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Highlights

- High order numerical schemes are developed by which highly accurate estimations for the ELI of the interpolated particles can be acquired.
- New evolution equations are derived for tracking the ELI of all the interfacial particles.
- Transformation formulae are derived for modifying the derivatives of the particles' location coordinates such that large amplitudes of which can be avoided.

A new front tracking method using particles with extended location information

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Abstract

A new front tracking method is developed through using Lagrangian particles marked by their extended location information (ELI) including the location coordinates and the spatial derivatives of the location coordinates. The new method is capable of providing more accurate descriptions for the geometrical features of the interface than the conventional front tracking (CFT) methods due to three key originalities. First, high order numerical schemes that can be used to evaluate the ELI of the interpolated particles with high order accuracy are developed based on the ELI of two given particles. Second, a series of evolution equations are derived on the need of tracking the ELI of all the particles during the interface evolving. Third, transformation formulae are derived for the use of modifying the spatial derivatives of the particles' location coordinates such that large amplitudes of which can be avoided. Performances of the new method are demonstrated through standard benchmark tests.

Keywords: moving interface; front tracking; numerical scheme; extended location information

1. Introduction

How to accurately and efficiently model the interface evolution is not only fundamental but also much challenging to a wide range of mathematical and engineering problems. The existing numerical methods for simulating the moving interface can be totally categorized into two kinds. The first kind is usually called the front capturing methods which define the interface implicitly by using a scalar field function and advect this function from solving a transport equation. As one typical of the capturing methods, the volume of fluid (VOF) method uses the volume fraction to discriminate each cell of the computational domain and reconstructs the interface

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from computing the fluxes across the cell boundary [Hirt & Nichols 1981; Rider & Kothe 1998; Gueyffier et al. 1998; Scardovelli & Zaleski 1999]. The other typical of the capturing methods, Level-Set method, defines the interface as the zero level of a signed distance function and modifies this function via a re-initialization process [Osher & Sethian 1988; Sethian 1996; Osher & Fedkiw 2001; Sethian 2001; Osher & Fedkiw 2003; Sethian & Smereka 2003]. One major benefit of the capturing methods is that the topological changes, such as merging and splitting, can be handled easily with few additional computational efforts. On the other hand, capturing methods are usually less accurate than the tracking methods because of the implicit inference. In the presence of thin filaments the capturing methods usually generate incorrect topologies by breaking the interface into numerous unphysical blobs.

The second kind is the front tracking methods which define the interface explicitly and track the interface from solving an ordinary differential equation for the particles' location coordinates [Unverdi & Tryggvason 1992; Glimm et al. 2000; Tryggvason et al. 2001; Sousa et al. 2004; Fan 2008]. These methods have the advantage of describing the interface more accurately than the capturing methods. On the other hand, there are still practical limitations in the CFT methods such as difficulty to achieve consistency between the interface advection and flow solvers. To obtain velocities at the interfacial points the CFT methods usually employ the kernel interpolation formula [Peskin 1977; Unverdi & Tryggvason 1992; Tryggvason et al. 2001; Hieber & Koumoutsakos 2005] which is practically 1st-order of accuracy due to the 1st-order discretization for the integral operator and the unavoidable asymmetrical distributions of the sampling grid points about each interfacial points. Furthermore, the approach used in the CFT methods for estimating the tangent and normal vectors of a 3D interface is 1st-order of accuracy as well because which is essentially based on 3-points elements, i.e., using the linear approximation for the tangent plane at the point of interest.

A variant tracking method was proposed by Tornberg & Engquist [2003] in which a third order ENO (essentially non-oscillatory) scheme was used for the interpolations of particles, however, limited on a same curve. The scheme they used has clearly only one independent variable and is hence inapplicable for the 3D problems in which the location function is relied on two independent variables. As a consequence, this method had to resort additionally to the kernel interpolation formula for the interpolations of new particles on a curved plane, which manifests this method is also 1st-order of accuracy for the 3D problems.

Recently, a lot of hybrid methods were developed in the attempt of suitably combining the best features of the capturing and tracking methods, such as the CLSVOF (coupled Level-Set and VOF) method [Sussman & Puckett 2000; Sussman 2003], the level contour reconstruction methods [Shin & Juric 2002], the marker-VOF method [Aulisa et al. 2003; Aulisa et al. 2004] and the particle Level-Set (PLS) method [Enright et al. 2002; Hieber & Koumoutsakos 2005; Ianniello & Mascio 2010;

Vartdal & Bøckmann 2013; Bøckmann & Vartdal 2014; Jiang et al. 2015]. Furthermore, in [Leung & Zhao 2009; Hon et al. 2014] the Lagrangian particles are associated to the grid nodes, while, in [Nave et al. 2010; Ianniello & Mascio 2010; Vartdal & Bøckmann 2013; Bøckmann & Vartdal 2014] the gradient or normal vector and curvature information are incorporated to the Level-Set function to improve the accuracy of the Level-Set methods.

In this paper a new front tracking method is developed which can provide more accurate descriptions for the geometrical features of the interface than the CFT methods. The new method, named as the extended location information particles (ELIP) method, employs Lagrangian particles marked by not only their location coordinates but also the spatial derivatives of the location coordinates. The new method is constructed based on three key originalities. First, based on the ELI of two given particles high order numerical schemes that can be used to achieve highly accurate estimations for the ELI of the interpolated particles are developed. Furthermore, a series of evolution equations are derived for tracking the ELI of all the particles during the interface evolving. Third, transformation formulae are derived for modifying the spatial derivatives of the particles' location coordinates such that large amplitudes of which can be avoided.

The outline of this paper is as follows. In section 2 the evolution equations and transformation formulae for tracking and modifying the ELI of all the interfacial particles are derived, respectively. The numerical schemes that can be used to estimate the ELI of the interpolated particles with high order accuracy are developed in section 3. In section 4 the reconnection and redistribution algorithms are specified. In section 5 we present validations of the new method by considering 2D and 3D benchmark problems and section 6 concludes this paper.

2. Evolution equations and transformation formulae for the ELI

2.1. Formulae for relating the ELI with the geometrical quantities of the interface

As a chief feature, the ELIP method uses not only the location coordinates of the interfacial particles but also the spatial derivatives of the location coordinates. Thus, in the ELIP method all of the interfacial particles are specified using the extended dimension data, such as (x, y, y_x, y_{xx}, k) for a 2D interface defined by $y = y(x)$ and $(x, y, z, z_x, z_y, z_{xx}, z_{xy}, z_{yy}, k)$ for a 3D interface defined by $z = z(x, y)$. Hereinafter, any variable with x, y and z appearing in the subscript represents the partial derivative of this variable with respect to x, y and z , respectively. The index k represents the axis-direction, i.e., $k = \pm 1, \pm 2$ and ± 3 representing the positive and negative x -, y - and

z -directions, respectively. Given the ELI of the interfacial particles, the geometrical quantities, such as the normal vector and curvature, can be computed from the following formulae.

For a 2D interface defined explicitly by $y = y(x)$ or $x = x(y)$, the unit normal vector and curvature can be calculated, respectively, by

$$\mathbf{n} = \begin{cases} \frac{k}{|k|} \frac{(-y_x, 1)}{\sqrt{1+y_x^2}}, & k = \pm 2; \\ \frac{k}{|k|} \frac{(1, -x_y)}{\sqrt{1+x_y^2}}, & k = \pm 1 \end{cases} \quad (1)$$

$$\kappa = \begin{cases} \frac{|y_{xx}|}{\sqrt{(1+y_x^2)^3}}, & k = \pm 2; \\ \frac{|x_{yy}|}{\sqrt{(1+x_y^2)^3}}, & k = \pm 1 \end{cases} \quad (2)$$

For a 3D interface specified explicitly by $z = z(x, y)$, $y = y(x, z)$ or $x = x(y, z)$, the local unit normal vector and mean curvature can be evaluated, respectively, by

$$\mathbf{n} = \begin{cases} \frac{k}{|k|} \frac{(-z_x, -z_y, 1)}{\sqrt{z_x^2 + z_y^2 + 1}}, & k = \pm 3; \\ \frac{k}{|k|} \frac{(-y_x, 1, -y_z)}{\sqrt{1+y_x^2+y_z^2}}, & k = \pm 2; \\ \frac{k}{|k|} \frac{(1, -x_y, -x_z)}{\sqrt{1+x_y^2+x_z^2}}, & k = \pm 1 \end{cases} \quad (3)$$

$$\kappa = \begin{cases} \frac{\left| (1+z_x^2)z_{yy} - 2z_xz_yz_{xy} + (1+z_y^2)z_{xx} \right|}{2\sqrt{(1+z_x^2+z_y^2)^3}}, & k = \pm 3; \\ \frac{\left| (1+y_x^2)y_{zz} - 2y_xy_zy_{xz} + (1+y_z^2)y_{xx} \right|}{2\sqrt{(1+y_x^2+y_z^2)^3}}, & k = \pm 2; \\ \frac{\left| (1+x_y^2)x_{zz} - 2x_yx_zx_{yz} + (1+x_z^2)x_{yy} \right|}{2\sqrt{(1+x_y^2+x_z^2)^3}}, & k = \pm 1 \end{cases} \quad (4)$$

2.2. Evolution equations of the ELI

Once the initial values of the ELI of all the interfacial particles are given, the instantaneous values of the ELI at any arbitrary time moment can be computed from solving the following evolution equations.

(1) 2D

From the definition of the vertical velocity component of a Lagrangian particle lying on an interface defined by $y = y(x)$, it is obvious that

$$y_t = v - uy_x \quad (5)$$

where t denotes the time variable; u and v are the horizontal and vertical components of the velocity, respectively. Hereinafter, any variable with t appearing in the subscript represents the partial derivative of this variable with respect to t . By taking derivatives on the above equation with respect to x , one can derive the following evolution equations for y_x and y_{xx}

$$\frac{dy_x}{dt} = y_{xt} + uy_{xx} = v_x + y_x(v_y - u_x) - y_x^2 u_y \quad (6)$$

$$\begin{aligned} \frac{dy_{xx}}{dt} = y_{xxt} + uy_{xxx} = v_{xx} + y_x(2v_{xy} - u_{xx}) + y_{xx}(v_y - 2u_x) + y_x^2(v_{yy} - 2u_{xy}) \\ - 3y_x y_{xx} u_y - y_x^3 u_{yy} \end{aligned} \quad (7)$$

Similarly, if an interface is defined by $x = x(y)$, the evolution equations for x_y and x_{yy} can be obtained, given by

$$\frac{dx_y}{dt} = u_y + x_y(u_x - v_y) - x_y^2 v_x \quad (8)$$

$$\begin{aligned} \frac{dx_{yy}}{dt} = u_{yy} + x_y(2u_{xy} - v_{yy}) + x_{yy}(u_x - 2v_y) + x_y^2(u_{xx} - 2v_{xy}) \\ - 3x_y x_{yy} v_x - x_y^3 v_{xx} \end{aligned} \quad (9)$$

(2) 3D

From the definition of the z -component of the velocity of a particle lying on an interface defined by $z = z(x, y)$, it can be yielded that

$$z_t = w - uz_x - vz_y \quad (10)$$

where w is the z -component of the velocity. By taking partial derivatives on the above equation with respect to x and y , respectively, one can derive the following evolution equations for z_x , z_y , z_{xx} , z_{xy} and z_{yy}

$$\begin{aligned} \frac{dz_x}{dt} = z_{xt} + uz_{xx} + vz_{xy} \\ = w_x + z_x(w_z - u_x) - z_y v_x - z_x z_y v_z - z_x^2 u_z \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{dz_y}{dt} &= z_{yt} + uz_{xy} + vz_{yy} \\ &= w_y - z_x u_y + z_y (w_z - v_y) - z_x z_y u_z - z_y^2 v_z \end{aligned} \quad (12)$$

$$\begin{aligned} \frac{dz_{xx}}{dt} &= z_{xxt} + uz_{xxx} + vz_{xxy} \\ &= w_{xx} + z_x (2w_{xz} - u_{xx}) - z_y v_{xx} + z_{xx} (w_z - 2u_x) - 2z_{xy} v_x \\ &\quad - 2z_x z_y v_{xz} - 3z_x z_{xx} u_z - 2z_x z_{xy} v_z - z_y z_{xx} v_z + z_x^2 (w_{zz} - 2u_{xz}) \\ &\quad - z_x^2 z_y v_{zz} - z_x^3 u_{zz} \end{aligned} \quad (13)$$

$$\begin{aligned} \frac{dz_{xy}}{dt} &= z_{xyt} + uz_{xxy} + vz_{xyy} \\ &= w_{xy} + z_x (w_{yz} - u_{xy}) + z_y (w_{xz} - v_{xy}) - z_{xx} u_y + z_{xy} (w_z - u_x - v_y) - z_{yy} v_x \\ &\quad + z_x z_y (w_{zz} - u_{xz} - v_{yz}) - 2z_x z_{xy} u_z - z_x z_{yy} v_z - z_y z_{xx} u_z - 2z_y z_{xy} v_z \\ &\quad - z_x^2 u_{yz} - z_y^2 v_{xz} - z_x z_y^2 v_{zz} - z_x^2 z_y u_{zz} \end{aligned} \quad (14)$$

$$\begin{aligned} \frac{dz_{yy}}{dt} &= z_{yyt} + uz_{xyy} + vz_{yyy} \\ &= w_{yy} - z_x u_{yy} + z_y (2w_{yz} - v_{yy}) - 2z_{xy} u_y + z_{yy} (w_z - 2v_y) \\ &\quad - 2z_x z_y u_{yz} - z_x z_{yy} u_z - 3z_y z_{yy} v_z - 2z_y z_{xy} u_z + z_y^2 (w_{zz} - 2v_{yz}) \\ &\quad - z_x z_y^2 u_{zz} - z_y^3 v_{zz} \end{aligned} \quad (15)$$

The evolution equations of the ELI for an interface defined by $y = y(x, z)$ and $x = x(y, z)$ are presented in the Appendix A for sake of concision.

Note that in the practical simulations, the velocities and their spatial derivatives on the right hand sides (RHS) of the above evolution equations should be obtained from the flow solvers. This process is simplified in the present paper by considering some oft studied benchmark tests in which the velocities and their spatial derivatives are specified analytically. The values of these quantities at the interfacial points are obtained directly by using their analytical values. Furthermore, to study effect of the discrete specification of the velocity field, special simulations are run additionally in section 5.4 with the velocities and their spatial derivatives acquired in the following way. First, the velocity field is specified analytically but discretely on the computational grids. Then, the spatial derivatives of the velocity field are evaluated numerically by using high order difference schemes. At last, the velocities and their numerically evaluated spatial derivatives are interpolated from the computational grids to the interfacial points though using high order Lagrangian interpolation formula.

2.3. Transformation formulae for the ELI

In the previous sub-section we have derived the evolution equations for the ELI of the interfacial particles. On the other hand, one may find in practical computations that the spatial derivatives of the particles' location coordinates, e.g., y_x , may become increasingly very large during the evolution of the interface, which eventually ceases the computation. To avoid such a singularity, an effective way is to change the definition of the interface to its inverse style. Specifically, if the amplitude of y_x exceeds 1.5 (one can also set other critical values that is slightly larger than 1), we can change the definition of the interface from $y = y(x)$ to $x = x(y)$, and, consequently, the spatial derivative of the particles' location coordinates is described by x_y , amplitude of which will be smaller than that of y_x . Apparently, from such a transformation implementation, the spatial derivatives of the particles' location coordinates can always be kept below a finite value 1.5 and the computation is hence kept stable. All of the transformation formulae for modifying the ELI are specified as follows.

(1) 2D

Consider a 2D interface defined by $y = y(x)$, the Taylor's series expansion of which about (x_0, y_0) is written by

$$y = y_0 + (x - x_0) y_{x0} + \sum_{n=2}^{\infty} \frac{(x - x_0)^n}{n!} y_{x0}^{(n)} \quad (16)$$

where $y_{x0}^{(n)}$ denotes the n^{th} derivative of y with respect to x about (x_0, y_0) . The above formula can also be used to describe the inverse function $x = x(y)$ in the vicinity of (x_0, y_0) . By taking derivatives on the above formula with respect to y and taking the results at (x_0, y_0) , one can have

$$x_{y0} = \frac{1}{y_{x0}}, \quad x_{yy0} = -\frac{y_{xx0}}{y_{x0}^3} \quad (17)$$

The above two formulae are just the transformation formulae for the ELI of the interfacial particles when definitions of which are modified from $y = y(x)$ to $x = x(y)$.

Similarly, when definition of a 2D interface is modified from $x = x(y)$ to $y = y(x)$ the transformation formulae are given by

$$y_x = \frac{1}{x_y}, \quad y_{xx} = -\frac{x_{yy}}{x_y^3} \quad (18)$$

(2) 3D

Consider a 3D interface specified by $z = z(x, y)$, the Taylor's series expansion of which about (x_0, y_0, z_0) can be expressed as

$$z = z_0 + (x - x_0) z_{x0} + (y - y_0) z_{y0} + \sum_{n=2}^{\infty} \frac{1}{n!} [(x - x_0) \partial_{x0} + (y - y_0) \partial_{y0}]^n z \quad (19)$$

1 where $(\partial_{x0})^n z$ and $(\partial_{y0})^n z$ represent the n^{th} partial-derivatives of z about (x_0, y_0, z_0) with
 2 respect to x and y , respectively. One can certainly use the above formula to describe
 3 the inverse function $x = x(y, z)$ in the vicinity of (x_0, y_0, z_0) . By taking partial
 4 derivatives of the above formula with respect to y and z , respectively, and taking the
 5 results at (x_0, y_0, z_0) , one can have

$$\begin{aligned} x_{y0} &= -\frac{z_{y0}}{z_{x0}}, \quad x_{z0} = \frac{1}{z_{x0}}, \\ x_{yy0} &= \frac{-z_{x0}^2 z_{yy0} + 2z_{x0} z_{y0} z_{xy0} - z_{y0}^2 z_{xx0}}{z_{x0}^3}, \\ x_{yz0} &= \frac{z_{y0} z_{xx0} - z_{x0} z_{xy0}}{z_{x0}^3}, \quad x_{zz0} = \frac{-z_{xx0}}{z_{x0}^3} \end{aligned} \quad (20)$$

7 The above five formulae are just the transformation formulae for the ELI of the
 8 interfacial particles when definitions of which are modified from $z = z(x, y)$ to $x = x(y, z)$.
 9 Similarly, if the definition of a 3D interface is modified from $z = z(x, y)$ to $y = y(x, z)$
 10 the transformation formulae read

$$\begin{aligned} y_x &= -\frac{z_x}{z_y}, \quad y_z = \frac{1}{z_y}, \\ y_{xx} &= \frac{-z_x^2 z_{yy} + 2z_x z_y z_{xy} - z_y^2 z_{xx}}{z_y^3}, \\ y_{xz} &= \frac{z_x z_{yy} - z_y z_{xy}}{z_y^3}, \quad y_{zz} = \frac{-z_{yy}}{z_y^3} \end{aligned} \quad (21)$$

12 In addition to the above two groups of formulae, there are four more groups formulae
 13 indispensable as well. Specifically, if the definition of a 3D interface is modified from
 14 $y = y(x, z)$ to $x = x(y, z)$ or from $y = y(x, z)$ to $z = z(x, y)$, the transformation formulae
 15 are given, respectively, by

$$\begin{aligned} x_y &= \frac{1}{y_x}, \quad x_z = -\frac{y_z}{y_x}, \\ x_{yy} &= \frac{-y_{xx}}{y_x^3}, \quad x_{yz} = \frac{y_z y_{xx} - y_x y_{xz}}{y_x^3}, \\ x_{zz} &= \frac{-y_x^2 y_{zz} + 2y_x y_z y_{xz} - y_z^2 y_{xx}}{y_x^3} \end{aligned} \quad (22)$$

17 and

$$\begin{aligned} z_x &= -\frac{y_x}{y_z}, \quad z_y = \frac{1}{y_z}, \\ z_{xx} &= \frac{-y_x^2 y_{zz} + 2y_x y_z y_{xz} - y_z^2 y_{xx}}{y_z^3}, \\ z_{xy} &= \frac{y_x y_{zz} - y_z y_{xz}}{y_z^3}, \quad z_{yy} = \frac{-y_{zz}}{y_z^3} \end{aligned} \quad (23)$$

Furthermore, if the definition of a 3D interface is modified from $x = x(y, z)$ to $y = y(x, z)$ or from $x = x(y, z)$ to $z = z(x, y)$ the transformation formulae are given, respectively, by

$$\begin{aligned} y_x &= \frac{1}{x_y}, \quad y_z = -\frac{x_z}{x_y}, \\ y_{xx} &= \frac{-x_{yy}}{x_y^3}, \quad y_{xz} = \frac{x_z x_{yy} - x_y x_{yz}}{x_y^3}, \\ y_{zz} &= \frac{-x_y^2 x_{zz} + 2x_y x_z x_{yz} - x_z^2 x_{yy}}{x_y^3} \end{aligned} \quad (24)$$

and

$$\begin{aligned} z_x &= \frac{1}{x_z}, \quad z_y = -\frac{x_y}{x_z}, \\ z_{xx} &= \frac{-x_{zz}}{x_z^3}, \quad z_{xy} = \frac{x_y x_{zz} - x_z x_{yz}}{x_z^3}, \\ z_{yy} &= \frac{-x_y^2 x_{zz} + 2x_y x_z x_{yz} - x_z^2 x_{yy}}{x_z^3} \end{aligned} \quad (25)$$

Note that all of the above transformation formulae can also be derived based on the implicit interface function which is presented in the Appendix B.

