Lecture 13: Differential Operations on Vectors

Reading:
Kreyszig Sections: 9.8, 9.9 (pages410–413, 414–416)

Generalizing the Derivative

The number of different ideas, whether from physical science or other disciplines, that can be understood with reference to the "meaning" of a derivative from the calculus of scalar functions, is very very large. Our ideas about many topics, such as price elasticity, strain, stability, and optimization, are connected to our understanding of a derivative.

In vector calculus, there are generalizations to the derivative from basic calculus that act on a scalar and give another scalar back:

gradient (∇): A derivative on a scalar that gives a vector.

curl ($\nabla\times$): A derivative on a vector that gives another vector.

divergence ($\nabla\cdot$): A derivative on a vector that gives scalar.

Each of these have "meanings" that can be applied to a broad class of problems.

The gradient operation on $f(\vec{x}) = f(x, y, z) = f(x_1, x_2, x_3)$,

$$\text{grad} f = \nabla f \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right) = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) f \tag{13-1}$$

has been discussed previously. The curl and divergence will be discussed below.

Lecture 13 MATHEMATICA® Example 1

Scalar Potentials and their Gradient Fields

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

An example of a scalar potential, due three point charges in the plane, is visualized. Methods for computing a gradient are presented.

Simple 2 D 1 / r potential

```
potential[x_ , y_, xo_ , yo_] :=
 -1 / Sqrt[ (x - xo) ^2 + (y - yo) ^2]
```
1

A field source located a distance 1 south of the origin

```
HoleSouth[x_, y_] :=
 potential[x, y, Cos[3 Pi / 2], Sin[3 Pi / 2]]
```
2

```
HoleNorthWest[x_ , y_] :=
 potential[x, y, Cos[Pi / 6], Sin[ Pi / 6]]
```
3

```
HoleNorthEast[x_ , y_] :=
 potential[x, y, Cos[ 5 Pi / 6], Sin[5 Pi / 6]]
```
4

Function that returns the two dimensional (x,y) gradient field of any function declared a function of two arguments:

```
gradfield[scalarfunction_] :=
 {D[scalarfunction[x, y], x] // Simplify,
  D[scalarfunction[x, y], y] // Simplify}
```
5

Generalizing the function to any arguments:

```
gradfield[scalarfunction_, x_ , y_] :=
 {D[scalarfunction[x, y], x] // Simplify,
  D[scalarfunction[x, y], y] // Simplify}
```
6

The sum of three potentials:

```
ThreeHolePotential[x_, y_] :=
 HoleSouth[x, y] +
  HoleNorthWest[x, y] + HoleNorthEast[x, y]
```
7

f(x,y) visualization of the scalar potential:

```
Plot3D[ThreeHolePotential[x, y],
 {x, -2, 2}, {y, -2, 2}]
```
8

Contour visualization of the three-hole potential

```
ContourPlot[ThreeHolePotential[x, y],
 {x, -2, 2}, {y, -2, 2}, PlotPoints → 40,
 ColorFunction → (Hue[1 - # * 0.66] &)]
```
9

1: This is the 2D $1/r$-potential; here *potential* takes four arguments: two for the location of the charge and two for the position where the "test" charge "feels" the potential.

2-4: These are three fixed charge potentials, arranged at the vertices of an equilateral triangle.

5: *gradfield* is an example of a function that takes a scalar function of x and y and returns a vector with component derivatives: the gradient vector of the scalar function of x and y.

6: However, the previous example only works for functions of x and y explicitly. This expands *gradfield* to other Cartesian coordinates other than x and y.

7: *ThreeHolePotential* is the superposition of the three potentials defined in 2–4.

8: `Plot3D` is used to visualize the superposition of the potentials due to the three charges.

9: `ContourPlot` is an alternative method to visualize this scalar field. The option `ColorFunction` points to an example of a *Pure Function*—a method of making functions that do not operate with the usual "square brackets." Pure functions are indicated with the & at the end; the # is a place-holder for the pure function's argument.

