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Assessment of a Log Stretch–Quaternion Decomposition of the Deformation Gradient to Reduce Advection Error

by Travis Wagner and Richard Becker

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Assessment of a Log Stretch–Quaternion Decomposition of the Deformation Gradient to Reduce Advection Error

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13. SUPPLEMENTARY NOTES * Travis Wagner wrote the code found in the Appendix while a student at the Aberdeen Science and Math Academy (Aberdeen, MD). He conducted further analysis and wrote the first draft of this report while enrolled in the Science and Engineering Apprenticeship Program (contract administered via the Academy of Applied Science, Concord, NH). At the time of publication, he was attending the Rochester Institute of Technology (Rochester, NY).					
14. ABSTRACT Alternative decompositions of the deformation gradient into distortion and rotation components are examined to determine whether advection error can be reduced. The distortion is described either by the right stretch tensor or logarithm of the right stretch tensor. The rotation is represented as quaternions, following earlier research. Accuracy of the decomposition schemes is assessed by using closed-form expressions for deformation fields that are spatially shifted to be consistent with the advected material motion. The results support prior findings where accuracy was improved by representing the deformation gradient as a stretch and quaternions. The results further suggest that additional benefit can be gained by using the log of the stretch. The improvement is credited to two factors: the diagonal and off-diagonal components are of similar magnitude for the log stretch, and the log volume strain is advected accurately.					
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1. Introduction

Simulations of solids using material models that account for hyper-elastic response, anisotropy, or specific microstructure deformation mechanisms often utilize the deformation gradient tensor in the model kinematics. The deformation gradient completely describes the material distortion and rotation. When used in numerical simulations of large strain deformation, where material advection through a computational grid is necessary, the deformation gradient must be advected along with the material. Advection of the deformation gradient in finite element (FE) or finite volume codes is typically accomplished by advecting the nine individual components. However, material models almost always use functions of the deformation gradient, such as separating distortion from rotation and tracking volume change with the determinant. These functions involve nonlinear combinations of the deformation gradient components, whereas the advection process creates a linear interpolation between two states. Consequently, advection introduces error into the nonlinear functions used by the material models.

The deformation gradient can be decomposed into rotation and strain fields using a polar decomposition. The deformation gradient is a continuous function, except at cracks, and for the vast majority of numerical simulations, the rotation and strain fields are also continuous functions. The rotation and strain are meaningful as independent fields, and they are usually more directly tied to constitutive relations than the deformation gradient. Hence, advecting the rotation and strain as independent quantities could be a reasonable alternative to advecting the deformation gradient if the error can be reduced.

The premise is that advecting meaningful quantities, each with fewer components than the original, would create less error. The deformation gradient has nine components. The stretch tensor has six unique components, and it takes three independent parameters to describe a general rotation. So while the total number of advected quantities would be the same, the decomposition ensures that both the strain and rotation fields are smooth and continuous. Robinson et al.¹ demonstrated that the error could be reduced by advecting the right stretch tensor and the rotation represented as quaternions. The quaternion representation of the rotation has four parameters rather than the minimum of three, but the decomposition still reduced advection error.

Here the decomposition is revisited with the hypothesis that part of the error in the advected stretch is due to the difference in magnitude between the diagonal and off-diagonal components. At zero deformation the diagonal components of the stretch tensor are unity and the off-diagonal components are zero. In this report, the

stretch tensor will be modified by taking the natural logarithm of the tensor, which results in all of the components being zero at zero deformation. If the magnitude difference between the diagonal and off-diagonal components affects advection accuracy, this approach should reduce error.

The other modification that will be explored is adjusting the determinant to be consistent with the advected determinant. The determinant of the deformation gradient is equal to the relative volume, which is the current specific volume divided by the initial specific volume. This determinant adjustment is common and is used to keep the volume change represented by the deformation gradient consistent with the volume change used elsewhere within the code. The adjustment is done for the control method as well as the rotation-stretch decomposition and the logarithm variation.

2. Methods, Assumptions, and Procedures

This project had two main goals: 1) to quantify the errors in the deformation gradient following the advection step and 2) to evaluate different decompositions of the deformation gradient to determine if any reduce the error. In order to evaluate the advection error apart from other solution aspects, analysis within common arbitrary Lagrange–Eulerian (ALE) FE codes would be unnecessarily complex. Therefore, a representative advection environment of an ALE–FE code was created. The full code and input are provided in the Appendix. The analysis is restricted to two spatial dimensions for this preliminary evaluation, with the software written in the C programming language.

The environment was constructed with arrays for the attributes that comprise the mesh. A user-defined input file is read by the code that then creates a regular mesh at the specified position in space with the given element size and number of nodes. This code calculates the coordinate values for each node, numbering nodes in bottom left to top right, row-based order. These nodes can be defined to start at any (x, y) position specified, which will place the lower-left origin at this point in space. The width and height of elements are read from the input file and used to space the nodes accordingly. The elements are numbered in the same lower-left to upper-right order in which the nodes were defined. The element connectivity is then created using the four nodes that bound each element. All arrays representing element-based quantities used by the code are ordered by the element number, and all looping is done by this same order.

Blank arrays are instantiated for the centroid coordinates, the deformation gradients, the invariants of the deformation gradients, and the various other variables for the different deformation gradient decompositions. The code has the

functionality to assign a spatially varying deformation gradient field throughout the mesh with specified analytic functions. The initial deformation gradient for the 2-D fields was calculated using derivatives of the current position with respect to the initial position:

$$F_{ij} = \begin{bmatrix} \frac{dx}{d\mathbb{X}} & \frac{dx}{d\mathbb{Y}} & 0 \\ \frac{dy}{d\mathbb{X}} & \frac{dy}{d\mathbb{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (1)$$

Here x and y are the current coordinates of material points initially at $\mathbb{X}$ and $\mathbb{Y}$, respectively.

2.1 Decomposition Methods

This research evaluated advection error for two variants on three decomposition methods for the deformation gradient. The three basic decomposition methods are as follows:

- 1) Control: the conventional advection method that advects the nine elements of the deformation gradient independently
- 2) Quaternion Stretch Tensor (QST): decomposing the deformation gradient into a rotation and a stretch, and advecting the rotation as four quaternion components and advecting the six right stretch tensor components individually
- 3) Quaternion Log Stretch Tensor (QLST): a variation of Method 2, but instead of advecting the right stretch tensor components, the components of the natural logarithm of the right stretch are used

A variant on these three methods was used to correct for the advected determinant, creating three additional solutions. This is described in detail in Section 2.1.4.

2.1.1 Polar Decomposition and Reconstruction

The first operation on the deformation gradient is a polar decomposition into a pure rotation, $\mathbf{R}$, and the right stretch tensor, $\mathbf{U}$, as

$$\mathbf{F} = \mathbf{R} \mathbf{U}. \quad (2)$$

The iterative method used for determining the rotation makes use of the property that the inverse of a pure rotation is equal to its transpose. Setting the initial iterate for the rotation as the deformation gradient, $\tilde{\mathbf{R}}_0 = \mathbf{F}$, the iteration runs over the relation

$$\tilde{\mathbf{R}}_{n+1} = \frac{1}{2}(\tilde{\mathbf{R}}_n + \tilde{\mathbf{R}}_n^{-T}). \quad (3)$$

The iterative solver is run until all components of $\tilde{\mathbf{R}}_{n+1}$ converge to $\tilde{\mathbf{R}}_n$ to within an absolute tolerance of 10^{-12} , which then results in $\tilde{\mathbf{R}}$ being a pure rotation. The loop is limited to 20 or less iterations, and an error is thrown if convergence does not occur. Once $\mathbf{R}$ is found, the right stretch tensor, $\mathbf{U}$, is determined by multiplying Eq. 2 by $\mathbf{R}^T$.

Following advection, the resulting rotation and right stretch tensor are used to reconstruct the deformation gradient according to Eq. 2.

2.1.2 Converting Between Rotations and Quaternions

Once the rotation is determined, it is converted to quaternions by

$$\begin{aligned} \rho &= \frac{1}{2} \sqrt{1 + R_{11} + R_{22} + R_{33}} \\ \lambda &= \frac{1}{4\rho} (R_{32} - R_{23}) \\ \mu &= \frac{1}{4\rho} (R_{13} - R_{31}) \\ v &= \frac{1}{4\rho} (R_{21} - R_{12}). \end{aligned} \quad (4)$$

Modified relations can be used if ρ is small, but the equations above cover all rotations for the simulations in this report.

Following advection, the advected quaternion (denoted with a tilde) is adjusted to ensure that it is a pure rotation by renormalizing as

$$\begin{aligned} \rho &= \tilde{\rho} / (\tilde{\rho}^2 + \tilde{\lambda}^2 + \tilde{\mu}^2 + \tilde{v}^2) \\ \lambda &= \tilde{\lambda} / (\tilde{\rho}^2 + \tilde{\lambda}^2 + \tilde{\mu}^2 + \tilde{v}^2) \\ \mu &= \tilde{\mu} / (\tilde{\rho}^2 + \tilde{\lambda}^2 + \tilde{\mu}^2 + \tilde{v}^2) \\ v &= \tilde{v} / (\tilde{\rho}^2 + \tilde{\lambda}^2 + \tilde{\mu}^2 + \tilde{v}^2). \end{aligned} \quad (5)$$

Once the quaternion components are properly normalized, the rotation matrix is calculated by

$$\mathbf{R} = \begin{bmatrix} \lambda^2 - \mu^2 - v^2 + \rho^2 & 2(\lambda\mu - v\rho) & 2(v\lambda + \mu\rho) \\ 2(\lambda\mu + v\rho) & -\lambda^2 + \mu^2 - v^2 + \rho^2 & 2(\mu v - \lambda\rho) \\ 2(v\lambda - \mu\rho) & 2(\mu v + \lambda\rho) & -\lambda^2 - \mu^2 + v^2 + \rho^2 \end{bmatrix}. \quad (6)$$

Orthogonality and the unitary property of the rotation are ensured by construction, providing that the quaternion is properly normalized.

2.1.3 Log of the Stretch Tensor and Exponentiation

The QLST method requires the logarithm of the stretch tensor, and the subsequent reconstruction of the deformation gradient requires exponentiation of the log form. The algorithm used here was developed by Xiao et al.,² and nearly the same coding is used to compute both the logarithm and exponential of a symmetric second rank tensor. This is accomplished without explicitly calculating the eigenvectors or performing a coordinate transformation. The equations and details of the algorithm are too involved to repeat here, and the reader is referred to the publication.

2.1.4 Correcting for the Determinant

The determinant of the deformation gradient is the ratio of the current volume to the initial volume. Deformation gradients advected in FE codes are often corrected so that the determinant is consistent with the density ratio, which is advected independently. An additional three deformation gradient reconstructions are created by adjusting the three solutions above to reflect an independently advected determinant.

To create these three additional solutions, all of the components of the deformation gradient resulting from the methods described above, $\tilde{\mathbf{F}}$, are multiplied by the cube root of the ratio of the advected determinant, D_{Adv} , to the calculated determinant, $Det(\tilde{\mathbf{F}})$.

$$\mathbf{F} = \left(\frac{D_{Adv}}{Det(\tilde{\mathbf{F}})} \right)^{1/3} \tilde{\mathbf{F}}. \quad (7)$$

This guarantees that the determinant of the resulting deformation gradient equals the independently advected determinant.