3. Numerical schemes for estimating the ELI of the interpolated particles

In this section the high order numerical schemes that can be used to achieve highly accurate estimations for the ELI of the interpolated particles are developed. The complete derivations of the schemes are presented in the Appendices C, D and E for concision.

3.1. 2D

3.1.1. Numerical schemes for approximating the function values

(i) 4th-order formulae based on stencil $\{y_1, y_2, y_{x1}, y_{x2}\}$

Given two function values y_1 and y_2 together with their first derivatives y_{x1} and y_{x2} , the 4th-order non-ENO approximation to the function value y at the given location x , denoted by $y^{intp-4th}$, can be written as

$$y^{intp-4th} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-3rd-1} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1} \right) y^{intp-3rd-2} \quad (26)$$

1 where $\delta_1 = x_1 - x$, $\delta_2 = x_2 - x$; $y^{intp-3rd-1}$ and $y^{intp-3rd-2}$ denote two 3rd-order
 2 approximations to y , defined, respectively, by

$$y^{intp-3rd-1} = \frac{-\delta_1}{\delta_2 - \delta_1} y^{intp-2nd-1} + \left(1 - \frac{-\delta_1}{\delta_2 - \delta_1}\right) y^{intp-2nd-2},$$

$$y^{intp-3rd-2} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-2nd-1} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y^{intp-2nd-3}$$

4 In the above formulae $y^{intp-2nd-1}$, $y^{intp-2nd-2}$ and $y^{intp-2nd-3}$ denote three 2nd-order
 5 approximations to y , defined, respectively, by

$$y^{intp-2nd-1} = \frac{\delta_2}{\delta_2 - \delta_1} y_1 + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y_2,$$

$$y^{intp-2nd-2} = y_1 - \delta_1 y_{x1},$$

$$y^{intp-2nd-3} = y_2 - \delta_2 y_{x2}$$

7
 8 **(ii) 6th-order formulae based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$**

9 Given two function values y_1 and y_2 together with their first and second derivatives y_{x1} ,
 10 y_{x2} , y_{xx1} and y_{xx2} , the 6th-order non-ENO approximation to the function value y at the
 11 given location x , denoted by $y^{intp-6th}$, is given by

$$y^{intp-6th} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-5th-1} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y^{intp-5th-2}$$

13 where $y^{intp-5th-1}$ and $y^{intp-5th-2}$ denote two 5th-order approximations to y , defined as

$$y^{intp-5th-1} = \frac{-\delta_1}{\delta_2 - \delta_1} y^{intp-4th-1} + \left(1 - \frac{-\delta_1}{\delta_2 - \delta_1}\right) y^{intp-4th-2},$$

$$y^{intp-5th-2} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-4th-1} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y^{intp-4th-3}$$

15 in which

$$y^{intp-4th-1} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-3rd-1} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y^{intp-3rd-2},$$

$$y^{intp-4th-2} = \frac{-\delta_1}{\delta_2 - \delta_1} y^{intp-3rd-1} + \left(1 - \frac{-\delta_1}{\delta_2 - \delta_1}\right) y^{intp-3rd-3},$$

$$y^{intp-4th-3} = \frac{\delta_2}{\delta_2 - \delta_1} y^{intp-3rd-2} + \left(1 - \frac{\delta_2}{\delta_2 - \delta_1}\right) y^{intp-3rd-4}$$

$$y^{intp-3rd-3} = y^{intp-2nd-2} + \frac{\delta_1^2}{2} y_{xx1},$$

$$y^{intp-3rd-4} = y^{intp-2nd-3} + \frac{\delta_2^2}{2} y_{xx2}$$

18 In the above formulae $y^{intp-4th-1}$, $y^{intp-4th-2}$ and $y^{intp-4th-3}$ denote three 4th-order

approximations to y ; $y^{intp-3rd-3}$ and $y^{intp-3rd-4}$ denote two more 3rd-order approximations to y in addition to the previously specified $y^{intp-3rd-1}$ and $y^{intp-3rd-2}$.

The ENO modifications of the above 4th-order and 6th-order formulae can be found in the Appendix C. Note that for sake of concision, we have used the simplified expressions in the Appendices to represent the approximations to the function value y for each orders of accuracy. For examples, the three 2nd-order approximations $y^{intp-2nd-1}$, $y^{intp-2nd-2}$ and $y^{intp-2nd-3}$ are simplified, respectively, to $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$ in the Appendix C.

3.1.2. Numerical schemes for approximating the first and second derivatives

The explicit expressions and derivations of the numerical schemes for approximating the first and second derivatives of the function value are presented in the Appendices D and E, respectively.

3.1.3. Accuracy tests

In this subsection numerical experiments are performed to test accuracies of the numerical schemes developed previously. Consider such a test function, $f(x) = \sin(2\pi x)$, $x \in [0, 1]$. The function values together with their first and second derivatives are specified on the cell edges of a uniform grid system and interpolated onto the midpoints of each cells. The numerical errors of the results of the ELI at the interpolated points are presented in Table 1 where the convergence rates are evaluated as well. In Table 1 (a) the computational stencil is $\{y_1, y_2, y_{x1}, y_{x2}\}$ and the results exhibit 4th-order convergence rates for y and y_x , while, 2nd-order for y_{xx} , which agree well with their respective theoretical values. In Table 1 (b) the computational stencil is $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$ and the results display 6th-order convergence rates for y and y_x , while, 4th-order for y_{xx} , which agree also with the theoretical values.

It is to be noted that the convergence rates are evaluated exclusively according to the following commonly used formula

$$r = -\frac{\log(err_1 / err_2)}{\log(N_1 / N_2)} \quad (33)$$

where r denotes the convergence rate; err_1 and err_2 are the numerical errors computed under two grid systems with total grid numbers N_1 and N_2 , respectively. It deserves a special remark that the above formula is just an approximated formula and able to describe the convergence rate accurately only in a limited range of the grid steps. Specifically, consider a r^{th} -order method the spatial discretization error of which can be described as $err = c_1 \Delta x^r + c_2 \Delta x^{r+1} + c_3 \Delta x^{r+2} + \dots$, where c_1 , c_2 and c_3 are constants independent of Δx . It is clear that (33) is accurate only when the higher order terms of err are negligible compared with the leading order term. This means (33) is applicable only in the asymptotic range, i.e., $\Delta x \ll 1$. On the other hand, when Δx is sufficiently

small and below a critical value, the round-off errors begin to dominate the total numerical errors which makes (33) inaccurate again. Therefore, it can be concluded that (33) can describe the convergence rate accurately only in the range where Δx is sufficient small but larger than a critical value at which the round-off errors begin to dominate.

From the above discussion, it can be interpreted that why in Table 1(a) the convergence rates of y_x for N larger than 2^{10} are absent. This is mostly because in this range of $N > 2^{10}$ the round-off errors of y_x are dominant and hence the convergence rates evaluated according to (33) are incorrect. Ascribed to a same reason, in Table 1(b) the convergence rates of y , y_x and y_{xx} are not presented for N larger than 2^9 , 2^8 and 2^{10} , respectively. Furthermore, it can be seen from Table 1 that all the convergence rates that agree with the theoretical results are almost independent of the grid resolutions which means the respective asymptotic ranges are reached. In addition, it can be noted that the critical N values in Table 1 (b) at which the round-off errors start to dominate are much smaller than those shown in Table 1 (a). This is mostly because the total numerical errors in Table 1 (b) are much smaller and simultaneously small enough for the round-off errors able to dominate earlier.

3.2. 3D

Assuming a 3D interface is defined by $z = z(x, y)$ and a new particle p_0 is to be interpolated between two given particles p_1 and p_2 located at (x_1, y_1, z_1) and (x_2, y_2, z_2) , respectively. It is clear that the three points are on a same plane and it is natural to prescribe the location coordinates (x, y) of p_0 at the center of (x_1, y_1) and (x_2, y_2) . Consequently, on this local 2D plane the three points can be redefined by using the local coordinates (s_1, z_1) , (s_2, z_2) and (s, z) , where

$$s_1 = 0, \quad s_2 = ds = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}, \quad s = \frac{ds}{2} \quad (34)$$

Accordingly, the ELI of the two given particles p_1 and p_2 in this local 2D coordinates system can be written by

$$z_{s1} = x_s z_{x1} + y_s z_{y1}, \quad (35)$$

$$z_{xs1} = x_s z_{xx1} + y_s z_{xy1}, \quad z_{ys1} = x_s z_{xy1} + y_s z_{yy1}$$

$$z_{s2} = x_s z_{x2} + y_s z_{y2}, \quad (36)$$

$$z_{xs2} = x_s z_{xx2} + y_s z_{xy2}, \quad z_{ys2} = x_s z_{xy2} + y_s z_{yy2}$$

where the subscript s represents the partial derivative operator with respect to s ; z_{x1} , z_{y1} , z_{xx1} , z_{xy1} , z_{yy1} and z_{x2} , z_{y2} , z_{xx2} , z_{xy2} , z_{yy2} denote, respectively, the ELI of p_1 and p_2 in the global coordinates system; x_s and y_s are defined, respectively, by

$$x_s = \frac{x_2 - x_1}{s_2 - s_1}, \quad y_s = \frac{y_2 - y_1}{s_2 - s_1} \quad (37)$$

At this stage, one can use the former 4th-order numerical scheme, Eq. (26), to estimate the z -coordinate of p_0 at the given location s in this local 2D plane based on the stencil $\{z_1, z_2, z_{s1}, z_{s2}\}$. It may be noted that as we can see in the following text the maximum order of accuracy for estimating the second partial derivatives of z are 2. This means the order of accuracy of the estimated value of z will not exceed 4 and consequently the 4th-order formulae are adequate for estimating the value of z .

The first partial derivatives of z , z_x and z_y , can be approximated using the 4th-order formulae, Eq. (26), as well except that the stencils should be replaced by $\{z_{x1}, z_{x2}, z_{xs1}, z_{xs2}\}$ and $\{z_{y1}, z_{y2}, z_{ys1}, z_{ys2}\}$, respectively. The second partial derivatives of z , z_{xx} , z_{xy} and z_{yy} , can be approximated straightforwardly using the following 2nd-order formulae

$$z_{xx} = \frac{z_{xx1} + z_{xx2}}{2}, \quad z_{xy} = \frac{z_{xy1} + z_{xy2}}{2}, \quad z_{yy} = \frac{z_{yy1} + z_{yy2}}{2} \quad (38)$$

4. Reconnection and redistribution algorithms

Similar as the CFT methods, the particles used in the ELIP method should also be redistributed frequently for a uniform distribution such that the interface configuration can be portrayed accurately even undergo a large topological deformation. This goal can be accomplished by the operations described in the following two subsections.

4.1. Reconnection operations

It is common to all the particles methods that in simulating the interface evolutions some situations such as particles over-aggregating or over-dispersing would be encountered inevitably. To get rid of these unwanted results we should delete some particles from the locations where they are over aggregated to save the memories or add new particles to the locations where particles are over dispersed to keep a continuous description for the interface. To accomplish these two goals the connection of each particle with the other neighboring ones should be identified frequently. The operation of constructing the connection structure for each particle is called the reconnection operation. Here, the reconnection operation is slightly different to that defined in the CFT method [Unverdi & Tryggvason 1992] in which each particle was connected in a way as that in the finite element method. In the present ELIP method, the reconnection operations are relatively simpler for no elements with more than 2 points and hence no complicated data structures are needed. Even if new particles are to be interpolated and geometric quantities on which should be estimated, only two sampling particles with the ELI on them are needed to establish high order numerical schemes.

4.1.1. 2D

The reconnection operation for a 2D interface is relatively simple. Consider an ELIP

p_0 on a 2D curve specified by, e.g., $y = y(x)$. The reconnection for p_0 is just to find the closest particles on its left and right sides. This can be done by first searching from all of the other particles, computing the distances to p_0 and finding out the minimums on each sides of p_0 . Furthermore, to make the result more precise, we can consider one more constraint by computing the normal vectors according to Eq. (1) for the two particles, i.e., p_0 and the closest one to it. The additional constraint is described as that the vector product of the two normal vectors should be positive. By adopting this additional constraint the two particles can be ensured to be on a same segment of the interface around p_0 .

4.1.2. 3D

The reconnection operation for a 3D interface is a bit more complex than the 2D cases. Consider an ELIP p_0 on a 3D plane specified by, e.g., $z = z(x, y)$. We first prescribe an influence circle for p_0 , the radius of which is defined by

$$r_{\text{inf}} = \alpha_{\text{inf}} \Delta x \cdot \min \left(1, \frac{\kappa_0}{\kappa_0'} \right) \quad (39)$$

The use of the influence circle is to reduce the computation cost in the reconnection procedure. κ_0 and κ_0' stand for the curvatures at p_0 (κ_0 is the curvature at the beginning of the simulation and κ_0' is the instantaneous curvature). Δx stands for the typical spatial step. α_{inf} is a non-dimensional parameter for regulating the amplitude of r_{inf} which is taken 5 in this paper. One can certainly take larger values for α_{inf} , which may increase the computation cost to some extent.

After establishing the influence circle for p_0 , we then partition the influence circle uniformly into 36 intervals with angle of each being 10 degree (see Fig. 1). These 36 intervals can be regarded as 36 boxes and each box can accommodate 1 ELIP at most which should have the smallest distance to p_0 compared with the other particles located in the same box. Next, we search from all of the given ELIP in the whole computational domain and find out the effective ELIP which locates in the influence circle of p_0 . If there is one ELIP p_1 that is effective, namely, the distance between p_0 and p_1 is less than r_{inf} , we then further determine which box p_1 falls into. Note that before it can be done, we should first ensure the definition of p_1 conformable to p_0 , that is, ensure p_1 defined by $z = z(x, y)$ as well, otherwise we should use the transformation formula to change p_1 to the same definition as p_0 .

Supposing p_1 falls into the l^{th} box and this box contains no other ELIP, then the sequence number of p_1 is related to the l^{th} box. On the other hand, if the l^{th} box has contained one ELIP p_{1a} already, we then compare the distance of p_{1a} to p_0 with that of p_1 to p_0 . One of p_{1a} and p_1 can be retained which should have the smaller distance to p_0 . After finishing the above implementations, the precise reconnection structure of p_0 is then obtained.

Figure 2 sketches a pattern of the influence circle for a particle on a spherical interface.

Plots (a), (b) and (c) show the interfacial particles defined by $x = x(y, z)$, $y = y(x, z)$ and $z = z(x, y)$, respectively. (d) gives the integrated sphere surface. (e) is one half of the sphere surface on which the particle of interest is marked by red color and all the effective particles in the influence circle (the red circle) are distinguished by yellow, cyan and blue colors. If during the interface evolving the curvature at the point of interest κ_0' becomes larger than its initial value κ_0 , there should be more particles aggregated in the influence circle. To keep the computation cost in searching the effective particles at a relatively stable level the radius of the influence circle should be decreased accordingly. On the other hand, the radius of the influence circle is set independent of the curvature if κ_0' is not greater than κ_0 . According to this rule the determination for the radius of the influence circle r_{inf} is formulated by (39). Plots (f), (g), (h) and (i) show, respectively, the effective particles in the 1st, 2nd, 3rd and 4th quarters of the influence circle. In each quarter of the influence circle the yellow, cyan and blue particles fall, in turns, into the 1st third, 2nd third and 3rd third of the sub region.

4.1.3. Deletion operations

During the reconnection operations, the deletion operations can in fact be done simultaneously. To initiate the deletion operation, it would be convenient to introduce a critical distance Δl_{del} , defined by

$$\Delta l_{del} = \max(\Delta l_{d0}, \Delta l_{d1}),$$

$$\Delta l_{d0} = \alpha_{del} \Delta x \cdot \min\left(1, \frac{\kappa_0}{\kappa_0'}\right), \quad \Delta l_{d1} = \alpha_{del} \Delta x \cdot \min\left(1, \frac{\kappa_1}{\kappa_1'}\right) \quad (40)$$

in which κ_1 and κ_1' stand for the curvatures at p_1 (κ_1 is the curvature at the beginning of the simulation and κ_1' is the instantaneous curvature); α_{del} is a parameter for regulating the amplitude of Δl_{del} . If the distance between p_0 and p_1 , Δl , is less than Δl_{del} , p_0 or p_1 can then be deleted.

To determine which of p_0 and p_1 should be deleted, we use such a rule. First, we introduce a new parameter μ to distinguish which particle is given originally at the initial moment. If a particle is an original one this particle is then labeled by $\mu = 1$, otherwise labeled by $\mu = 2$. The rule for determining which of p_0 and p_1 should be deleted is described as: (1) if $\mu_0 \neq \mu_1$, the particle labeled by $\mu = 2$ is deleted; (2) if $\mu_0 = \mu_1 = 2$, we delete the particle which has a larger κ ; (3) if $\mu_0 = \mu_1 = 1$ both of the two particles are retained. Here, μ_0 and μ_1 denote the μ values of p_0 and p_1 , respectively.

4.2. Addition operations

In the previous subsection, we have specified the reconnection operations for each ELIP. In this subsection, we shall specify when and where a new ELIP can be interpolated based on the obtained reconnection structures.

4.2.1. 2D

To determine whether a new ELIP should be interpolated between p_0 and p_1 , it would be helpful to introduce the following critical distance Δl_{add}

$$\Delta l_{add} = \max(\Delta l_{a0}, \Delta l_{a1}),$$

$$\Delta l_{a0} = \alpha_{add} \Delta x \cdot \min\left(1, \frac{\kappa_0}{\kappa_0'}\right), \quad \Delta l_{a1} = \alpha_{add} \Delta x \cdot \min\left(1, \frac{\kappa_1}{\kappa_1'}\right) \quad (41)$$

Here α_{add} is a parameter for regulating the amplitude of Δl_{add} . If the distance between p_0 and p_1 , Δl , is longer than Δl_{add} , then a new ELIP is to be interpolated between p_0 and p_1 . Before it can be done, we should ensure the definition of p_1 conformable to p_0 , otherwise the transformation formulae should be used to fulfill this requirement. The ELI of the newly interpolated particle can be evaluated using the high order numerical schemes specified in section 3.

4.2.2. 3D

For a 3D case the process for determining where to interpolate new ELIP can be specified as follows. Suppose we have established a reconnection structure for p_0 (see Fig. 1). We first search from the 36 boxes to find the closest particle to p_0 . Assume the closest particle to p_0 is in the l_1^{th} box and named as p_1 . We then search from the l_1^{th} to $(l_1+9)^{\text{th}}$ boxes, e.g., in the clockwise direction, and may encounter the following two possible results:

(1) If there is a particle p_s found in the l_s^{th} box ($l_1 < l_s < l_1+9$) the distance of which to p_0 is less than the critical distance Δl_{add} , we then set the l_s^{th} box as the new start point and restart the search from the l_s^{th} to $(l_s+9)^{\text{th}}$ boxes.

(2) If in the region from the l_1^{th} to $(l_1+9)^{\text{th}}$ boxes the distances of all of the particles to p_0 are greater than the critical distance Δl_{add} , we then search the effective particle p_e in the sub-region from the $(l_1+4)^{\text{th}}$ to $(l_1+7)^{\text{th}}$ boxes. This effective particle p_e should have a maximum distance to p_0 compared with other particles in the same sub-region. A new ELIP p_a can then be interpolated between p_0 and p_e (see Fig. 1 where p_3 is the effective particle and p_a is the new particle). Fig. 2 (j) shows a new particle (denoted by purple color) interpolated between the red and cyan particles on a spherical interface and similarly Fig. 2 (k) shows another new particle (denoted by purple color) interpolated between the red and yellow particles. To reduce the computation cost the reconnection operations can be performed every 20 time steps.