Divergence and Its Interpretation

The divergence operates on a vector field that is a function of position, $\vec{v}(x, y, z) = \vec{v}(\vec{x}) = (v_1(\vec{x}), v_2(\vec{x}), v_3(\vec{x}))$, and returns a scalar that is a function of position. The scalar field is often called the divergence field of $\vec{v}$, or simply the divergence of $\vec{v}$.

$$\text{div } \vec{v}(\vec{x}) = \nabla \cdot \vec{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \cdot (v_1, v_2, v_3) = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \cdot \vec{v} \tag{13-2}$$

Think about what the divergence means.

Lecture 13 MATHEMATICA® Example 2

Visualizing the Gradient Field and its Divergence: The Laplacian

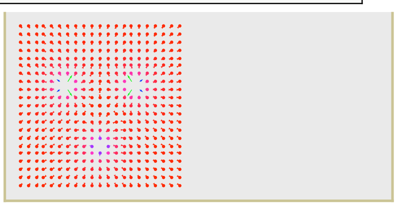
Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

A visualization gradient field of the potential defined in the previous example is presented. The divergence of the gradient $\nabla \cdot \nabla\phi = \nabla^2\phi$ (i.e., the result of the Laplacian operator ∇^2) is computed and visualized.

Gradient field of three-hole potential

```
gradthreehole = gradfield[ThreeHolePotential]
```
1

```
Needs["VectorFieldPlots`"];
VectorFieldPlots`VectorFieldPlot[
 gradthreehole, {x, -2, 2}, {y, -2, 2},
 ScaleFactor → 0.2`, ColorFunction →
  (Hue[1 - #1 0.66`] &), PlotPoints → 21]
```
2



Function that takes a two-dimensional vector function of (x,y) as an argument and returns its divergence

```
divergence[{xcomp_ , ycomp_}] :=
 Simplify[D[xcomp, x] + D[ycomp, y]]
```
3

```
divgradthreehole = divergence[
   gradfield[ThreeHolePotential]] // Simplify
```
4

Plotting the divergence of the gradient

($\nabla \cdot (\nabla f)$ is the "Laplacian" $\nabla^2 f$, sometimes indicated with symbol Δf)

```
Plot3D[divgradthreehole,
 {x, -2, 2}, {y, -2, 2}, PlotPoints -> 60]
```
5

1: We use our previously defined function *gradfield* to compute the gradient of *ThreeHolePotential* everywhere in the plane.

2: `PlotVectorField` is in the `VectorFieldPlots` package. Because a gradient produces a vector field from a scalar potential, arrows are used at discrete points to visualize it.

3: The divergence operates on a vector and produces a scalar. Here, we define a function, *divergence* , that operates on a 2D-vector field of x and y and returns the sum of the component derivatives. Therefore, taking the divergence of the gradient of a scalar field returns a scalar field that is naturally associated with the original—its physical interpretation is (minus) the rate at which gradient vectors "diverge" from a point.

4–5: We compute the divergence of the gradient of the scalar potential. This is used to visualize the Laplacian field of *ThreeHolePotential* .

Coordinate Systems

The above definitions are for a Cartesian (x, y, z) system. Sometimes it is more convenient to work in other (spherical, cylindrical, etc) coordinate systems. In other coordinate systems, the derivative operations ∇, $\nabla\cdot$, and $\nabla\times$ have different forms. These other forms can be derived, or looked up in a mathematical handbook, or specified by using the MATHEMATICA® package "VectorAnalysis."

Lecture 13 MATHEMATICA® Example 3

Coordinate Transformations

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

Examples of *Coordinate Transformations* obtained from the `VectorAnalysis` package are presented.