2.2 Simulated Advection and Data Analysis

The simulated advection process in this study is the same for all six decomposition methods. It handles components of the tensors and quaternions as independent scalars, which is consistent with advection methods in ALE-FE codes.

A shifted mesh was created with a slight displacement in both the positive x and y directions. For all of the analyses discussed here, the shift was 0.1 of the element size in each orthogonal direction. This shift creates the same advection as material flow down and to the left through the mesh. Advected results are stored at the centroids of the shifted mesh, and analytical forms are also recalculated at the shifted element centroids. This analytic solution serves as the correct result, and it provides a metric to which the advected results can be compared to calculate error.

The simulated advection through the 2-D rectangular mesh consists of a linear interpolation by a weighted average of the two values within adjacent elements. The x -direction is advected first, and then the y -direction. For the 0.1 element size mesh motion simulated here, 0.1 of the quantity in the element to the right is added to 0.9 of the original value for all elements. Then 0.1 of the new quantity in the element above is added to 0.9 of this modified value. Overall, for a variable ψ , the advected value is

$$\psi = 0.81\check{\psi}_0 + 0.09\check{\psi}_r + 0.09\check{\psi}_a + 0.01\check{\psi}_{ar}, \quad (8)$$

where $\check{\psi}_0$ is the original value in the element of interest, $\check{\psi}_r$ is the original value in the element to the right, $\check{\psi}_a$ is the original value in the element above, and $\check{\psi}_{ar}$ is the original value in the element diagonally above and to the right.

The invariants of the deformation gradient are calculated and compared to assess the effectiveness of the decomposition. The three invariants are calculated as

$$\begin{aligned} IV_I &= F_{11} + F_{22} + F_{33} \\ IV_{II} &= F_{32}F_{23} + F_{13}F_{31} + F_{21}F_{12} - F_{22}F_{33} - F_{33}F_{11} - F_{11}F_{22} \\ IV_{III} &= F_{11}(F_{22}F_{33} - F_{32}F_{23}) - F_{12}(F_{21}F_{33} - F_{31}F_{23}) + F_{13}(F_{21}F_{32} - F_{31}F_{22}). \end{aligned} \quad (9)$$

The third invariant, IV_{III} , is the determinant, so the error in IV_{III} for the determinant corrected solutions is not a function of the specific decomposition.

The deformation gradients and the invariants for each case were output in .xmf files for graphing with VisIt.³ The invariants from the advected methods were then compared to the invariants of the analytically shifted result, and the error was computed. These errors were also output in .xmf files for visualization. Since all of the invariants are unitless and order unity, the error values were not normalized.

Additionally, the absolute errors from each element were aggregated and placed on a logarithmic scale for display as box and whisker plots. The absolute error was scaled by 10^{10} , and an offset was added so that the logarithmic measure goes to zero as the error approaches zero. The resulting expression for the box and whisker plotted error is

$$E_{BW} = \ln(10^{10}|E| + 1), \quad (10)$$

where E is the signed error between the advected and the analytic result. With this scheme, E_{BW} values for a few errors are as listed in Table 1.

Table 1 Error values on box and whisker plots as a function of measured error

E	0	10^{-10}	10^{-8}	10^{-6}	10^{-4}	10^{-2}	1
E_{BW}	0	0.693	4.62	9.21	13.82	18.42	23.03

With this scaling, errors differing by a factor of 2 will not be noticeable on the plots. Note that errors of 5 or less would generally have a small effect on the solution, whereas error values above 15 could significantly alter the results.

2.3 Evaluation Functions

Four functions were coded and used to evaluate the advection error associated with the different decompositions of the deformation gradient:

1. Hyperbolic tangent that resembles a shear band
2. Isochoric, plane strain hole closure
3. Radially dependent rotation field resembling a vortex
4. Square root conformal map that distorts the volume significantly

These functions are described in detail in the following subsections.

2.3.1 Hyperbolic Tangent Function

The hyperbolic tangent function creates a displacement field with a single band of deformation in the mesh. The deformed coordinates are given by

$$x = \mathbb{X} . \quad (11)$$

$$y = \mathbb{Y} + a \tanh[\gamma(\mathbb{X} - x_c)] . \quad (12)$$

Here, $a = 1.0$ is the magnitude of the shear centered at $x_c = 1.0$, and the width of the band is controlled by the normalization constant $\gamma = 5.0$. The derivative of the hyperbolic tangent function provides the value of the F_{21} component of the deformation gradient. The deformation gradient is given by Eq. 13, where it is evident that the field only varies in the y -direction.

$$F_{HT} = \begin{bmatrix} \frac{1}{a\gamma} & 0 & 0 \\ \frac{1}{\cosh^2(\gamma(\mathbb{X} - x_c))} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} . \quad (13)$$

This band of the F_{21} component runs vertically in the mesh, as shown in Fig. 1, and the function only varies in the x -direction. All of the invariants are constant across the domain as they are not affected by this deformation field. The corner coordinates of the rectangular region for this example span from $(0.5, -1.0)$ to $(2.5, 1.0)$, with 75 elements in each direction. The function is the steepest at x_c , the center of the shear.

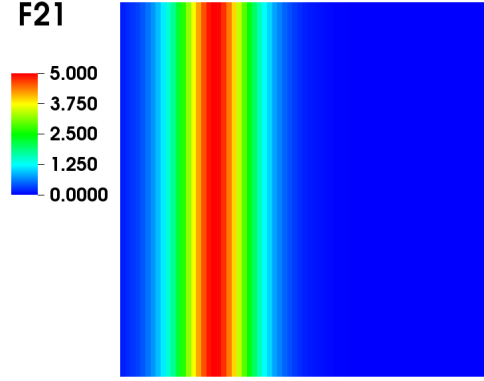


Fig. 1 The F_{21} component of the deformation gradient for the hyperbolic tangent function

2.3.2 Hole Closure Function

The current coordinates of the partially closed hole, given in terms of the initial coordinates, are

$$x = r \cos(\theta) = \frac{r}{\mathbb{R}} \mathbb{X}, \quad (14)$$

$$y = r \sin(\theta) = \frac{r}{\mathbb{R}} \mathbb{Y}, \quad (15)$$

where

$$r = \sqrt{\mathbb{R}^2 + a^2 - \mathbb{A}^2} \text{ and } \mathbb{R} = \sqrt{\mathbb{X}^2 + \mathbb{Y}^2}. \quad (16)$$

Here, $a = 0.2$ is the current radius of the hole, which had an initial radius of $\mathbb{A} = 0.5$. The function has a location with no material, the inside of the hole. It experiences sharp gradients near the hole and gentle gradients in the far field. The deformation gradient is given by

$$F_{EH} = \begin{bmatrix} \frac{1}{r \mathbb{R}} \left(\frac{r^2}{\mathbb{R}^2} \mathbb{Y}^2 + \mathbb{X}^2 \right) & \frac{\mathbb{X} \mathbb{Y}}{r \mathbb{R}} \left(1 - \frac{r^2}{\mathbb{R}^2} \right) & 0 \\ \frac{\mathbb{X} \mathbb{Y}}{r \mathbb{R}} \left(1 - \frac{r^2}{\mathbb{R}^2} \right) & \frac{1}{r \mathbb{R}} \left(\frac{r^2}{\mathbb{R}^2} \mathbb{X}^2 + \mathbb{Y}^2 \right) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (17)$$

The first and second invariants of the deformation gradient are plotted in Fig. 2 for a rectangular domain spanning from $(0.0, -1.0)$ to $(2.0, 1.0)$ to illustrate the deformation field. The third invariant is identically 1.0. The analyses used 75 elements in each direction.

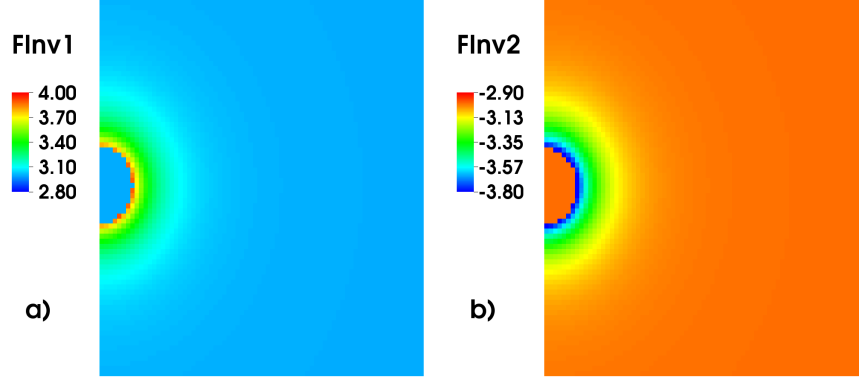


Fig. 2 Plots of the a) first and b) second invariants of the deformation gradient for the collapsing hole

2.3.3 Vortex Function

The third function resembles a planar vortex in which the deformation field is a radially dependent rotation.

$$x = \mathbb{X} \cos(a\mathbb{R}) - \mathbb{Y} \sin(a\mathbb{R}). \quad (18)$$

$$y = \mathbb{X} \sin(a\mathbb{R}) + \mathbb{Y} \cos(a\mathbb{R}). \quad (19)$$

The radius is the same in both the initial and current coordinates,

$$\mathbb{R} = \sqrt{\mathbb{X}^2 + \mathbb{Y}^2} = \sqrt{x^2 + y^2}, \quad (20)$$

rendering the deformation isochoric. The normalization factor, $a = 0.5$, scales the deformation. Note that the deformation is periodic, but the scaling factor is set such that the function increases continuously over the domain, which spans from a rectangular region from $(0.0, -1.0)$ to $(2.0, 1.0)$. The corresponding deformation gradient is given by

$$F_{Vor} = \begin{bmatrix} \left(1 - \frac{a\mathbb{X}\mathbb{Y}}{\mathbb{R}}\right) \cos(a\mathbb{R}) - \frac{a\mathbb{X}^2}{\mathbb{R}} \sin(a\mathbb{R}) & -\left(1 + \frac{a\mathbb{X}\mathbb{Y}}{\mathbb{R}}\right) \sin(a\mathbb{R}) - \frac{a\mathbb{Y}^2}{\mathbb{R}} \cos(a\mathbb{R}) & 0 \\ \left(1 - \frac{a\mathbb{X}\mathbb{Y}}{\mathbb{R}}\right) \sin(a\mathbb{R}) + \frac{a\mathbb{X}^2}{\mathbb{R}} \cos(a\mathbb{R}) & \left(1 + \frac{a\mathbb{X}\mathbb{Y}}{\mathbb{R}}\right) \cos(a\mathbb{R}) - \frac{a\mathbb{Y}^2}{\mathbb{R}} \sin(a\mathbb{R}) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (21)$$

and the deformation field is illustrated by the first and second invariants of the deformation gradient plotted in Fig. 3. Since the deformation is isochoric, the third invariant is constant at 1.0.