To estimate the ELI of the new interpolated particle, the ELIP method uses the ELI of two old neighboring particles on two sides of the interpolated particle to establish the numerical schemes developed in section 3. The geometric quantities on the new interpolated particle can then be evaluated directly according to Eq. (3) and Eq. (4) based on the obtained ELI.

It may be noted that there should be other methods suitable as well for establishing the reconnection structure for the particle with ELI and compared with them the method used in this paper may be not the optimal. Specifically, the influence circle is divided into 36 intervals in this paper. However, one may select a larger or less interval number to divide the influence circle. The fact is that a larger interval number implies a more accurate description for the reconnection structure, while, more computation costs are needed. Furthermore, in searching locations where new particles should be interpolated, this paper uses a sub region of a quarter of the influence circle, i.e., 9 boxes, which actually is not the only way for the aim. One can certainly select a larger sub region with more boxes contained. Anyhow, one rule may be guidable, that is, there should be adequate spaces between each of the new particles and the old neighboring particles otherwise the new particles may be deleted by the deletion operation of the next step.

5. Numerical examples

In this section performances of the ELIP method are tested by considering several benchmark problems. For the temporal discretization the 4th-order Runge-Kutta method is used with the CFL number taken as 0.4.

5.1. Solid body rotation

Before running benchmark tests for interface shapes that may suffer significant distortions, a simple test of solid body rotation which induces no topology changes is considered as an elementary validation for the evolution equations and transformation formulae derived previously. For the 2D case, the following constant-vorticity velocity field is imposed

$$\begin{aligned} u &= \pi(y - 0.5), \\ v &= \pi(0.5 - x) \end{aligned} \tag{42}$$

which rotates the fluid body around the center (0.5, 0.5) in the clockwise direction. In figure 3 four stages of one full rotation of a circular interface are presented. The initial circle is centered at (0.5, 0.75) with a radius 0.15. The numerical errors of the ELI of the interfacial points after one fourth of a full rotation are given in Table 2. It is seen that the theoretical 4th-order temporal convergence rate is reached in the asymptotical range. Furthermore, because of the effects of the round-off errors, the convergence rates of y , y_x and y_{xx} are not presented for N larger than 2^{10} , 2^{11} and 2^{12} , respectively. The results of the 3D cases are quite similar and not presented for concision.

5.2. Single vortex test

To test capability of the method on resolving thin filaments occurring in stretching flows the single vortex flow introduced in [Bell et al. 1989] is considered. The initial circular interface is centered at $(0.5, 0.75)$ and has a radius $r = 0.15$, while the velocity field is defined by the stream function

$$\psi = \frac{1}{\pi} \sin^2(\pi x) \sin^2(\pi y) \quad (43)$$

which is reversed at $t = T/2$, where T is the period.

Figure 4 presents the initial setup under a mesh $(2^7 \times 2^7)$. It may deserve a clarification for why a mesh is needed to specify the initial condition in this tracking method. This is because the initial inputs of the particles are distributed on the gridlines. The initial particles' locations can be determined by scanning the interface in the x - and y - directions and finding the intersections of the interface with the gridlines. For $|y_x| < 1.5$ the particles lying on the y -gridlines, specified by $y=y(x_i)$, are retained, while, the particles lying on the x -gridlines, specified by $x=x(y_i)$, are retained for $|x_y| < 1.5$. It is clear that the density of the mesh determines the total particle number. The initial values of y_x and y_{xx} for $k = \pm 1$ and ± 2 can be evaluated by using the derivative forms of the Lagrangian interpolation formulae based on the stencils $\{x(y_i)\}$ and $\{y(x_i)\}$, respectively.

Figure 4 (a) and (b) depict the particles defined by $x = x(y)$ and $y = y(x)$, respectively. The particles represented by the red, green, blue and purple circles correspond to $k = 1, -1, 2$ and -2 , respectively. Fig. 4 (c) is the initial input without applying the addition operation and the total particle number is $N_{original} = 108$. Fig. 4 (d) gives the result after carrying out an addition operation with the addition parameter $\alpha_{add} = 1$ and the total particle number $N_{total} = 216$.

Numerical experiments are conducted to test accuracy of the results for the obtained ELI and geometric quantities of the interpolated particles. Before it can be done, analytical values of the ELI and geometric quantities should be known in advance. Consider a circular interface centered at (x_c, y_c) with radius r , the implicit definition of which can be expressed as

$$\Phi(x, y) = (x - x_c)^2 + (y - y_c)^2 - r^2 = 0 \quad (44)$$

The analytical values of the ELI of particles defined explicitly by $y = y(x)$ and $x = x(y)$ can be calculated, respectively, according to the following formulae (see Appendix B)

$$\begin{aligned} y_x &= -\frac{x - x_c}{y - y_c}, & y_{xx} &= -\frac{1 + y_x^2}{y - y_c}, \\ x_y &= -\frac{y - y_c}{x - x_c}, & x_{yy} &= -\frac{1 + x_y^2}{x - x_c} \end{aligned} \quad (45)$$

The analytical values of the curvature can then be computed according to Eq. (2).

The L_2 and L_∞ errors of the ELI and curvature of the interpolated particles under various grid sizes are presented in Table 3. Clearly, the numerical errors decrease with the increase of the grid numbers. Note that it is inappropriate to use (33) to evaluate the convergence rates for the results given in Table 3. This is because (33) is applicable only for uniform grids, while, in this computational setup the particles' distribution is not completely uniform and the grid spaces vary not linearly with the increase of the grid numbers. To partly prove this opinion, additional numerical experiments are conducted with selecting the equally spaced interfacial points ($k = \pm 2$) taken as the sampling points. The L_∞ errors and convergence rates of the ELI and curvature of the interpolated particles are presented in Table 4. It is seen that the convergence rates of y , y_x and κ attain approximately 6th-order, 6th-order and 4th-order, respectively, which agree with the theoretical values.

It can also be noted that the asymptotical range in which the convergence rate should be independent of the grid sizes is not obvious in Table 4. This may be ascribed to the following reasons. First, as in the previous discussions the spatial discretization error of a r^{th} -order method can be described as $err = c_1\Delta x^r + c_2\Delta x^{r+1} + c_3\Delta x^{r+2} + \dots$ where c_1 , c_2 and c_3 are constants independent of Δx . The absolute value of c_2/c_1 for the interface profile of this case may be a bit large, which delays the reach of the asymptotical range. On the other hand, with the increase of the grid number, the total numerical errors decrease at a high rate due to the large r value. The high decreasing rate of the total numerical errors makes the total numerical errors become sufficiently small very quickly and consequently the round-off errors become dominant very quickly even before the asymptotical range is reached. The combination of the above factors results in the shrinks or even absences of the asymptotical range.

Figure 5 shows the results of the single vortex test under a mesh ($2^9 \times 2^9$). The flow starts at $t = 0$ with total particle number $N_{\text{original}} = 436$ and ends at $t = 40$ with total particle number $N_{\text{total}} = 624$. At $t = 20$ the flow is reversed. The addition and deletion parameters are taken as $\alpha_{\text{add}} = 1.5$ and $\alpha_{\text{del}} = 0.5$, respectively. The total particle numbers at various time moments are labeled under each plot. It is obvious from this figure that the interface suffers a strong thinning and is stretched into a filament that spirals around the vortex center. At $t = 40$ the starting circle is perfectly rebuilt. Good performance of the ELIP method is evidenced by the extreme pattern at $t = 20$ where the thinnest tail develops.

Figure 6 presents the separated results distinguishing the original particles (a) and the interpolated particles (b) of the result obtained at $t = 20$. The particles marked by $k = 1$, -1 , 2 and -2 are distinguished by the red, green, blue and purple colors, respectively. It is seen that the number of the interpolated particles is 25302, far more than that of the original particles. This manifests that quality of the addition operation is crucial for the global accuracy of a tracking method. The L_2 and L_∞ errors of the ELI and curvature of the result obtained at $t = 40$ are presented and compared in Table 5 for

various mesh sizes. As previously, the numerical errors are reduced with the increase of the grid numbers. Furthermore, there are three reasons for why convergence studies are not performed for this case as well as the latter cases any more. First, the spatial and temporal convergence rates of the method have been tested separately and the results are shown in Table 1, Table 4 and Table 2, respectively. Second, to simulate the evolution of the interface the temporal and spatial discretizations should be done simultaneously. The interplay of the temporal and spatial discretization errors may cause the evaluated spatial convergence rate unequal to the theoretical value. Although effects of the temporal discretization errors can be eliminated by taking a sufficiently small time step, such a way is not economical in time because the total computation time would be elongated significantly. Third, also the most important, even if the temporal discretization errors are eliminated, it is still impracticable to do the convergence studies for this case because during the interface evolving all of the interpolations of new particles are done actually on non-uniform grids due to the irregular distributions of the interfacial particles and under the non-uniform grids the commonly used formula (33) is inapplicable. Due to the above three accounts convergence studies are not performed any more for this as well as the latter cases.

5.3. Deformation field test

To further test ability of the new method in tracking thin filaments, the deformation field test introduced in [Smolarkiewicz 1982] is considered. The initial circle of radius $r = 0.15$ centered at $(0.5, 0.75)$ is entrained by the velocity field determined by the stream function

$$\psi = \frac{1}{n_v \pi} \sin[n_v \pi(x + 0.5)] \cos[n_v \pi(y + 0.5)] \quad (46)$$

in which n_v denotes the vortex number.

Figure 7 presents the results of the deformation field test under a mesh $(2^9 \times 2^9)$ with the vortex number taken as $n_v = 4$. The flow starts at $t = 0$ with total particle number $N_{original} = 436$ and ends at $t = 2$ with total particle number $N_{total} = 638$. At $t = 1$ the flow is reversed. The addition and deletion parameters are taken as $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively. Figure 8 presents the separated results distinguishing the original particles (a) and interpolated particles (b) of the result obtained at $t = 1$. The L_2 and L_∞ errors of the ELI and curvature of the result obtained at $t = 2$ are presented and compared in Table 6 for various mesh sizes. It is seen that the errors of the curvature κ exceed the acceptable range, which may be ascribed to the deformation field test is more challenge and more tough than the single vortex test. At cusps of the thin filaments, the interface profiles represented by the discrete particles are not smooth any longer and as a consequence pronounced numerical errors produced.

As an additional case, the simulation is run with the vortex number taken as $n_v = 8$.

The results are presented in Figures 9 and 10. It can be seen that the configurations obtained in this example are more complex than those in the previous case. The thin filament structures are smaller and the curvatures are hence larger. As a result, the numerical errors are more significant which are found to be 6.282E-06, 2.526E-03 and 2.018E+03 for y , y_x and κ , respectively.

5.4. Cases on discretely specified velocity field

To study effect of the discrete specifications of the velocity field, more simulations are performed with the velocities specified analytically but discretely on the computational grids. The spatial derivatives of the velocity components are evaluated numerically by using high order difference schemes specified as follows.

Given a stencil consisting of 7 successively specified function values $\{y_1, y_2, y_3, y_4, y_5, y_6, y_7\}$ on uniform grids, the first derivative of the function can be evaluated according to the following 6th-order difference schemes

$$y'_j = \frac{1}{60\Delta x} \sum_{k=1}^7 a_{jk} y_k, \quad j \in [1, 7] \quad (47)$$

where

$$\begin{aligned} \{a_{1k}\} &= \{-147, 360, -450, 400, -225, 72, -10\}, \\ \{a_{2k}\} &= \{-10, -77, 150, -100, 50, -15, 2\}, \\ \{a_{3k}\} &= \{2, -24, -35, 80, -30, 8, -1\}, \\ \{a_{4k}\} &= \{-1, 9, -45, 0, 45, -9, 1\}, \\ \{a_{5k}\} &= \{1, -8, 30, -80, 35, 24, -2\}, \\ \{a_{6k}\} &= \{-2, 15, -50, 100, -150, 77, 10\}, \\ \{a_{7k}\} &= \{10, -72, 225, -400, 450, -360, 147\} \end{aligned} \quad (48)$$

In the above formulae, y'_j denotes the first derivative of y at x_j , $j \in [1, 7]$. The schemes are right-biased for $j \in [1, 3]$, left-biased for $j \in [5, 7]$, and central type for $j = 4$, respectively.

Given a stencil consisting of 8 successively specified function values $\{y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8\}$ on uniform grids, the second derivative of the function can be evaluated according to the following 6th-order difference schemes

$$y''_j = \frac{1}{180\Delta x^2} \sum_{k=1}^8 b_{jk} y_k \quad (49)$$

where

$$\begin{aligned}
 \{b_{1k}\} &= \{938, -4014, 7911, -9490, 7380, -3618, 1019, -126\}, \\
 \{b_{2k}\} &= \{126, -70, -486, 855, -670, 324, -90, 11\}, \\
 \{b_{3k}\} &= \{-11, 214, -378, 130, 85, -54, 16, -2\}, \\
 \{b_{4k}\} &= \{2, -27, 270, -490, 270, -27, 2, 0\}, \\
 \{b_{5k}\} &= \{0, 2, -27, 270, -490, 270, -27, 2\}, \\
 \{b_{6k}\} &= \{-2, 16, -54, 85, 130, -378, 214, -11\}, \\
 \{b_{7k}\} &= \{11, -90, 324, -670, 855, -486, -70, 126\}, \\
 \{b_{8k}\} &= \{-126, 1019, -3618, 7380, -9490, 7911, -4014, 938\}
 \end{aligned} \tag{50}$$

In the above formulae, y_j'' denotes the second derivative of y at x_j , $j \in [1, 8]$. The schemes are right-biased for $j \in [1, 3]$, left-biased for $j \in [6, 8]$, and central type for $j \in [4, 5]$, respectively.

In this study, the spatial derivatives of the velocities are evaluated exclusively using the above 6th-order difference schemes, usages of which are specified as follows.

i) For the inner grid points x_i ($4 \leq i \leq N-3$): the first partial derivatives of the velocity components, such as u_x , v_x , u_y and v_y , can be evaluated using the central scheme defined in (47) with $j = 4$; the second partial derivatives of the velocity components, such as u_{xx} , v_{xx} , u_{yy} and v_{yy} , can be evaluated using the central scheme defined in (49) with $j = 4$ or $j = 5$.

ii) For the boundary grid point x_i ($i = 1$ or $i = N$): u_x , v_x , u_y and v_y can be evaluated using the right-biased or left-biased scheme defined in (47) with $j = 1$ or $j = 7$; u_{xx} , v_{xx} , u_{yy} and v_{yy} can be evaluated using the right-biased or left-biased scheme defined in (49) with $j = 1$ or $j = 8$.

iii) For the first inner grid point x_i adjacent to the boundary ($i = 2$ or $i = N-1$): u_x , v_x , u_y and v_y can be evaluated using the right-biased or left-biased schemes defined in (47) with $j = 2$ or $j = 6$; u_{xx} , v_{xx} , u_{yy} and v_{yy} can be evaluated using the right-biased or left-biased schemes defined in (49) with $j = 2$ or $j = 7$.

iv) For the second inner grid point x_i adjacent to the boundary ($i = 3$ or $i = N-2$): u_x , v_x , u_y and v_y can be evaluated using the right-biased or left-biased schemes defined in (47) with $j = 3$ or $j = 5$; u_{xx} , v_{xx} , u_{yy} and v_{yy} can be evaluated using the right-biased or left-biased schemes defined in (49) with $j = 3$ or $j = 6$.

v) The cross partial derivatives terms u_{xy} and v_{xy} can be obtained, respectively, by evaluating the partial derivatives of u_y and v_y with respect to x .

For the purpose of assisting the readers the explicit expressions for the difference schemes with accuracies from 2nd-order to 5th-order are also presented which are

summarized in the Appendix F.

Note that all of the above difference schemes can be derived by using the Taylor's series expansions and matching the coefficients or, alternatively, by evaluating the derivatives of the corresponding Lagrangian interpolation polynomials and implementing the uniform grids assumption. The latter method is somewhat easier than the former, both of which are not presented in this paper for sake of concision. Furthermore, accuracies of the above difference schemes have been tested and the testing results are not presented for concision as well.

The discretely specified velocity field together with their numerically evaluated spatial derivatives can be interpolated from the Eulerian grids onto the interfacial points by using the following 6th-order bi-variate Lagrangian interpolation formula

$$f(x, y) = \sum_{n=1}^6 \sum_{m=1}^6 f_{i+m, j+n} \prod_{l=1, l \neq m}^6 \frac{x - x_{i+l}}{x_{i+m} - x_{i+l}} \prod_{k=1, k \neq n}^6 \frac{y - y_{j+k}}{y_{j+n} - y_{j+k}} \quad (51)$$

in which $f(x, y)$ denotes the function value at an arbitrary point (x, y) ; $f_{i+m, j+n}$ denotes the function value at the grid node (x_{i+m}, y_{j+n}) . The above formula can be evaluated practically in the following way.

Supposing an interfacial particle, the location coordinates of which are (x, y) , falls into the (i, j) cell, i.e., $x_i \leq x < x_{i+1}$ and $y_j \leq y < y_{j+1}$. Then, we can select 36 grid nodes, (x_{i+s}, y_{j+t}) ($-2 \leq s, t \leq 3$), and based on which run the following 6th-order univariate Lagrangian interpolation formula 6 times to obtain 6 intermediate values $f_{x, j+t}$ at 6 intermediate nodes (x, y_{j+t}) ($-2 \leq t \leq 3$)

$$f_{x, j+t} = \sum_{m=-2}^3 f_{i+m, j+t} \prod_{l=-2, l \neq m}^3 \frac{x - x_{i+l}}{x_{i+m} - x_{i+l}}, \quad -2 \leq t \leq 3 \quad (52)$$

Based on the 6 intermediate values, the function value at (x, y) can then be obtained from using the 6th-order univariate Lagrangian interpolation formula again

$$f(x, y) = \sum_{n=-2}^3 f_{x, j+n} \prod_{k=-2, k \neq n}^3 \frac{y - y_{j+k}}{y_{j+n} - y_{j+k}} \quad (53)$$

Clearly, substituting the univariate Lagrangian interpolation formula (52) into (53) gives immediately the bi-variate Lagrangian interpolation formula (51). As a chief advantage, order of accuracy of the above multi-variate Lagrangian interpolation formula is much higher than that of the kernel interpolation formula used in the CFT method. The strict proof for the accuracy of the univariate Lagrangian interpolation polynomial is presented in the Appendix G. Note that in real situations the velocity field may be not sufficiently smooth. To ensure the numerical solutions smooth and stable, all of the aforementioned difference schemes and interpolation formulae can be modified to the ENO styles, which will not be discussed in this paper for brevity.

The single vortex test ($\alpha_{add} = 1.5$, $\alpha_{del} = 0.5$) and the deformation field test ($n_v = 4$, α_{add}

($\alpha_{del} = 1.5$, $\alpha_{del} = 0.5$) are re-performed with the velocities and their spatial derivatives obtained in the abovementioned way. The computation times are 4 and 0.8, respectively. The L_2 and L_∞ errors of the ELI and curvature of the results for the two tests are presented in Table 7 and Table 8, respectively. It can be seen that the numerical errors in Table 7 (b) and Table 8 (b) are higher than those in Table 7 (a) and Table 8 (a), respectively. This manifests the aforementioned interpolation procedures and numerical evaluations for the spatial derivatives of the velocities do introduce additional numerical errors to the final results. In particular, it can be identified from Table 8 (b) that the numerical errors of y for $N = 2^8$ is abnormally higher than those for $N = 2^7$, which can be attributed mostly to the interplay of the temporal and spatial discretization errors. To validate such a conjecture, more simulations are conducted additionally with CFL number taken as 0.1, less than the previously used CFL number 0.4. The numerical errors obtained with the smaller CFL number are presented in Table 8 (c), in which the abnormal results are not seen any longer.

5.5. Enright test

To demonstrate the ability of the method in accurately portraying the three-dimensional deformations, we consider a well-known and also challenging test case introduced originally by LeVeque [1996] and used again by Enright et al. [2002]. This problem, named as the Enright test in [Osher & Fedkiw 2003], uses an initial sphere centered at (0.35, 0.35, 0.35) with radius 0.15. The velocity field is given by

$$\begin{aligned} u &= 2 \sin^2(\pi x) \sin(2\pi y) \sin(2\pi z), \\ v &= -\sin(2\pi x) \sin^2(\pi y) \sin(2\pi z), \\ w &= -\sin(2\pi x) \sin(2\pi y) \sin^2(\pi z) \end{aligned} \quad (54)$$

Figure 11 presents the initial input of the 3D interface under a mesh ($2^6 \times 2^6 \times 2^6$), in which (a), (b) and (c) show the particles defined by $x = x(y, z)$, $y = y(x, z)$ and $z = z(x, y)$, respectively. (d) is the integrated result combined by (a), (b) and (c). (e) is the same as (d) except that all of the particles are described by a single color. The total particle number in (e) is $N_{original} = 978$.