It is no surprise that many of these differential operations already exist in Mathematica packages.

```
<< "VectorAnalysis`"
```
1

Converting between coordinate systems

The spherical coordinates expressed in terms of the cartesian x,y,z

```
CoordinatesFromCartesian[
 {x, y, z}, Spherical[r, theta, phi]]
```
2

$$\left\{\sqrt{x^2+y^2+z^2},\ \mathrm{ArcCos}\left[\frac{z}{\sqrt{x^2+y^2+z^2}}\right],\ \mathrm{ArcTan}[x, y]\right\}$$

The cartesian coordinates expressed in terms of the spherical r θ φ

```
CoordinatesToCartesian[
 {r, theta, phi}, Spherical[r, theta, phi]]
```
3

```
{r Cos[phi] Sin[theta],
 r Sin[phi] Sin[theta], r Cos[theta]}
```

The equation of a line through the origin in spherical coodinates

```
Simplify[
 CoordinatesFromCartesian[{a t, b t, c t},
  Spherical[r, theta, phi]], t > 0]
```
4

1–2: `CoordinatesFromCartesian` from the `VectorAnalysis` package transforms three Cartesian coordinates, named in the first argument-list, into one of many coordinate systems named by the second argument.

3: `CoordinatesToCartesian` transforms one of many different coordinate systems, named in the second argument, into the three Cartesian coordinates, named in the first argument (which is a list).

4: For example, this would be the equation of a line radiating from the origin in spherical coordinates.

Lecture 13 Mathematica® Example 4

Frivolous Example Using `Geodesy`, `VectorAnalysis`, and `CityData`.

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

We compute distances from Boston to Paris along different routes.

(The following will not work unless you have an active internet connection)

```
CityData["Boston", "Latitude"]                                    1

CityData["Marseille", "Latitude"]                                 2

CityData["Paris", "Longitude"]                                    3

SphericalCoordinatesofCity[
  cityname_String] := {
  6378.1 , CityData[cityname, "Latitude"]
   Degree,
  CityData[cityname, "Longitude"] Degree}                         4

SphericalCoordinatesofCity["Boston"]                              5

LatLong[city_String] :=
 {CityData[city, "Latitude"],
  CityData[city, "Longitude"]}                                    6

CartesianCoordinatesofCity[
  cityname_String] := CoordinatesToCartesian[
  SphericalCoordinatesofCity[cityname],
  Spherical[r, theta, phi]]                                       7

CartesianCoordinatesofCity["Paris"]                               8

MinimumTunnel[city1_String, city2_String] :=
 Norm[CartesianCoordinatesofCity[city1] -
   CartesianCoordinatesofCity[city2]]                             9

MinimumTunnel["Boston", "Paris"]                                  10

Needs["Geodesy`"]                                                 11

SphericalDistance[
 LatLong["Paris"], LatLong["Boston"]]                             12

SpheroidalDistance[
 LatLong["Paris"], LatLong["Boston"]]                             13
```

1–3: `CityData` provides downloadable data. The data includes—among many other things—the latitude and longitude of many cities in the database. This show that Marseilles is north of Boston (which I found to be surprising).

4–5: *SphericalCoordinatesofCity* takes the string-argument of a city name and uses `CityData` to compute its spherical coordinates (i.e., $(r_{\text{earth}}, \theta, \phi)$ are same as (average earth radius = 6378.1 km, latitude, longitude)). We use `Degree` which is numerically $\pi/180$.

6: *LatLong* takes the string-argument of a city name and uses `CityData` to return a list-structure for its latitude and longitude. We will use this function below.

7–8: *CartesianCoordinatesofCity* uses a coordinate transform and *SphericalCoordinatesofCity*

9–10: If we imagine traveling *through* the earth instead of around it, we would use the `Norm` of the difference of the Cartesian coordinates of two cities.

11–12: Comparing the great circle route using `SphericalDistance` (from the `Geodesy` package) to the Euclidean distance, is a result that surprises me. It would save only about 55 kilometers to dig a tunnel to Paris—sigh.

13: `SpheroidalDistance` accounts for the earth's extra waistline for computing great-circle distances.