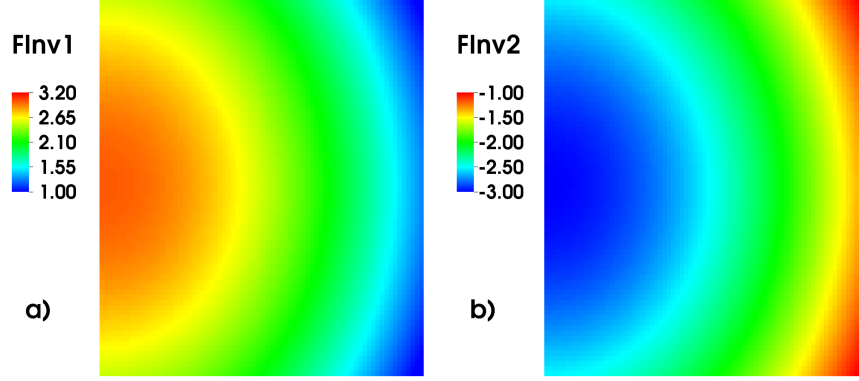


Fig. 3 Plot of the a) first and b) second invariants of the deformation gradient for the vortex function

2.3.4 Square Root Conformal Map Function

The square root conformal map function is included to assess the deformation gradient decompositions under large volume changes. The particular complex variable mapping obtains the current coordinates from the square root of the initial coordinates. As this function is more complicated than the earlier examples, more details are provided. The basic mapping is provided as

$$\left(\frac{\mathbb{Z}}{\mathbb{A}}\right)^{1/2} = \frac{\omega}{a}, \quad (22)$$

where the complex numbers $\mathbb{Z}$ and ω can be represented, respectively, in terms of the initial and final rectangular coordinates and the polar decompositions. These are

$$\mathbb{Z} = \mathbb{X} + i\mathbb{Y} = \mathbb{R} e^{i\theta} \text{ and } \omega = x + iy = r e^{i\varphi}, \quad (23)$$

where the radii are given by

$$\mathbb{R}^2 = \mathbb{X}^2 + \mathbb{Y}^2 \text{ and } r^2 = x^2 + y^2. \quad (24)$$

The normalization constants $\mathbb{A} = 2$ and $a = 2$ in Eq. 22 are needed to nondimensionalize the coordinates and permit the square root operation. The relationship between the initial and current coordinates can be determined using the polar form

$$\left(\frac{\mathbb{Z}}{\mathbb{A}}\right)^{1/2} = \left(\frac{\mathbb{R}}{\mathbb{A}} e^{i\theta}\right)^{1/2} = \left(\frac{\mathbb{R}}{\mathbb{A}}\right)^{1/2} e^{i\frac{\theta}{2}} = \frac{r}{a} e^{i\frac{\theta}{2}} = \frac{\omega}{a}. \quad (25)$$

Also, from term matching by squaring Eq. 22 and using the Cartesian definitions of $\mathbb{Z}$ and ω from Eq. 23,

$$\frac{\mathbb{X}}{\mathbb{A}} = \frac{x^2 - y^2}{a^2} \text{ and } \frac{\mathbb{Y}}{\mathbb{A}} = \frac{2xy}{a^2}. \quad (26)$$

By using the Euler relations in Eq. 25, the current coordinates are expressed in terms of the initial coordinates as

$$x = r \cos\left(\frac{\theta}{2}\right) = a \left(\frac{\mathbb{R}}{\mathbb{A}}\right)^{1/2} \cos\left(\frac{\theta}{2}\right), \quad (27)$$

$$y = r \sin\left(\frac{\theta}{2}\right) = a \left(\frac{\mathbb{R}}{\mathbb{A}}\right)^{1/2} \sin\left(\frac{\theta}{2}\right), \quad (28)$$

with the polar angle given by

$$\theta = \arctan\left(\frac{\mathbb{Y}}{\mathbb{X}}\right). \quad (29)$$

The derivatives required for the deformation gradient can be greatly simplified, as illustrated below for the F_{11} component:

$$\begin{aligned} F_{11} &= \frac{a}{\sqrt{\mathbb{A}}} \left\{ \left[\frac{1}{4} (\mathbb{X}^2 + \mathbb{Y}^2)^{-3/4} 2\mathbb{X} \cos\left(\frac{\theta}{2}\right) \right] - \left[\sin\left(\frac{\theta}{2}\right) \frac{1}{2} \frac{d\theta}{d\mathbb{X}} (\mathbb{X}^2 + \mathbb{Y}^2)^{1/4} \right] \right\} \\ &= \frac{1}{2} \frac{a}{\sqrt{\mathbb{A}}} (\mathbb{X}^2 + \mathbb{Y}^2)^{-3/4} \left[\mathbb{X} \cos\left(\frac{\theta}{2}\right) + \mathbb{Y} \sin\left(\frac{\theta}{2}\right) \right] \\ &= \frac{1}{2} \frac{a}{\sqrt{\mathbb{A}}} (\mathbb{R})^{-3/2} \left[\frac{\mathbb{A}}{a^2} (x^2 - y^2) \frac{x}{r} + \frac{\mathbb{A}}{a^2} 2xy \frac{y}{r} \right] \\ &= \frac{1}{2} \frac{a^4}{\mathbb{A}^2 r^3} \left(\frac{\mathbb{A}}{a^2} \frac{x^3 - xy^2 + 2xy^2}{r} \right) \\ &= \frac{1}{2} \frac{a^2}{\mathbb{A}}. \end{aligned} \quad (30)$$

The result is dimensionally correct, yielding the ratio of a current coordinate over an initial coordinate. The deformation gradient is then simply

$$F_{CM} = \frac{1}{2} \frac{a^2}{\mathbb{A}} \frac{1}{r^2} \begin{bmatrix} x & y & 0 \\ -y & x & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (31)$$

The function is evaluated on a rectangular domain ranging from (0.9, -0.1) to (1.1, 0.1) with 75 elements in each direction. The three invariants of the deformation gradient are plotted in Fig. 4 to illustrate the spatial variation.

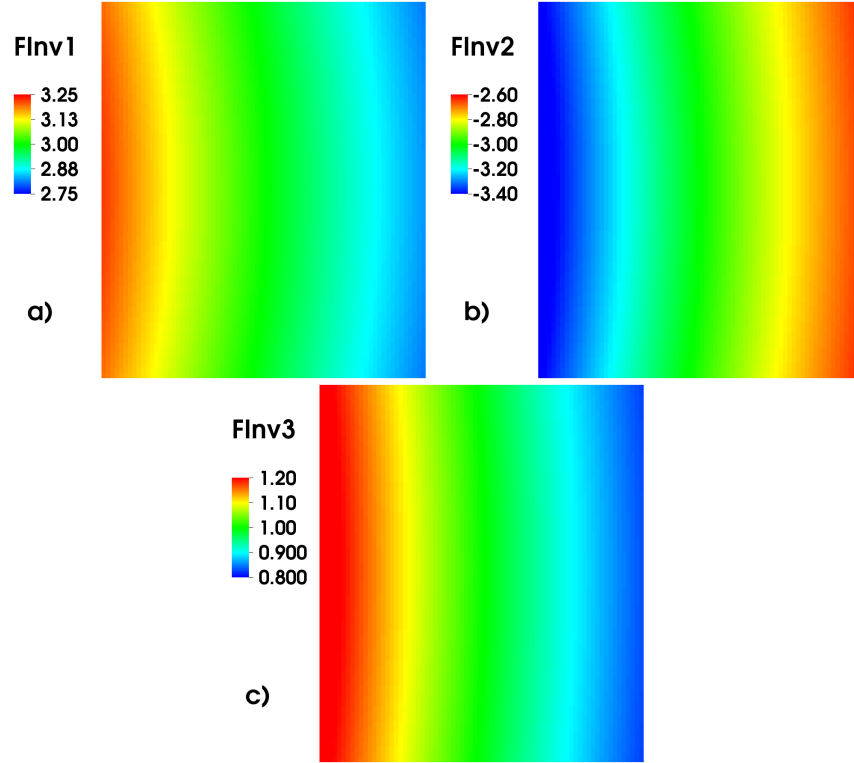


Fig. 4 The a) first, b) second, and c) third invariant of the deformation gradient for the conformal mapping function

3. Results

Detailed spatial maps of the error in the invariants are calculated for the four deformation fields. A comparison of the error in the three invariants will be presented for the six different advection methods. This will be followed by box and whisker plots, which summarize the error over the domains.

3.1 Detailed Error Distributions

3.1.1 Hyperbolic Tangent Function

The hyperbolic tangent function creates a variation in a single component of the deformation gradient, and it provides a simple 1-D example. The F_{21} component of the deformation gradient is depicted in Fig. 1, and all of the invariants are constant: $IV_I = 3$, $IV_{II} = -3$, and $IV_{III} = 1$.

The error in the first invariant computed following the advection of the deformation gradients by the six different methods is shown in Fig. 5. The three base algorithms are shown in the left column, and the determinant corrected versions are shown on the right. Since only a single component of the deformation gradient, F_{21} , is varied

spatially, advection of individual components by the default methods results in an accurate advected solution, as shown by Fig. 5a. However, when F was decomposed for the other two methods, the components were convolved and error was introduced. Of these two, the QLST method, which involved taking the log of the stretch, introduced less error. Correcting for the determinant by Eq. 7 reduced the error substantially for the QST method but not the QLST method. The reason for little change with the determinant correction for the QLST result is that the method advected the determinant accurately, so little alteration is necessary. This is described below.

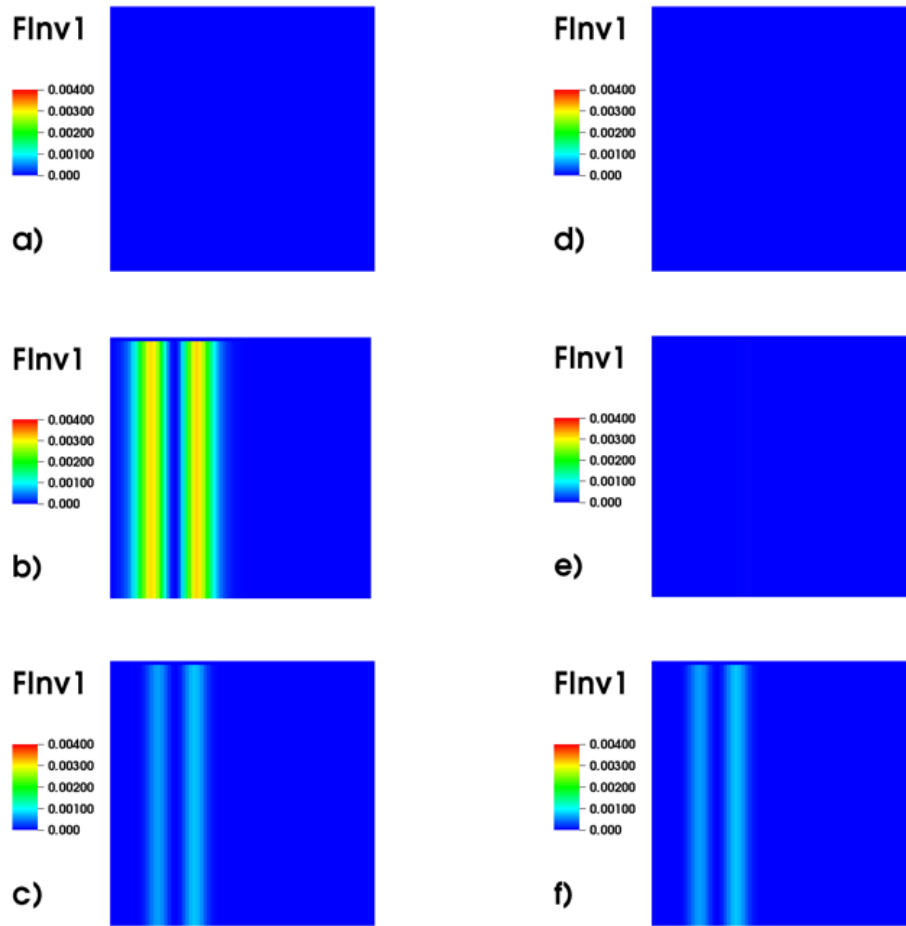


Fig. 5 Error in the first invariant of F for the hyperbolic tangent function following simulated advection. a) Control, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

The error results for the second invariant have a pattern similar to those of the first invariant, with the error magnitude being approximately double. For brevity, these will not be shown.

