors: 7.1% (top), 0.88% (bottom).

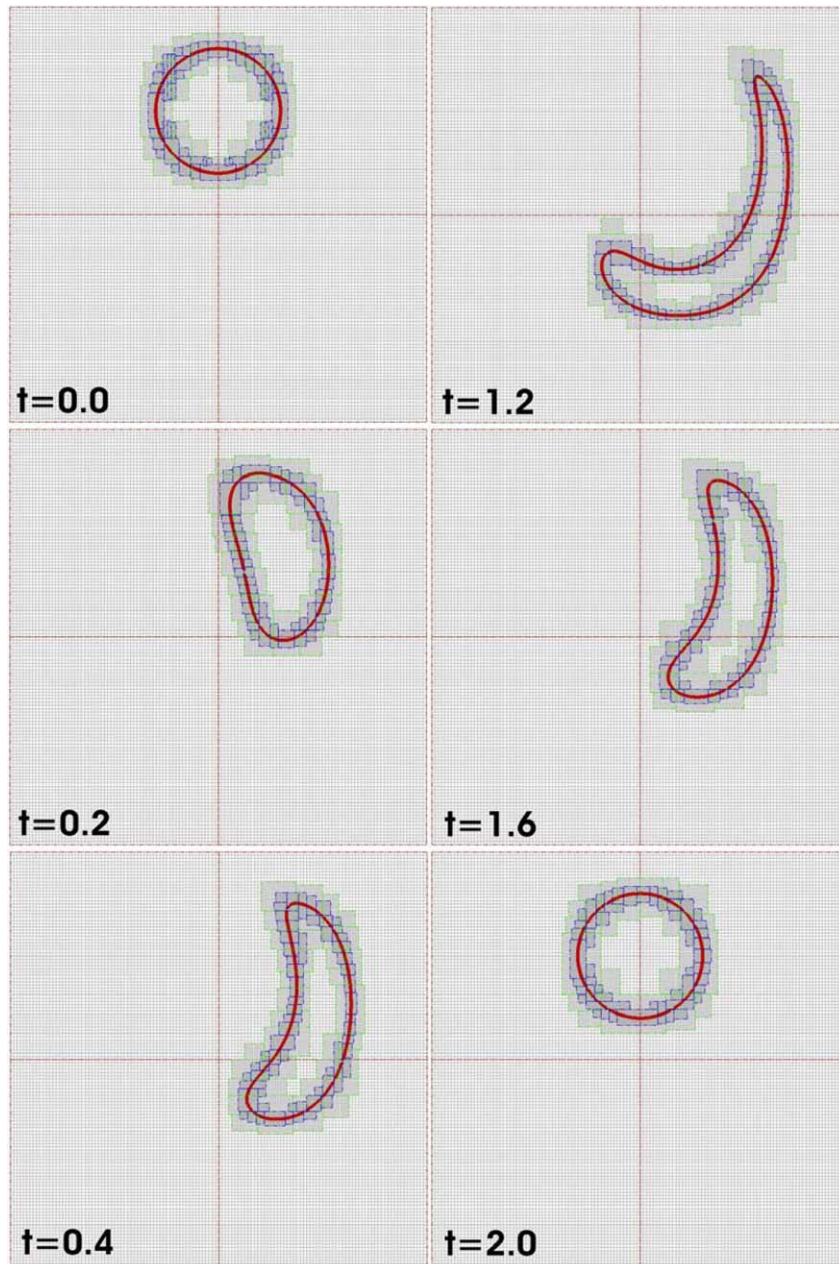


Fig. 6. One cycle of a “time-reversed single-vortex” numerical test (Rider and Kothe, 1998). Solution using $\text{SAMR}_{512^2}^{2/3}$ with LWENO₅-RK₃. AMR patches are shown in blue and green (for color version of this figure, the reader is referred to the web version of the article), computational mesh—in grey. Mass conservation error: 0.005%.