Figure 12 presents comparisons of the interface configurations after applying addition operations with different addition parameters used. The original data is that shown in Figure 11 (e). (a1), (a2) and (a3) present the interpolated particles with the addition parameter α_{add} taken as 1.3, 1.2 and 1, respectively. (b1), (b2) and (b3) present the integrated results in which the original and interpolated particles are distinguished by red and green colors, respectively. (c1), (c2) and (c3) are the same as (b1), (b2) and (b3), respectively, except that all of the particles are described by a single color. The total particle numbers in (c1), (c2) and (c3) are $N_{total} = 1188$, 1413 and 3055, respectively. It is evident that with the decrease of the addition parameter the number of interpolated particles increases and consequently the interface becomes smoother

and continuous.

For comparisons, we show more initial setups in figures 13 –16 with meshes enriched to $(2^7 \times 2^7 \times 2^7)$ and $(2^8 \times 2^8 \times 2^8)$, respectively. The L_2 and L_∞ errors of the ELI and curvature of the interpolated particles under the above three meshes are compared in Table 9 and Table 10 with α_{add} taken as 1.3 and 1.2, respectively. It is seen that the numerical errors are reduced with the increase of the grid numbers.

It may be worthy of remark that as in the 2D cases to calculate the numerical errors of the ELI and curvatures of the interpolated particles, the analytical values of these quantities should be known a priori. For a sphere interface defined implicitly by

$$\Phi(x, y) = (x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2 - r^2 = 0 \quad (55)$$

the analytical values of the ELI of a particle defined explicitly by $z = z(x, y)$, $y = y(x, z)$ and $x = x(y, z)$ can be calculated, respectively, according to the following formulae (see Appendix B)

$$\begin{aligned} z_x &= -\frac{x - x_c}{z - z_c}, \quad z_y = -\frac{y - y_c}{z - z_c}, \\ z_{xx} &= -\frac{1 + z_x^2}{z - z_c}, \quad z_{xy} = -\frac{z_x z_y}{z - z_c}, \quad z_{yy} = -\frac{1 + z_y^2}{z - z_c} \end{aligned} \quad (56)$$

$$\begin{aligned} y_x &= -\frac{x - x_c}{y - y_c}, \quad y_z = -\frac{z - z_c}{y - y_c}, \\ y_{xx} &= -\frac{1 + y_x^2}{y - y_c}, \quad y_{xz} = -\frac{y_x y_z}{y - y_c}, \quad y_{zz} = -\frac{1 + y_z^2}{y - y_c} \end{aligned} \quad (57)$$

$$\begin{aligned} x_y &= -\frac{y - y_c}{x - x_c}, \quad x_z = -\frac{z - z_c}{x - x_c}, \\ x_{yy} &= -\frac{1 + x_y^2}{x - x_c}, \quad x_{yz} = -\frac{x_y x_z}{x - x_c}, \quad x_{zz} = -\frac{1 + x_z^2}{x - x_c} \end{aligned} \quad (58)$$

By substituting the above formulae into Eq. (4), the analytical value of the curvature can be obtained.

Figure 17 presents results of the Enright test under a mesh $(2^8 \times 2^8 \times 2^8)$. The flow starts at $t = 0$ with total particle number $N_{original} = 15408$ and ends at $t = 2$ with total particle number $N_{total} = 15500$. At $t = 1$ the flow is reversed. The addition and deletion parameters are $\alpha_{add} = 2.5$ and $\alpha_{del} = 1$, respectively.

Figure 18 presents separated results distinguishing the original particles and interpolated particles from the integrated results obtained at $t = 1$ under a mesh $(2^6 \times 2^6 \times 2^6)$. In plots (a1), (a2), (a3) and (a4) only the original particles are presented, while, (b1), (b2), (b3) and (b4) present the integrated results in which the original and interpolated particles are described by red and green colors, respectively. Plots (c1),

(c2), (c3) and (c4) are the same as (b1), (b2), (b3) and (b4), respectively, except that all of the particles are described by using a single color. Plots (a2), (b2) and (c2) show a different view for (a1), (b1) and (c1), respectively, while, (a4), (b4) and (c4) show a different view for (a3), (b3) and (c3), respectively. For the results on the upper two rows the addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively, with total particle number $N_{total} = 14403$, while, for the results on the lower two rows the addition and deletion parameters are $\alpha_{add} = 1$ and $\alpha_{del} = 0.2$, respectively, with total particle number $N_{total} = 44325$. Obviously, decreasing the addition and deletion parameters makes the interface configuration smoother and continuous.

Figures 19 and 20 present comparisons with figure 18, in which meshes are enriched to $(2^7 \times 2^7 \times 2^7)$ and $(2^8 \times 2^8 \times 2^8)$, respectively. Again, one can find that the smaller the addition and deletion parameters the smoother and continuous the results. Furthermore, increasing the initial particle number, i.e. using a densified mesh, is also beneficial for improving the results. The L_2 and L_∞ errors of the ELI and curvature of the result obtained at $t = 2$ are presented and compared in Table 11 for various mesh sizes. As previously, the numerical errors are reduced with the increase of the grid numbers.

5.6. Comparisons of the ELIP method with other hybrid tracking methods

To further demonstrate the high accuracy performance of the ELIP method, we compare results of this method with other various hybrid tracking methods. First, the results of the single vortex test are compared. Two indices are selected for comparisons, which are (1) the max durations of the computation and (2) whether the initial circle is perfectly rebuilt at the end of simulation. It is understandable that these two indices are good criterions for assessing qualities of the methods. The comparisons are presented in Table 12, from which the high accuracy performance of the ELIP method is obvious.

Furthermore, the results of the Enright test are compared. Here, we select such two indices for comparisons: (1) whether the initial sphere is perfectly rebuilt at the end of simulation, (2) whether the interface configuration is smooth and continuous at the maximum stretched state. Note that we do not compare the max durations of the computation in this case. This is because the velocity fields used in some of the methods were multiplied by a time factor $\cos(\pi t/T)$, while, in some other methods the time factor was $\text{sign}(T/2 - t)$. Although the max durations are not coincident precisely, it can still be observed that the interface patterns at the maximum stretched states are close. Therefore, we select whether the interface configuration is smooth and continuous at the maximum stretched state as an alternative reasonable index to assess quality of the numerical result. From the comparisons presented in Table 13 the high

accuracy features of the present ELIP method are substantiated. Note that the advantages of the new ELIP method should be further validated from simulating the practical problems of multiphase flows such as the bubbles and drops movements and comparing the results with that of the CFT methods.

6. Conclusions

In this work a new front tracking method, which can provide more accurate descriptions for the geometrical features of the interface than the CFT methods, is developed with the employment of Lagrangian particles marked by their ELI. The method is built successfully due to three key originalities. First, to acquire highly accurate estimations for the ELI of the interpolated particles, high order numerical schemes are developed based on ELI of two given particles. Second, a series of evolution equations are derived for tracking the ELI of all the particles during the interface evolving. Third, transformation formulae are derived for modifying the spatial derivatives of the particles' location coordinates such that large amplitudes of which can be avoided. The efficiency and accuracy of the method are demonstrated from modeling the two- and three-dimensional benchmark problems.

How to correctly delineate the topological changes such as merging and splitting is a common difficulty for the front tracking methods. The topological changes could be detected and handled by this method from the step of searching the closest particle in the reconnection operations. Furthermore, when topological changes happen singularities may be generated on the spatial derivatives of the location coordinates between two different segments of the interface. This singularity would be a challenge in accurately evaluating the geometrical features of the interface. This topic can be discussed systematically in the future studies.

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Appendix A. Evolution equations for the ELI of the particles on the

3D interface specified by $y = y(x, z)$ and $x = x(y, z)$

For an interface specified by $y = y(x, z)$, the evolution equations for the ELI y_x, y_z, y_{xx}, y_{xz} and y_{zz} can be given, respectively, by

$$\frac{dy_x}{dt} = v_x + y_x (v_y - u_x) - y_z w_x - y_x^2 u_y - y_x y_z w_y \quad (1)$$

$$\frac{dy_z}{dt} = v_z + y_z (v_y - w_z) - y_x u_z - y_x y_z u_y - y_z^2 w_y \quad (2)$$

$$\begin{aligned} \frac{dy_{xx}}{dt} = & v_{xx} + y_x (2v_{xy} - u_{xx}) - y_z w_{xx} + y_{xx} (v_y - 2u_x) - 2y_{xz} w_x \\ & + y_x^2 (v_{yy} - 2u_{xy}) - 2y_x y_z w_{xy} - 3y_x y_{xx} u_y - 2y_x y_{xz} w_y - y_z y_{xx} w_y \\ & - y_x^3 u_{yy} - y_x^2 y_z w_{yy} \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{dy_{xz}}{dt} = & v_{xz} + y_x (v_{yz} - u_{xz}) + y_z (v_{xy} - w_{xz}) - y_{xx} u_z - y_{zz} w_x + y_{xz} (v_y - u_x - w_z) \\ & + y_x y_z (v_{yy} - u_{xy} - w_{yz}) - 2y_x y_{xz} u_y - y_x y_{zz} w_y - y_z y_{xx} u_y - 2y_z y_{xz} w_y \\ & - y_x^2 u_{yz} - y_z^2 w_{xy} - y_x y_z^2 w_{yy} - y_x^2 y_z u_{yy} \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{dy_{zz}}{dt} = & v_{zz} - y_x u_{zz} + y_z (2v_{yz} - w_{zz}) - 2y_{xz} u_z + y_{zz} (v_y - 2w_z) \\ & - 2y_x y_z u_{yz} - y_x y_{zz} u_y - 2y_z y_{xz} u_y - 3y_z y_{zz} w_y + y_z^2 (v_{yy} - 2w_{yz}) \\ & - y_x y_z^2 u_{yy} - y_z^3 w_{yy} \end{aligned} \quad (5)$$

Similarly, if an interface is specified by $x = x(y, z)$, the evolution equations for the ELI x_y, x_z, x_{yy}, x_{yz} and x_{zz} are given, respectively, by

$$\frac{dx_y}{dt} = u_y + x_y (u_x - v_y) - x_z w_y - x_y^2 v_x - x_y x_z w_x \quad (6)$$

$$\frac{dx_z}{dt} = u_z - x_y v_z + x_z (u_x - w_z) - x_y x_z v_x - x_z^2 w_x \quad (7)$$

$$\begin{aligned} \frac{dx_{yy}}{dt} = & u_{yy} + x_y (2u_{xy} - v_{yy}) - x_z w_{yy} + x_{yy} (u_x - 2v_y) - 2x_{yz} w_y \\ & + x_y^2 (u_{xx} - 2v_{xy}) - 2x_y x_z w_{xy} - 3x_y x_{yy} v_x - 2x_y x_{yz} w_x - x_z x_{yy} w_x \\ & - x_y^3 v_{xx} - x_y^2 x_z w_{xx} \end{aligned} \quad (8)$$

$$\begin{aligned} \frac{dx_{yz}}{dt} = & u_{yz} + x_y (u_{xz} - v_{yz}) + x_z (u_{xy} - w_{yz}) - x_{yy} v_z - x_{zz} w_y + x_{yz} (u_x - v_y - w_z) \\ & + x_y x_z (u_{xx} - v_{xy} - w_{xz}) - 2x_y x_{yz} v_x - x_y x_{zz} w_x - x_z x_{yy} v_x - 2x_z x_{yz} w_x \\ & - x_y^2 v_{xz} - x_z^2 w_{xy} - x_y x_z^2 w_{xx} - x_y^2 x_z v_{xx} \end{aligned} \quad (9)$$

$$\begin{aligned}
\frac{dx_{zz}}{dt} = & u_{zz} - x_y v_{zz} + x_z (2u_{xz} - w_{zz}) - 2x_{yz} v_z + x_{zz} (u_x - 2w_z) \\
& - 2x_y x_z v_{xz} - x_y x_{zz} v_x - 2x_z x_{yz} v_x - 3x_z x_{zz} w_x + x_z^2 (u_{xx} - 2w_{xz}) \\
& - x_y x_z^2 v_{xx} - x_z^3 w_{xx}
\end{aligned} \tag{10}$$

Appendix B. Verifications of the transformation formulae by using the implicit interface function

In what follows, we will show that the previously derived transformation formulae can also be yielded based on the implicit interface function.

(1) 2D

Considering a 2D curve defined implicitly by $\Phi[x, y(x)] = 0$ and taking the 1st and 2nd derivatives of which gives

$$\begin{aligned}\Phi_x + \Phi_y y_x &= 0, \\ \Phi_{xx} + 2\Phi_{xy} y_x + \Phi_{yy} y_x^2 + \Phi_y y_{xx} &= 0\end{aligned}\tag{1}$$

From the above equations one can obtain

$$\begin{aligned}y_x &= -\frac{\Phi_x}{\Phi_y}, \\ y_{xx} &= -\frac{\Phi_{xx} \Phi_y^2 - 2\Phi_{xy} \Phi_x \Phi_y + \Phi_{yy} \Phi_x^2}{\Phi_y^3}\end{aligned}\tag{2}$$

Similarly, for a 2D curve defined implicitly by $\Phi[y, x(y)] = 0$, one can obtain the following relations to express x_y and x_{yy} , given by

$$\begin{aligned}x_y &= -\frac{\Phi_y}{\Phi_x}, \\ x_{yy} &= -\frac{\Phi_{yy} \Phi_x^2 - 2\Phi_{xy} \Phi_x \Phi_y + \Phi_{xx} \Phi_y^2}{\Phi_x^3}\end{aligned}\tag{3}$$

Consequently, it is not difficult to verify from the above four equations that

$$x_y = \frac{1}{y_x}, \quad x_{yy} = -\frac{y_{xx}}{y_x^3}\tag{4}$$

(2) 3D

Considering a 3D surface defined implicitly by $\Phi[x, y, z(x, y)] = 0$, the 1st and 2nd partial derivatives of which read

$$\begin{aligned}\Phi_x + \Phi_z z_x &= 0, \\ \Phi_y + \Phi_z z_y &= 0, \\ \Phi_{xx} + 2\Phi_{xz} z_x + \Phi_{zz} z_x^2 + \Phi_z z_{xx} &= 0, \\ \Phi_{xy} + \Phi_{xz} z_y + \Phi_{yz} z_x + \Phi_{zz} z_x z_y + \Phi_z z_{xy} &= 0, \\ \Phi_{yy} + 2\Phi_{yz} z_y + \Phi_{zz} z_y^2 + \Phi_z z_{yy} &= 0\end{aligned}\tag{5}$$

From the above equations, one can have the following relations to express the partial derivatives of z with respect to x and y , given by

$$\begin{aligned}
 z_x &= -\frac{\Phi_x}{\Phi_z}; \quad z_y = -\frac{\Phi_y}{\Phi_z} \\
 z_{xx} &= -\frac{\Phi_{xx}\Phi_z^2 - 2\Phi_{xz}\Phi_x\Phi_z + \Phi_{zz}\Phi_x^2}{\Phi_z^3} \\
 z_{xy} &= -\frac{\Phi_{xy}\Phi_z^2 - \Phi_{xz}\Phi_y\Phi_z - \Phi_{yz}\Phi_x\Phi_z + \Phi_{zz}\Phi_x\Phi_y}{\Phi_z^3} \\
 z_{yy} &= -\frac{\Phi_{yy}\Phi_z^2 - 2\Phi_{yz}\Phi_y\Phi_z + \Phi_{zz}\Phi_y^2}{\Phi_z^3}
 \end{aligned} \tag{6}$$

Similarly, for a 3D surface defined implicitly by $\Phi[x, z, y(x, z)] = 0$, one can have

$$\begin{aligned}
 y_x &= -\frac{\Phi_x}{\Phi_y}; \quad y_z = -\frac{\Phi_z}{\Phi_y} \\
 y_{xx} &= -\frac{\Phi_{xx}\Phi_y^2 - 2\Phi_{xy}\Phi_x\Phi_y + \Phi_{yy}\Phi_x^2}{\Phi_y^3} \\
 y_{xz} &= -\frac{\Phi_{xz}\Phi_z^2 - \Phi_{xy}\Phi_y\Phi_z - \Phi_{yz}\Phi_x\Phi_y + \Phi_{yy}\Phi_x\Phi_z}{\Phi_y^3} \\
 y_{zz} &= -\frac{\Phi_{zz}\Phi_y^2 - 2\Phi_{yz}\Phi_y\Phi_z + \Phi_{yy}\Phi_z^2}{\Phi_y^3}
 \end{aligned} \tag{7}$$

and for a 3D surface defined implicitly by $\Phi[y, z, x(y, z)] = 0$ the following relations can be derived

$$\begin{aligned}
 x_y &= -\frac{\Phi_y}{\Phi_x}; \quad x_z = -\frac{\Phi_z}{\Phi_x} \\
 x_{yy} &= -\frac{\Phi_{yy}\Phi_x^2 - 2\Phi_{xy}\Phi_x\Phi_y + \Phi_{xx}\Phi_y^2}{\Phi_x^3} \\
 x_{yz} &= -\frac{\Phi_{yz}\Phi_x^2 - \Phi_{xy}\Phi_x\Phi_z - \Phi_{xz}\Phi_x\Phi_y + \Phi_{xx}\Phi_y\Phi_z}{\Phi_x^3} \\
 x_{zz} &= -\frac{\Phi_{zz}\Phi_x^2 - 2\Phi_{xz}\Phi_x\Phi_z + \Phi_{xx}\Phi_z^2}{\Phi_x^3}
 \end{aligned} \tag{8}$$

By combining the above equations, it is not difficult to verify the previously derived transformation formulae for the ELI of a 3D interface presented in the section 2.3.