The error for the third invariant is shown in Fig. 6 using the same layout as the previous plot. As stated previously, the results for the control method have low

error because only a single component of $\mathbf{F}$ varies with the deformation. Advection by the QST method introduces error in the third invariant, which is the determinant. The error is near zero when taking the log of the stretch in the QLST method. The determinant error in the QST method is removed by the determinant correction, which is expected since the correction is exact in these cases. There is little correction for the QLST method since the third invariant was advected with little error.

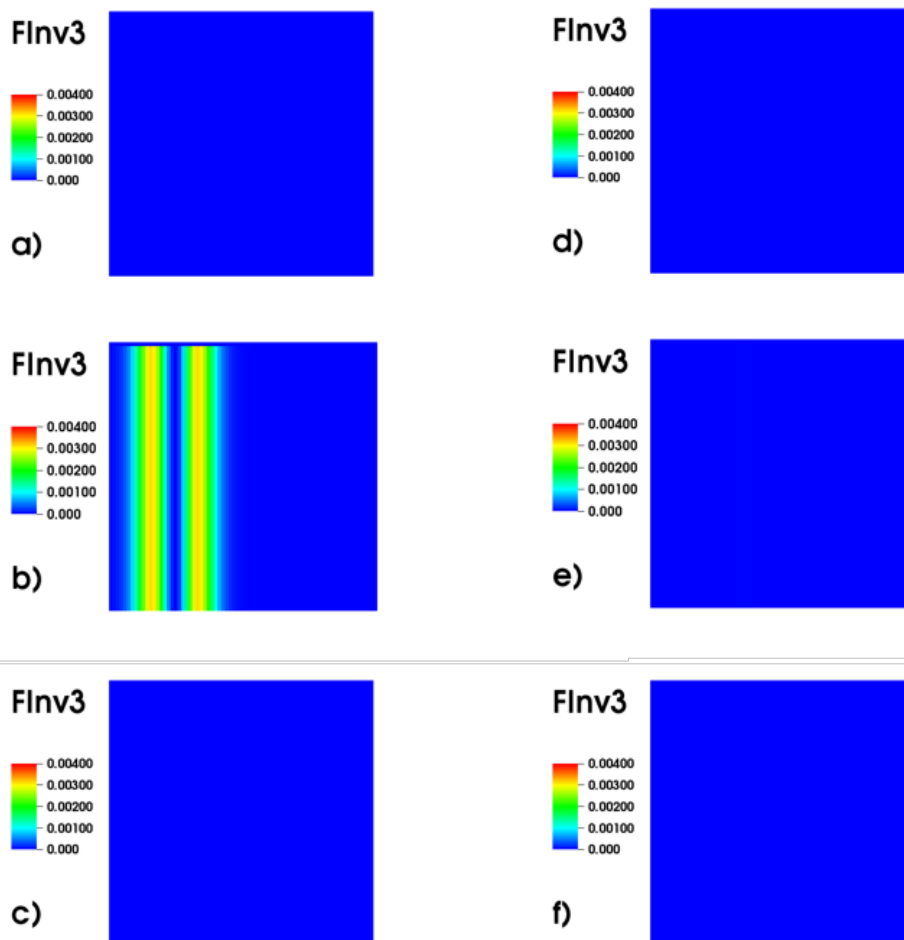


Fig. 6 Error in the third invariant of F for the hyperbolic tangent function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

3.1.2 Hole Closure Function

The collapsing hole function presents a 2-D assessment of the advection methods. The deformation is intense near the hole and then fairly gradual throughout, as shown by the plots of the first and second invariants in Fig. 2. The displacement field is isochoric, so the determinant remains 1.0 throughout. Also, there is no rotation in the deformation field, which is evident by the symmetry of the

deformation gradient in Eq. 17. Hence, $\mathbf{R}$ is the identity tensor, $\mathbf{U} = \mathbf{F}$, and there is no difference between the control and the QST method.

The advection error is greatest near the hole, following the regions with the steepest function gradients. The error plots in Figs. 7–9 show that both the control and the QST method yield higher error than the QLST function for all three invariants. As with the hyperbolic tangent function, using the log of the stretch in the QLST method advects the determinant more accurately than the control or the QST method, Fig. 9. It also introduces slightly less error for the first and second invariants. For this functional form, the determinant correction reduces the error so that the methods perform similarly well for all three of the invariants. The determinant correction is exact for this isochoric function, and it removes all error in the third invariant, as is evident in Fig. 9.

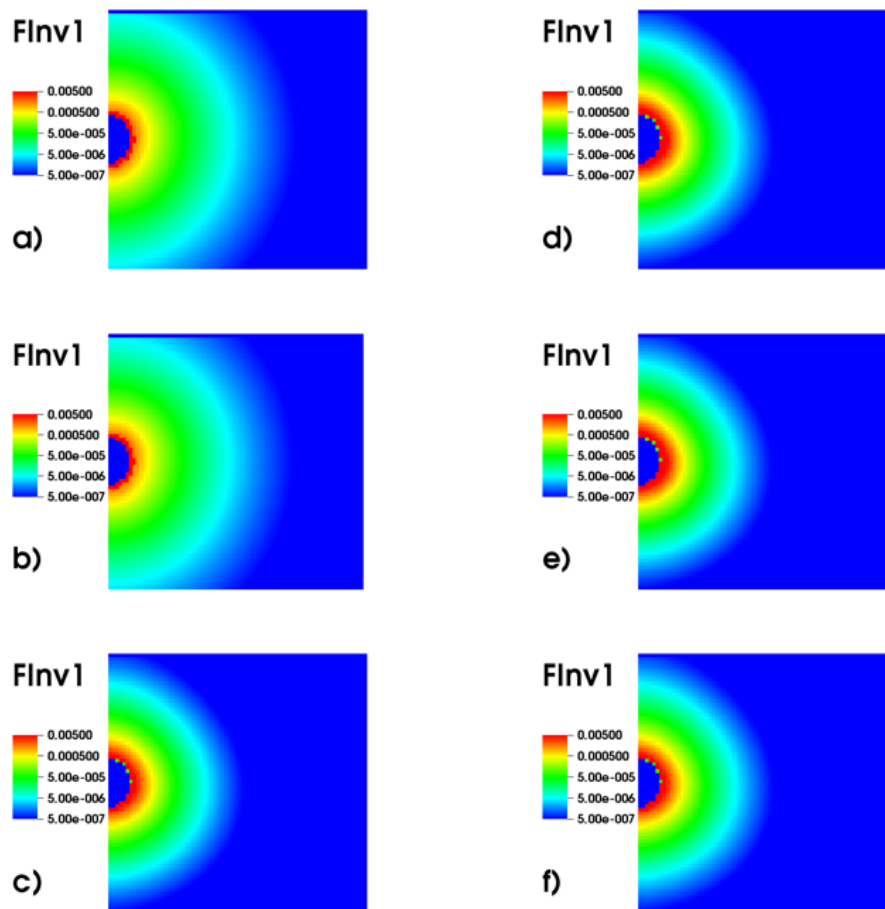


Fig. 7 Error in the first invariant of F for the hole collapse function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

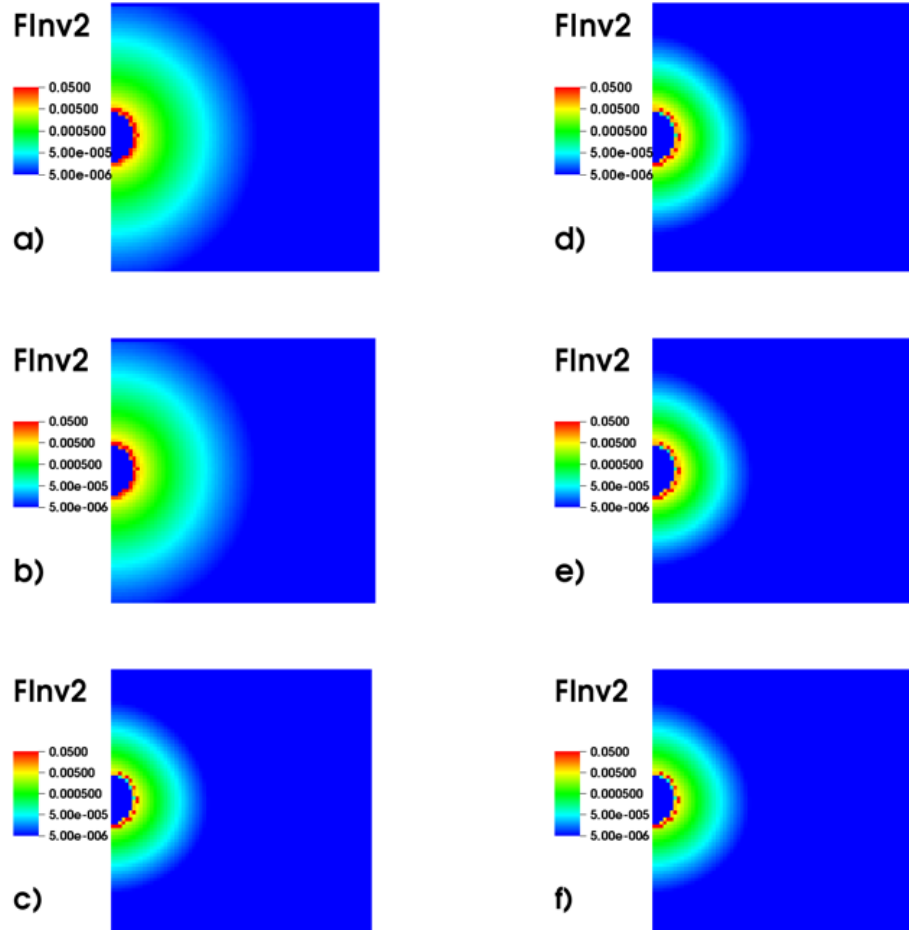


Fig. 8 Error in the second invariant of F for the hole collapse function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left