Lecture 13 MATHEMATICA® Example 5

Gradient and Divergence Operations in Other Coordinate Systems

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

A $1/r^n$-potential is used to demonstrate how to obtain gradients and divergences in other coordinate systems.

```
SimplePot[x_ , y_ , z_, n_] :=
        1
  ─────────────────────
  (x^2 + y^2 + z^2)^(n/2)                                  1

gradsp = Grad[
  SimplePot[x, y, z, 1], Cartesian[x, y, z]]               2
```

$$\left\{-\frac{x}{(x^2+y^2+z^2)^{3/2}},\ -\frac{y}{(x^2+y^2+z^2)^{3/2}},\ -\frac{z}{(x^2+y^2+z^2)^{3/2}}\right\}$$

The above is equal to $\vec{r}\big/\left(\|\vec{r}\|\right)^3$

```
SimplePot[r_, n_] := 1/r^n                                 3

gradsphere =
  Grad[SimplePot[r, 1], Spherical[r, θ, φ]]                4

Grad[SimplePot[r, 1], Cylindrical[r, θ, z]]                5

Grad[SimplePot[r, 1],
  ProlateSpheroidal[r, θ, φ]]                              6

GradSimplePot[x_, y_, z_, n_] :=
  Evaluate[Grad[SimplePot[x, y, z, n],
    Cartesian[x, y, z]]]                                   7

Div[GradSimplePot[x, y, z, n],
  Cartesian[x, y, z]] // Simplify                          8

Div[GradSimplePot[x, y, z, 1],
  Cartesian[x, y, z]] // Simplify                          9

0
```

1: *SimplePot* is the simple $1/r^n$ potential in Cartesian coordinates.

2: `Grad` is defined in the `VectorAnalysis`: in this form it takes a scalar function and returns its gradient in the coordinate system defined by the second argument.

3: An alternate form of *SimplePot* is defined in terms of a single coordinate; *if* r is the spherical coordinate $r^2 = x^2 + y^2 + z^2$ (referring back to a Cartesian (x, y, z)), then this is equivalent the function in **1**.

4: Here, the gradient of $1/r$ is obtained in spherical coordinates; it is equivalent to the gradient in **2**, but in spherical coordinates.

5: Here, the gradient of $1/r$ is obtained in cylindrical coordinates, but it is not equivalent to **2** nor **4**, because in cylindrical coordinates, (r, θ, z), $r^2 = x^2+y^2$, even though the form appears to be the same.

6: Here, the gradient of $1/r$ is obtained in prolate spheroidal coordinates.

7: We define a function for the x–y–z gradient of the $1/r^n$ scalar potential. `Evaluate` is used in the function definition, so that `Grad` is not called each time the function is used.

8: The Laplacian ($\nabla^2(1/r^n)$) has a particularly simple form, $n(n-1)/r^{2+n}$

9: By inspection of $\nabla^2(1/r^n)$ or by direct calculation, it follows that $\nabla^2(1/r)$ vanishes identically.

Curl and Its Interpretation

The curl is the vector-valued derivative of a vector function. As illustrated below, its operation can be geometrically interpreted as the rotation of a field about a point.

For a vector-valued function of (x, y, z):

$$\vec{v}(x,y,z) = \vec{v}(\vec{x}) = (v_1(\vec{x}), v_2(\vec{x}), v_3(\vec{x})) = v_1(x,y,z)\hat{\imath} + v_2(x,y,z)\hat{\jmath} + v_3(x,y,z)\hat{k} \qquad (13\text{-}3)$$

the curl derivative operation is another vector defined by:

$$\text{curl } \vec{v} = \nabla \times \vec{v} = \left(\left(\frac{\partial v_3}{\partial y} - \frac{\partial v_2}{\partial z} \right), \left(\frac{\partial v_1}{\partial z} - \frac{\partial v_3}{\partial x} \right), \left(\frac{\partial v_2}{\partial x} - \frac{\partial v_1}{\partial y} \right) \right) \qquad (13\text{-}4)$$

or with the memory-device:

$$\text{curl } \vec{v} = \nabla \times \vec{v} = \det \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_1 & v_2 & v_3 \end{pmatrix} \tag{13-5}$$

For an example, consider the vector function that is often used in Brakke's Surface Evolver program:

$$\vec{w} = \frac{z^n}{(x^2+y^2)(x^2+y^2+z^2)^{\frac{n}{2}}}(y\hat{i} - x\hat{j}) \tag{13-6}$$

This will be shown below, in a MATHEMATICA® example, to have the property:

$$\nabla \times \vec{w} = \frac{nz^{n-1}}{(x^2+y^2+z^2)^{1+\frac{n}{2}}}(x\hat{i} + y\hat{j} + z\hat{k}) \tag{13-7}$$

which is spherically symmetric for $n = 1$ and convenient for turning surface integrals over a portion of a sphere, into a path-integral, over a curve, on a sphere.