Appendix C. Numerical schemes for evaluating y based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

(i) 2nd-order solutions based on stencils $\{y_1, y_2\}$, $\{y_1, y_{x1}\}$ and $\{y_2, y_{x2}\}$

From the following Taylor series expansions of y_1 and y_2

$$\begin{cases} y_1 = y + \sum_{n=1}^{\infty} \frac{(x_1 - x)^n}{n!} y_x^{(n)} = y + \sum_{n=1}^{\infty} \frac{\delta_1^n}{n!} y_x^{(n)} = y + \sum_{n=1}^{\infty} C_{1,1}^{(n)} y_x^{(n)}; \\ y_2 = y + \sum_{n=1}^{\infty} \frac{(x_2 - x)^n}{n!} y_x^{(n)} = y + \sum_{n=1}^{\infty} \frac{\delta_2^n}{n!} y_x^{(n)} = y + \sum_{n=1}^{\infty} C_{2,1}^{(n)} y_x^{(n)} \end{cases} \quad (1)$$

one can obtain a 2nd-order approximation to y , denoted by $A_{1,2}$, via using the following weighting operation

$$A_{1,2} = \omega_{1,2} y_1 + (1 - \omega_{1,2}) y_2 = y + \sum_{n=2}^{\infty} C_{1,2}^{(n)} y_x^{(n)} \quad (2)$$

where the weight is obtained from

$$\omega_{1,2} = \frac{C_{2,1}^{(1)}}{C_{2,1}^{(1)} - C_{1,1}^{(1)}} = \frac{\delta_2}{\delta_2 - \delta_1} \quad (3)$$

and the coefficients of the truncation error (TE) can be obtained from

$$C_{1,2}^{(n)} = \omega_{1,2} C_{1,1}^{(n)} + (1 - \omega_{1,2}) C_{2,1}^{(n)} = \frac{-\delta_1 \delta_2}{n!} \frac{\delta_2^{n-1} - \delta_1^{n-1}}{\delta_2 - \delta_1} \quad (4)$$

with the leading order term given by

$$C_{1,2}^{(2)} = \frac{-\delta_2 \delta_1}{2!} \quad (5)$$

In addition to $A_{1,2}$, another two 2nd-order approximations to y , denoted, respectively, by $A_{2,2}$ and $A_{3,2}$, can be acquired from the following weighting operations

$$\begin{aligned} A_{2,2} &= y_1 - \delta_1 y_{x1}^{(1)} = y + \sum_{n=2}^{\infty} C_{2,2}^{(n)} y_x^{(n)}, \\ A_{3,2} &= y_2 - \delta_2 y_{x2}^{(1)} = y + \sum_{n=2}^{\infty} C_{3,2}^{(n)} y_x^{(n)} \end{aligned} \quad (6)$$

where the coefficients of TE are

$$C_{2,2}^{(n)} = \frac{1-n}{n!} \delta_1^n, \quad C_{3,2}^{(n)} = \frac{1-n}{n!} \delta_2^n \quad (7)$$

(ii) 3rd-order solutions based on stencils $\{y_1, y_2, y_{x1}\}$, $\{y_1, y_2, y_{x2}\}$, $\{y_1, y_{x1}, y_{xx1}\}$ and $\{y_2, y_{x2}, y_{xx2}\}$

By using the following weighting operations one can obtain four 3rd-order approximations to y , denoted, respectively, by $A_{1,3}$, $A_{2,3}$, $A_{3,3}$ and $A_{4,3}$, given by

$$\begin{aligned} A_{1,3} &= \omega_{1,3} A_{1,2} + (1 - \omega_{1,3}) A_{2,2} = y + \sum_{n=3}^{\infty} C_{1,3}^{(n)} y_x^{(n)}, \\ A_{2,3} &= \omega_{2,3} A_{1,2} + (1 - \omega_{2,3}) A_{3,2} = y + \sum_{n=3}^{\infty} C_{2,3}^{(n)} y_x^{(n)}, \\ A_{3,3} &= A_{2,2} + \frac{\delta_1^2}{2} y_{x1}^{(2)} = y + \sum_{n=3}^{\infty} C_{3,3}^{(n)} y_x^{(n)}, \\ A_{4,3} &= A_{3,2} + \frac{\delta_2^2}{2} y_{x2}^{(2)} = y + \sum_{n=3}^{\infty} C_{4,3}^{(n)} y_x^{(n)} \end{aligned} \quad (8)$$

where the weights are

$$\begin{aligned} \omega_{1,3} &= \frac{C_{2,2}^{(2)}}{C_{2,2}^{(2)} - C_{1,2}^{(2)}} = \frac{-\delta_1}{\delta_2 - \delta_1}, \\ \omega_{2,3} &= \frac{C_{3,2}^{(2)}}{C_{3,2}^{(2)} - C_{1,2}^{(2)}} = \frac{\delta_2}{\delta_2 - \delta_1} \end{aligned} \quad (9)$$

and the leading order terms of TE are

$$\begin{aligned} C_{1,3}^{(3)} &= \frac{\delta_2 \delta_1^2}{3!}, \quad C_{2,3}^{(3)} = \frac{\delta_1 \delta_2^2}{3!}, \\ C_{3,3}^{(3)} &= \frac{\delta_1^3}{3!}, \quad C_{4,3}^{(3)} = \frac{\delta_2^3}{3!} \end{aligned} \quad (10)$$

To achieve ENO modifications for higher order approximations, we introduce here the following smoothness parameters for assessing the smoothness of $A_{1,3}$ and $A_{2,3}$, which are defined, respectively, as

$$\begin{aligned} S_{1,3} &= (A_{1,2} - A_{2,2})^2, \\ S_{2,3} &= (A_{1,2} - A_{3,2})^2 \end{aligned} \quad (11)$$

It is apparent that if $A_{1,3}$ and $A_{2,3}$ are smooth approximations for y , the scales of $S_{1,3}$ and $S_{2,3}$ satisfy $O(S_{1,3}) = O(S_{2,3}) = O(\Delta^4)$ where $\Delta = |x_2 - x_1|$.

(iii) 4th-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}\}$, $\{y_1, y_2, y_{x1}, y_{xx1}\}$

and $\{y_1, y_2, y_{x2}, y_{xx2}\}$

By using the following weighting operations one can achieve three 4th-order approximations to y , denoted, respectively, by $A_{1,4}$, $A_{2,4}$ and $A_{3,4}$, given by

$$\begin{aligned}
 A_{1,4} &= \omega_{1,4} A_{1,3} + (1 - \omega_{1,4}) A_{2,3} = y + \sum_{n=4}^{\infty} C_{1,4}^{(n)} y_x^{(n)}, \\
 A_{2,4} &= \omega_{2,4} A_{1,3} + (1 - \omega_{2,4}) A_{3,3} = y + \sum_{n=4}^{\infty} C_{2,4}^{(n)} y_x^{(n)}, \\
 A_{3,4} &= \omega_{3,4} A_{2,3} + (1 - \omega_{3,4}) A_{4,3} = y + \sum_{n=4}^{\infty} C_{3,4}^{(n)} y_x^{(n)}
 \end{aligned} \tag{12}$$

where

$$\begin{aligned}
 \omega_{1,4} &= \frac{C_{2,3}^{(3)}}{C_{2,3}^{(3)} - C_{1,3}^{(3)}} = \frac{\delta_2}{\delta_2 - \delta_1}, \\
 \omega_{2,4} &= \frac{C_{3,3}^{(3)}}{C_{3,3}^{(3)} - C_{1,3}^{(3)}} = \frac{-\delta_1}{\delta_2 - \delta_1}, \\
 \omega_{3,4} &= \frac{C_{4,3}^{(3)}}{C_{4,3}^{(3)} - C_{2,3}^{(3)}} = \frac{\delta_2}{\delta_2 - \delta_1}
 \end{aligned} \tag{13}$$

The leading order terms of TE are given by

$$C_{1,4}^{(4)} = \frac{-\delta_2^2 \delta_1^2}{4!}, \quad C_{2,4}^{(4)} = \frac{-\delta_2 \delta_1^3}{4!}, \quad C_{3,4}^{(4)} = \frac{-\delta_1 \delta_2^3}{4!} \tag{14}$$

The smoothness of $A_{1,4}$, $A_{2,4}$ and $A_{3,4}$ can be assessed by using the following smoothness parameters

$$\begin{aligned}
 S_{1,4} &= (A_{1,3} - A_{2,3})^2, \\
 S_{2,4} &= (A_{1,3} - A_{3,3})^2, \\
 S_{3,4} &= (A_{2,3} - A_{4,3})^2
 \end{aligned} \tag{15}$$

Clearly, if $A_{1,4}$, $A_{2,4}$ and $A_{3,4}$ are smooth approximations to y , the scales of $S_{1,4}$, $S_{2,4}$ and $S_{3,4}$ satisfy $O(S_{1,4}) = O(S_{2,4}) = O(S_{3,4}) = O(\Delta^6)$. Consequently, the ENO modifications of $A_{1,4}$, $A_{2,4}$ and $A_{3,4}$, denoted, respectively, by $B_{1,4}$, $B_{2,4}$ and $B_{3,4}$, can be defined as

$$\begin{cases} \text{if } S_{1,4} < \min(S_{1,3}, S_{2,3}), & B_{1,4} = A_{1,4} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,3} < S_{2,3}, & B_{1,4} = A_{1,3}, S_{1,4} = S_{1,3} \\ \text{otherwise,} & B_{1,4} = A_{2,3}, S_{1,4} = S_{2,3} \end{cases} \end{cases} \tag{16}$$

$$\begin{cases} \text{if } S_{2,4} < S_{1,3}, & B_{2,4} = A_{2,4} \\ \text{otherwise,} & B_{2,4} = A_{1,3}, S_{2,4} = S_{1,3} \end{cases} \tag{17}$$

$$\begin{cases} \text{if } S_{3,4} < S_{2,3}, & B_{3,4} = A_{3,4} \\ \text{otherwise,} & B_{3,4} = A_{2,3}, S_{3,4} = S_{2,3} \end{cases} \tag{18}$$

(iv) 5th-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}\}$ and $\{y_1, y_2,$

$y_{x1}, y_{x2}, y_{xx2}\}$

From the following weighting operations one can obtain two 5th-order approximations to y , denoted, respectively, by $A_{1,5}$ and $A_{2,5}$, given by

$$\begin{aligned} A_{1,5} &= \omega_{1,5} A_{1,4} + (1 - \omega_{1,5}) A_{2,4} = y + \sum_{n=5}^{\infty} C_{1,5}^{(n)} y_x^{(n)}, \\ A_{2,5} &= \omega_{2,5} A_{1,4} + (1 - \omega_{2,5}) A_{3,4} = y + \sum_{n=5}^{\infty} C_{2,5}^{(n)} y_x^{(n)} \end{aligned} \quad (19)$$

where the weights are

$$\begin{aligned} \omega_{1,5} &= \frac{C_{2,4}^{(4)}}{C_{2,4}^{(4)} - C_{1,4}^{(4)}} = \frac{-\delta_1}{\delta_2 - \delta_1}, \\ \omega_{2,5} &= \frac{C_{3,4}^{(4)}}{C_{3,4}^{(4)} - C_{1,4}^{(4)}} = \frac{\delta_2}{\delta_2 - \delta_1} \end{aligned} \quad (20)$$

The leading order terms of TE are given by

$$C_{1,5}^{(5)} = \frac{\delta_2^2 \delta_1^3}{5!}, \quad C_{2,5}^{(5)} = \frac{\delta_1^2 \delta_2^3}{5!} \quad (21)$$

The smoothness parameters for $A_{1,5}$ and $A_{2,5}$ are defined as

$$\begin{aligned} S_{1,5} &= (A_{1,4} - A_{2,4})^2, \\ S_{2,5} &= (A_{1,4} - A_{3,4})^2 \end{aligned} \quad (22)$$

Obviously, if $A_{1,5}$ and $A_{2,5}$ are smooth approximations to y , the scales of $S_{1,5}$ and $S_{2,5}$ satisfy $O(S_{1,5}) = O(S_{2,5}) = O(\Delta^8)$. Therefore, the ENO modifications for $A_{1,5}$ and $A_{2,5}$, denoted, respectively, by $B_{1,5}$ and $B_{2,5}$, can be defined as

$$\begin{cases} \text{if } S_{1,5} < \min(S_{1,4}, S_{2,4}), & B_{1,5} = A_{1,5} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,4} < S_{2,4}, & B_{1,5} = B_{1,4}, S_{1,5} = S_{1,4} \\ \text{otherwise,} & B_{1,5} = B_{2,4}, S_{1,5} = S_{2,4} \end{cases} \end{cases} \quad (23)$$

$$\begin{cases} \text{if } S_{2,5} < \min(S_{1,4}, S_{3,4}), & B_{2,5} = A_{2,5} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,4} < S_{3,4}, & B_{2,5} = B_{1,4}, S_{2,5} = S_{1,4} \\ \text{otherwise,} & B_{2,5} = B_{3,4}, S_{2,5} = S_{3,4} \end{cases} \end{cases} \quad (24)$$

(v) 6th-order solution based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

A 6th-order approximation to y , denoted by $A_{1,6}$, can be yielded from the following weighting operation

$$A_{1,6} = \omega_{1,6} A_{1,5} + (1 - \omega_{1,6}) A_{2,5} \quad (25)$$

where the weight is

$$\omega_{1,6} = \frac{C_{2,5}^{(5)}}{C_{2,5}^{(5)} - C_{1,5}^{(5)}} = \frac{\delta_2}{\delta_2 - \delta_1} \quad (26)$$

The smoothness parameter for $A_{1,6}$ can be defined as

$$S_{1,6} = (A_{1,5} - A_{2,5})^2 \quad (27)$$

which satisfies $O(S_{1,6}) = O(\Delta^{10})$ if $A_{1,6}$ is a smooth approximation to y . Hence, the ENO modification for $A_{1,6}$, denoted by $B_{1,6}$, can be defined as

$$\begin{cases} \text{if } S_{1,6} < \min(S_{1,5}, S_{2,5}), & B_{1,6} = A_{1,6} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,5} < S_{2,5}, & B_{1,6} = B_{1,5} \\ \text{otherwise,} & B_{1,6} = B_{2,5} \end{cases} \end{cases} \quad (28)$$

Appendix D. Numerical schemes for evaluating y_x based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

(i) 1st-order solutions based on stencils $\{y_1, y_2\}$, $\{y_{x1}\}$ and $\{y_{x2}\}$

It is straightforward to obtain the following three 1st-order approximations to y_x , denoted, respectively, by $A_{1,1}$, $A_{2,1}$ and $A_{3,1}$, given by

$$\begin{aligned} A_{1,1} &= \frac{y_2 - y_1}{x_2 - x_1} = y_x^{(1)} + \sum_{n=2}^{\infty} \frac{\delta_2^n - \delta_1^n}{n! (\delta_2 - \delta_1)} y_x^{(n)} = y_x^{(1)} + \sum_{n=2}^{\infty} C_{1,1}^{(n)} y_x^{(n)}, \\ A_{2,1} &= y_{x1}^{(1)} = y_x^{(1)} + \sum_{n=2}^{\infty} \frac{\delta_1^{n-1}}{(n-1)!} y_x^{(n)} = y_x^{(1)} + \sum_{n=2}^{\infty} C_{2,1}^{(n)} y_x^{(n)}, \\ A_{3,1} &= y_{x2}^{(1)} = y_x^{(1)} + \sum_{n=2}^{\infty} \frac{\delta_2^{n-1}}{(n-1)!} y_x^{(n)} = y_x^{(1)} + \sum_{n=2}^{\infty} C_{3,1}^{(n)} y_x^{(n)} \end{aligned} \quad (1)$$

By noticing that

$$C_{1,1}^{(2)} = \frac{\delta_2 + \delta_1}{2} \quad (2)$$

one can realize that $A_{1,1}$ can be 2nd-order accurate provided $\delta_1 + \delta_2 = 0$.

(ii) 2nd-order solutions based on stencils $\{y_1, y_2, y_{x1}\}$, $\{y_1, y_2, y_{x2}\}$, $\{y_{x1}, y_{xx1}\}$, $\{y_{x2}, y_{xx2}\}$ and $\{y_{x1}, y_{x2}\}$

From the following weighting operations, one can obtain five 2nd-order approximations to y_x , denoted, respectively, by $A_{1,2}$, $A_{2,2}$, $A_{3,2}$, $A_{4,2}$ and $A_{5,2}$, given by

$$\begin{aligned} A_{1,2} &= \omega_{1,2} A_{1,1} + (1 - \omega_{1,2}) A_{2,1} = y_x^{(1)} + \sum_{n=3}^{\infty} C_{1,2}^{(n)} y_x^{(n)}, \\ A_{2,2} &= \omega_{2,2} A_{1,1} + (1 - \omega_{2,2}) A_{3,1} = y_x^{(1)} + \sum_{n=3}^{\infty} C_{2,2}^{(n)} y_x^{(n)}, \\ A_{3,2} &= y_{x1}^{(1)} - \delta_1 y_{x1}^{(2)} = y_x^{(1)} + \sum_{n=3}^{\infty} C_{3,2}^{(n)} y_x^{(n)}, \\ A_{4,2} &= y_{x2}^{(1)} - \delta_2 y_{x2}^{(2)} = y_x^{(1)} + \sum_{n=3}^{\infty} C_{4,2}^{(n)} y_x^{(n)}, \\ A_{5,2} &= \omega_{5,2} A_{2,1} + (1 - \omega_{5,2}) A_{3,1} = y_x^{(1)} + \sum_{n=3}^{\infty} C_{5,2}^{(n)} y_x^{(n)} \end{aligned} \quad (3)$$

where the weights are

$$\begin{aligned}\omega_{1,2} &= \frac{C_{2,1}^{(2)}}{C_{2,1}^{(2)} - C_{1,1}^{(2)}} = \frac{2\delta_1}{\delta_1 - \delta_2}, \quad \omega_{2,2} = \frac{C_{3,1}^{(2)}}{C_{3,1}^{(2)} - C_{1,1}^{(2)}} = \frac{2\delta_2}{\delta_2 - \delta_1}, \\ \omega_{5,2} &= \frac{C_{3,1}^{(2)}}{C_{3,1}^{(2)} - C_{2,1}^{(2)}} = \frac{\delta_2}{\delta_2 - \delta_1}\end{aligned}\tag{4}$$

and

$$\begin{aligned}C_{1,2}^{(3)} &= \frac{-\delta_1(2\delta_2 + \delta_1)}{3!}, \quad C_{2,2}^{(3)} = \frac{-\delta_2(2\delta_1 + \delta_2)}{3!}, \\ C_{3,2}^{(n)} &= \frac{(2-n)}{(n-1)!} \delta_1^{n-1}, \quad C_{4,2}^{(n)} = \frac{(2-n)}{(n-1)!} \delta_2^{n-1}, \\ C_{5,2}^{(n)} &= \frac{-\delta_1\delta_2}{\delta_2 - \delta_1} \frac{\delta_2^{n-2} - \delta_1^{n-2}}{(n-1)!}\end{aligned}\tag{5}$$

It is clear that $A_{1,2}$ and $A_{2,2}$ can attain 3rd-order of accuracy provided $\delta_1 + 2\delta_2 = 0$ and $\delta_2 + 2\delta_1 = 0$, respectively. To achieve ENO solutions for higher order approximations, we introduce here smoothness parameters for assessing the smoothness of $A_{1,2}$ and $A_{2,2}$, which are defined, respectively, as

$$\begin{aligned}S_{1,2} &= (A_{1,1} - A_{2,1})^2, \\ S_{2,2} &= (A_{1,1} - A_{3,1})^2\end{aligned}\tag{6}$$

It is apparent that if $A_{1,2}$ and $A_{2,2}$ are smooth approximations to y_x , the scales of $S_{1,2}$ and $S_{2,2}$ satisfy $O(S_{1,2}) = O(S_{2,2}) = O(\Delta^2)$.

(iii) 3rd-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}\}$, $\{y_1, y_2, y_{x1}, y_{xx1}\}$, $\{y_1, y_2, y_{x2}, y_{xx2}\}$, $\{y_{x1}, y_{x2}, y_{xx1}\}$ and $\{y_{x1}, y_{x2}, y_{xx2}\}$

$\{y_{xx1}\}$, $\{y_1, y_2, y_{x2}, y_{xx2}\}$, $\{y_{x1}, y_{x2}, y_{xx1}\}$ and $\{y_{x1}, y_{x2}, y_{xx2}\}$

From the following weighting operations one can obtain five 3rd-order approximations to y_x , denoted, respectively, by $A_{1,3}$, $A_{2,3}$, $A_{3,3}$, $A_{4,3}$ and $A_{5,3}$, given by

$$\begin{aligned}A_{1,3} &= \omega_{1,3}A_{1,2} + (1 - \omega_{1,3})A_{5,2} = y_x^{(1)} + \sum_{n=4}^{\infty} C_{1,3}^{(n)} y_x^{(n)}, \\ A_{2,3} &= \omega_{2,3}A_{1,2} + (1 - \omega_{2,3})A_{3,2} = y_x^{(1)} + \sum_{n=4}^{\infty} C_{2,3}^{(n)} y_x^{(n)}, \\ A_{3,3} &= \omega_{3,3}A_{2,2} + (1 - \omega_{3,3})A_{4,2} = y_x^{(1)} + \sum_{n=4}^{\infty} C_{3,3}^{(n)} y_x^{(n)}, \\ A_{4,3} &= \omega_{4,3}A_{3,2} + (1 - \omega_{4,3})A_{5,2} = y_x^{(1)} + \sum_{n=4}^{\infty} C_{4,3}^{(n)} y_x^{(n)}, \\ A_{5,3} &= \omega_{5,3}A_{4,2} + (1 - \omega_{5,3})A_{5,2} = y_x^{(1)} + \sum_{n=4}^{\infty} C_{5,3}^{(n)} y_x^{(n)}\end{aligned}\tag{7}$$

where the weights are

$$\begin{aligned}
 \omega_{1,3} &= \frac{C_{5,2}^{(3)}}{C_{5,2}^{(3)} - C_{1,2}^{(3)}} = \frac{3\delta_2}{\delta_2 - \delta_1}, \quad \omega_{2,3} = \frac{C_{3,2}^{(3)}}{C_{3,2}^{(3)} - C_{1,2}^{(3)}} = \frac{-3\delta_1}{2(\delta_2 - \delta_1)}, \\
 \omega_{3,3} &= \frac{C_{4,2}^{(3)}}{C_{4,2}^{(3)} - C_{2,2}^{(3)}} = \frac{3\delta_2}{2(\delta_2 - \delta_1)}, \quad \omega_{4,3} = \frac{C_{5,2}^{(3)}}{C_{5,2}^{(3)} - C_{3,2}^{(3)}} = \frac{\delta_2}{\delta_2 - \delta_1}, \\
 \omega_{5,3} &= \frac{C_{5,2}^{(3)}}{C_{5,2}^{(3)} - C_{4,2}^{(3)}} = \frac{-\delta_1}{\delta_2 - \delta_1}
 \end{aligned} \tag{8}$$

and the leading order terms of TE are

$$\begin{aligned}
 C_{1,3}^{(4)} &= \frac{2\delta_1\delta_2(\delta_1 + \delta_2)}{4!}, \\
 C_{2,3}^{(4)} &= \frac{\delta_1^2(3\delta_2 + \delta_1)}{4!}, \quad C_{3,3}^{(4)} = \frac{\delta_2^2(3\delta_1 + \delta_2)}{4!}, \\
 C_{4,3}^{(4)} &= \frac{\delta_2\delta_1^2}{3!}, \quad C_{5,3}^{(4)} = \frac{\delta_1\delta_2^2}{3!}
 \end{aligned} \tag{9}$$