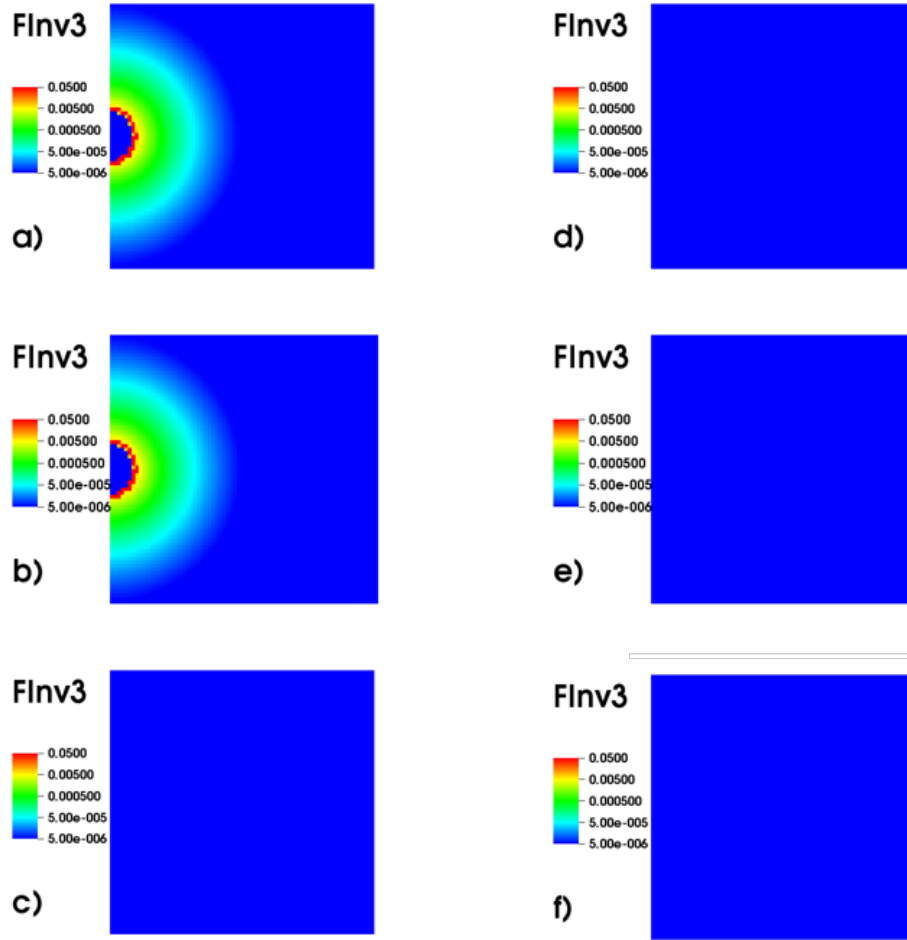


Fig. 9 Error in the third invariant of F for the hole collapse function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

3.1.3 Vortex Function

The vortex function combines shear and rotation gradients over the full domain, and it assesses the effects of their coupling in two dimensions. The vortex function is also isochoric, so the determinant is identically 1.0 throughout.

The advection error plots for the three invariants are presented in Figs. 10–12, respectively. The first and second invariants, Figs. 10 and 11, show that the two methods involving decomposition produce less error than the control. However, the QST method has significantly lower error than the QLST. In contrast to the first two invariants, the error in the third invariant, Fig. 12, is higher for the QST method than the control, and the QLST method has a very low error for the third invariant.

As with the earlier functions, the determinant correction shown in the right-hand columns substantially modifies the error for the control and the QST method. The determinant correction reduces the error for the control algorithm, but the error is

increased for the QST method since it was low before the adjustment. As with the earlier functions, the log used in the QLST method appears to maintain the correct determinant during advection so the determinant correction makes little difference.

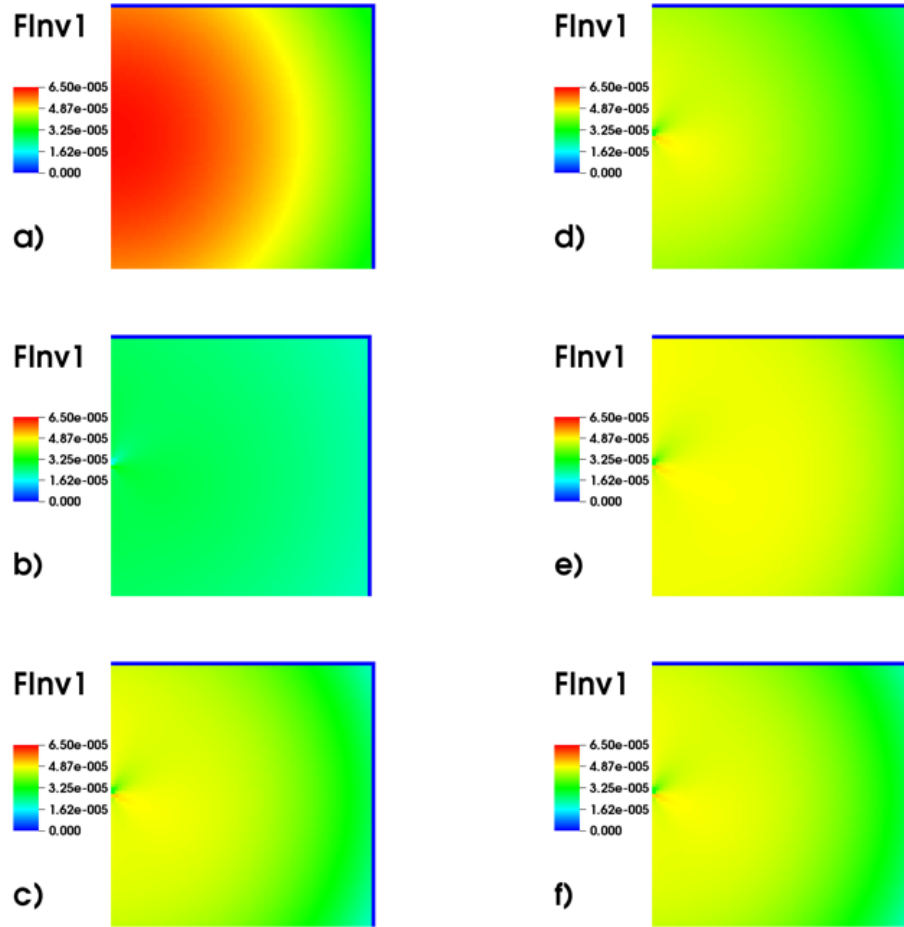


Fig. 10 Error in the first invariant of F for the vortex function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

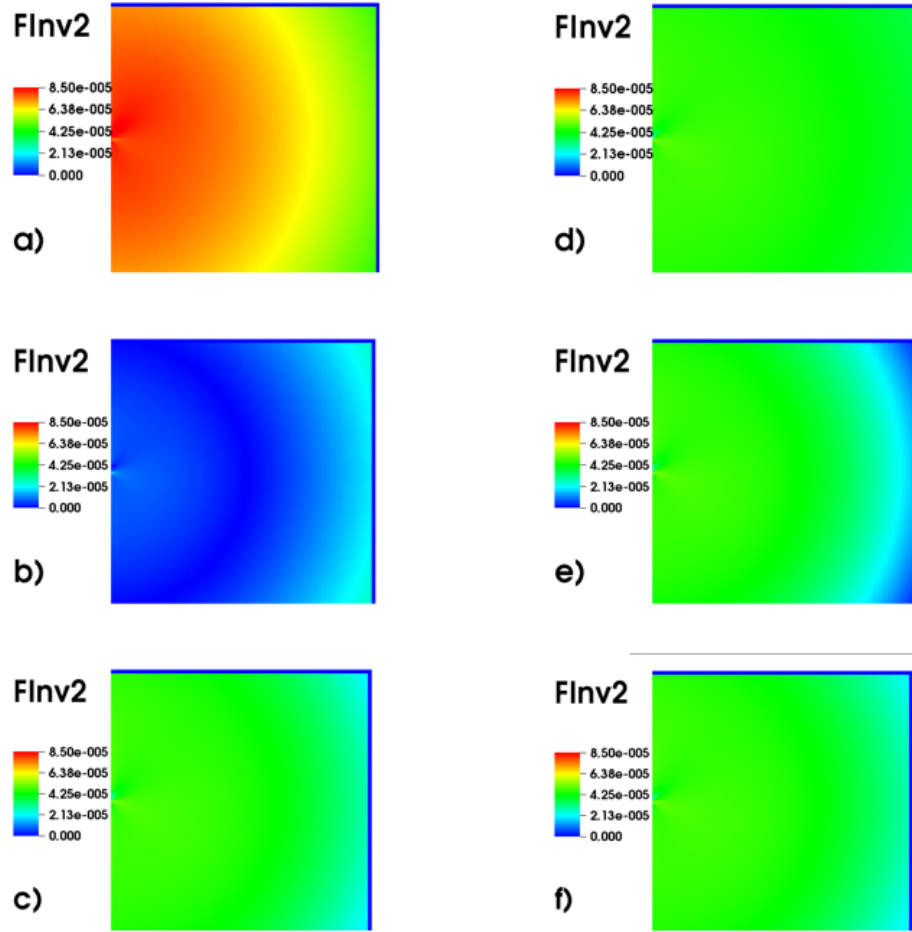


Fig. 11 Error in the second invariant of F for the vortex function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

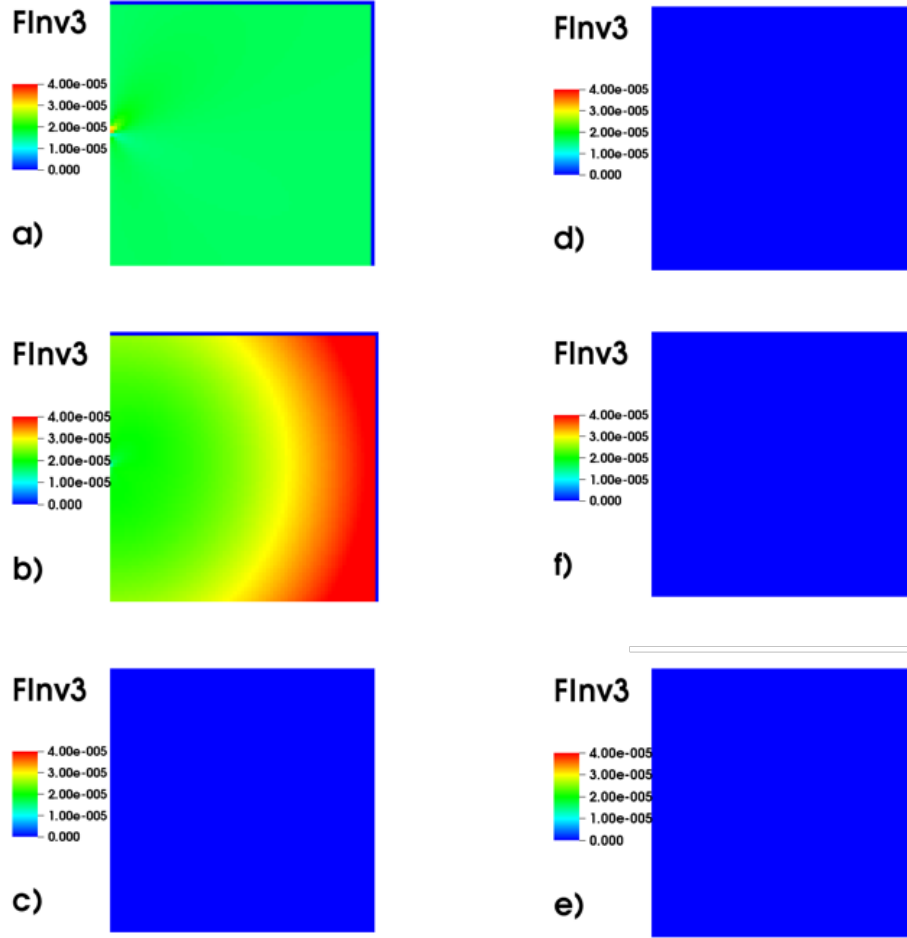


Fig. 12 Error in the third invariant of F for the vortex function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left.