Lecture 13 MATHEMATICA® Example 6

Computing and Visualizing Curl Fields

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2011.

Examples of curls are computing for a particular family of vector fields. Visualization is produced with the `VectorFieldPlot3D` function from the `VectorFieldPlots` package.

```
LeavingKansas[x_, y_, z_ , n_] :=
                      z^n
  ------------------------------------ {y, -x, 0}      1
  (x^2 + y^2) (x^2 + y^2 + z^2)^(n/2)
```

```
Needs["VectorFieldPlots`"];

VectorFieldPlot3D[LeavingKansas[x, y, z, 3],
 {x, -1, 1}, {y, -1, 1},
 {z, -0.5, 0.5}, VectorHeads → True,
 ColorFunction → (Hue[#1 0.66`] &),
 PlotPoints → 21, ScaleFactor → 0.5`]      2
```

```
VectorFieldPlot3D[
 LeavingKansas[x, y, z, 3], {x, 0, 1},
 {y, 0, 1}, {z, 0.0, 0.5}, VectorHeads → True,
 ColorFunction → (Hue[#1 0.66] &),
 PlotPoints → 15, ScaleFactor → 0.5]      3
```

```
Curl[LeavingKansas[x, y, z, 3],
  Cartesian[x, y, z]] // Simplify      4
```

```
Glenda[x_, y_, z_, n_] :=
 Simplify[Curl[LeavingKansas[x, y, z, n],
   Cartesian[x, y, z]]]      5
```

```
VectorFieldPlot3D[
 Evaluate[Glenda[x, y, z, 1]],
 {x, -0.5, 0.5}, {y, -0.5, 0.5},
 {z, -0.25, 0.25}, VectorHeads → True,
 ColorFunction → (Hue[#1 0.66`] &),
 PlotPoints → 21]      6
```

Demonstrate that the divergence of the curl vanishes for the above function independent of n

```
DivCurl =
 Div[Glenda[x, y, z, n], Cartesian[x, y, z]]      7
```

```
Simplify[DivCurl]      8
```

1: *LeavingKansas* is the family of vector fields indicated by 13-6.

2–3: The function will be singular for $n > 1$ along the $z - axis$. This singularity will be reported during the numerical evaluations for visualization. There are two visualizations—the second one is over a sub-region but is equivalent because of the cylindrical symmetry of *LeavingKansas* . The singularity in the second case could be removed easily by excluding points near $z = 0$, but MATHEMATICA® seems to handle this fine without doing so.

4–6: This demonstrates the assertion, that for Eq. 13-7, the curl has cylindrical symmetry for arbitrary n, and spherical symmetry for $n = 1$.

7–8: This demonstrates that the divergence of the curl of $\vec{w}$ vanishes for any n; this is true for any differentiable vector field.

One important result that has physical implications is that the curl of a gradient is always zero: $f(\vec{x}) = f(x, y, z)$:

$$\nabla \times (\nabla f) = 0 \tag{13-8}$$

Therefore *if some vector function* $\vec{F}(x, y, z) = (F_x, F_y, F_z)$ *can be derived from a scalar potential,* $\nabla f = \vec{F}$, *then the curl of* $\vec{F}$ *must be zero.* This is the property of an *exact* differential $df = (\nabla f) \cdot$