Clearly, $A_{1,3}$, $A_{2,3}$ and $A_{3,3}$ can attain 4th-order of accuracy provided $\delta_1 + \delta_2 = 0$, $\delta_1 + 3\delta_2 = 0$ and $3\delta_1 + \delta_2 = 0$, respectively. The smoothness parameters for $A_{1,3}$, $A_{2,3}$ and $A_{3,3}$ can be defined by

$$\begin{aligned}
 S_{1,3} &= (A_{1,2} - A_{2,2})^2, \\
 S_{2,3} &= (A_{1,2} - A_{3,2})^2, \\
 S_{3,3} &= (A_{2,2} - A_{4,2})^2
 \end{aligned} \tag{10}$$

It is seen that if $A_{1,3}$, $A_{2,3}$ and $A_{3,3}$ are smooth approximations to y_x , the scales of $S_{1,3}$, $S_{2,3}$ and $S_{3,3}$ satisfy $O(S_{1,3}) = O(S_{2,3}) = O(S_{3,3}) = O(\Delta^4)$. Thus, the ENO modifications for $A_{1,3}$, $A_{2,3}$ and $A_{3,3}$, denoted, respectively, by $B_{1,3}$, $B_{2,3}$ and $B_{3,3}$, can be defined by

$$\begin{cases} \text{if } S_{1,3} < \min(S_{1,2}, S_{2,2}), & B_{1,3} = A_{1,3} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,2} < S_{2,2}, & B_{1,3} = A_{1,2}, S_{1,3} = S_{1,2} \\ \text{otherwise,} & B_{1,3} = A_{2,2}, S_{1,3} = S_{2,2} \end{cases} \end{cases} \tag{11}$$

$$\begin{cases} \text{if } S_{2,3} < S_{1,2}, & B_{2,3} = A_{2,3} \\ \text{otherwise,} & B_{2,3} = A_{1,2}, S_{2,3} = S_{1,2} \end{cases} \tag{12}$$

$$\begin{cases} \text{if } S_{3,3} < S_{2,2}, & B_{3,3} = A_{3,3} \\ \text{otherwise,} & B_{3,3} = A_{2,2}, S_{3,3} = S_{2,2} \end{cases} \tag{13}$$

It may be noted that $A_{1,3}$ can also be yielded from the following weighting operation

$$A_{1,3} = \omega_{1,3}A_{1,2} + (1 - \omega_{1,3})A_{2,2} \tag{14}$$

where the weight is

$$\omega_{1,3} = \frac{C_{2,2}^{(3)}}{C_{2,2}^{(3)} - C_{1,2}^{(3)}} = \frac{\delta_2(2\delta_1 + \delta_2)}{\delta_2^2 - \delta_1^2} \quad (15)$$

which is singular for $\delta_1 + \delta_2 = 0$.

(iv) 4th-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}\}$, $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx2}\}$ and $\{y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

From the following weighting operations one can acquire three 4th-order approximations to y_x , denoted, respectively, by $A_{1,4}$, $A_{2,4}$, and $A_{3,4}$, given by

$$\begin{aligned} A_{1,4} &= \omega_{1,4}A_{1,3} + (1 - \omega_{1,4})A_{4,3} = y_x^{(1)} + \sum_{n=5}^{\infty} C_{1,4}^{(n)} y_x^{(n)}, \\ A_{2,4} &= \omega_{2,4}A_{1,3} + (1 - \omega_{2,4})A_{5,3} = y_x^{(1)} + \sum_{n=5}^{\infty} C_{2,4}^{(n)} y_x^{(n)}, \\ A_{3,4} &= \omega_{3,4}A_{4,3} + (1 - \omega_{3,4})A_{5,3} = y_x^{(1)} + \sum_{n=5}^{\infty} C_{3,4}^{(n)} y_x^{(n)} \end{aligned} \quad (16)$$

where the weights are

$$\begin{aligned} \omega_{1,4} &= \frac{C_{4,3}^{(4)}}{C_{4,3}^{(4)} - C_{1,3}^{(4)}} = \frac{2\delta_1}{\delta_1 - \delta_2}, \\ \omega_{2,4} &= \frac{C_{5,3}^{(4)}}{C_{5,3}^{(4)} - C_{1,3}^{(4)}} = \frac{2\delta_2}{\delta_2 - \delta_1}, \\ \omega_{3,4} &= \frac{C_{5,3}^{(4)}}{C_{5,3}^{(4)} - C_{4,3}^{(4)}} = \frac{\delta_2}{\delta_2 - \delta_1} \end{aligned} \quad (17)$$

and the leading order terms of TE given by

$$\begin{aligned} C_{1,4}^{(5)} &= \frac{-\delta_2\delta_1^2(3\delta_2 + 2\delta_1)}{5!}, \\ C_{2,4}^{(5)} &= \frac{-\delta_1\delta_2^2(3\delta_1 + 2\delta_2)}{5!}, \\ C_{3,4}^{(5)} &= \frac{-\delta_2^2\delta_1^2}{4!} \end{aligned} \quad (18)$$

It can be seen that $A_{1,4}$ and $A_{2,4}$ can attain 5th-order of accuracy provided $2\delta_1 + 3\delta_2 = 0$ and $3\delta_1 + 2\delta_2 = 0$, respectively. The smoothness parameters for $A_{1,4}$ and $A_{2,4}$ can be defined as

$$\begin{aligned} S_{1,4} &= (A_{1,3} - A_{2,3})^2, \\ S_{2,4} &= (A_{1,3} - A_{3,3})^2 \end{aligned} \quad (19)$$

It is clear that if $A_{1,4}$ and $A_{2,4}$ are smooth approximations to y_x , the scales of $S_{1,4}$ and $S_{2,4}$ satisfy $O(S_{1,4}) = O(S_{2,4}) = O(\Delta^6)$. Hence, the ENO modifications for $A_{1,4}$ and $A_{2,4}$,

denoted, respectively, by $B_{1,4}$ and $B_{2,4}$, can be defined by

$$\begin{cases} \text{if } S_{1,4} < \min(S_{1,3}, S_{2,3}), & B_{1,4} = A_{1,4} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,3} < S_{2,3}, & B_{1,4} = B_{1,3}, S_{1,4} = S_{1,3} \\ \text{otherwise,} & B_{1,4} = B_{2,3}, S_{1,4} = S_{2,3} \end{cases} \end{cases} \quad (20)$$

$$\begin{cases} \text{if } S_{2,4} < \min(S_{1,3}, S_{3,3}), & B_{2,4} = A_{2,4} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,3} < S_{3,3}, & B_{2,4} = B_{1,3}, S_{2,4} = S_{1,3} \\ \text{otherwise,} & B_{2,4} = B_{3,3}, S_{2,4} = S_{3,3} \end{cases} \end{cases} \quad (21)$$

It may be noted that $A_{1,4}$ and $A_{2,4}$ can also be yielded from the following weighting operations

$$\begin{aligned} A_{1,4} &= \omega_{1,4} A_{1,3} + (1 - \omega_{1,4}) A_{2,3} = y_x^{(1)} + \sum_{n=5}^{\infty} C_{1,4}^{(n)} y_x^{(n)}, \\ A_{2,4} &= \omega_{2,4} A_{1,3} + (1 - \omega_{2,4}) A_{3,3} = y_x^{(1)} + \sum_{n=5}^{\infty} C_{2,4}^{(n)} y_x^{(n)} \end{aligned} \quad (22)$$

where

$$\begin{aligned} \omega_{1,4} &= \frac{C_{2,3}^{(4)}}{C_{2,3}^{(4)} - C_{1,3}^{(4)}} = \frac{-\delta_1}{\delta_2 - \delta_1} \frac{3\delta_2 + \delta_1}{2\delta_2 + \delta_1} \\ \omega_{2,4} &= \frac{C_{3,3}^{(4)}}{C_{3,3}^{(4)} - C_{1,3}^{(4)}} = \frac{\delta_2}{\delta_2 - \delta_1} \frac{3\delta_1 + \delta_2}{2\delta_1 + \delta_2} \end{aligned} \quad (23)$$

which are singular for $\delta_1 + 2\delta_2 = 0$ and $2\delta_1 + \delta_2 = 0$, respectively.

(v) 5th-order solution based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

A 5th-order approximation to y_x , denoted by $A_{1,5}$, can be yielded from the following weighting operation

$$A_{1,5} = \omega_{1,5} A_{1,4} + (1 - \omega_{1,5}) A_{3,4} = y_x^{(1)} + \sum_{n=6}^{\infty} C_{1,5}^{(n)} y_x^{(n)} \quad (24)$$

where the weight is

$$\omega_{1,5} = \frac{C_{3,4}^{(5)}}{C_{3,4}^{(5)} - C_{1,4}^{(5)}} = \frac{5\delta_2}{2(\delta_2 - \delta_1)} \quad (25)$$

and the leading order term of TE is given by

$$C_{1,5}^{(6)} = \frac{3\delta_2^2 \delta_1^2 (\delta_2 + \delta_1)}{6!} \quad (26)$$

Evidently, $A_{1,5}$ can attain 6th-order of accuracy provided $\delta_1 + \delta_2 = 0$. The smoothness parameter of $A_{1,5}$ can be defined as

$$S_{1,5} = (A_{1,4} - A_{2,4})^2 \quad (27)$$

which satisfies $O(S_{1,5}) = O(\Delta^8)$ if $A_{1,5}$ is a smooth approximation to y_x . Therefore, the ENO modification for $A_{1,5}$, denoted by $B_{1,5}$, can be defined as

$$\begin{cases} \text{if } S_{1,5} < \min(S_{1,4}, S_{2,4}), & B_{1,5} = A_{1,5} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,4} < S_{2,4}, & B_{1,5} = B_{1,4} \\ \text{otherwise,} & B_{1,5} = B_{2,4} \end{cases} \end{cases} \quad (28)$$

It may be noted that $A_{1,5}$ can also be obtained from the following weighting operation

$$A_{1,5} = \omega_{1,5} A_{1,4} + (1 - \omega_{1,5}) A_{2,4} \quad (29)$$

where

$$\omega_{1,5} = \frac{C_{2,4}^{(5)}}{C_{2,4}^{(5)} - C_{1,4}^{(5)}} = \frac{\delta_2 (3\delta_1 + 2\delta_2)}{2(\delta_2^2 - \delta_1^2)} \quad (30)$$

which is singular for $\delta_1 + \delta_2 = 0$.

Appendix E. Numerical schemes for evaluating y_{xx} based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

(i) 1st-order solutions based on stencils $\{y_1, y_2, y_{x1}\}$, $\{y_1, y_2, y_{x2}\}$, and $\{y_{x1}, y_{x2}\}$

It is straightforward to achieve the following three 1st-order approximations to y_{xx} , denoted, respectively, by $A_{1,1}$, $A_{2,1}$ and $A_{3,1}$, from

$$\begin{aligned} A_{1,1} &= \frac{2}{x_2 - x_1} \left(\frac{y_2 - y_1}{x_2 - x_1} - y_{x1}^{(1)} \right) = y_x^{(2)} + \sum_{n=3}^{\infty} C_{1,1}^{(n)} y_x^{(n)}, \\ A_{2,1} &= \frac{2}{x_1 - x_2} \left(\frac{y_2 - y_1}{x_2 - x_1} - y_{x2}^{(1)} \right) = y_x^{(2)} + \sum_{n=3}^{\infty} C_{2,1}^{(n)} y_x^{(n)}, \\ A_{3,1} &= \frac{y_{x2}^{(1)} - y_{x1}^{(1)}}{\delta_2 - \delta_1} = y_x^{(2)} + \sum_{n=3}^{\infty} C_{3,1}^{(n)} y_x^{(n)} \end{aligned} \quad (1)$$

where the coefficients of TE are

$$\begin{aligned} C_{1,1}^{(n)} &= \frac{2/n!}{\delta_2 - \delta_1} \left(\frac{\delta_2^n - \delta_1^n}{\delta_2 - \delta_1} - n\delta_1^{n-1} \right), \\ C_{2,1}^{(n)} &= \frac{-2/n!}{\delta_2 - \delta_1} \left(\frac{\delta_2^n - \delta_1^n}{\delta_2 - \delta_1} - n\delta_2^{n-1} \right), \\ C_{3,1}^{(n)} &= \frac{\delta_2^{n-1} - \delta_1^{n-1}}{(n-1)!(\delta_2 - \delta_1)} \end{aligned} \quad (2)$$

with the leading order terms given by

$$C_{1,1}^{(3)} = \frac{2}{3!}(\delta_2 + 2\delta_1), \quad C_{2,1}^{(3)} = \frac{2}{3!}(\delta_1 + 2\delta_2), \quad C_{3,1}^{(3)} = \frac{\delta_2 + \delta_1}{2} \quad (3)$$

Evidently, the above solutions $A_{1,1}$, $A_{2,1}$ and $A_{3,1}$ can attain 2nd-order of accuracy provided $2\delta_1 + \delta_2 = 0$, $\delta_1 + 2\delta_2 = 0$ and $\delta_1 + \delta_2 = 0$, respectively.

(ii) 2nd-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}\}$, $\{y_1, y_2, y_{x1}, y_{xx1}\}$ and $\{y_1, y_2, y_{x2}, y_{xx2}\}$

From the following weighting operations one can obtain three 2nd-order approximations to y_{xx} , denoted, respectively, by $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$, given by

$$\begin{aligned}
 A_{1,2} &= \omega_{1,2} A_{1,1} + (1 - \omega_{1,2}) A_{2,1} = y_x^{(2)} + \sum_{n=4}^{\infty} C_{1,2}^{(n)} y_x^{(n)}, \\
 A_{2,2} &= \omega_{2,2} A_{1,1} + (1 - \omega_{2,2}) y_{x1}^{(2)} = y_x^{(2)} + \sum_{n=4}^{\infty} C_{2,2}^{(n)} y_x^{(n)}, \\
 A_{3,2} &= \omega_{3,2} A_{2,1} + (1 - \omega_{3,2}) y_{x2}^{(2)} = y_x^{(2)} + \sum_{n=4}^{\infty} C_{3,2}^{(n)} y_x^{(n)}
 \end{aligned} \tag{4}$$

where the weights are

$$\begin{aligned}
 \omega_{1,2} &= \frac{C_{2,1}^{(3)}}{C_{2,1}^{(3)} - C_{1,1}^{(3)}} = \frac{\delta_1 + 2\delta_2}{\delta_2 - \delta_1}, \\
 \omega_{2,2} &= \frac{-3\delta_1}{\delta_2 - \delta_1}, \quad \omega_{3,2} = \frac{3\delta_2}{\delta_2 - \delta_1}
 \end{aligned} \tag{5}$$

and the leading order terms of TE given by

$$\begin{aligned}
 C_{1,2}^{(4)} &= \frac{-2}{4!} [(\delta_1 + \delta_2)^2 + 2\delta_1\delta_2], \\
 C_{2,2}^{(4)} &= \frac{-\delta_1(\delta_2 + \delta_1)}{4}, \quad C_{3,2}^{(4)} = \frac{-\delta_2(\delta_2 + \delta_1)}{4}
 \end{aligned} \tag{6}$$

It can be seen that $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$ can attain 3rd-order of accuracy provided $(\delta_1 + \delta_2)^2 + 2\delta_1\delta_2 = 0$ and $\delta_1 + \delta_2 = 0$. The smoothness of $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$ can be assessed by using the following smoothness parameters

$$\begin{aligned}
 S_{1,2} &= (A_{1,1} - A_{2,1})^2, \\
 S_{2,2} &= (A_{2,2} - A_{1,1})^2, \\
 S_{3,2} &= (A_{3,2} - A_{2,1})^2
 \end{aligned} \tag{7}$$

Clearly, if $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$ are smooth approximations to y_{xx} , the scales of $S_{1,2}$, $S_{2,2}$ and $S_{3,2}$ satisfy $O(S_{1,2}) = O(S_{2,2}) = O(S_{3,2}) = O(\Delta^2)$. Note that since the smoothness parameters for assessing the smoothness of $A_{1,1}$ and $A_{2,1}$ expressed in terms of $A_{1,1}$ and $A_{2,1}$ are unavailable, we then use the smoothness parameters designed for approximating y_x to test the smoothness of the same stencils. Due to this reason, the ENO modifications for $A_{1,2}$, $A_{2,2}$ and $A_{3,2}$, denoted, respectively, by $B_{1,2}$, $B_{2,2}$ and $B_{3,2}$, are defined as

$$\begin{cases} \text{if } s_{1,3} < \min(s_{1,2}, s_{2,2}), & B_{1,2} = A_{1,2} \\ \text{otherwise,} & \begin{cases} \text{if } s_{1,2} < s_{2,2}, & B_{1,2} = A_{1,1} \\ \text{otherwise,} & B_{1,2} = A_{2,1} \end{cases} \end{cases} \tag{8}$$

$$\begin{cases} \text{if } s_{2,3} < s_{1,2}, & B_{2,2} = A_{2,2} \\ \text{otherwise,} & B_{2,2} = A_{1,1} \end{cases} \tag{9}$$

$$\begin{cases} \text{if } s_{3,3} < s_{2,2}, & B_{3,2} = A_{3,2} \\ \text{otherwise,} & B_{3,2} = A_{2,1} \end{cases} \quad (10)$$

where $s_{1,2}$, $s_{2,2}$, $s_{1,3}$, $s_{2,3}$ and $s_{3,3}$ are smoothness parameters for approximating y_x based on stencils $\{y_1, y_2, y_{x1}\}$, $\{y_1, y_2, y_{x2}\}$, $\{y_1, y_2, y_{x1}, y_{x2}\}$, $\{y_1, y_2, y_{x1}, y_{xx1}\}$ and $\{y_1, y_2, y_{x2}, y_{xx2}\}$, respectively.