3.1.4 Square Root Conformal Map Function

The conformal map function was the most strenuous deformation field tested. The deformation is substantial and the gradients are sharp, partly because the range of values in Fig. 4 occurs over a domain that is only 10% of the size of the other test functions. There is also a considerable volume change, making this the only no-isochoric test function.

Unlike all of the earlier error plots, those in Figs. 13–15 for the conformal mapping function are not all to the same scale. The control and the QLST methods produce approximately the same error, with the QLST error being about half of the control. The error for the QST method, however, is more than 2 orders of magnitude greater. Some feature of this function does not play well with the QST decomposition.

In addition, the determinant correction did not reduce error. In fact, it increased the error for the control and QLST methods to the same level as the QST method. All

of the legend scales are the same for the determinant corrected error plotted in Figs. 13–15. The determinant corrected error increases because of error in the advected determinant compared to the determinant computed from the function reevaluated on the shifted mesh. Since the determinant varies as r^{-2} , linear interpolation resulted in an approximate prediction of the determinant used in the adjustment. When the various methods were corrected with this determinant, their entries were scaled to this incorrect value, which produced a larger error compared to the analytically shifted result.

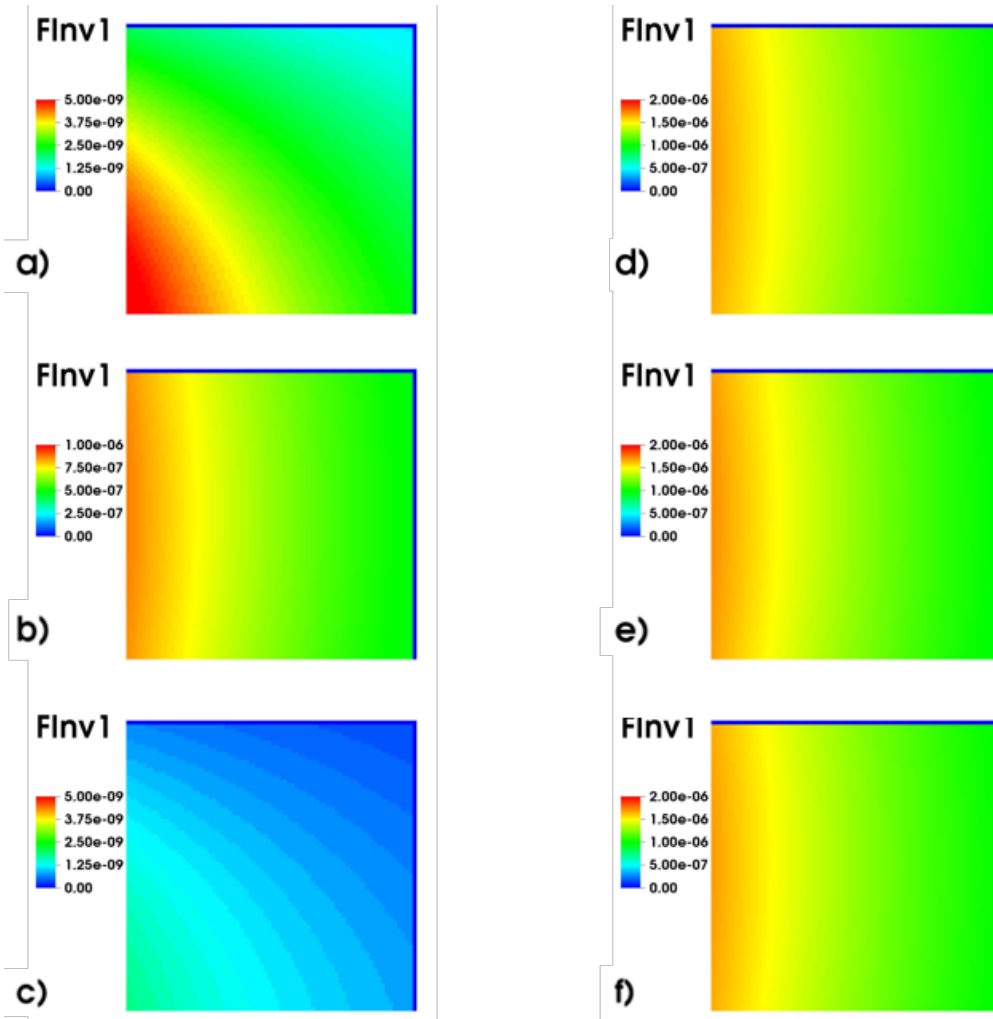


Fig. 13 Error in the first invariant of F for the conformal mapping function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left. Note that the scale for b) differs from a) and c).

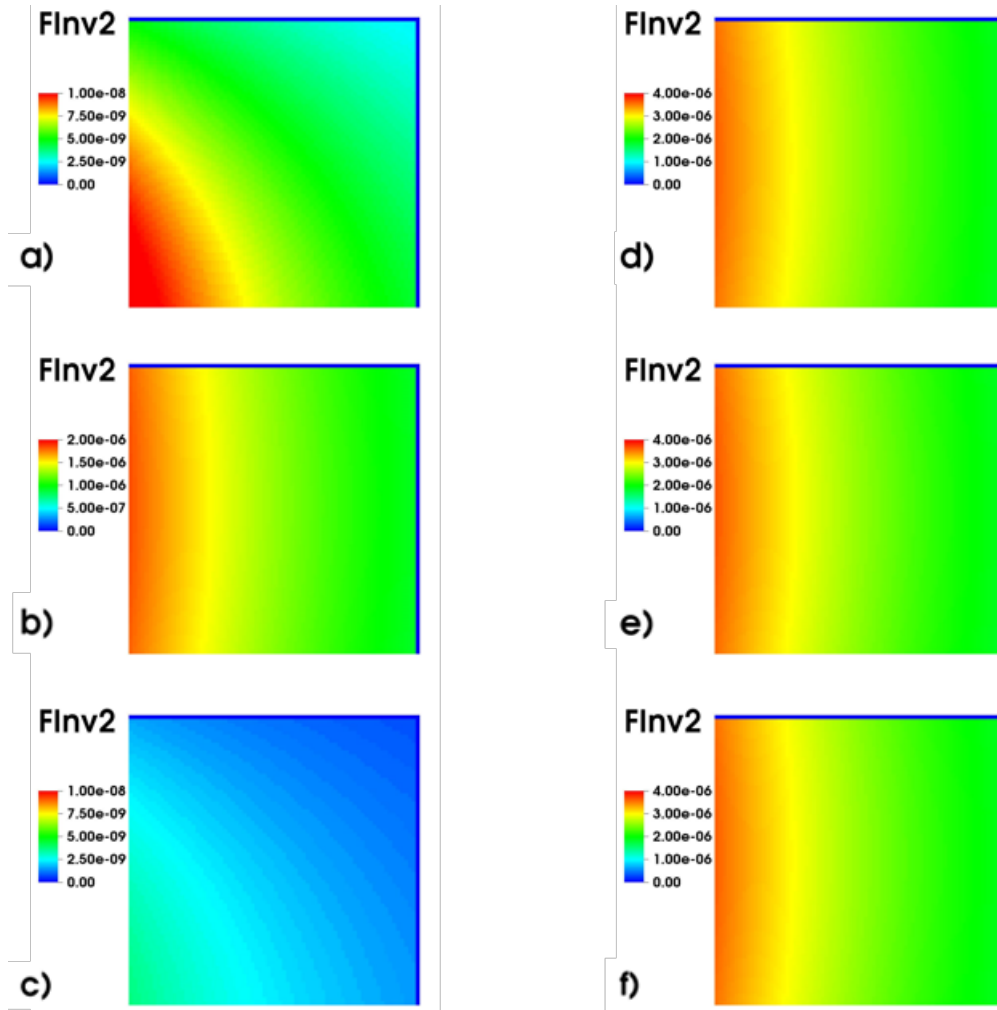


Fig. 14 Error in the second invariant of F for the conformal mapping function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left. Note that the scale for b) differs from a) and c).

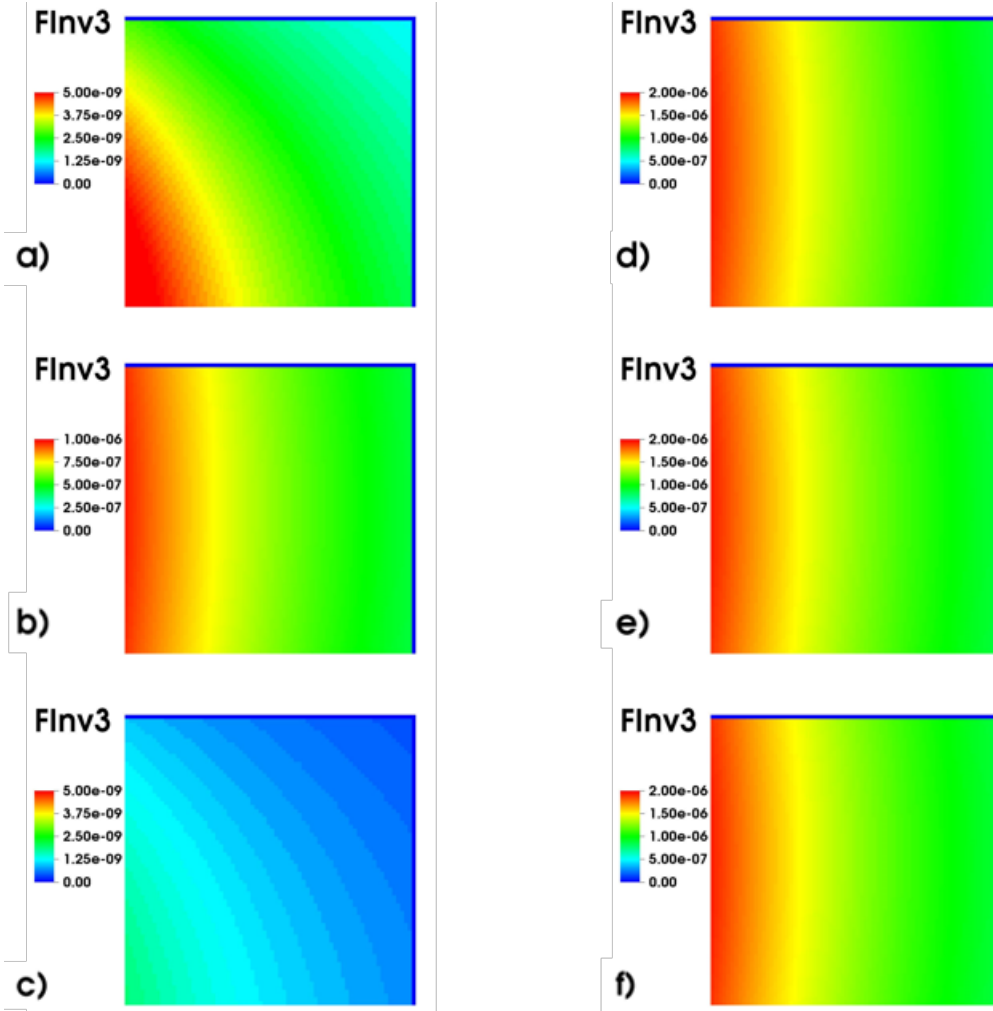


Fig. 15 Error in the third invariant of F for the conformal mapping function following simulated advection. a) Control method, b) QST, c) QLST. Plots d), e), and f) are determinant corrected solutions for the plots on the left. Note that the scale for b) differs from a) and c).