$(dx, dy, dz) = \vec{F} \cdot (dx, dy, dz)$. Maxwell's relations follow from equation 13-8:

$$
\begin{aligned}
0 =& \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} = \frac{\partial \frac{\partial f}{\partial z}}{\partial y} - \frac{\partial \frac{\partial f}{\partial y}}{\partial z} = \frac{\partial^2 f}{\partial z \partial y} - \frac{\partial^2 f}{\partial y \partial z} \\
0 =& \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} = \frac{\partial \frac{\partial f}{\partial x}}{\partial z} - \frac{\partial \frac{\partial f}{\partial z}}{\partial x} = \frac{\partial^2 f}{\partial x \partial z} - \frac{\partial^2 f}{\partial z \partial x} \\
0 =& \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} = \frac{\partial \frac{\partial f}{\partial y}}{\partial x} - \frac{\partial \frac{\partial f}{\partial x}}{\partial y} = \frac{\partial^2 f}{\partial y \partial x} - \frac{\partial^2 f}{\partial x \partial y}
\end{aligned} \qquad (13\text{-}9)
$$

Another interpretation is that gradient fields are *curl-free, irrotational, or conservative.*

The notion of "conservative" means that, if a vector function can be derived as the gradient of a scalar potential, then integrals of the vector function over any path is zero for a closed curve—meaning that there is no change in "state;" energy is a common state function.

Here is a picture that helps visualize why the curl invokes names associated with spinning, rotation, etc.

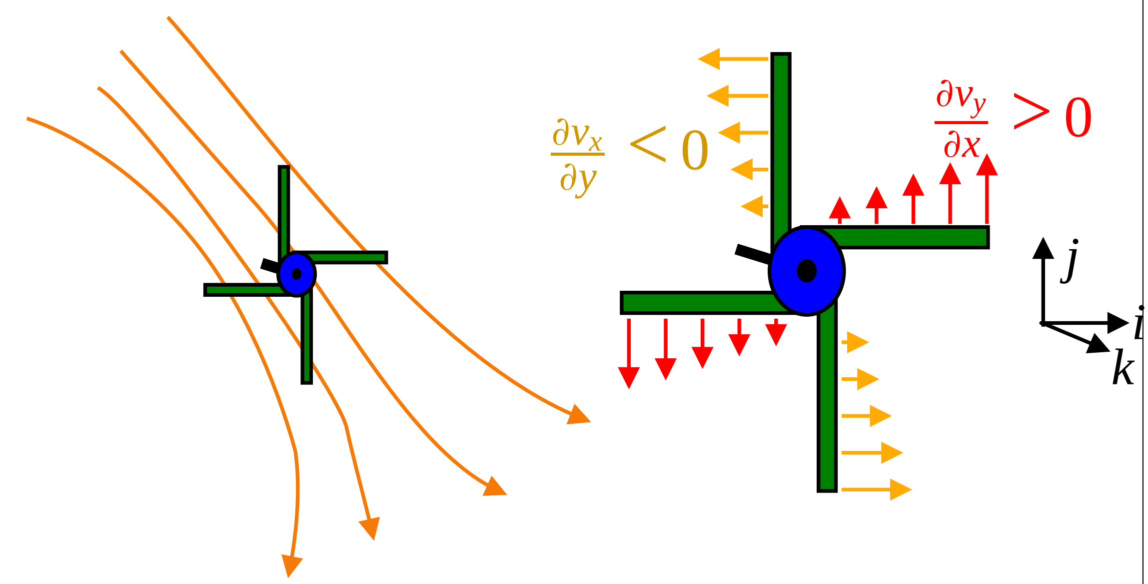


Figure 13-11: Consider a small paddle wheel placed in a set of stream lines defined by a vector field of position. If the v_y component is an increasing function of x, this tends to make the paddle wheel want to spin (positive, counter-clockwise) about the $\hat{k}$-axis. If the v_x component is a decreasing function of y, this tends to make the paddle wheel want to spin (positive, counter-clockwise) about the $\hat{k}$-axis. The net impulse to spin around the $\hat{k}$-axis is the sum of the two.
Note that this is independent of the reference frame because a constant velocity $\vec{v} =$ const. and the local acceleration $\vec{v} = \nabla f$ can be subtracted because of Eq. 13-10.

Another important result is that divergence of any curl is also zero, for $\vec{v}(\vec{x}) = \vec{v}(x, y, z)$:

$$\nabla \cdot (\nabla \times \vec{v}) = 0 \qquad (13\text{-}10)$$