(iii) 3rd-order solutions based on stencils $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}\}$ and $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx2}\}$

Using the following weighting operations one can achieve two 3rd-order approximations to y_{xx} , denoted, respectively, by $A_{1,3}$ and $A_{2,3}$, given by

$$\begin{aligned} A_{1,3} &= \omega_{1,3} A_{1,2} + (1 - \omega_{1,3}) A_{2,2} = y_x^{(2)} + \sum_{n=5}^{\infty} C_{1,3}^{(n)} y_x^{(n)}, \\ A_{2,3} &= \omega_{2,3} A_{1,2} + (1 - \omega_{2,3}) A_{3,2} = y_x^{(2)} + \sum_{n=5}^{\infty} C_{2,3}^{(n)} y_x^{(n)} \end{aligned} \quad (11)$$

where the weights are

$$\begin{aligned} \omega_{1,3} &= \frac{C_{2,2}^{(4)}}{C_{2,2}^{(4)} - C_{1,2}^{(4)}} = \frac{3(-\delta_1)(\delta_2 + \delta_1)}{(\delta_2 - \delta_1)(\delta_2 + 2\delta_1)}, \\ \omega_{2,3} &= \frac{C_{3,2}^{(4)}}{C_{3,2}^{(4)} - C_{1,2}^{(4)}} = \frac{3\delta_2(\delta_2 + \delta_1)}{(\delta_2 - \delta_1)(\delta_1 + 2\delta_2)} \end{aligned} \quad (12)$$

and the leading order terms of TE are

$$\begin{aligned} C_{1,3}^{(5)} &= \frac{2\delta_1(3\delta_2^2 + \delta_1^2 + 6\delta_2\delta_1)}{5!}, \\ C_{2,3}^{(5)} &= \frac{2\delta_2(3\delta_1^2 + \delta_2^2 + 6\delta_2\delta_1)}{5!} \end{aligned} \quad (13)$$

Note that $\omega_{1,3}$ and $\omega_{2,3}$ are singular for $2\delta_1 + \delta_2 = 0$ and $2\delta_2 + \delta_1 = 0$, respectively. However, if the interpolated variable is at the mid point, that is, $\delta_1 + \delta_2 = 0$, the above solutions $A_{1,3}$ and $A_{2,3}$ can still be applicable. The smoothness of $A_{1,3}$ and $A_{2,3}$ can be assessed by using the following smoothness parameters

$$\begin{aligned} S_{1,3} &= (A_{1,2} - A_{2,2})^2, \\ S_{2,3} &= (A_{1,2} - A_{3,2})^2 \end{aligned} \quad (14)$$

It is apparent that if $A_{1,3}$ and $A_{2,3}$ are smooth approximations to y_{xx} , the scales of $S_{1,3}$ and $S_{2,3}$ satisfy $O(S_{1,3}) = O(S_{2,3}) = O(\Delta^4)$. Consequently, the ENO modifications for $A_{1,3}$ and $A_{2,3}$, denoted, respectively, by $B_{1,3}$ and $B_{2,3}$, can be defined in the following manner

$$\begin{cases} \text{if } S_{1,3} < \min(S_{1,2}, S_{2,2}), & B_{1,3} = A_{1,3} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,2} < S_{2,2}, & B_{1,3} = B_{1,2}, S_{1,3} = S_{1,2} \\ \text{otherwise,} & B_{1,3} = B_{2,2}, S_{1,3} = S_{2,2} \end{cases} \end{cases} \quad (15)$$

$$\begin{cases} \text{if } S_{2,3} < \min(S_{1,2}, S_{3,2}), & B_{2,3} = A_{2,3} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,2} < S_{3,2}, & B_{2,3} = B_{1,2}, S_{2,3} = S_{1,2} \\ \text{otherwise,} & B_{2,3} = B_{3,2}, S_{2,3} = S_{3,2} \end{cases} \end{cases} \quad (16)$$

(iv) 4th-order solution based on stencil $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$

A 4th-order approximation to y_{xx} , denoted by $A_{1,4}$, can be yielded from the following weighting operation

$$A_{1,4} = \omega_{1,4} A_{1,3} + (1 - \omega_{1,4}) A_{2,3} \quad (17)$$

where the weight is

$$\omega_{1,4} = \frac{C_{2,3}^{(5)}}{C_{2,3}^{(5)} - C_{1,3}^{(5)}} = \frac{\delta_2 (3\delta_1^2 + \delta_2^2 + 6\delta_2\delta_1)}{(\delta_2 - \delta_1)(\delta_2^2 + 4\delta_2\delta_1 + \delta_1^2)} \quad (18)$$

Note that although $\omega_{1,4}$ is singular for $\delta_1^2 + 4\delta_1\delta_2 + \delta_2^2 = 0$, if the interpolated variable is taken at the mid point, that is, $\delta_1 + \delta_2 = 0$, the above solution $A_{1,4}$ can still be used. The smoothness of $A_{1,4}$ can be assessed by using the following smoothness parameter

$$S_{1,4} = (A_{1,3} - A_{2,3})^2 \quad (19)$$

which satisfies $O(S_{1,4}) = O(\Delta^6)$ if $A_{1,4}$ is a smooth approximation to y_{xx} . Consequently, the ENO modification for $A_{1,4}$, denoted by $B_{1,4}$, can be defined as

$$\begin{cases} \text{if } S_{1,4} < \min(S_{1,3}, S_{2,3}), & B_{1,4} = A_{1,4} \\ \text{otherwise,} & \begin{cases} \text{if } S_{1,3} < S_{2,3}, & B_{1,4} = B_{1,3} \\ \text{otherwise,} & B_{1,4} = B_{2,3} \end{cases} \end{cases} \quad (20)$$

Appendix F. Difference schemes for evaluating the first and second derivatives (2nd-order to 5th-order)

The 2nd-order difference schemes for evaluating y_j' , $j \in [1, 3]$, are given by

$$y_j' = \frac{1}{2\Delta x} \sum_{k=1}^3 a_{jk} y_k, \quad j \in [1, 3] \quad (1)$$

where

$$\begin{aligned} \{a_{1k}\} &= \{-3, 4, -1\}, \\ \{a_{2k}\} &= \{-1, 0, 1\}, \\ \{a_{3k}\} &= \{1, -4, 3\} \end{aligned} \quad (2)$$

The 2nd-order difference schemes for evaluating y_j'' , $j \in [1, 4]$, are given by

$$y_j'' = \frac{1}{\Delta x^2} \sum_{k=1}^4 b_{jk} y_k \quad (3)$$

where

$$\begin{aligned} \{b_{1k}\} &= \{2, -5, 4, -1\}, \\ \{b_{2k}\} &= \{1, -2, 1, 0\}, \\ \{b_{3k}\} &= \{0, 1, -2, 1\}, \\ \{b_{4k}\} &= \{-1, 4, -5, 2\} \end{aligned} \quad (4)$$

The 3rd-order difference schemes for evaluating y_j' , $j \in [1, 4]$, are given by

$$y_j' = \frac{1}{6\Delta x} \sum_{k=1}^4 a_{jk} y_k, \quad j \in [1, 4] \quad (5)$$

where

$$\begin{aligned} \{a_{1k}\} &= \{-11, 18, -9, 2\}, \\ \{a_{2k}\} &= \{-2, -3, 6, -1\}, \\ \{a_{3k}\} &= \{1, -6, 3, 2\}, \\ \{a_{4k}\} &= \{-2, 9, -18, 11\} \end{aligned} \quad (6)$$

The 3rd-order difference schemes for evaluating y_j'' , $j \in [1, 5]$, are given by

$$y_j'' = \frac{1}{12\Delta x^2} \sum_{k=1}^5 b_{jk} y_k \quad (7)$$

where

$$\begin{aligned}
\{b_{1k}\} &= \{35, -104, 114, -56, 11\}, \\
\{b_{2k}\} &= \{11, -20, 6, 4, -1\}, \\
\{b_{3k}\} &= \{-1, 16, -30, 16, -1\}, \\
\{b_{4k}\} &= \{-1, 4, 6, -20, 11\}, \\
\{b_{5k}\} &= \{11, -56, 114, -104, 35\}
\end{aligned} \tag{8}$$

The 4th-order difference schemes for evaluating y_j' , $j \in [1, 5]$, are given by

$$y_j' = \frac{1}{12\Delta x} \sum_{k=1}^5 a_{jk} y_k, \quad j \in [1, 5] \tag{9}$$

where

$$\begin{aligned}
\{a_{1k}\} &= \{-25, 48, -36, 16, -3\}, \\
\{a_{2k}\} &= \{-3, -10, 18, -6, 1\}, \\
\{a_{3k}\} &= \{1, -8, 0, 8, -1\}, \\
\{a_{4k}\} &= \{-1, 6, -18, 10, 3\}, \\
\{a_{5k}\} &= \{3, -16, 36, -48, 25\}
\end{aligned} \tag{10}$$

The 4th-order difference schemes for evaluating y_j'' , $j \in [1, 6]$, are given by

$$y_j'' = \frac{1}{12\Delta x^2} \sum_{k=1}^6 b_{jk} y_k \tag{11}$$

where

$$\begin{aligned}
\{b_{1k}\} &= \{45, -154, 214, -156, 61, -10\}, \\
\{b_{2k}\} &= \{10, -15, -4, 14, -6, 1\}, \\
\{b_{3k}\} &= \{-1, 16, -30, 16, -1, 0\}, \\
\{b_{4k}\} &= \{0, -1, 16, -30, 16, -1\}, \\
\{b_{5k}\} &= \{1, -6, 14, -4, -15, 10\}, \\
\{b_{6k}\} &= \{-10, 61, -156, 214, -154, 45\}
\end{aligned} \tag{12}$$

The 5th-order difference schemes for evaluating y_j' , $j \in [1, 6]$, are given by

$$y_j' = \frac{1}{60\Delta x} \sum_{k=1}^6 a_{jk} y_k, \quad j \in [1, 6] \tag{13}$$

where

$$\begin{aligned}
\{a_{1k}\} &= \{-137, 300, -300, 200, -75, 12\}, \\
\{a_{2k}\} &= \{-12, -65, 120, -60, 20, -3\}, \\
\{a_{3k}\} &= \{3, -30, -20, 60, -15, 2\}, \\
\{a_{4k}\} &= \{-2, 15, -60, 20, 30, -3\}, \\
\{a_{5k}\} &= \{3, -20, 60, -120, 65, 12\}, \\
\{a_{6k}\} &= \{-12, 75, -200, 300, -300, 137\}
\end{aligned} \tag{14}$$

The 5th-order difference schemes for evaluating y_j'' , $j \in [1, 7]$, are given by

$$y_j'' = \frac{1}{180\Delta x^2} \sum_{k=1}^7 b_{jk} y_k \tag{15}$$

where

$$\begin{aligned}
\{b_{1k}\} &= \{812, -3132, 5265, -5080, 2970, -972, 137\}, \\
\{b_{2k}\} &= \{137, -147, -255, 470, -285, 93, -13\}, \\
\{b_{3k}\} &= \{-13, 228, -420, 200, 15, -12, 2\}, \\
\{b_{4k}\} &= \{2, -27, 270, -490, 270, -27, 2\}, \\
\{b_{5k}\} &= \{2, -12, 15, 200, -420, 228, -13\}, \\
\{b_{6k}\} &= \{-13, 93, -285, 470, -255, -147, 137\}, \\
\{b_{7k}\} &= \{137, -972, 2970, -5080, 5265, -3132, 812\}
\end{aligned} \tag{16}$$

Appendix G. Accurate error analysis for the Lagrangian interpolation polynomial

Based on a k -points stencil $S_k = \{y_1, \dots, y_k\}$ which is a set of k discretely given function values, the value of a smooth function $y(x)$ at an arbitrary point x can be approximated using the following Lagrangian interpolation polynomial, defined by

$$P_k(x) = \sum_{m=0}^{k-1} y_{1+m} \prod_{l=0, l \neq m}^{k-1} \frac{x - x_{1+l}}{x_{1+m} - x_{1+l}} \quad (1)$$

As pointed out in [Phillips 2003], the conventional error estimation for the Lagrangian interpolation polynomial is of limited use for the error is expressed in an uncertain form with an unknown value used. Below, an accurate error analysis will be conducted by using the mathematical induction method, which is more mathematically strict than the conventional method.

(i) 2-points stencil $\{y_1, y_2\}$

In section (i) of Appendix C we have derived that the 2nd-order Lagrangian interpolation polynomial based on a 2-points stencil $\{y_1, y_2\}$ (see $A_{1,2}$ in Appendix C) can be expanded in the Taylor's series about x as

$$P_2(x) = y(x) + \sum_{n=2}^{\infty} C_2^{(n)} y_x^{(n)} \quad (2)$$

where

$$C_2^{(n)} = \frac{-\delta_1 \delta_2}{n!} \frac{\delta_2^{n-1} - \delta_1^{n-1}}{\delta_2 - \delta_1} = \frac{-\delta_1 \delta_2}{n!} \sum_{l=0}^{n-2} \delta_1^{n-2-l} \delta_2^l \quad (3)$$

in which $\delta_i = x_i - x$. The leading order term of $C_2^{(n)}$ is given by

$$C_2^{(2)} = \frac{-\delta_1 \delta_2}{2!} \quad (4)$$

manifesting $P_2(x)$ is a 2nd-order approximation for $y(x)$.

(ii) 3-points stencil $\{y_1, y_2, y_3\}$

Similar as in (i), the 2nd-order Lagrangian interpolation polynomial based on the 2-points stencil $\{y_1, y_3\}$ can be expanded in the Taylor's series about x as

$$P_{2,a}(x) = y(x) + \sum_{n=2}^{\infty} C_{2,a}^{(n)} y_x^{(n)} \quad (5)$$

where

$$C_{2,a}^{(n)} = \frac{-\delta_1 \delta_3}{n!} \sum_{l=0}^{n-2} \delta_1^{n-2-l} \delta_3^l \quad (6)$$

with the leading order term given by

$$C_{2,a}^{(2)} = \frac{-\delta_1 \delta_3}{2!} \quad (7)$$

Then, one can obtain the 3rd-order Lagrangian interpolation polynomial based on the 3-points stencil $\{y_1, y_2, y_3\}$ via using the following weighting operation

$$P_3(x) = \omega_3 P_2(x) + (1 - \omega_3) P_{2,a}(x) = y(x) + \sum_{n=3}^{\infty} C_3^{(n)} y_x^{(n)} \quad (8)$$

where the weight is obtained from

$$\omega_3 = \frac{C_{2,a}^{(2)}}{C_{2,a}^{(2)} - C_2^{(2)}} = \frac{\delta_3}{\delta_3 - \delta_2} \quad (9)$$

and $C_3^{(n)}$ can be obtained from

$$\begin{aligned} C_3^{(n)} &= \omega_3 C_2^{(n)} + (1 - \omega_3) C_{2,a}^{(n)} \\ &= \frac{\delta_1 \delta_2 \delta_3}{n!} \sum_{l_1=0}^{n-2} \delta_1^{n-2-l_1} \frac{\delta_3^{l_1} - \delta_2^{l_1}}{\delta_3 - \delta_2} \\ &= \frac{\delta_1 \delta_2 \delta_3}{n!} \sum_{l_1=1}^{n-2} \sum_{l_2=0}^{l_1-1} \delta_1^{n-2-l_1} \delta_2^{l_1-1-l_2} \delta_3^{l_2} \end{aligned} \quad (10)$$

The leading order term of $C_3^{(n)}$ is given by

$$C_3^{(3)} = \frac{\delta_1 \delta_2 \delta_3}{3!} \quad (11)$$

which manifests $P_3(x)$ is a 3rd-order approximation for $y(x)$. It is straightforward to verify that $P_3(x)$ obtained by (8) has the same form as the 3rd-order case of the Lagrangian interpolation polynomial defined by (1).

(iii) p -points stencil $\{y_1, y_2, y_3, \dots, y_p\}$ ($p \geq 3$)

According to the features of $C_2^{(n)}$ and $C_3^{(n)}$ we can assume that the p^{th} -order Lagrangian interpolation polynomial based on the p -points stencil $\{y_1, y_2, y_3, \dots, y_p\}$ can be expanded as

$$P_p(x) = y(x) + \sum_{n=p}^{\infty} C_p^{(n)} y_x^{(n)} \quad (12)$$

where

$$C_p^{(n)} = (-1)^{n+1} \frac{\prod_{k=1}^p \delta_k}{n!} \sum_{l_1=p-2}^{n-2} \sum_{l_2=p-3}^{l_1-1} \dots \sum_{l_{p-1}=0}^{l_{p-2}-1} \delta_1^{n-2-l_1} \delta_2^{l_1-1-l_2} \dots \delta_{p-1}^{l_{p-2}-1-l_{p-1}} \delta_p^{l_{p-1}} \quad (13)$$

with the leading order term given by

$$C_p^{(p)} = (-1)^{p+1} \frac{\prod_{k=1}^p \delta_k}{p!} \quad (14)$$

(iv) $(p+1)$ -points stencil $\{y_1, y_2, y_3, \dots, y_p, y_{p+1}\}$ ($p \geq 3$)

Similar as in (iii), the p^{th} -order Lagrangian interpolation polynomial based on the p -points stencil $\{y_1, y_2, y_3, \dots, y_{p-1}, y_{p+1}\}$ can be expanded as

$$P_{p,a}(x) = y(x) + \sum_{n=p}^{\infty} C_{p,a}^{(n)} y_x^{(n)} \quad (15)$$

where

$$C_{p,a}^{(n)} = (-1)^{n+1} \frac{\delta_{p+1} \prod_{k=1}^{p-1} \delta_k}{n!} \sum_{l_1=p-2}^{n-2} \sum_{l_2=p-3}^{l_1-1} \dots \sum_{l_{p-1}=0}^{l_{p-2}-1} \delta_1^{n-2-l_1} \delta_2^{l_1-1-l_2} \dots \delta_{p-1}^{l_{p-2}-1-l_{p-1}} \delta_{p+1}^{l_{p-1}} \quad (16)$$

and the leading order term is given by

$$C_{p,a}^{(p)} = (-1)^{p+1} \frac{\delta_{p+1} \prod_{k=1}^{p-1} \delta_k}{p!} \quad (17)$$

Then, the $(p+1)^{\text{th}}$ -order Lagrangian interpolation polynomial based on the $(p+1)$ -points stencil $\{y_1, y_2, y_3, \dots, y_p, y_{p+1}\}$ can be obtained via using the following weighting operation

$$P_{p+1}(x) = \omega_{p+1} P_p(x) + (1 - \omega_{p+1}) P_{p,a}(x) = y(x) + \sum_{n=p+1}^{\infty} C_{p+1}^{(n)} y_x^{(n)} \quad (18)$$

where the weight is obtained from

$$\omega_{p+1} = \frac{C_{p,a}^{(p)}}{C_{p,a}^{(p)} - C_p^{(p)}} = \frac{\delta_{p+1}}{\delta_{p+1} - \delta_p} \quad (19)$$

and $C_{p+1}^{(n)}$ can be obtained from

$$\begin{aligned} C_{p+1}^{(n)} &= \omega_{p+1} C_p^{(n)} + (1 - \omega_{p+1}) C_{p,a}^{(n)} \\ &= (-1)^{n+1} \frac{\prod_{k=1}^{p+1} \delta_k}{n!} \sum_{l_1=p-2}^{n-2} \sum_{l_2=p-3}^{l_1-1} \dots \sum_{l_{p-1}=0}^{l_{p-2}-1} \delta_1^{n-2-l_1} \delta_2^{l_1-1-l_2} \dots \delta_{p-1}^{l_{p-2}-1-l_{p-1}} \frac{\delta_{p+1}^{l_{p-1}} - \delta_p^{l_{p-1}}}{\delta_{p+1} - \delta_p} \\ &= (-1)^{n+1} \frac{\prod_{k=1}^{p+1} \delta_k}{n!} \sum_{l_1=p-1}^{n-2} \sum_{l_2=p-2}^{l_1-1} \dots \sum_{l_p=0}^{l_{p-1}-1} \delta_1^{n-2-l_1} \delta_2^{l_1-1-l_2} \dots \delta_{p-1}^{l_{p-2}-1-l_{p-1}} \delta_p^{l_{p-1}-1-l_p} \delta_{p+1}^{l_p} \end{aligned} \quad (20)$$

The leading order term of $C_{p+1}^{(n)}$ is given by

$$C_{p+1}^{(p+1)} = (-1)^{p+2} \frac{\prod_{k=1}^{p+1} \delta_k}{(p+1)!} \quad (21)$$

By comparing the features between (13) and (20) it is obvious that the previous

assumed $C_p^{(n)}$ is proven correct which just gives the accurate error estimation for an arbitrary p^{th} -order Lagrangian interpolation polynomial. Also, Eq. (18) has presented a proof for the known Neville-Aitken relation for the Lagrangian interpolation polynomial.

Table 1. Accuracy tests for the numerical schemes developed in section 3. The computational stencils are $\{y_1, y_2, y_{x1}, y_{x2}\}$ in (a) and $\{y_1, y_2, y_{x1}, y_{x2}, y_{xx1}, y_{xx2}\}$ in (b).

Table 1 (a).

N	y		y_x		y_{xx}	
	L_∞ error	Order	L_∞ error	order	L_∞ error	order
2^4	6.059E-05	–	7.619E-05	–	2.483E-01	–
2^5	3.850E-06	3.98	4.838E-06	3.98	6.308E-02	1.98
2^6	2.416E-07	3.99	3.036E-07	3.99	1.583E-02	1.99
2^7	1.511E-08	4.00	1.899E-08	4.00	3.962E-03	2.00
2^8	9.449E-10	4.00	1.187E-09	4.00	9.908E-04	2.00
2^9	5.906E-11	4.00	7.458E-11	3.99	2.477E-04	2.00
2^{10}	3.691E-12	4.00	5.015E-12	–	6.193E-05	2.00
2^{11}	2.308E-13	4.00	2.065E-12	–	1.548E-05	2.00
2^{12}	1.454E-14	3.99	4.563E-12	–	3.871E-06	2.00

Table 1 (b).

N	y		y_x		y_{xx}	
	L_∞ error	Order	L_∞ error	order	L_∞ error	order
2^4	7.790E-08	–	7.000E-08	–	4.787E-04	–
2^5	1.237E-09	5.98	1.110E-09	5.98	3.040E-05	3.98
2^6	1.940E-11	5.99	1.746E-11	5.99	1.908E-06	3.99
2^7	3.034E-13	6.00	3.144E-13	5.80	1.193E-07	4.00
2^8	4.885E-15	5.96	3.828E-13	–	7.461E-09	4.00
2^9	4.580E-16	–	4.778E-13	–	4.686E-10	3.99
2^{10}	4.996E-16	–	1.260E-12	–	3.150E-11	–
2^{11}	4.996E-16	–	2.224E-12	–	1.305E-11	–
2^{12}	5.551E-16	–	5.682E-12	–	2.863E-11	–

Table 2. Errors of the ELI of the 2D interface particles after one fourth of a full solid body rotation for various time steps Δt (defined by T/N).