3.2 Error Summaries

Errors for the six functions are summarized in the following subsection as box and whisker plots. These plots show the natural log of the error as determined by Eq. 10. The boxes are color-coded by the decomposition method, and the method is indicated below each bar. The “-d” in the name indicates the determinant corrected method. The range of the boxes includes the values between the first and third quartile. The bar in the box represents the mean, and the whiskers indicate the full range of the data. The columns that appear empty have near zero error. The specific invariant being plotted is indicated at the top of each graph.

3.2.1 Hyperbolic Tangent Function

The invariant errors for the hyperbolic tangent function are plotted in Fig. 16. As shown previously in Figs. 5 and 6, the control method has zero error for this function. Of note is that the other methods have tall boxes, indicating that the error is distributed over the volume and not just a small subset of the elements. The error for the QST method is unacceptably high, but it is improved appreciably following determinant correction. These plots also show that by taking the log of the stretch, the QLST method gives lower error than QST. However, as demonstrated previously, the results are not improved with determinant correction and would likely be considered marginal.

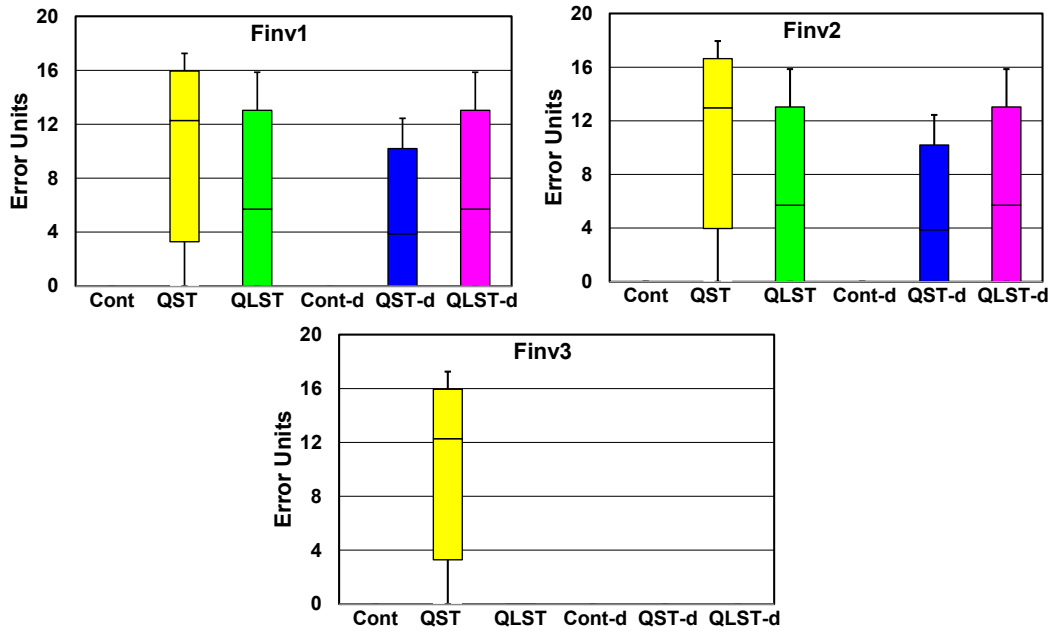


Fig. 16 Box and whisker plots of the logarithmic error in the three invariants of the deformation gradient for the six advection methods for the hyperbolic tangent function

3.2.2 Hole Closure Function

Results of the hole closure function are shown in Fig. 17. For this function only, error values greater than 20 were filtered from the plot. These were likely associated with elements in the hole, and advection of something into nothing would produce substantial error. Some of the filtered errors were greater than 24.4, which corresponds to the largest invariant value on the plots in Fig. 2. Even with the filtering, the maximum error is large.

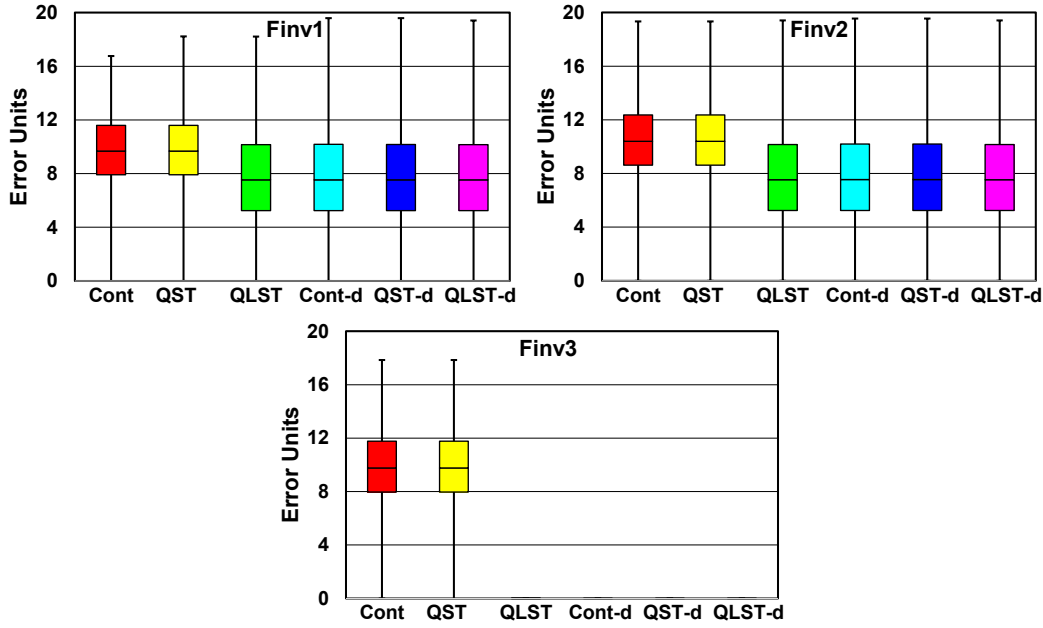


Fig. 17 Box and whisker plots of the logarithmic error in the three invariants of the deformation gradient for the six advection methods for the collapsing hole function

Unlike the hyperbolic tangent function, the whisker extent from the top of the boxes indicates the significant error in a small fraction of the elements near the hole where the gradient is very sharp. These extreme values were not mitigated by the determinant correction, and some appear to have gotten worse. The whiskers indicating the first quartile of data are also rather long, indicating a wide error range. The error in regions most remote from the hole is near zero, as the lower end of the whiskers is at zero.

The error for the middle two quartiles of data is less spread, indicating modest error over most of the domain. For this midrange error, the control and the QST methods produce similar error, which is a bit higher than the error from the QLST decomposition. The determinant correction does not change the QLST result, but it does reduce the midrange error of the control and QST methods to approximately the same level as the QLST method. As mentioned earlier, the determinant correction for these isochoric examples creates the exact solution for the third invariant, so the third invariant errors go to zero following the adjustment.

3.2.3 Vortex Function

The error plots for the vortex function are shown in Fig. 18. The error for the first invariant is rather tightly clustered, so the scale for that particular subplot has been modified to accentuate the differences. The second and third invariants are on the same scale as the previous results.

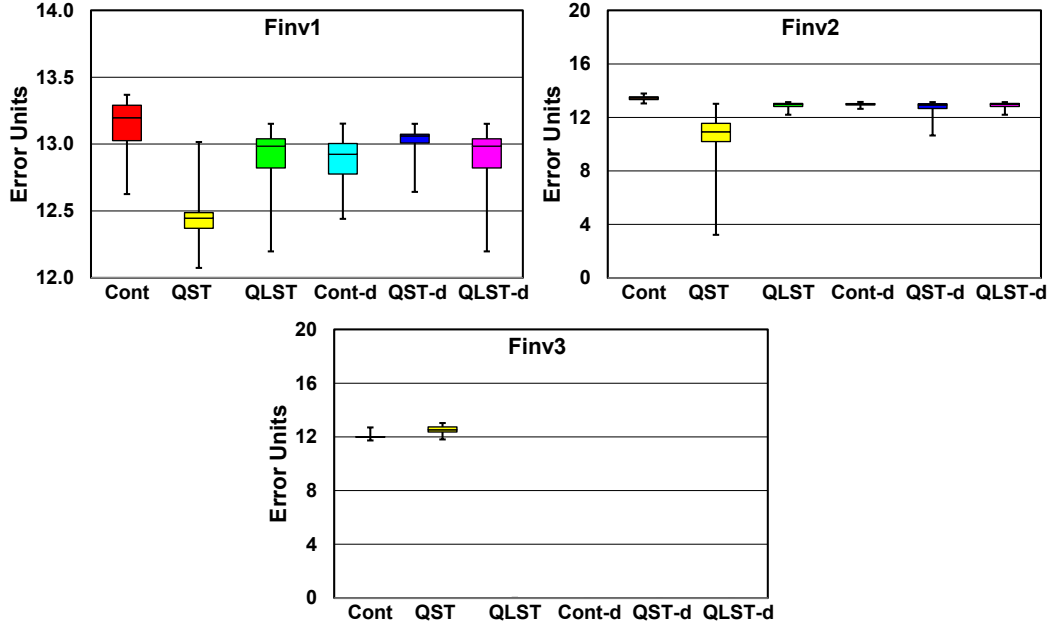


Fig. 18 Box and whisker plots of the logarithmic error in the three invariants of the deformation gradient for the six advection methods for the vortex function

The first invariant data show some advantage to decomposing the deformation gradient for advection for this example, but not much. The error for the control is only slightly higher than the other methods. The QST performed better than the QLST for the first and second invariants. However, the QLST method again advected the constant determinant with nearly zero error.

As with the previous isochoric examples, the determinant correction removes all of the error for the third invariant and removes much of the difference between the QST and QLST results. In this case, the correction increases the QST error for the first and second invariants.

3.2.4 Square Root Conformal Map Function

The summary plots in Fig. 19 for the conformal mapping function clearly depict the substantial error difference between the QST method and the control and QLST. Recall that this is a natural log scale so the higher error value for QST represents more than 2 orders of magnitude higher error. As described in Section 3.1.4, the determinant correction increases the error markedly due to error in the independently advected determinant. This was not an issue for the other functions since all of the earlier functional forms described isochoric deformation. Advection of the determinant in these earlier cases was exact since it was a constant.