accurate LWENO with AMR is still not quite satisfactory. While formally conserving mass within 1–2%, the final shape of the interface at the end of the time-reversed cycle is different from its original (spherical) shape, see Fig. 7(a) vs. (f). The reason is in irreversible deformation of the interface when an infinitely thin sheet of advected material is formed at the middle of the cycle, Fig. 7(c). As a result of numerical discretization errors, blobby structures are created (Fig. 7(e)), very similar to those reported by Rider and Kothe for their VOF computations (Rider and Kothe, 1998). The final result of this “numerical surface tension” is a formation of a “slot” at one side of a sphere and “bulge” on the other, see Fig. 7(f). For these types of flows the

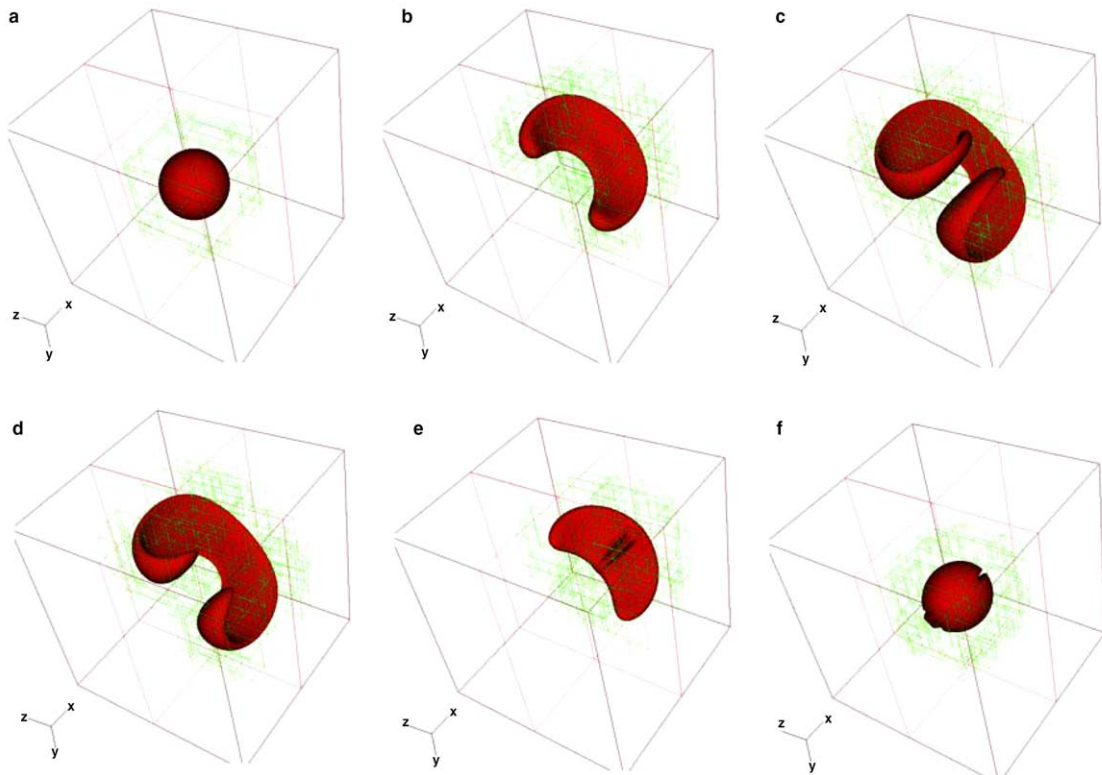


Fig. 7. One cycle of a “time-reversed 3D deformation” numerical test (Enright et al., 2002). Solution using SAMR $_{200}^{4/2}$ with LWENO $_9$ -RK $_3$. AMR patches are shown in red and green. Mass conservation error: 1.8%.

PLS method (Enright et al., 2002, 2005) could be better, provided sufficiently large numbers of particles were seeded. Moreover, in principle, pure front-tracking methods may still have the accuracy advantage more broadly, however, no direct quantitative comparison exists that pit levels of accuracy against amounts of computational effort. Even then, there would remain the issue of accessibility (simplicity) of the numerical scheme, as discussed at the beginning of this note.

Acknowledgments

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