N	y		y_x		y_{xx}	
	L_∞ error	Order	L_∞ error	order	L_∞ error	order
2^4	4.864E-07	–	2.047E-06	–	1.108E-03	–
2^5	3.040E-08	4.00	1.287E-07	3.99	5.903E-05	4.23
2^6	1.900E-09	4.00	8.241E-09	3.97	2.606E-06	4.50
2^7	1.188E-10	4.00	5.241E-10	3.97	1.321E-07	4.30
2^8	7.421E-12	4.00	3.309E-11	3.99	7.339E-09	4.17
2^9	4.653E-13	4.00	2.082E-12	3.99	4.514E-10	4.02
2^{10}	3.305E-14	–	1.326E-13	3.97	2.798E-11	4.01
2^{11}	6.125E-15	–	1.199E-14	–	1.728E-12	4.02
2^{12}	9.100E-15	–	5.884E-15	–	2.593E-13	–

Table 3. L_2 and L_∞ errors of the ELI and curvature of the interpolated particles ($\alpha_{add} = 1$) on an initial 2D circle under various meshes.

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	1.281E-07	6.370E-07	7.439E-05	3.813E-04	3.753E-03	1.657E-02
$2^7 \times 2^7$	2.523E-10	1.763E-09	1.135E-06	7.525E-06	3.009E-05	1.966E-04
$2^8 \times 2^8$	1.837E-12	9.920E-12	4.350E-08	2.239E-07	1.185E-06	5.934E-06
$2^9 \times 2^9$	2.901E-14	1.722E-13	2.743E-09	1.536E-08	7.464E-08	4.040E-07
$2^{10} \times 2^{10}$	6.773E-16	1.066E-14	2.091E-10	2.486E-09	5.608E-09	6.464E-08

Table 4. L_∞ errors and convergence rates of the ELI and curvature of the interpolated particles ($\alpha_{add} = 1$) on an initial 2D circle between equally spaced points with $k = \pm 2$.

Mesh	y		y_x		κ	
	L_∞ error	order	L_∞ error	order	L_∞ error	Order
$2^6 \times 2^6$	8.163E-09	—	6.491E-08	—	5.385E-04	—
$2^7 \times 2^7$	3.502E-10	4.54	3.419E-09	4.25	7.932E-05	2.76
$2^8 \times 2^8$	9.920E-12	5.14	1.103E-10	4.95	8.172E-06	3.28
$2^9 \times 2^9$	1.722E-13	5.85	1.956E-12	5.82	5.576E-07	3.87
$2^{10} \times 2^{10}$	2.859E-15	5.91	2.169E-13	—	3.646E-08	3.93
$2^{11} \times 2^{11}$	1.943E-16	—	4.759E-13	—	2.442E-09	3.90
$2^{12} \times 2^{12}$	1.665E-16	—	9.729E-13	—	1.549E-10	3.98

Table 5. L_2 and L_∞ errors of the ELI and curvature of the results obtained at $t = 40$ in the single vortex test ($\alpha_{add} = 1.5$, $\alpha_{del} = 0.5$) under various meshes.

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^7 \times 2^7$	3.076E-07	3.251E-06	1.679E-04	1.549E-03	8.737E-01	2.503E-00
$2^8 \times 2^8$	1.447E-08	1.438E-07	1.200E-05	1.990E-04	8.255E-02	1.112E-00
$2^9 \times 2^9$	2.704E-10	3.497E-09	3.337E-07	4.694E-06	4.701E-03	8.378E-02

Table 6. L_2 and L_∞ errors of the ELI and curvature of the results obtained at $t = 2$ in the deformation field test ($n_v = 4$, $\alpha_{add} = 1.5$, $\alpha_{del} = 0.5$) under various meshes.

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^7 \times 2^7$	4.887E-06	4.450E-05	6.203E-02	6.548E-01	2.624E+02	2.819E+03
$2^8 \times 2^8$	5.717E-08	7.911E-07	1.558E-03	2.727E-02	3.239E+01	5.671E+02
$2^9 \times 2^9$	2.643E-08	6.609E-07	8.810E-05	2.225E-03	1.136E+01	2.869E+02

Table 7. L_2 and L_∞ errors of the ELI and curvature of the results obtained at $t = 4$ in the single vortex test ($\alpha_{add} = 1.5$, $\alpha_{del} = 0.5$) under various meshes. In Table 7 (a) the velocities and their spatial derivatives are obtained analytically; in Table 7 (b) the velocities are specified discretely on the computational grids and their spatial derivatives are evaluated numerically.

Table 7 (a).

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	2.496E-07	1.605E-06	7.701E-05	4.008E-04	9.208E-03	5.048E-02
$2^7 \times 2^7$	4.029E-09	3.522E-08	2.653E-06	2.193E-05	8.096E-04	9.006E-03
$2^8 \times 2^8$	2.196E-10	3.088E-09	2.676E-07	3.203E-06	3.123E-04	4.591E-03

Table 7 (b).

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	1.268E-06	7.595E-06	3.731E-04	1.984E-03	6.778E-02	4.761E-01
$2^7 \times 2^7$	4.187E-08	2.967E-07	5.148E-05	5.968E-04	6.914E-03	8.166E-02
$2^8 \times 2^8$	1.953E-09	1.567E-08	4.703E-06	6.205E-05	9.854E-04	1.463E-02

Table 8. L_2 and L_∞ errors of the ELI and curvature of the results obtained at $t = 0.8$ in the deformation field test ($n_v = 4$, $\alpha_{add} = 1.5$, $\alpha_{del} = 0.5$) under various meshes. In Table 8 (a) the velocities and their spatial derivatives are obtained analytically; in Table 8 (b) and (c) the velocities are specified discretely on the computational grids and their spatial derivatives are evaluated numerically. The CFL numbers used in Table 8 (a), (b) and (c) are 0.4, 0.4 and 0.1, respectively.

Table 8 (a).

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	7.898E-06	4.682E-05	9.499E-04	7.773E-03	3.349E-01	2.325E-00
$2^7 \times 2^7$	1.946E-07	1.994E-06	8.041E-05	9.031E-04	2.016E-01	2.201E-00
$2^8 \times 2^8$	1.035E-08	1.326E-07	2.285E-06	3.691E-05	6.938E-04	8.848E-03

Table 8 (b).

Mesh	y		y_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	1.648E-05	9.811E-05	7.428E-03	4.292E-02	7.047E-01	5.203E-00
$2^7 \times 2^7$	4.024E-06	3.713E-05	2.794E-03	3.007E-02	3.640E-01	2.416E-00
$2^8 \times 2^8$	7.774E-06	6.765E-05	1.177E-03	1.407E-02	1.019E-01	1.267E-00

Table 8 (c).

Mesh	y		y'_x		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6$	1.342E-05	7.752E-05	1.072E-02	5.687E-02	8.514E-01	6.608E-00
$2^7 \times 2^7$	2.607E-06	1.773E-05	2.508E-03	3.041E-02	4.698E-01	5.345E-00
$2^8 \times 2^8$	1.644E-06	1.377E-05	3.177E-04	3.117E-03	9.814E-02	1.456E-00

Table 9. L_2 and L_∞ errors of the ELI and curvature of the interpolated particles ($\alpha_{add} = 1.3$) on an initial 3D sphere under various meshes.

Mesh	z		z_x		z_y		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6 \times 2^6$	1.278E-06	1.871E-05	1.696E-03	2.924E-02	1.712E-03	2.800E-02	2.459E-01	2.591E-00
$2^7 \times 2^7 \times 2^7$	3.604E-08	1.365E-06	1.077E-04	4.952E-03	1.084E-04	5.552E-03	4.547E-02	9.113E-01
$2^8 \times 2^8 \times 2^8$	1.851E-09	1.014E-07	7.948E-06	3.371E-04	6.282E-06	2.135E-04	9.729E-03	1.676E-01

Table 10. L_2 and L_∞ errors of the ELI and curvature of the interpolated particles ($\alpha_{add} = 1.2$) on an initial 3D sphere under various meshes.

Mesh	z		z_x		z_y		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6 \times 2^6$	1.178E-06	1.730E-05	1.421E-03	1.967E-02	1.300E-03	2.025E-02	2.373E-01	1.993E-00
$2^7 \times 2^7 \times 2^7$	3.923E-08	1.365E-06	1.090E-04	4.952E-03	1.029E-04	5.552E-03	4.837E-02	9.113E-01
$2^8 \times 2^8 \times 2^8$	1.748E-09	8.180E-08	7.910E-06	3.371E-04	6.592E-06	2.384E-04	1.053E-02	1.676E-01

Table 11. L_2 and L_∞ errors of the ELI and curvature of the results obtained at $t = 2$ in the Enright test under various meshes.

Mesh	z		z_x		z_y		κ	
	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error	L_2 error	L_∞ error
$2^6 \times 2^6 \times 2^6$	1.611E-05	4.407E-04	4.388E-03	6.479E-02	3.669E-03	5.276E-02	1.171E+01	3.795E+02
$2^7 \times 2^7 \times 2^7$	7.971E-08	2.105E-06	5.881E-05	2.171E-03	2.559E-04	1.445E-02	7.153E-02	3.816E-00
$2^8 \times 2^8 \times 2^8$	3.147E-09	3.084E-07	6.800E-06	4.997E-04	8.949E-06	6.787E-04	2.589E-02	1.890E-00

Table 12. Comparisons of the performances of the ELIP method with other various hybrid tracking methods on the single vortex test.

Methods	The max durations	Is the initial circle rebuilt perfectly at the end of simulation?
Enright et al. [2002]	T=5	No
Aulisa et al. [2004]	T=8	No

Hieber & Koumoutsakos [2005]	T=8	No
Leung & Zhao [2009]	T=8	No
Hon et al. [2014]	T=8	No
Jiang et al. [2015]	T=8	Yes
Ianniello & Mascio [2010]	T=20	Yes
ELIP	T=40	Yes

Table 13. Comparisons of the performances of the ELIP method with other various hybrid tracking methods on the Enright test.

Methods	Is the initial sphere rebuilt perfectly at the end of simulation?	Is the interface configuration smooth and continuous at the maximum stretched state?
Enright et al. [2002]	Yes	No
Hieber & Koumoutsakos [2005]	No	No
Leung & Zhao [2009]	Yes	No
Ianniello & Mascio [2010]	Yes	No
Vartdal & Bøckmann [2013]	Yes	No
Bøckmann & Vartdal [2014]	No	No
Jiang et al. [2015]	Yes	No
ELIP	Yes	Yes

Figure 1. A schematic of influence circle and reconnection structure of p_0 .

Figure 2. A pattern of the influence circle for a particle of interest on a spherical interface. (a), (b) and (c) show the interfacial particles defined by $x = x(y, z)$, $y = y(x, z)$ and $z = z(x, y)$, respectively. (d) gives the integrated sphere surface. (e) presents one half of the sphere surface on which the particle of interest is marked by the red color and all the effective particles in the influence circle (the red circle) are distinguished by yellow, cyan and blue colors. (f), (g), (h) and (i) show, respectively, the effective particles in the 1st, 2nd, 3rd and 4th quarters of the influence circle. In each quarter of the influence circle the yellow, cyan and blue particles fall, in turns, into the 1st third, 2nd third and 3rd third of the sub region. In (j) a new particle (denoted by purple color) is interpolated between the red and cyan particles. In (k) another new particle (denoted

by purple color) is interpolated between the red and yellow particles.

Figure 3. The 2D circular shapes after 1/4 rotation, 1/2 rotation, 3/4 rotation and one rotation.

(a) $k = \pm 1$

(b) $k = \pm 2$

Figure 4. The initial input of a 2D circular interface under a mesh $(2^7 \times 2^7)$. (a) and (b) present the particles defined by $x = x(y)$ and $y = y(x)$, respectively. The particles represented by the red, green, blue and purple circles correspond to $k = 1, -1, 2$ and -2 , respectively. (c) is the initial input without applying the addition operation and the total particle number is $N_{original} = 108$. (d) is the result after applying an addition operation with the addition parameter $\alpha_{add} = 1$ and the total particle number $N_{total} = 216$.

 $t = 1 (N_{total} = 1689)$

 $t = 2 (N_{total} = 2936)$

 $t = 4 (N_{total} = 5467)$

 $t = 8 (N_{total} = 10642)$

 $t = 12 (N_{total} = 17426)$

 $t = 16 (N_{total} = 20530)$

Figure 5. Results of the single vortex test under a mesh ($2^9 \times 2^9$). The flow starts at $t = 0$ with a total particle number $N_{original} = 436$ and ends at $t = 40$ with a total particle number $N_{total} = 624$. At $t = 20$ the flow is reversed. The addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively.

Figure 6. Separated results distinguishing the original particles (a) and interpolated particles (b) of those obtained at $t = 20$ shown in figure 5.

$t = 0.2$ ($N_{total} = 1788$)

$t = 0.4$ ($N_{total} = 4168$)

$t = 0.6$ ($N_{total} = 6493$)

$t = 0.8$ ($N_{total} = 8779$)

$t = 1$ ($N_{total} = 11283$)

$t = 1.4$ ($N_{total} = 7049$)

Figure 7. Results of the deformation field test ($n_v = 4$) under a mesh ($2^9 \times 2^9$). The flow starts at $t = 0$ with a total particle number $N_{original} = 436$ and ends at $t = 2$ with a total particle number $N_{total} = 638$. At $t = 1$ the flow is reversed. The addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively.

Figure 8. Separated results distinguishing the original particles (a) and interpolated particles (b) of those obtained at $t = 1$ shown in figure 7.

 $t = 0.1 (N_{total} = 2878)$

 $t = 0.2 (N_{total} = 6194)$

 $t = 0.3 (N_{total} = 9641)$

 $t = 0.4 (N_{total} = 12998)$

 $t = 0.5 (N_{total} = 16327)$

 $t = 0.7 (N_{total} = 10317)$

Figure 9. Results of the deformation field test ($n_v = 8$) under a mesh ($2^9 \times 2^9$). The flow starts at $t = 0$ with a total particle number $N_{original} = 436$ and ends at $t = 1$ with a total particle number $N_{total} = 604$. At $t = 0.5$ the flow is reversed. The addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively.

Figure 10. Separated results distinguishing the original particles (a) and interpolated particles (b) of those obtained at $t = 0.5$ shown in figure 9.

Figure 11. The initial input of a 3D interface under a mesh $(2^6 \times 2^6 \times 2^6)$. (a), (b) and (c) present the particles marked by $k = \pm 1$, $k = \pm 2$ and $k = \pm 3$, respectively. (d) shows the integrated result combined by (a), (b) and (c). (e) is the same as (d) except that all of the particles are described by a single color. The total particle number in (e) is $N_{original} = 978$.

Figure 12. Comparisons of the interface configurations for different addition parameters under a same mesh ($2^6 \times 2^6 \times 2^6$). The original data is that shown in Figure 11 (e). (a1), (a2) and (a3) present the interpolated particles with the addition parameter α_{add} taken as 1.3, 1.2 and 1, respectively. (b1), (b2) and (b3) present the integrated results in which the original and interpolated particles are distinguished by red and green colors, respectively. (c1), (c2) and (c3) are the same as (b1), (b2) and (b3), respectively, except that all of the particles are described by a single color. The total particle numbers in (c1), (c2) and (c3) are $N_{total} = 1188, 1413$ and 3055 , respectively.

Figure 13. The initial input of a 3D interface under a mesh ($2^7 \times 2^7 \times 2^7$). (a), (b) and (c) present the particles marked by $k = \pm 1$, $k = \pm 2$ and $k = \pm 3$, respectively. (d) shows the integrated result combined by (a), (b) and (c). (e) is the same as (d) except that all of the particles are described by a single color. The total particle number in (e) is $N_{original} = 3864$.

Figure 14. Comparisons of the interface configurations for different addition parameters under a same mesh ($2^7 \times 2^7 \times 2^7$). The original data is that shown in Figure 13(e). (a1), (a2) and (a3) present the interpolated particles with the addition parameter α_{add} taken as 1.3, 1.2 and 1, respectively. (b1), (b2) and (b3) present the integrated results in which the original and interpolated particles are distinguished by red and green colors, respectively. (c1), (c2) and (c3) are the same as (b1), (b2) and (b3), respectively, except that all of the particles are described by a single color. The total particle numbers in (c1), (c2) and (c3) are $N_{total} = 4704, 5801$ and 12115 , respectively.

Figure 15. The initial input of a 3D interface under a mesh ($2^8 \times 2^8 \times 2^8$). (a), (b) and (c) present the particles marked by $k = \pm 1$, $k = \pm 2$ and $k = \pm 3$, respectively. (d) shows the integrated result combined by (a), (b) and (c). (e) is the same as (d) except that all of the particles are described by a single color. The total particle number in (e) is

$$N_{original} = 15408.$$

Figure 16. Comparisons of the interface configurations for different addition parameters under a same mesh ($2^8 \times 2^8 \times 2^8$). The original data is that shown in Figure 15 (e). (a1), (a2) and (a3) present the interpolated particles with the addition parameter α_{add} taken as 1.3, 1.2 and 1, respectively. (b1), (b2) and (b3) present the integrated results in which the original and interpolated particles are distinguished by red and green colors, respectively. (c1), (c2) and (c3) are the same as (b1), (b2) and (b3), respectively, except that all of the particles are described by a single color. The total particle numbers in (c1), (c2) and (c3) are $N_{total} = 18628$, 23023 and 48289, respectively.

$t = 0.2$ ($N_{total} = 18289$)

$t = 0.4$ ($N_{total} = 28207$)

$t = 0.6$ ($N_{total} = 56104$)

$t = 0.8$ ($N_{total} = 110647$)

$t = 1$ ($N_{total} = 168903$)

$t = 1.2$ ($N_{total} = 144580$)

Figure 17. Results of the Enright test under a mesh $(2^8 \times 2^8 \times 2^8)$. The flow starts at $t = 0$ with total particle number $N_{original} = 15408$ and ends at $t = 2$ with total particle number $N_{total} = 15500$. At $t = 1$ the flow is reversed. The addition and deletion parameters are $\alpha_{add} = 2.5$ and $\alpha_{del} = 1$, respectively.

Figure 18. Separated results distinguishing the original particles and interpolated particles from the integrated results obtained at $t = 1$ under a mesh $(2^6 \times 2^6 \times 2^6)$. In plots (a1), (a2), (a3) and (a4) only the original particles are presented, while, (b1), (b2), (b3) and (b4) present the integrated results in which the original and interpolated particles are described by red and green colors, respectively. Plots (c1), (c2), (c3) and (c4) are the same as (b1), (b2), (b3) and (b4), respectively, except that all of the particles on the right column are described using a single color. Plots (a2), (b2) and (c2) show a different view for (a1), (b1) and (c1), respectively, while, (a4), (b4) and (c4) show a different view for (a3), (b3) and (c3), respectively. For the results on the upper two rows the addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively, with total particle number $N_{total} = 14403$, while, for the results on the lower two rows the addition and deletion parameters are $\alpha_{add} = 1$ and $\alpha_{del} = 0.2$, respectively, with total particle number $N_{total} = 44325$.

Figure 19. Separated results distinguishing the original particles and interpolated particles from the integrated results obtained at $t = 1$ under a mesh $(2^7 \times 2^7 \times 2^7)$. The illustrations are the same as those of figure 18 except for the following differences: for the results on the upper two rows the addition and deletion parameters are $\alpha_{add} = 2.5$ and $\alpha_{del} = 1$, respectively, with total particle number $N_{total} = 27214$, while, for the results on the lower two rows the addition and deletion parameters are $\alpha_{add} = 1.5$ and $\alpha_{del} = 0.5$, respectively, with total particle number $N_{total} = 103483$.

Figure 20. Separated results distinguishing the original particles and interpolated particles from the integrated results obtained at $t = 1$ under a mesh $(2^8 \times 2^8 \times 2^8)$. The illustrations are the same as those of figure 19 except for the following differences: for the results on the upper two rows the addition and deletion parameters are $\alpha_{add} = 4$ and $\alpha_{del} = 1$, respectively, with total particle number $N_{total} = 49213$, while, for the results on the lower two rows the addition and deletion parameters are $\alpha_{add} = 2.5$ and $\alpha_{del} = 1$, respectively, with total particle number $N_{total} = 168903$.