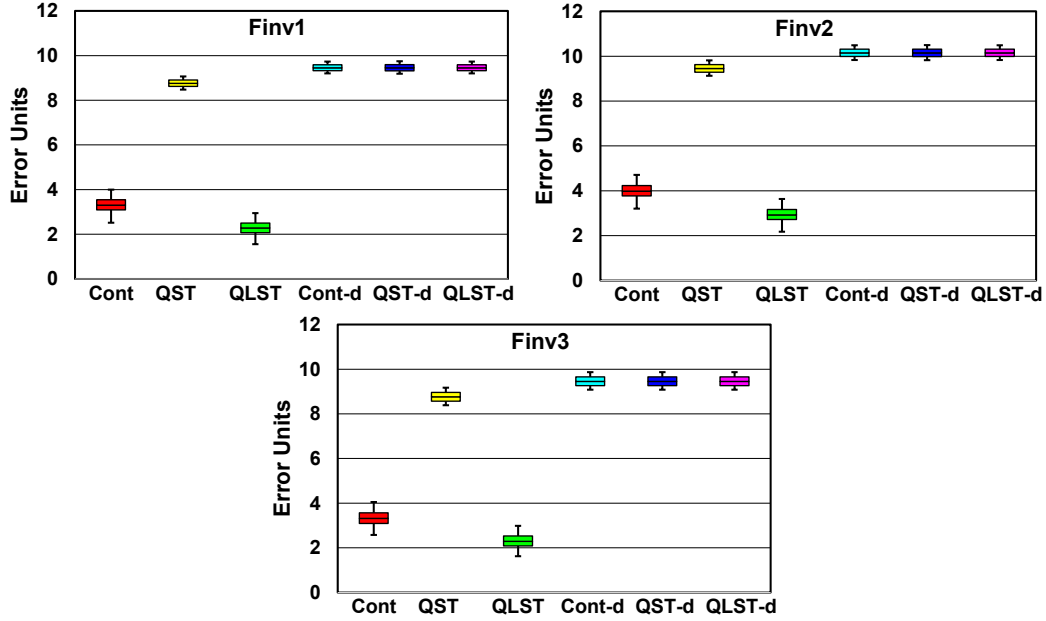


Fig. 19 Box and whisker plots of the logarithmic error in the three invariants of the deformation gradient for the six advection methods for the conformal map function

Also of note in Fig. 19 is the tight error range. This is partly due to the domain for this example being 10% of the linear extent of the other domains. As long as the functions are continuous, the error range over a small domain is less than over a larger domain, since it is sampling a smaller volume.

4. Discussion

It had been shown previously¹ that advecting a deformation gradient decomposed into a stretch tensor and a rotation represented as quaternions would improve advection accuracy. In the examples presented above, this result was verified by examining additional deformation fields. The above examples also illustrated that the advection error may be reduced further if the logarithm of the stretch tensor were advected rather than the stretch itself. The greatest benefit for using the logarithm appears to be in the advection of the third invariant, or determinant, which captures the volume change.

Before examining the logarithmic result in more detail, it is instructive to show the magnitude of the error that advection can introduce to a fundamental quantity like the determinant. To simplify the illustration, it will be assumed that there is no rotation ($\mathbf{F} = \mathbf{U}$), the deformation is 2-D, and as with the examples in this report, 10% new material is advected into the finite element. The quantities for the original element are designated by Greek symbols with a subscript 1 and the new material has a subscript 2. With these assumptions, the new stretch is given by

$$\begin{bmatrix} U_{11} & U_{12} \\ U_{12} & U_{22} \end{bmatrix} = 0.9 \begin{bmatrix} 1 - \delta_1 & \alpha_1 \\ \alpha_1 & 1 - \varepsilon_1 \end{bmatrix} + 0.1 \begin{bmatrix} 1 - \delta_2 & \alpha_2 \\ \alpha_2 & 1 - \varepsilon_2 \end{bmatrix}. \quad (32)$$

If the components of the stretch are advected, and then the determinant constructed from the advected components, the determinant would be

$$\begin{aligned} \text{Det}_{AC} = & 1 - 0.9(\delta_1 + \varepsilon_1) - 0.1(\delta_2 + \varepsilon_2) \\ & - 0.81\alpha_1^2 - 0.18\alpha_1\alpha_2 - 0.01\alpha_2^2 \\ & + 0.81\delta_1\varepsilon_1 + 0.09(\delta_1\varepsilon_2 + \delta_2\varepsilon_1) + 0.01\delta_2\varepsilon_2. \end{aligned} \quad (33)$$

If, on the other hand, the determinant for each neighboring element is computed and then advected as a single scalar, the resulting determinant is

$$\begin{aligned} \text{Det}_{AD} = & 1 - 0.9(\delta_1 + \varepsilon_1) - 0.1(\delta_2 + \varepsilon_2) \\ & - 0.9\alpha_1^2 - 0.1\alpha_2^2 \\ & + 0.9\delta_1\varepsilon_1 + 0.1\delta_2\varepsilon_2. \end{aligned} \quad (34)$$

The results in Eqs. 33 and 34 differ by second order terms. To make this example a bit more concrete, the deformation field will be assumed isochoric, as it was for the first three examples above, by applying the constraint $\text{Det}(\mathbf{U}) = 1$. This gives the constraints

$$-(\delta_1 + \varepsilon_1) = \alpha_1^2 - \delta_1\varepsilon_1 \text{ and } -(\delta_2 + \varepsilon_2) = \alpha_2^2 - \delta_2\varepsilon_2. \quad (35)$$

Substituting these constraints in Eqs. 33 and 34 yields

$$\text{Det}_{AC} = 1 + 0.09[(\alpha_1 - \alpha_2)^2 - (\delta_1 - \delta_2)(\varepsilon_1 - \varepsilon_2)] \quad (36)$$

for the determinant of the advected components, and

$$\text{Det}_{AD} = 1 \quad (37)$$

for the advected determinant. The numerical factor in Eq. 39 results from $\phi - \phi^2 = 0.09$, where ϕ , is the fraction advected. It is apparent that advecting components results in error even for an isochoric deformation field. In this 2-D isochoric example, the determinant error resulting from advecting the components is related to the square of the difference between components in the neighboring elements. Hence, if the fields are smooth, the error is quadratic with mesh resolution.

Now consider the advected volume change associated with the logarithmic strain tensor. The log volume strain is obtained from the trace of the log strain tensor. The trace is a simple sum of the diagonal components, and rudimentary advection is a linear interpolation between values in adjacent finite elements. Since both are linear

operations, the trace should be advected with the same accuracy as any individual scalar component. This is illustrated with the following assumed advection

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{12} & \varepsilon_{22} \end{bmatrix} = 0.9 \begin{bmatrix} \chi_1 & \gamma_1 \\ \gamma_1 & \beta_1 \end{bmatrix} + 0.1 \begin{bmatrix} \chi_2 & \gamma_2 \\ \gamma_2 & \beta_2 \end{bmatrix}. \quad (38)$$

Taking the trace following advection is

$$Tr(\boldsymbol{\varepsilon}) = (0.9\chi_1 + 0.1\chi_2) + (0.9\beta_1 + 0.1\beta_2), \quad (39)$$

and the trace of the log strain advects as

$$Tr(\boldsymbol{\varepsilon}) = 0.9(\chi_1 + \beta_1) + 0.1(\chi_2 + \beta_2). \quad (40)$$

Equations 39 and 40 are equivalent. Hence, when the log of the stretch tensor is advected, the volume change is advected with the same accuracy as the scalar log volume change. This consistency is in contrast to advecting the stretch tensor itself, as was shown by Eqs. 33 and 34.

While advecting the log stretch tensor appears to offer some advantage, it is still not the same as advecting the determinant of the deformation gradient. This is demonstrated by considering a pure small-strain volume strain with advection in a single dimension. Assume a stretch in the element of interest as λ , and that the material being advected in has a perturbed stretch of $\lambda + \xi$, where ξ is small. Again assuming 10% advected material, the advected determinant would be

$$\begin{aligned} \text{Det}_U &= 0.9\lambda^3 + 0.1(\lambda + \xi)^3 \\ &= 0.9\lambda^3 + 0.1\lambda^3 + 0.3\lambda^2\xi + 0.3\lambda\xi^2 + 0.01\xi^3 \\ &= \lambda^3 + 0.3\lambda^2\xi + 0.3\lambda\xi^2 + 0.01\xi^3. \end{aligned} \quad (41)$$

This can be compared to the determinant calculated from the advected log strain

$$\begin{aligned} \text{Det}_\varepsilon &= \exp\{3[0.9 \ln(\lambda) + 0.1 \ln(\lambda + \xi)]\} \\ &= \exp\left\{\ln(\lambda^{2.7}) + \ln\left(\lambda^{0.3} \left(1 + \frac{\xi}{\lambda}\right)^{0.3}\right)\right\} \\ &= \exp\left\{\ln\left(\lambda^{2.7} \lambda^{0.3} \left(1 + \frac{\xi}{\lambda}\right)^{0.3}\right)\right\} \\ &= \lambda^3 \left(1 + \frac{\xi}{\lambda}\right)^{0.3} = \lambda^3 \left(1 + 0.3 \frac{\xi}{\lambda} - 0.105 \frac{\xi^2}{\lambda^2} + 0.357 \frac{\xi^3}{\lambda^3} + \dots\right) \\ &= \lambda^3 + 0.3\lambda^2\xi - 0.105\lambda\xi^2 + 0.357\xi^3 + \dots \end{aligned} \quad (42)$$

Equations 41 and 42 both give a determinant of 1.0 when the deformation field is isochoric, as it was for the first three example deformation fields. This is the reason

for the low determinant error for the QLST method. For nonisochoric deformations, the determinants are the same to first order, but they differ in higher-order terms. The difference is evident in the conformal mapping function where the determinant correction affected the QLST result.

The conformal mapping example was the only function evaluated that had a volume change. The volume change was substantial for a solid. The results exhibited an increased error for the QLST method following the determinant correction. This is because the simulation produced a larger error for advecting the determinant than it did for advecting the trace of the log of the stretch. Whether the determinant or the log volume strain advects more accurately will depend on the gradients in the deformation field. Regardless of which is advected more accurately, if other aspects of the finite element or finite volume code are using an advected relative volume for the equation of state or other purposes, the determinant correction is likely best practice to maintain consistency.

The results support the hypothesis that advecting the deformation gradient as multiple physically meaningful quantities will reduce advection error. This has been demonstrated by the prior¹ and current results for advecting the stretch tensor and the rotation represented as quaternions. The current results also suggest that taking the logarithm of the stretch tensor will further reduce the error. One reason is that the magnitude of the diagonal and off-diagonal components is similar. Another reason is that advecting the log of the stretch tensor is akin to advecting the log volume strain, as was shown by Eqs. 39 and 40.

If the volume strain is advected more accurately, the magnitude of the determinant correction will also be reduced. A smaller correction will change the advected tensor less, and this will likely introduce lower error for other tensor quantities. For example, correcting the determinant for the QST method in the vortex function increased the error in the first and second invariants while the error was unchanged for the QLST method.

The results have also shown that the error accrued can depend on the specific functional form. The control method gave lower error for the hyperbolic tangent function. On the other hand, for the vortex function the error in the first two invariants for all of the methods was similar. Both of these deformation fields produced rather tight error bands. Real deformations are generally more complex and are likely to have a wide range of error, like the hole-collapse function. The best method for the particular problem cannot be known ahead of time. The QLST method gave better results in several of the examples and was never the worst, unlike the control and the QST.

5. Conclusions

Advecting the deformation gradient decomposed into two independent fields, the log of the stretch tensor and rotations represented as quaternions, is shown to introduce less error than advecting the deformation gradient as a single entity. This work corroborates prior results¹ that used a similar decomposition without taking the logarithm. The use of the log further reduces the advection error in general. While not conclusive, this is thought to result from a combination of two factors: making the diagonal components similar in magnitude to the off-diagonal component and having the volume strain be a linear combination of the diagonal components of the log strain. Further comparisons on real, large-scale simulations are needed to assess improvements in production simulations and whether the expense of evaluating the logarithm and exponential is justified.

6. References

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Appendix. Log Stretch–Quaternion Analysis Code*

* This appendix appears as an attachment to this .pdf.

List of Symbols, Abbreviations, and Acronyms

1-D	one-dimensional
2-D	two-dimensional
ALE	arbitrary Lagrangian-Eulerian
FE	finite element
QST	quaternion stretch tensor
QLST	quaternion log stretch tensor

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